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Supplementary material for

Role of Spin-State and Ligand-Charge in Coordination Patterns in Complexes of 2,6-Diacetylpyridinebis(semioxamazide) with 3d-Block Metal Ions: A Density Functional Theory Study

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Table S1. Relative energies (kcal·mol^{-1}) of isomeric structures depicted in Figure 2, compared to the most stable one; single-point energy calculations (on LDA/TZP geometries) with LDA/TZP, OPBE/TZP, SSB-D/TZP and S12g/TZP.

CM	Ligand	Vxc	I	II	III	V	VI	VII	VIII	IX	X	XI	XII
Fe^{III}	dapsox	LDA	0	-0.3	1.2	-2.1	-1.1	3.1	12.4	6.2	11.5	24.2	61.2
		OPBE	0	-1.0	0.8	5.2	6.4	12.1	29.4	12.4	22.4	32.9	76.9
		SSB-D	0	-1.0	0.6	7.2	5.3	8.5	22.8	9.2	16.1	26.1	61.9
		S12g	0	-0.8	0.9	6.6	5.8	9.3	22.7	9.2	17.6	25.2	64.7
	Hdapsox	LDA	0	-1.6	11.7	2.3	-2.0	6.4	14.1	3.6	7.4	30.6	71.4
		OPBE	0	-2.0	10.1	4.9	3.9	14.1	29.5	8.5	17.7	34.4	87.5
		SSB-D	0	-2.3	9.6	8.2	3.6	8.6	22.1	4.9	11.1	26.8	71.5
		S12g	0	-1.4	10.6	6.5	3.2	10.2	22.0	5.4	12.2	28.4	76.1
	H_2dapsox	LDA	0	0.0	2.0	4.2	-	5.5	20.9	3.1	7.1	35.2	87.7
		OPBE	0	6.0	13.4	8.9	-	11.1	31.6	7.0	14.9	42.6	102.8
		SSB-D	0	3.8	8.7	11.2	-	5.0	19.7	2.2	6.8	35.4	84.8
		S12g	0	4.4	9.8	10.6	-	7.3	22.2	3.4	8.5	35.4	91.0
Fe^{II}	dapsox	LDA	0	9.4	2.4	1.7	6.7	4.2	12.2	6.5	14.5	15.3	46.6
		OPBE	0	3.1	2.0	0.8	6.9	13.1	26.9	11.8	22.9	24.5	56.9
		SSB-D	0	0.3	1.4	4.4	5.2	6.8	18.8	8.3	15.7	14.9	40.0
		S12g	0	3.1	2.1	3.7	6.0	9.4	19.8	8.5	16.8	16.3	44.3
	Hdapsox	LDA	0	-1.4	14.4	0.1	-0.5	3.0	17.2	3.6	9.6	16.6	59.4
		OPBE	0	-1.4	11.6	3.6	1.8	11.8	29.7	8.2	18.4	22.6	68.6
		SSB-D	0	-1.8	11	6.6	0.8	7.9	22.2	5.0	12.0	16.4	53.2
		S12g	0	-1.7	12.4	5.3	1.3	8.3	23.2	5.3	12.6	16.8	56.9
	H_2dapsox	LDA	0	4.1	21.2	3.1	-	4.9	11.5	2.1	7.5	22.6	66.4
		OPBE	0	16.4	15.8	4.2	-	12.4	17.9	8.5	16.4	31.2	80.2
		SSB-D	0	7.5	16.1	7.8	-	7.9	16.8	5.7	9.9	24.7	64.0
		S12g	0	7.5	17.9	6.9	-	8.4	16.6	6.0	10.7	25.4	67.7
Mn^{II}	dapsox	LDA	0	2.8	3.8	1.7	-0.1	1.3	8.6	5.6	13.2	24.0	41.3
		OPBE	0	0.9	2.3	3.5	13.6	12.9	23.6	10.4	21.6	27.4	52.1
		SSB-D	0	0.2	1.5	5.0	10.5	7.5	14.4	6.4	13.3	18.4	34.4
		S12g	0	0.8	2.3	5.1	9.8	8.9	16.0	7.8	15.7	21.1	39.5
	Hdapsox	LDA	0	0.5	14.5	0.1	-4.3	4.0	13.1	6.2	8.0	24.1	52.6
		OPBE	0	2.1	11.7	1.9	8.4	12.4	25.6	9.1	15.5	24.8	62.4
		SSB-D	0	1.9	11.3	4.8	6.7	7.1	17.0	6.1	8.7	18.2	46.0
		S12g	0	1.9	12.2	4.0	5.1	8.6	18.2	6.4	10.2	19.5	50.6
	H_2dapsox	LDA	0	4.1	23.8	-0.7	-	5.4	12.0	2.1	6.5	22.0	61.6
		OPBE	0	11.0	19.3	5.4	-	13.3	28.7	9.4	16.1	30.6	77.0
		SSB-D	0	7.5	18.7	7.9	-	7.4	19.8	5.0	9.1	23.4	59.5
		S12g	0	8.4	19.7	7.8	-	8.8	20.9	6.1	10.1	24.7	64.7
Co^{II}	dapsox	LDA	0	0.4	3.4	-0.2	-1.1	3.6	25.7	8.2	14.0	25.2	44.0
		OPBE	0	0.5	2.6	0.2	14.0	13.2	30.4	13.0	24.5	28.5	55.2
		SSB-D	0	0.9	2.2	0.6	16.5	10.4	22.5	10.4	16.5	19.2	39.4
		S12g	0	1.0	2.7	0.6	13.8	10.5	23.6	10.3	17.5	21.6	42.8
	Hdapsox	LDA	0	-3.7	11.8	-2.3	-10.2	1.3	18.5	2.4	6.6	19.8	50.6
		OPBE	0	-3.0	9.5	0.5	2.4	12.6	33.2	8.5	17.2	24.2	63.5
		SSB-D	0	-4.2	8.4	3.2	3.9	7.9	23.9	4.4	9.9	15.6	46.7
		S12g	0	-3.5	9.7	1.8	2.1	8.3	25.6	5.0	10.8	17.7	51.5
	H_2dapsox	LDA	0	10.4	22.6	1.3	-	5.2	25.1	-2.4	8.3	23.8	61.3

		OPBE	0	9.8	17.7	4.0	-	13.2	39.0	6.3	17.9	31.4	76.6
		SSB-D	0	7.6	17.4	8.1	-	9.2	28.3	5.3	10.8	24.5	59.1
		S12g	0	7.8	18.4	6.5	-	9.3	30.5	5.9	11.6	25.5	64.1
Zn^{II}	dapsox	LDA	0	0.8	2.7	14.6	16.0	15.1	27.9	17.2	23.1	32.4	53.9
		OPBE	0	0.8	2.5	4.4	7.0	13.0	30.0	11.3	19.0	24.9	53.2
		SSB-D	0	0.5	1.7	6.4	5.4	9.7	22.4	11.3	16.0	19.6	38.1
		S12g	0	0.7	2.1	6.9	6.9	10.8	22.4	11.6	16.6	21.2	41.8
	Hdapsox	LDA	0	-0.5	16.1	3.6	5.9	13.5	28.6	15.1	19.8	30.5	56.9
		OPBE	0	-0.6	12.0	-2.0	27.1	1.2	29.4	9.5	14.2	24.7	57.4
		SSB-D	0	-1.4	10.8	3.4	25.6	9.3	20.4	8.8	12.4	19.7	42.5
		S12g	0	-0.9	12.1	2.1	26.0	10.6	23.2	9.4	12.8	21.1	46.3
	H_2dapsox	LDA	0	14.9	5.3	-0.4	-	15.3	28.1	8.4	19.3	36.8	63.6
		OPBE	0	10.7	3.4	-4.7	-	12.2	23.0	2.5	14.2	28.3	63.4
		SSB-D	0	9.9	3.5	1.0	-	8.3	19.5	2.2	8.3	24.3	49.3
		S12g	0	11.4	3.5	0.5	-	10.3	20.5	3.3	10.6	26.0	53.8

Table S2. Selected average bond lengths (Å) and valence angles (º) for DFT energy-minimized structures of $[Fe^{III}(dapsox)(H_2O)_2]^+$, $[Fe^{II}(H_2dapsox)(H_2O)_2]^{2+}$, $[Mn^{II}(H_2dapsox)(H_2O)_2]^{2+}$ and $[Co^{II}(H_2dapsox)(H_2O)_2]^{2+}$ and comparison to available crystallographic data.

	XC	M-N	M-O_{eq}	M-O_{ax}	N-M-N	O_{eq}-M-N	O_{eq}-M-O_{eq}	O_{ax}-M-O_{eq}
$[Fe^{III}(dapsox)(H_2O)_2]^+$	LDA /COSMO	2.17	2.05	2.10	70.7	71.7	77.6	88.9
	LDA	2.15	2.06	2.11	71.4	71.9	78.1	86.7
	OPBE	2.19	2.08	2.27	70.8	71.1	78.6	88.7
	X-ray[29]	2.20	2.05	2.03	70.0	71.8	76.8	90.7
$[Fe^{II}(H_2dapsox)(H_2O)_2]^{2+}$	LDA /COSMO	2.16	2.16	2.08	70.1	73.1	73.6	90.3
	LDA	2.13	2.26	2.07	71.5	72.3	72.9	81.3
	OPBE	2.21	2.29	2.27	70.3	71.3	76.9	85.9
	X-ray[26]	2.22	2.19	2.15	70.0	71.5	77.1	90.3
$[Mn^{II}(H_2dapsox)(H_2O)_2]^{2+}$	LDA /COSMO	2.22 2.23	2.26 2.28	2.16 2.16	69.4 69.0	71.3 71.6	79.5 78.5	84.7 83.2
	LDA	2.23	2.58	2.16	69.0	71.7	78.5	83.2
	OPBE	2.31	2.30	2.36	67.7	70.4	83.7	83.7

	X-ray[26]	2.29	2.29	2.17	68.3	69.6	84.3	88.8
$[Co^{II}(H_2dapsox)(H_2O)_2]^{2+}$	LDA /COSMO	2.10	2.18	2.09	71.4	73.1	70.9	86.1
	LDA	2.11	2.21	2.08	71.7	73.4	70.9	82.7
	OPBE	2.17	2.26	2.28	71.1	72.2	73.4	86.3
	X-ray[27]	2.19	2.25	2.11	70.0	71.0	77.4	87.5

Table S3. Relative energies ($kcal \cdot mol^{-1}$)[a] of isomers **I** and **V** for different 3d-metal ions in high spin; Calculations were performed on the OPBE, OPBE/SSB-D and OPBE/S12g level of theory

3d-metal ion	Ligand	Isomer	OPBE	OPBE/SSB-D	OPBE/S12g
Mn^{II}	H_2dapsox	I	0	0	0
		V	8.99	12.06	10.9
	Hdapsox	I	0	0	0
		V	6.30	8.55	7.68
	dapsox	I	0	0	0
		V	6.29	9.16	8.09
Fe^{III}	H_2dapsox	I	0	0	0
		V	11.42	12.49	11.75
	Hdapsox	I	0	0	0
		V	4.00	4.72	4.04
	dapsox	I	0	0	0
		V	0.60	1.19	0.02
Fe^{II}	H_2dapsox	I	0	0	0
		V*	-	-	-
	Hdapsox	I	0	0	0
		V	7.03	9.04	7.99
	dapsox	I	0	0	0
		V	0.88	3.48	2.55
Co^{II}	H_2dapsox	I	0	0	0
		V	4.63	5.81	5.58
	Hdapsox	I	0	0	0
		V	1.22	2.73	2.31
	dapsox	I	0	0	0
		V	1.23	3.96	3.2
Zn^{II}	H_2dapsox	I	0	0	0
		V	-1.64	2.65	1.56
	Hdapsox	I	0	0	0
		V	1.31	5.88	3.88
	dapsox	I	0	0	0
		V	1.87	3.97	5.38

* OPBE failed to optimize this isomer; Starting from different initial geometries, the optimization always resulted in Isomer **I**

Table S4. Relative energetics of available spin states for some hepta-coordinated 3d-block metal complexes with H_2dapsox and its deprotonated analogues; Single point calculations were performed using LDA optimized geometries with SSB-D, OPBE and S12g functional, as well as with included solvent; Energies are given in kcal·mol^{-1}.

V_{XC}		OPBE / COSMO			SSB-D / COSMO			S12g / COSMO		
Spin State		**HS**	**IS**	**LS**	**HS**	**IS**	**LS**	**HS**	**IS**	**LS**
Fe^{III}	$[Fe^{III}(H_2dapsox)(H_2O)_2]^{3+}$	0	22.3	24.0	0	22.6	35.4	0	20.3	27.0
	$[Fe^{III}(Hdapsox)(H_2O)_2]^{2+}$	0	16.2	15.9	0	23.1	26.8	0	18.4	18.7
	$[Fe^{III}(dapsox)(H_2O)_2]^{+}$	0	17.1	15.8	0	21.2	25.8	0	17.8	17.4
Fe^{II}	$[Fe^{II}(H_2dapsox)(H_2O)_2]^{2+}$	0	29.4	15.7	0	31.6	27.4	0	28.7	19.9
	$[Fe^{II}(Hdapsox)(H_2O)_2]^{+}$	0	9.4	10.1	0	17.5	22.9	0	13.0	15.5
	$[Fe^{II}(dapsox)(H_2O)_2]$	0	10.1	5.3	0	17.3	15.4	0	13.1	9.1
Mn^{II}	$[Mn^{II}(H_2dapsox)(H_2O)_2]^{2+}$	0	33.2	43.2	0	39.2	52.2	0	31.7	41.7
	$[Mn^{II}(Hdapsox)(H_2O)_2]^{+}$	0	14.8	27.4	0	19.1	35.0	0	12.7	25.1
	$[Mn^{II}(dapsox)(H_2O)_2]$	0	14.9	24.9	0	21.2	32.5	0	15.0	22.9
Co^{II}	$[Co^{II}(H_2dapsox)(H_2O)_2]^{2+}$	0	-	5.5	0	-	16.3	0	-	9.6
	$[Co^{II}(Hdapsox)(H_2O)_2]^{+}$	0	-	-5.4	0	-	4.6	0	-	-1.1
	$[Co^{II}(dapsox)(H_2O)_2]$	0	-	-6.7	0	-	3.0	0	-	-3.4

Table S5. Relative spin-state energies (kcal·mol^{-1})[a] for some metal complexes with $H_n$dapsox ligands; Single point calculations were performed using OPBE optimized geometries with SSB-D, and S12g functional

V_{XC}		OPBE			OPBE/SSB-D			OPBE/S12g		
Spin State		HS	IS	LS	HS	IS	LS	HS	IS	LS
Mn^{II}	$[Mn^{II}(H_2dapsox)(H_2O)_2]^{2+}$	0	31.0	48.8	0	34.5	50.4	0	27.6	41.5
	$[Mn^{II}(Hdapsox)(H_2O)_2]^{+}$	0	16.7[†]	32.6	0	18.4	34.8	0	11.0	25.9
	$[Mn^{II}(dapsox)(H_2O)_2]$	0	12.7[†]	26.5	0	15.4	31.6	0	7.6	21.6
Fe^{III}	$[Fe^{III}(H_2dapsox)(H_2O)_2]^{3+}$	0	28.2	19.2	0	27.1	30.1	0	17.1	22.0
	$[Fe^{III}(Hdapsox)(H_2O)_2]^{2+}$	0	11.0	16.7	0	18.6	25.5	0	13.0	17.8
	$[Fe^{III}(dapsox)(H_2O)_2]^{+}$	0	9.7	14.6	0	18.6	25.2	0	12.1	16.8
Fe^{II}	$[Fe^{II}(H_2dapsox)(H_2O)_2]^{2+}$	0	32.8	21.6	0	32.8	30.5	0	29.0	22.6
	$[Fe^{II}(Hdapsox)(H_2O)_2]^{+}$	0	11.7[†]	18.4	0	19.2	29.3	0	10.8	20.7
	$[Fe^{II}(dapsox)(H_2O)_2]$	0	9.4[†]	9.0	0	17.2	20.1	0	8.8	11.6
Co^{II}	$[Co^{II}(H_2dapsox)(H_2O)_2]^{2+}$	0	-	5.9[†]	0	-	15.8	0	-	7.7
	$[Co^{II}(Hdapsox)(H_2O)_2]^{+}$	0	-	-4.1[†]	0	-	5.2	0	-	-2.7
	$[Co^{II}(dapsox)(H_2O)_2]$	0	-	-5.1[†]	0	-	4.4	0	-	-3.0

[†]These structures could not be optimized with OPBE, because apical water tends to dissociate. We obtained reasonable geometries with PBE-D, that can take dispersion interactions into account more adequately, and subsequently performed single point OPBE, SSB-D and S12g calculations.

Table S6. Selected average bond lengths (Å) and valence angles (º) for LDA energy-minimized structures of $[Cu^{II}(dapsox)H_2O]$ and $[Cu^{II}(Hdapsox)H_2O]^+$ and comparison to available crystallographic data.

		M-N	M-O_{eq}	M-O_{ax}	N-M-N_6	N-M-N_5	O_{eq}-M-N	O_{ax}-M-O_{eq}
$[Cu^{II}(dapsox)H_2O]$	DFT	1.95	2.01	2.10	90.5	83.5	83.5	96.3
	X-ray[33]	1.95	1.99	2.30	90.8	82.9	83.5	95.4
$[Cu^{II}(Hdapsox)H_2O]^+$	DFT	1.94	1.97	2.25	92.1	82.2	84.4	87.9
	X-ray[28]	1.95	1.99	2.33	92.4	81.8	84.5	94.8

Table S7. Relative energetics of available spin states for penta-coordinated Fe^{III} complexes with mono- and di-anionic forms of H_2dapsox. Single point calculations were performed using optimized geometries with SSB-D, OPBE and S12g functional, as well as with included solvent. The energy is given in kcal·mol^{-1}.

V_{XC}	LDA/ OPBE / COSMO			LDA/SSB-D / COSMO			LDA/S12g / COSMO		
Spin State	**HS**	**IS**	**LS**	**HS**	**IS**	**LS**	**HS**	**IS**	**LS**
$[Fe^{III}(dapsox)Cl]$	0	-10.5	8.1	0	-7.4	11.3	0	-12.7	3.5
$[Fe^{III}(Hdapsox)Cl]^+$	0	0.6	11.7	0	2.7	18.2	0	-0.4	12.6
$[Fe^{III}(dapsox)H_2O]^+$	0	-1.5	4.8	0	1.5	10.7	0	-3.8	3.9
$[Fe^{III}(Hdapsox)H_2O]^{2+}$	0	-6.4	8.8	0	-4.9	12.9	0	-7.9	6.6

Table S8. Relative spin-state energies (kcal·mol^{-1})[a] for penta-coordinated Fe^{III} with Hdapsox and dapsox ligands; Calculations were performed on the OPBE, OPBE/SSB-D and OPBE/S12g level of theory

V_{XC}	OPBE			LDA/SSB-D			LDA/S12g		
Spin State	HS	IS	LS	HS	IS	LS	HS	IS	LS
$[Fe^{III}(dapsox)Cl]$	0	-4.7	8.4	0	-0.7	15.3	0	-5.7	8.2
$[Fe^{III}(Hdapsox)Cl]^+$	0	0.6	13.3	0	5.9	22.3	0	0.6	14.8
$[Fe^{III}(dapsox)H_2O]^+$	0	-5.1	4.1	0	-0.6	10.3	0	-5.5	4.2
$[Fe^{III}(Hdapsox)H_2O]^{2+}$	0	-6.0	9.5	0	-2.6	15.9	0	-7.2	9.2

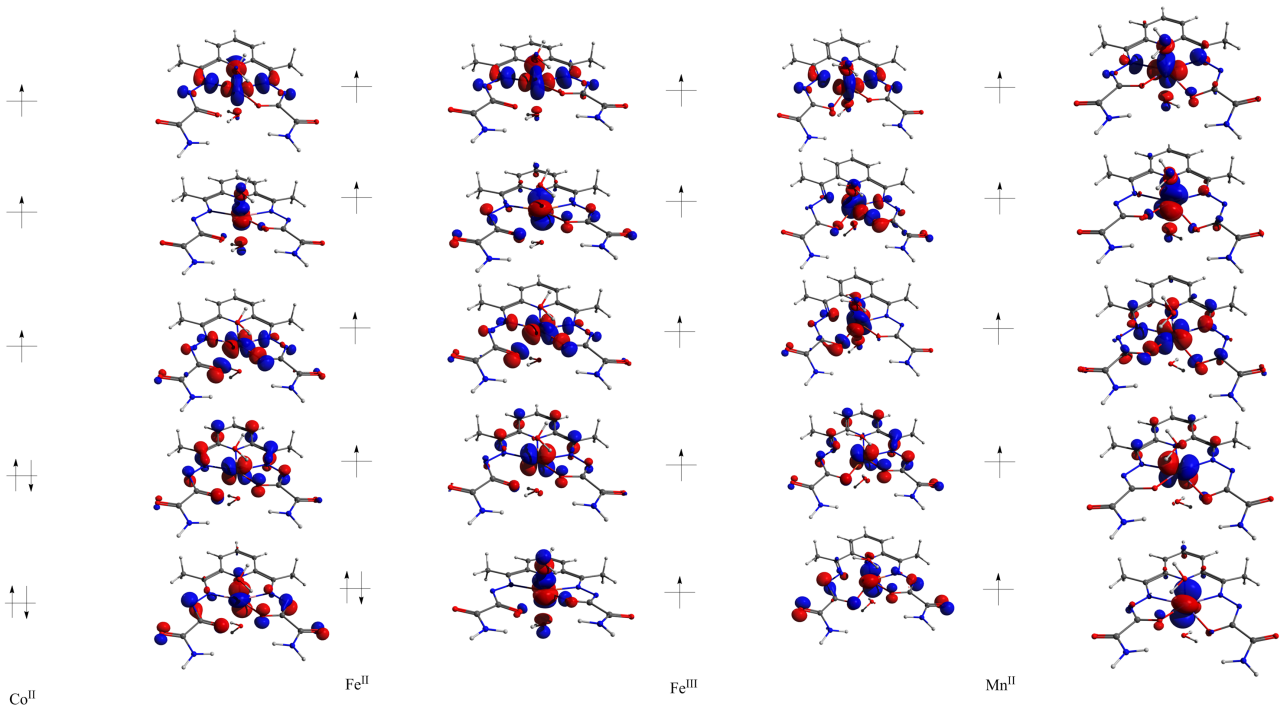

Figure S1. Molecular orbitals for $[M(dapsox)(H_2O)_2]^q$, where q=0,1 and M = Fe^{II}, Fe^{III}, Mn^{II} and Co^{II}.

Fe^{3+} dapsox Isomer I HS LDA

Fe	0.049067	2.322035	2.615371
O	-0.955499	3.552989	1.276507
O	-0.079304	6.147211	-0.922824
O	-1.593370	2.887569	3.711690
O	-3.789722	1.388695	6.006630
O	-0.947478	0.934510	1.379882
H	-0.503586	0.149795	0.999570
H	-1.263639	1.500718	0.639817
O	0.823182	3.921204	3.745440
H	-0.004106	4.269619	4.149083
H	1.230749	4.650715	3.231361
N	1.817067	1.130315	2.746508
N	1.465258	3.022875	1.149530
N	1.100839	4.034018	0.363333
N	-2.089485	5.560677	-0.010679
H	-2.556775	4.880535	0.587451
H	-2.599296	6.309568	-0.475159
N	-0.205045	0.899111	4.197845
N	-1.323563	0.947319	4.909791
N	-3.949993	3.338576	4.830739
H	-4.877755	3.561673	5.185008
H	-3.488390	3.920882	4.133840
C	2.851812	1.387855	1.941063
C	4.022119	0.639893	2.014082
H	4.855482	0.864153	1.343671
C	4.100099	-0.382058	2.944486
H	5.007788	-0.986280	3.021075
C	3.026567	-0.632522	3.781153
H	3.062107	-1.424669	4.533107
C	1.886641	0.154886	3.658054
C	2.636393	2.474492	1.009690
C	3.626308	2.888377	0.008663
H	3.826191	2.071976	-0.706658
H	3.247489	3.760336	-0.542257
H	4.588122	3.140130	0.485717
C	-0.186786	4.254151	0.524189
C	-0.772474	5.428422	-0.230481
C	0.716577	0.030901	4.498710
C	0.606489	-0.934581	5.596644
H	0.802142	-1.960941	5.245044
H	-0.399955	-0.874459	6.033604
H	1.348198	-0.714415	6.384283
C	-2.002791	2.016185	4.562785
C	-3.349079	2.205747	5.223650

Fe^{3+} dapsox IS LDA

Fe	0.168322	1.971477	2.755647
O	-1.296230	3.227235	0.079270
O	-0.121556	6.509047	0.297704
O	-1.409011	2.788929	3.519636
O	-3.679259	1.780158	6.010191
O	-0.970285	1.178596	1.349632
H	-0.583479	0.462586	0.806695
H	-1.138606	2.063015	0.687525
O	1.022947	3.862721	3.730170
H	0.278688	4.156792	4.296467
H	1.024479	4.501946	2.976385
N	1.786612	1.067463	2.811772
N	1.162252	2.894116	1.306889
N	0.755019	4.056147	0.829167
N	-1.978945	5.649899	-0.719964
H	-2.479917	4.787547	-0.933149
H	-2.319160	6.556154	-1.034941
N	-0.062320	0.944644	4.322457
N	-1.202133	1.070659	5.004886
N	-3.803249	3.442523	4.449947
H	-4.725765	3.749535	4.753012
H	-3.337655	3.873851	3.652370
C	2.732789	1.343487	1.891302
C	3.913636	0.617861	1.881020
H	4.675959	0.834470	1.128544
C	4.111240	-0.368115	2.840443
H	5.040286	-0.943280	2.844048
C	3.143719	-0.613262	3.799194
H	3.287354	-1.367411	4.577017
C	1.970059	0.130009	3.769777
C	2.367188	2.446236	1.045330
C	3.241154	3.094693	0.064589
H	3.009284	2.757948	-0.961001
H	3.048258	4.181403	0.083352
H	4.301873	2.890874	0.263567
C	-0.461612	4.148479	0.316873
C	-0.829625	5.577436	-0.040225
C	0.859702	0.061813	4.663763
C	0.730371	-0.838739	5.808894
H	0.799657	-1.892328	5.489334
H	-0.235407	-0.672755	6.305390
H	1.545334	-0.663339	6.532166
C	-1.874441	2.066496	4.488766
C	-3.225332	2.407686	5.075884

Fe^{3+} dapsox LS LDA

Fe	0.305075	2.172406	2.889434
O	-1.420801	3.174024	0.465712
O	-0.139594	6.346688	-0.248384
O	-1.278628	2.955979	3.588963
O	-3.818217	1.730260	5.698821
O	-0.817302	1.181753	1.713991
H	-0.317686	0.544059	1.163116
H	-1.117120	2.039771	1.053352
O	1.152113	3.543855	4.004932
H	0.353249	3.976651	4.395473
H	1.577899	4.226181	3.437193
N	1.821182	1.124957	2.821217
N	1.192412	2.957486	1.363670
N	0.725486	4.052104	0.782273
N	-2.237310	5.476718	-0.497902
H	-2.789437	4.623018	-0.417215
H	-2.609424	6.312811	-0.943910
N	-0.081665	0.946191	4.241622
N	-1.289629	1.023793	4.815687
N	-3.723894	3.587736	4.376056
H	-4.660504	3.894332	4.632304
H	-3.178219	4.087854	3.676028
C	2.775062	1.408737	1.918559
C	3.934300	0.643216	1.871763
H	4.701868	0.864526	1.126117
C	4.081266	-0.400505	2.772396
H	4.986604	-1.011942	2.751428
C	3.081970	-0.680537	3.693744
H	3.175381	-1.504109	4.405833
C	1.940870	0.107743	3.699870
C	2.399185	2.515139	1.081189
C	3.245941	3.097274	0.036588
H	3.306061	2.429984	-0.841491
H	2.821193	4.057835	-0.291402
H	4.275010	3.245218	0.402154
C	-0.547288	4.090930	0.423436
C	-0.945801	5.438847	-0.149324
C	0.775399	-0.002155	4.535318
C	0.547721	-1.029150	5.552532
H	0.705934	-2.037013	5.133962
H	-0.476903	-0.946077	5.940979
H	1.255634	-0.909816	6.391364
C	-1.864110	2.116735	4.399183
C	-3.249922	2.448628	4.903849

Fe^{3+} dapsox Isomer II LDA

Fe	-1.966253	4.023093	11.175133
N	-2.819875	5.955076	10.979822
N	-2.609152	4.276861	9.127239
N	-2.443612	3.250978	8.301869
N	-1.942396	1.002787	6.940459
N	-1.889323	4.987574	13.096750

N	-1.329539	4.334759	14.114085
N	0.386826	1.220689	14.094084
O	-1.814611	2.233364	10.252933
O	-1.331106	-0.058888	8.867854
O	-0.669802	2.941735	12.410505
O	-0.111736	2.591145	15.854212
O	-0.030742	4.628764	10.540070
O	-3.654607	3.038508	11.933794
H	-3.460553	2.111553	11.651629
C	-3.289803	6.355067	9.793449
C	-3.882056	7.603561	9.641408
C	-3.986781	8.430382	10.747664
C	-3.502810	8.002193	11.971786
C	-2.917598	6.744931	12.056201
C	-3.154187	5.385594	8.727585
C	-3.624516	5.637846	7.360625
C	-2.005105	2.213031	8.997062
C	-1.721104	0.918268	8.262681
C	-2.359529	6.188076	13.270089
C	-2.310043	6.914840	14.543476
H	-3.321783	7.202170	14.874725
H	-1.726192	7.844930	14.444296
H	-1.842692	6.276103	15.307778
C	-0.734365	3.255628	13.650180
C	-0.112924	2.324054	14.668692
H	-4.451153	9.414779	10.654469
H	-4.260646	7.913027	8.663710
H	0.293572	1.102095	13.085186
H	-3.572088	8.631535	12.862254
H	0.812064	0.503101	14.678053
H	-3.367940	4.787656	6.716752
H	0.266455	5.543283	10.732520
H	-1.769664	0.186523	6.357952
H	-2.270962	1.883224	6.545052
H	-4.721209	5.775158	7.344022
H	0.445715	4.035023	11.170782
H	-3.178082	6.558072	6.949684
H	-3.773671	3.028441	12.907460

Fe^{3+} dapsox Isomer III LDA

Fe	-1.955695	4.017111	11.187721
N	-2.815082	5.948032	10.992932
N	-2.548607	4.297773	9.121634
N	-2.383107	3.280241	8.287132
N	-1.929197	1.032125	6.912532
N	-1.966866	4.961121	13.140136
N	-1.398674	4.303075	14.149835
N	-0.202518	2.686427	15.916727
O	-1.829278	2.222063	10.239533
O	-1.686527	-0.133788	8.859288
O	-0.711754	2.950264	12.431071
O	0.814573	1.555435	14.215031
O	-0.010145	4.499933	10.487826
O	-3.646900	2.969726	11.874153
H	-3.371036	2.076074	11.553843
C	-3.225783	6.372540	9.791880
C	-3.806247	7.627001	9.632746
C	-3.970732	8.430663	10.746079
C	-3.557907	7.975228	11.986410
C	-2.974935	6.716221	12.076575
C	-3.052287	5.424201	8.714921
C	-3.463024	5.705061	7.333875
C	-2.013587	2.214670	8.984948
C	-1.854493	0.900293	8.246476
C	-2.473891	6.145510	13.308760
C	-2.499224	6.868447	14.586846
H	-3.534463	7.097035	14.891718
H	-1.967580	7.831240	14.504149
H	-2.019450	6.261103	15.364651
C	-0.744090	3.256442	13.659410
C	0.048658	2.399905	14.628543
H	-4.427473	9.418969	10.647733
H	-4.129220	7.954578	8.641440
H	-0.820226	3.464416	16.144771
H	-3.678359	8.585492	12.884668
H	0.291860	2.168491	16.640832
H	-3.193704	4.858811	6.689414
H	0.375980	5.382112	10.660608
H	-1.838853	0.201531	6.330583
H	-2.124611	1.948034	6.510015
H	-4.554544	5.858340	7.275824
H	0.476768	3.854887	11.058397
H	-2.985422	6.623404	6.955317
H	-3.772168	2.906143	12.843562

Fe^{3+} dapsox Isomer V LDA

Fe	-2.037988	4.001324	10.938294
N	-2.827720	5.932387	10.904861
N	-2.801667	4.299646	9.011988
N	-2.705088	3.304063	8.140061
N	-1.456401	0.004116	8.583121
N	-1.836591	4.832809	12.950975
N	-1.505584	4.042745	13.971373
N	1.012247	1.866696	15.131214
O	-2.019690	2.175137	10.015198
O	-2.287273	1.010173	6.711876
O	0.578791	3.456331	13.084601
O	-1.085018	2.285792	15.932441
O	-0.149355	4.146185	10.886679
O	-3.194115	2.795450	12.159401
H	-3.142756	1.881949	11.800343
C	-3.332980	6.395802	9.755767
C	-3.823356	7.691895	9.664678
C	-3.770538	8.500242	10.787162
C	-3.241355	8.008441	11.968417
C	-2.778758	6.698372	11.998079
C	-3.326472	5.439696	8.668542
C	-3.864196	5.724248	7.335762
C	-2.259505	2.232281	8.755437
C	-2.007585	1.013209	7.893655
C	-2.242648	6.042720	13.175849
C	-2.201673	6.664652	14.504826
H	-3.043746	7.353469	14.661048
H	-1.266691	7.234407	14.646817
H	-2.213429	5.869856	15.268822
C	-0.376607	3.389877	13.947030
C	-0.191366	2.451688	15.121298
H	-4.148163	9.525139	10.742378
H	-4.241771	8.051779	8.721486
H	1.680157	2.075505	14.389773
H	-3.187940	8.627653	12.866763
H	1.247289	1.233330	15.893102
H	-3.673997	4.867426	6.674713
H	0.242795	4.985128	10.567991
H	-1.203880	-0.850782	8.091161
H	-1.213788	0.141740	9.562633
H	-4.952623	5.902414	7.386231
H	0.289755	3.859970	12.057445
H	-3.406998	6.632973	6.910251
H	-2.893820	2.802725	13.106623

Fe^{3+} dapsox Isomer VI LDA

Fe	0.191172	0.502886	-0.071288
O	2.014399	0.417312	0.476864
O	-1.986672	0.497533	0.286928
O	-0.055375	2.166278	1.022107
O	-0.318495	4.094084	-1.859672
O	1.814600	-0.256193	2.787899
O	-0.837987	-1.073027	4.922870
N	-0.282898	4.417540	0.760178
N	-0.021883	1.783199	-1.594166
N	-0.003683	1.673584	-2.911291
N	0.023906	-0.981869	-1.590916
N	-0.044661	-1.273980	1.002335
N	-0.250664	-1.247003	2.315872
N	1.223992	-0.184291	5.336087
C	-0.171223	3.192560	0.316208
C	-0.181889	3.091357	-1.189305
C	0.063771	0.534763	-3.520524
C	0.110527	0.636494	-5.002401
C	0.077029	-0.796530	-2.923619
C	0.128518	-1.898827	-3.787117
C	0.114809	-3.179051	-3.284331
C	0.034361	-3.356839	-1.916826
C	-0.014394	-2.240525	-1.097647
C	-0.109418	-2.384879	0.342592
C	-0.276554	-3.686256	1.007490
C	0.647170	-0.712532	3.094557
C	0.253963	-0.679634	4.556293
H	-0.286724	4.636089	1.755640
H	-0.369328	5.136692	0.030165
H	0.082112	1.698199	-5.275515
H	1.029028	0.189684	-5.416761
H	-0.748414	0.131372	-5.474315
H	0.176266	-1.727897	-4.862992
H	0.160511	-4.039541	-3.956782
H	0.014991	-4.354220	-1.472209
H	-0.643199	-3.517587	2.032555
H	-0.975839	-4.337116	0.461956
H	2.099130	0.119689	4.911763
H	1.070554	-0.123836	6.340418
H	0.686452	-4.220293	1.083299
H	-2.148973	0.132251	1.186748
H	-2.470757	-0.088696	-0.331405
H	2.738775	0.078365	-0.083660
H	1.990668	-0.011837	1.686663

Fe^{3+} dapsox Isomer VII LDA

Fe	10.613905	6.379733	1.997177
O	9.433457	5.555866	3.429900
O	9.328550	2.545986	5.246545
O	10.470196	10.593859	3.532261
O	8.722147	7.666794	2.103077
O	11.618115	7.294165	3.440447
N	11.989454	5.983830	0.445239
N	11.162495	4.350884	2.134193
N	10.609727	3.616054	3.086088
N	8.161510	4.484398	5.517880
H	7.662757	4.140595	6.335976
H	8.025383	5.430800	5.170881
N	11.124050	8.262323	1.084372
N	10.662753	9.411248	1.590697
N	11.890676	8.981701	4.916882
H	11.612518	9.965023	5.066525
H	12.310951	8.391541	5.634491
C	12.422913	4.731706	0.265112
C	13.258283	4.419464	-0.802825
H	13.608239	3.394699	-0.946082
C	13.629293	5.432324	-1.669507
H	14.283287	5.212595	-2.517566
C	13.179282	6.725859	-1.460658
H	13.472689	7.541228	-2.125973
C	12.346713	6.974376	-0.374414
C	11.933425	3.788507	1.247128
C	12.222034	2.352175	1.246352
H	12.268500	1.990642	2.285608
H	13.148813	2.110509	0.709490
H	11.391110	1.797959	0.772757
C	9.726983	4.344327	3.736427
C	9.051848	3.680709	4.914851
C	11.853744	8.283370	0.010280
C	12.230467	9.521000	-0.685183
H	12.288522	9.375380	-1.773964
H	11.503009	10.310167	-0.441016
H	13.219858	9.875237	-0.343539
C	10.825540	9.594332	2.908919
C	11.504333	8.503044	3.761250
O	9.191247	5.808485	0.488343
H	9.056445	8.601984	1.945233
H	8.294614	7.615649	2.981887
H	8.537914	6.504172	0.765458
H	9.431835	5.986346	-0.443039

Fe^{3+} dapsox Isomer VIII LDA

Fe	11.223889	6.454781	2.158589
O	8.351640	3.257228	3.701841
O	9.213877	6.008382	1.717848
O	12.438857	10.601073	3.662703
O	10.008083	8.006824	2.973332
O	12.850175	7.138414	3.331759
N	12.192416	5.905936	0.358419
N	11.118584	4.278315	1.947071
N	10.443542	3.542290	2.832039
N	7.255013	4.971488	2.154307
H	6.681685	5.684387	1.704792
H	6.869437	4.189005	2.707562
N	11.956154	8.272598	1.189190
N	11.830396	9.460474	1.782801
N	13.848484	8.707300	4.617852
H	13.806738	9.721822	4.812199
H	14.359115	8.038538	5.192964
C	12.405881	4.616918	0.085107
C	13.056746	4.225606	-1.078590
H	13.234452	3.165672	-1.274421
C	13.446536	5.199966	-1.980660
H	13.946763	4.918887	-2.911239
C	13.199040	6.531577	-1.699144
H	13.494207	7.324944	-2.389847
C	12.580615	6.853877	-0.496879
C	11.828999	3.691838	1.035582
C	11.939358	2.233381	0.900666
H	11.649027	1.757211	1.848218
H	12.959471	1.933573	0.616679
H	11.254411	1.859671	0.118718
C	9.148736	3.855148	2.984149
C	8.562149	5.047976	2.200970
C	12.389083	8.208922	-0.031078
C	12.765324	9.382988	-0.829893
H	13.861898	9.446308	-0.943564
H	12.335385	9.325285	-1.842778

H	12.420219	10.295263	-0.323575
C	12.391611	9.571380	2.995185
C	13.059590	8.338931	3.639274
O	10.980063	5.733646	4.145467
H	11.836387	6.011523	4.542618
H	10.943951	4.732724	4.112213
H	9.118832	7.745219	2.644652
H	10.273625	8.866134	2.531739

Fe^{3+} dapsox Isomer IX LDA

Fe	10.510997	6.553229	2.165909
O	9.909831	5.778527	4.023589
O	9.225740	2.612856	5.384791
O	10.155236	10.992991	3.445169
O	8.954958	7.789095	2.663848
O	8.877991	6.046861	0.872632
O	11.958829	7.145131	3.565248
N	11.718505	6.104438	0.514215
N	10.854181	4.437100	2.164712
N	10.374572	3.700842	3.159344
N	8.859123	4.708059	6.210408
H	8.426127	4.370286	7.067521
H	8.939477	5.702617	6.003353
N	11.204685	8.481355	1.334485
N	11.073872	9.679658	1.846119
N	8.149660	9.518892	3.875361
H	8.413270	10.478011	4.163314
H	7.304089	9.032244	4.169362
C	11.972917	4.822828	0.213087
C	12.683524	4.478038	-0.927787
H	12.888475	3.427387	-1.146489
C	13.121561	5.493472	-1.764095
H	13.678538	5.252840	-2.673476
C	12.859702	6.809919	-1.444038
H	13.197464	7.621421	-2.091246
C	12.155600	7.099294	-0.271236
C	11.480607	3.867073	1.177927
C	11.696900	2.419732	1.067875
H	11.151996	1.907741	1.872867
H	12.770368	2.178723	1.159216
H	11.362366	2.039924	0.088885
C	9.888753	4.496838	4.084260
C	9.286459	3.823208	5.298089
C	11.874911	8.422766	0.199551
C	12.335826	9.646855	-0.467310
H	13.087397	9.453578	-1.241952
H	11.488129	10.189905	-0.919442
H	12.738913	10.334300	0.295587
C	10.195751	9.932790	2.818982
C	9.052590	8.957770	3.110591
H	12.910386	7.311243	3.410127
H	11.838521	6.552664	4.339613
H	9.020663	6.062866	-0.095138
H	8.259846	6.778562	1.100223

Fe^{3+} dapsox Isomer X LDA

Fe	10.518941	6.670816	2.142868
O	9.727440	3.725628	5.497939
O	8.744633	5.657783	2.745549
O	10.008647	11.301144	3.033026
O	9.940879	7.838330	3.583997
O	8.883000	7.075117	0.782594
O	12.439398	6.978100	3.129820
N	11.634781	6.181128	0.504506
N	11.132090	4.641997	2.485444
N	10.953928	3.962574	3.595116
N	7.675615	4.876886	4.590120
H	7.885482	4.305838	5.430439
H	6.780228	5.318305	4.387883
N	11.065699	8.624964	1.144646
N	10.787666	9.858050	1.490623
N	9.440728	9.657051	4.813473
H	9.425192	10.691228	4.730441
H	9.162806	9.124184	5.636452
C	12.053560	4.913093	0.374910
C	12.734711	4.513390	-0.771176
H	13.048142	3.474144	-0.885005
C	13.003562	5.456684	-1.749753
H	13.534989	5.161293	-2.658361
C	12.626488	6.773565	-1.567505
H	12.868878	7.542705	-2.305093
C	11.944762	7.119266	-0.400005
C	11.770842	4.057107	1.496327
C	12.176245	2.646620	1.555414
H	12.264998	2.345888	2.611741
H	13.122475	2.465834	1.025661
H	11.406936	1.994310	1.104232
C	9.903200	4.205157	4.376431
C	8.721872	5.000761	3.813664
C	11.583151	8.465008	-0.059430
C	11.822792	9.586272	-0.984130
H	12.901416	9.805254	-1.070676
H	11.455314	9.355209	-1.996266
H	11.325971	10.485725	-0.597846
C	10.241804	10.146186	2.674842
C	9.868538	9.081315	3.719376
H	12.974651	6.155751	3.108672
H	12.955332	7.664344	2.657658
H	8.257976	6.416863	1.175578
H	9.019373	6.842033	-0.157632

Fe^{3+} dapsox Isomer XI LDA

Fe	10.606801	6.520882	2.126954
O	9.302843	5.697702	3.483710
O	9.092729	2.770032	5.397202
O	10.048960	11.056597	3.238810
N	8.531710	8.229097	3.029120
O	8.825778	6.222536	0.940673
O	11.908931	6.946471	3.613066
N	11.765156	6.085423	0.512665
N	11.054352	4.468799	2.254738
N	10.545490	3.776793	3.275858
N	8.442521	4.898616	5.898635
H	8.070352	4.625685	6.807579
H	8.562067	5.884832	5.668536
N	11.033370	8.483123	1.208288
N	10.794129	9.719227	1.569889
O	10.135956	8.365271	4.611746
C	12.205006	4.830652	0.326431
C	12.976451	4.497821	-0.773309
H	13.325754	3.471051	-0.906345
C	13.278133	5.494426	-1.694092
H	13.870955	5.258297	-2.581601
C	12.838703	6.782839	-1.483623
H	13.080800	7.576077	-2.192853
C	12.086134	7.074320	-0.337274
C	11.785135	3.894006	1.346202
C	12.127837	2.468229	1.344544
H	11.754864	2.002118	2.267209

H	13.218616	2.327520	1.270701
H	11.675653	1.953638	0.479602
C	9.656029	4.519505	3.888616
C	9.035375	3.955866	5.145576
C	11.661897	8.384838	0.037202
C	11.955774	9.589653	-0.745444
H	12.461578	9.373561	-1.693172
H	11.027832	10.151951	-0.942323
H	12.572366	10.279751	-0.142545
C	10.193298	9.942279	2.769381
C	9.623002	8.784206	3.563989
H	12.240235	6.188654	4.138333
H	11.370706	7.572199	4.238221
H	8.082567	8.627787	2.203339
H	8.104588	7.432357	3.514653
H	8.950492	5.743999	0.094306
H	8.389331	5.591889	1.559901

Fe^{3+} dapsox Isomer XII LDA

Fe	10.682885	6.673961	2.156393
O	8.982331	3.221909	4.906874
O	8.180185	5.940255	4.377467
O	10.013079	11.292538	2.925200
N	9.013789	8.034058	2.858479
O	8.996333	6.029662	1.079570
O	12.556473	7.177546	2.999512
N	11.763600	6.136857	0.516420
N	10.905506	4.455359	2.312542
N	10.389285	3.587208	3.178030
N	10.429427	6.266111	4.345918
H	13.195802	6.434031	3.067730
H	11.298664	5.794868	4.624945
N	11.063202	8.565429	1.080310
N	10.774379	9.831649	1.377690
O	10.100466	8.952131	4.631261
C	12.136629	4.863226	0.372240
C	12.894842	4.464751	-0.726059
H	13.198302	3.421239	-0.828487
C	13.243340	5.410206	-1.671158
H	13.831830	5.121472	-2.544543
C	12.844090	6.723954	-1.508494
H	13.111033	7.483208	-2.244373
C	12.099505	7.068179	-0.382417
C	11.684237	3.944215	1.381633
C	12.047833	2.524231	1.312781
H	11.642930	1.987294	2.177847
H	13.143869	2.411403	1.280558
H	11.654161	2.069142	0.388065
C	9.568709	4.003422	4.145358
C	9.315043	5.475202	4.341164
C	11.673082	8.407313	-0.079072
C	11.933783	9.546025	-0.961510
H	12.408884	9.250266	-1.902417
H	10.989754	10.074533	-1.173254
H	12.571781	10.281370	-0.442124
C	10.195988	10.128673	2.545608
C	9.741078	9.020577	3.459524
H	13.003725	7.844642	2.432096
H	10.309830	7.229634	4.758995
H	8.517731	8.315739	2.004298
H	8.452172	7.412441	3.500594
H	8.750265	6.575955	0.300268
H	9.146373	5.126231	0.721889

Fe^{3+} Hdapsox Isomer I HS LDA

Fe	0.034481	2.352483	2.697241
O	-1.040072	3.787662	1.391557
O	0.204068	5.798009	-1.190235
O	-1.614217	2.850702	3.771843
O	-3.816196	1.131170	5.882553
O	-0.971940	1.085920	1.376234
H	-1.212781	0.175173	1.650330
H	-1.789640	1.510355	1.037110
O	0.794886	3.902284	3.843056
H	0.171417	4.208755	4.535219
H	1.702934	4.173888	4.088399
N	1.826356	1.177544	2.770968
N	1.422997	3.021695	1.145499
N	0.963845	3.999755	0.372311
N	-1.930593	5.872553	-0.350919
H	-2.570350	5.481247	0.340191
H	-2.248900	6.610389	-0.982717
N	-0.195577	0.872761	4.216110
N	-1.316910	0.889355	4.923989
N	-3.974609	3.244842	5.037570
H	-4.891528	3.421021	5.449135
H	-3.508731	3.955812	4.476558
C	2.835321	1.413242	1.927787
C	4.001340	0.662404	1.960148
H	4.815716	0.874310	1.262112
C	4.109269	-0.358942	2.892009
H	5.017827	-0.965382	2.941689
C	3.058407	-0.604143	3.754895
H	3.111809	-1.401974	4.500769
C	1.916881	0.188581	3.667228
C	2.592357	2.493705	0.981426
C	3.582636	2.870208	-0.034771
H	3.780028	2.016397	-0.707114
H	3.279267	3.721631	-0.658309
H	4.545085	3.127879	0.439612
C	-0.314172	4.337085	0.547837
C	-0.684515	5.435351	-0.430109
C	0.757886	0.035826	4.521764
C	0.683359	-0.929248	5.618190
H	0.897139	-1.951139	5.260940
H	-0.313078	-0.898912	6.079371
H	1.439529	-0.700176	6.390727
C	-2.016463	1.952568	4.596989
C	-3.374500	2.073546	5.251124
H	1.438368	4.518254	-0.400684

Fe^{3+} Hdapsox IS LDA

Fe	0.149310	1.984146	2.829678
O	-1.527430	3.442361	0.303516
O	0.392213	6.275421	-0.370547
O	-1.452461	2.754400	3.625665
O	-3.661024	1.552001	6.083931
O	-0.969547	1.224152	1.345458
H	-1.759573	0.691721	1.577407
H	-1.292256	2.084480	0.845333
O	0.959543	3.755109	3.938343
H	0.180325	4.144712	4.389690
H	1.667186	3.703307	4.613733
N	1.791118	1.124457	2.831877
N	1.108511	2.971563	1.319886
N	0.673867	4.061732	0.671989
N	-1.818529	5.939716	-0.901009
H	-2.585798	5.266026	-0.866788

H	-1.945030	6.838465	-1.370365
N	-0.081666	0.887199	4.334589
N	-1.204161	0.984473	5.041750
N	-3.853338	3.349140	4.688256
H	-4.775782	3.613004	5.036496
H	-3.411450	3.873206	3.934581
C	2.714919	1.434695	1.910325
C	3.910334	0.730531	1.865090
H	4.670607	0.981565	1.120356
C	4.126793	-0.286990	2.785392
H	5.065726	-0.847067	2.766464
C	3.158879	-0.591848	3.729833
H	3.313774	-1.386893	4.465049
C	1.977406	0.137745	3.735108
C	2.316679	2.536544	1.058959
C	3.199776	3.107605	0.040519
H	3.816572	2.325124	-0.427053
H	2.635849	3.625767	-0.749743
H	3.899480	3.837267	0.491936
C	-0.585199	4.233198	0.245640
C	-0.645816	5.617066	-0.390788
C	0.856287	-0.002607	4.623528
C	0.744386	-0.967449	5.709923
H	0.964279	-1.988842	5.353988
H	-0.259847	-0.933039	6.153969
H	1.485419	-0.743206	6.500600
C	-1.890599	2.000024	4.581545
C	-3.243823	2.282186	5.210101
H	1.232237	4.933421	0.435695

Fe^{3+} Hdapsox LS LDA

Fe	0.281829	2.160020	2.966405
O	-1.545575	3.288010	0.517243
O	0.152795	6.131247	-0.584202
O	-1.258204	2.979475	3.758462
O	-3.898403	1.458295	5.485930
O	-0.781519	1.252886	1.706617
H	-1.483210	0.665220	2.065509
H	-1.209878	2.061791	1.154600
O	1.225864	3.433293	4.110941
H	0.516975	3.915274	4.598559
H	1.832022	3.063532	4.791019
N	1.805644	1.167973	2.837794
N	1.144717	3.057349	1.399067
N	0.625309	4.072409	0.685116
N	-2.058518	5.616095	-0.936011
H	-2.783197	4.913763	-0.777766
H	-2.264036	6.448656	-1.491922
N	-0.113477	0.899818	4.241109
N	-1.315689	0.955998	4.826514
N	-3.646883	3.647841	4.891542
H	-4.577443	3.917058	5.214400
H	-3.038856	4.332884	4.446279
C	2.753666	1.510875	1.953836
C	3.922906	0.772494	1.877930
H	4.696347	1.033171	1.149936
C	4.083349	-0.315757	2.732129
H	5.000711	-0.908743	2.685733
C	3.085146	-0.661454	3.626326
H	3.192650	-1.522031	4.292650
C	1.926501	0.108268	3.665965
C	2.348292	2.629893	1.116943
C	3.208892	3.149830	0.052723
H	3.641031	2.314944	-0.525144
H	2.676944	3.809827	-0.647078
H	4.061832	3.710381	0.479925
C	-0.656205	4.121744	0.311941
C	-0.841447	5.417770	-0.467601
C	0.760925	-0.056153	4.497517
C	0.548113	-1.122409	5.471622
H	0.697109	-2.112541	5.007471
H	-0.466129	-1.060637	5.889949
H	1.275996	-1.047601	6.299847
C	-1.860884	2.103701	4.504035
C	-3.257030	2.379872	5.025043
H	1.122514	4.935275	0.318753

Fe^{3+} Hdapsox Isomer II LDA

Fe	-1.997873	3.988539	11.282684
N	-2.810485	5.941509	10.998692
N	-2.637830	4.211077	9.196225
N	-2.412870	3.156999	8.421457
N	-1.161982	-0.138752	8.513846
N	-1.850856	5.073739	13.152529
N	-1.288075	4.439185	14.174754
N	-0.039488	2.747698	15.947347
O	-1.625034	2.073017	10.236862
O	-2.029107	1.220593	6.874658
O	-1.112132	2.807302	12.585433
O	0.538631	1.436810	14.168005
O	-0.054240	4.413043	10.644492
O	-3.784673	3.157766	11.909388
H	-3.694976	2.253664	12.280114
C	-3.280878	6.314427	9.802588
C	-3.854883	7.560939	9.603126
C	-3.946318	8.431945	10.678640
C	-3.458999	8.042614	11.911006
C	-2.886011	6.779826	12.041146
C	-3.145899	5.313286	8.751408
C	-3.554595	5.585165	7.367501
C	-1.886062	2.087239	9.028875
C	-1.685338	0.972593	8.024167
C	-2.331365	6.275136	13.282229
C	-2.321296	7.052546	14.522827
H	-3.349697	7.301258	14.838582
H	-1.791419	8.010488	14.381644
H	-1.829977	6.484763	15.322537
C	-0.889444	3.250095	13.760211
C	-0.054921	2.376226	14.665975
H	-4.400322	9.418546	10.550673
H	-4.231292	7.844640	8.616716
H	-0.554165	3.573404	16.251663
H	-3.514668	8.707053	12.777500
H	0.514112	2.208153	16.614035
H	-3.400954	4.737378	6.686848
H	0.367813	5.291387	10.546116
H	-0.990580	-0.934400	7.895770
H	-0.910534	-0.196220	9.501938
H	-4.624008	5.855678	7.326848
H	0.582072	3.823274	11.106704
H	-2.994531	6.446424	6.963261
H	-4.691848	3.256481	11.555262
H	-2.577552	3.031070	7.398438

Fe^{3+} Hdapsox Isomer III LDA

Fe	0.052797	2.310731	2.529364
O	-0.863689	3.600882	1.308566
O	-2.029914	5.292600	-0.435491
O	-1.791408	2.731321	3.572598

O	-3.298485	3.450706	5.850030
O	-0.998777	1.078211	1.236947
H	-1.432419	0.204181	1.319998
H	-1.601615	1.693079	0.755886
O	0.523740	3.858374	3.863229
H	1.115743	4.576714	3.553993
H	-0.336004	4.283318	4.094347
N	1.831464	1.150002	2.758312
N	1.538197	3.100673	1.198529
N	1.175455	4.109440	0.410541
N	0.023094	6.103779	-1.024741
H	1.030731	5.983353	-0.927212
H	-0.357592	6.816835	-1.647733
N	-0.228597	0.816059	4.131050
N	-1.388659	0.899565	4.798043
H	-1.575755	0.342913	5.643384
N	-4.077311	1.295369	5.792687
H	-4.851391	1.523466	6.425042
H	-4.215194	0.490141	5.180103
C	2.898602	1.450347	2.011037
C	4.080334	0.719943	2.109771
H	4.937825	0.984215	1.485102
C	4.143031	-0.332818	3.001056
H	5.057682	-0.924358	3.096519
C	3.034154	-0.630130	3.779003
H	3.060831	-1.450953	4.500448
C	1.891391	0.141142	3.631798
C	2.721198	2.565166	1.102277
C	3.762656	2.997653	0.169484
H	4.033065	2.177759	-0.519186
H	3.416451	3.855422	-0.419871
H	4.684138	3.274231	0.710917
C	-0.130930	4.282172	0.522692
C	-0.815195	5.294712	-0.372547
C	0.686576	-0.043611	4.431893
C	0.607741	-1.072383	5.478451
H	0.940038	-2.047332	5.085595
H	-0.401912	-1.217507	5.888010
H	1.281435	-0.820211	6.317414
C	-2.141576	1.979693	4.486774
C	-3.286247	2.319048	5.423837

Fe^{3+} Hdapsox Isomer V LDA

Fe	-0.038310	2.188491	2.903634
O	-1.397667	3.696637	0.058629
O	0.860925	6.191714	-0.860945
O	-1.653269	2.671652	4.044292
O	-3.562024	0.963245	6.439815
O	-1.244126	1.674580	1.460221
H	-2.138549	1.366491	1.721198
H	-1.353145	2.500719	0.787959
O	0.484196	4.008797	3.718720
H	1.379746	4.371419	3.881363
H	-0.087993	4.210485	4.491364
N	1.767735	1.153760	2.823935
N	1.180125	3.034686	1.190985
N	0.853844	4.098254	0.437702
H	1.508962	4.863975	0.097670
N	-1.365290	6.058487	-1.411500
H	-2.211639	5.494268	-1.318266
H	-1.377719	6.912248	-1.973066
N	-0.126845	0.764993	4.415341
N	-1.189124	0.752748	5.209101
N	-3.977707	2.956823	5.410323
H	-4.875321	3.093401	5.876702
H	-3.625880	3.648450	4.750628
C	2.707593	1.455606	1.923782
C	3.887690	0.726046	1.849796
H	4.658593	0.986354	1.121251
C	4.072461	-0.342315	2.712742
H	4.992935	-0.931077	2.668670
C	3.085116	-0.657159	3.626968
H	3.199644	-1.493580	4.321932
C	1.933353	0.120400	3.660653
C	2.386671	2.570007	1.043842
C	3.342338	3.109284	0.066383
H	4.128420	2.387456	-0.187757
H	2.833282	3.404891	-0.865825
H	3.849718	4.009826	0.462453
C	-0.360169	4.359864	-0.047945
C	-0.247948	5.660294	-0.836606
C	0.845987	-0.086939	4.596205
C	0.852592	-1.115654	5.631830
H	1.020770	-2.114033	5.191056
H	-0.100400	-1.108876	6.178116
H	1.678103	-0.943735	6.346736
C	-1.954269	1.781053	4.923941
C	-3.259864	1.866687	5.682211

Fe^{3+} Hdapsox Isomer VI LDA

Fe	0.009123	0.537057	-0.102491
O	1.877429	0.896954	0.512526
O	-2.097994	0.236132	0.100383
O	-0.480816	2.208557	0.883403
O	0.240963	4.095941	-1.942346
O	1.633842	0.337360	2.924417
O	-0.375609	-1.856504	4.751468
N	-0.234082	4.467613	0.659221
N	0.066518	1.775825	-1.642879
N	0.191815	1.637536	-2.946639
N	-0.024706	-0.987490	-1.560718
N	0.113903	-1.260361	1.051218
N	0.088145	-1.310653	2.392144
N	1.127428	-0.332551	5.580655
C	-0.234918	3.246242	0.211944
C	0.065476	3.115250	-1.262316
C	0.181941	0.481453	-3.531717
C	0.299890	0.543520	-5.007106
C	0.053601	-0.830294	-2.897084
C	0.003965	-1.947633	-3.743091
C	-0.141083	-3.210134	-3.223853
C	-0.215424	-3.357444	-1.850512
C	-0.140722	-2.234843	-1.045457
C	-0.143125	-2.357586	0.407368
C	-0.390764	-3.624012	1.113087
C	0.813586	-0.539354	3.209371
C	0.466685	-0.968553	4.632678
H	-0.431360	4.698754	1.634791
H	-0.026733	5.199974	-0.034399
H	0.411787	1.592955	-5.305599
H	1.170364	-0.022930	-5.377276
H	-0.596946	0.135951	-5.504457
H	0.071004	-1.799137	-4.821823
H	-0.191739	-4.082227	-3.881432
H	-0.319557	-4.349824	-1.408965
H	-1.401624	-3.625968	1.563839
H	-0.327544	-4.504374	0.465504
H	1.820068	0.374349	5.328352
H	0.971357	-0.571897	6.561653

H	0.330003	-3.754982	1.938358
H	-0.482233	-1.978007	2.989031
H	-2.624559	0.097665	-0.714904
H	-2.516182	0.983684	0.580388
H	2.708862	0.684135	0.043044
H	1.924481	0.651174	1.532586

Fe^{3+} Hdapsox Isomer VII LDA

Fe	10.632758	6.414528	1.973751
O	9.267816	5.461380	3.269482
O	9.666483	2.713175	5.411603
O	10.702311	10.742096	3.471602
O	8.962289	7.766468	2.427159
O	11.433150	7.291549	3.542696
N	11.956378	5.987712	0.385687
N	11.186583	4.389934	2.149056
N	10.664574	3.661713	3.125865
N	7.966481	4.226227	5.372742
H	7.514681	3.829811	6.197735
H	7.548655	5.020931	4.894716
N	11.303064	8.306776	1.065812
N	11.013273	9.481550	1.634813
N	11.460319	8.897210	5.130125
H	11.308695	9.900457	5.305653
H	11.728961	8.251313	5.875781
C	12.392231	4.730302	0.233356
C	13.186352	4.376549	-0.854166
H	13.532550	3.346140	-0.968247
C	13.514624	5.347516	-1.780765
H	14.126124	5.093813	-2.651064
C	13.077254	6.651000	-1.595494
H	13.348582	7.432529	-2.308846
C	12.305160	6.944562	-0.480066
C	11.948280	3.810752	1.259413
C	12.271670	2.385663	1.294213
H	12.257202	2.030968	2.336675
H	13.240730	2.167053	0.824667
H	11.499311	1.799414	0.760795
C	9.687087	4.321814	3.697214
C	9.088709	3.665031	4.920301
C	11.896045	8.285552	-0.087296
C	12.231524	9.504636	-0.837041
H	12.743265	9.293097	-1.782917
H	11.325578	10.088080	-1.084202
H	12.893120	10.158031	-0.238230
C	10.935922	9.658483	2.985425
C	11.290531	8.484393	3.902141
O	9.128923	5.892482	0.495370
H	10.984062	10.349059	1.077826
H	8.355640	7.887639	1.665120
H	8.530312	7.105581	3.025945
H	9.412154	5.579007	-0.389718
H	8.578111	5.175470	0.879166

Fe^{3+} Hdapsox Isomer VIII LDA

Fe	11.292366	6.435147	2.193215
O	8.272317	3.327204	3.512151
O	9.368472	6.103600	1.713921
O	12.353829	10.659432	3.593662
O	10.219347	7.919868	3.415556
O	12.852828	7.178122	3.331070
N	12.178762	5.886600	0.347192
N	11.196682	4.306718	2.023465
N	10.458591	3.629159	2.910480
N	7.372045	5.042248	1.803766
H	6.859323	5.766911	1.298764
H	6.896827	4.244123	2.255031
N	11.918465	8.256414	1.124519
N	11.860158	9.439782	1.762131
N	13.701815	8.747356	4.722372
H	13.694902	9.752776	4.945099
H	14.250224	8.082421	5.271525
C	12.401223	4.594734	0.099797
C	13.002352	4.183351	-1.083675
H	13.187624	3.120986	-1.263207
C	13.329249	5.137376	-2.030876
H	13.788111	4.839453	-2.977796
C	13.063544	6.472982	-1.775334
H	13.301000	7.244560	-2.512187
C	12.499913	6.813635	-0.553987
C	11.845364	3.686547	1.088986
C	11.898063	2.229490	0.949903
H	11.554699	1.748511	1.876547
H	12.918912	1.895207	0.703809
H	11.241750	1.889442	0.127856
C	9.140823	3.915790	2.889135
C	8.651114	5.120146	2.048342
C	12.301857	8.186406	-0.109246
C	12.649796	9.317618	-0.978947
H	13.725931	9.281891	-1.227620
H	12.102465	9.253935	-1.934515
H	12.450061	10.304056	-0.540667
C	12.329256	9.588150	3.031823
C	12.973734	8.369667	3.703007
O	11.050837	5.685229	4.288590
H	11.931469	5.762087	4.715052
H	10.846796	4.692535	4.155696
H	10.076262	7.285125	4.164428
H	9.332026	8.157928	3.072163
H	11.672836	10.313351	1.251413

Fe^{3+} Hdapsox Isomer IX LDA

Fe	10.542170	6.543892	2.209321
O	9.981603	5.751778	4.065131
O	8.995542	2.578498	5.168036
O	10.011567	11.175412	3.164312
O	9.036649	7.816109	2.846454
O	8.890407	6.143103	0.955746
O	12.049750	7.109339	3.550089
N	11.768048	6.107551	0.533590
N	10.817540	4.429036	2.141449
N	10.316894	3.689204	3.121325
N	8.966515	4.567215	6.286043
H	8.536059	4.177017	7.125001
H	9.187463	5.559601	6.225921
N	11.173768	8.476197	1.259375
N	10.959599	9.695464	1.773323
N	8.165208	9.563428	3.994251
H	8.288529	10.567282	4.188928
H	7.387710	9.028419	4.384644
C	11.993998	4.824534	0.221370
C	12.690787	4.469895	-0.929246
H	12.874041	3.415281	-1.151702
C	13.142575	5.470040	-1.767544
H	13.690670	5.221787	-2.680501
C	12.895722	6.793039	-1.440935
H	13.244905	7.594727	-2.094831
C	12.200053	7.080821	-0.272726
C	11.487147	3.863169	1.175940

C	11.728233	2.422767	1.081781
H	11.186968	1.898735	1.881127
H	12.806498	2.202410	1.181076
H	11.414468	2.029224	0.100110
C	9.883472	4.473862	4.081246
C	9.232512	3.769725	5.251976
C	11.899825	8.425916	0.180911
C	12.387930	9.635384	-0.502235
H	12.880275	9.410310	-1.454809
H	11.555737	10.330535	-0.714343
H	13.131417	10.177453	0.113617
C	10.065276	10.041091	2.737673
C	9.051604	9.013162	3.204398
H	13.018443	7.124997	3.405395
H	11.855280	6.576034	4.354635
H	8.630432	5.220604	0.748177
H	8.112853	6.581683	1.366997
H	11.517973	10.490208	1.425713

Fe^{3+} Hdapsox Isomer X LDA

Fe	10.637826	6.728944	2.203476
O	9.397960	3.161135	5.115924
O	8.925368	6.113050	3.274033
O	9.211182	11.135537	2.674100
O	10.551374	8.070483	3.692507
O	8.966882	6.753169	0.875581
O	12.559532	6.667322	3.176059
N	11.752994	6.204670	0.540838
N	10.941960	4.543549	2.291831
N	10.591294	3.746844	3.311965
N	7.777679	5.167196	4.987599
H	7.760557	4.344880	5.608567
H	7.076633	5.907027	5.050814
N	10.895435	8.596893	1.055014
N	10.328538	9.751529	1.274405
N	9.790396	9.892539	4.802876
H	9.393781	10.832361	4.624455
H	9.920233	9.505440	5.738354
C	12.134410	4.935990	0.349842
C	12.886953	4.571389	-0.756369
H	13.186497	3.533375	-0.913711
C	13.251881	5.552163	-1.668870
H	13.852073	5.290268	-2.544591
C	12.854503	6.854606	-1.462967
H	13.136267	7.647871	-2.159690
C	12.081774	7.160538	-0.338107
C	11.702634	4.010781	1.379326
C	12.101592	2.594006	1.409932
H	12.741464	2.373590	2.286225
H	12.676376	2.300212	0.524601
H	11.216243	1.934954	1.464767
C	9.618959	3.965167	4.234295
C	8.750599	5.203417	4.113332
C	11.592324	8.480205	-0.062561
C	11.826412	9.606885	-0.974075
H	12.868255	9.967844	-0.895722
H	11.661229	9.319676	-2.024389
H	11.165285	10.442829	-0.706438
C	9.824640	10.096427	2.468010
C	10.092069	9.242033	3.713549
H	13.389951	6.652439	2.656354
H	12.591872	7.452420	3.765539
H	8.177926	6.549114	1.425334
H	8.770863	7.570627	0.369294
H	11.066000	2.837545	3.422242

Fe^{3+} Hdapsox Isomer XI LDA

Fe	10.489460	6.509579	2.113979
O	9.674418	5.768684	3.826827
O	8.980327	2.636280	5.180368
O	10.247792	11.108288	3.250731
N	8.852912	7.962834	2.796996
O	8.883590	6.026640	0.795005
O	11.920834	7.133590	3.463766
N	11.763515	6.087770	0.499069
N	10.931132	4.428433	2.192651
N	10.454481	3.710384	3.199622
N	8.715113	4.691706	6.139798
H	8.264999	4.321367	6.978560
H	8.899600	5.691391	6.060354
N	11.039161	8.470532	1.117647
N	10.715052	9.694747	1.560412
O	9.742954	8.684850	4.775662
C	12.135153	4.813715	0.288728
C	12.920010	4.459237	-0.802618
H	13.214667	3.416160	-0.946465
C	13.314759	5.447114	-1.684293
H	13.931859	5.198964	-2.552355
C	12.930112	6.758153	-1.456705
H	13.245176	7.548307	-2.141344
C	12.150200	7.054123	-0.343855
C	11.675678	3.865241	1.280826
C	12.015869	2.443393	1.263401
H	11.511657	1.925346	2.090260
H	13.106874	2.302230	1.365213
H	11.725891	1.978670	0.305051
C	9.791493	4.503247	4.011871
C	9.120314	3.846802	5.192710
C	11.737516	8.398622	0.020465
C	12.127004	9.596723	-0.742647
H	12.654186	9.356269	-1.672494
H	11.242969	10.201404	-1.015056
H	12.804334	10.243088	-0.151560
C	10.214321	9.986533	2.824527
C	9.578355	8.841817	3.594689
H	12.845582	7.433339	3.344364
H	11.723660	7.071932	4.424335
H	8.409274	8.358100	1.957525
H	8.233686	7.356285	3.352750
H	9.110632	5.880819	-0.148489
H	8.307199	5.273392	1.050670
H	11.111966	10.518915	1.081962

Fe^{3+} Hdapsox Isomer XII LDA

Fe	10.673167	6.693255	2.142171
O	8.949242	3.187881	4.871095
O	8.161984	5.934647	4.441096
O	10.052758	11.292417	2.925874
N	9.015592	8.039868	2.862917
O	9.013067	6.035948	1.083144
O	12.517237	7.184577	3.014230
N	11.776182	6.125791	0.518732
N	10.952162	4.459968	2.302702
N	10.428912	3.643532	3.233287
N	10.413025	6.262559	4.349201
H	13.180663	6.458661	2.989824
H	11.291650	5.796456	4.609088
N	11.055195	8.559306	1.081679
N	10.774889	9.820349	1.372700

O	10.115927	8.945588	4.634434
C	12.146920	4.856769	0.359683
C	12.906762	4.463562	-0.734073
H	13.207971	3.420449	-0.846922
C	13.265682	5.416543	-1.670386
H	13.861765	5.133736	-2.539974
C	12.862007	6.725022	-1.501489
H	13.130824	7.490288	-2.230211
C	12.107356	7.060694	-0.378123
C	11.684067	3.924097	1.368725
C	12.028008	2.504146	1.240790
H	11.606076	1.846710	2.008798
H	13.124022	2.389516	1.271193
H	11.692370	2.129673	0.260299
C	9.532151	4.005214	4.182778
C	9.293689	5.483964	4.367045
C	11.665126	8.395024	-0.085286
C	11.906484	9.527828	-0.972788
H	12.360325	9.231797	-1.923373
H	10.958457	10.059145	-1.159134
H	12.555437	10.263026	-0.465064
C	10.209116	10.128843	2.551926
C	9.749968	9.023099	3.467883
H	12.955784	7.941878	2.566516
H	10.305382	7.228564	4.765021
H	8.512020	8.329764	2.015961
H	8.440228	7.440546	3.506378
H	8.718605	6.592489	0.328090
H	9.128213	5.134383	0.707877
H	10.594981	2.631160	3.140650

Fe^{3+} H_2dapsox Isomer I HS LDA

Fe	0.021196	2.376786	2.626225
O	-0.984255	3.784132	1.379722
O	0.337522	5.853726	-1.117331
O	-1.779292	2.853536	3.651890
O	-3.447250	1.066477	6.160407
O	-0.886936	1.062898	1.341444
H	-0.850116	0.083004	1.311492
H	-1.598733	1.365010	0.736231
O	0.753599	3.853802	3.845770
H	1.672081	4.171074	3.982837
H	0.151346	4.412053	4.383375
N	1.802624	1.170151	2.760902
N	1.446695	3.015511	1.120088
N	1.001029	3.995793	0.341938
H	1.476923	4.557207	-0.411984
N	-1.828784	5.977564	-0.376742
H	-2.531800	5.594387	0.255205
H	-2.085050	6.747318	-1.004060
N	-0.201789	0.922619	4.224657
N	-1.349714	1.023554	4.885995
H	-1.764765	0.435396	5.655312
N	-4.286865	2.957168	5.170500
H	-5.152270	2.961443	5.720904
H	-4.132187	3.691646	4.479643
C	2.821913	1.384553	1.920646
C	3.982040	0.621281	1.974762
H	4.802262	0.812144	1.275943
C	4.079099	-0.383272	2.923427
H	4.981463	-0.999529	2.987341
C	3.020877	-0.598229	3.790909
H	3.071086	-1.382960	4.551984
C	1.890343	0.201990	3.680997
C	2.605543	2.456562	0.955752
C	3.599085	2.800104	-0.062054
H	3.834642	1.914452	-0.680786
H	3.287938	3.605999	-0.740036
H	4.549390	3.106960	0.413130
C	-0.265026	4.354478	0.534215
C	-0.600960	5.500147	-0.413149
C	0.724170	0.073446	4.547429
C	0.668321	-0.896139	5.641840
H	0.754392	-1.927260	5.250679
H	-0.248733	-0.842062	6.243691
H	1.525816	-0.752237	6.324750
C	-2.126665	2.043511	4.535954
C	-3.398989	2.004491	5.373545

Fe^{3+} H_2dapsox IS LDA

Fe	0.020568	2.356558	2.624852
O	-0.920492	3.994512	1.544310
O	0.309074	5.748560	-1.222659
O	-1.885981	2.670123	3.485174
O	-3.390331	1.184439	6.271624
O	-0.789210	1.179612	1.382654
H	-1.768431	1.173190	1.287017
H	-0.410799	0.323313	1.083850
O	0.645297	3.656011	3.862382
H	1.590420	3.916250	3.938444
H	0.080308	4.457060	3.961582
N	1.795257	1.162230	2.758122
N	1.413961	2.985478	1.100285
N	0.969744	3.963480	0.319765
H	1.413466	4.441992	-0.507405
N	-1.750319	6.125939	-0.290518
H	-2.413302	5.854800	0.435710
H	-2.005395	6.867024	-0.951912
N	-0.172589	0.936670	4.269223
N	-1.317150	1.046433	4.935891
H	-1.663466	0.535107	5.784295
N	-4.343340	2.866124	5.037602
H	-5.197925	2.914676	5.602236
H	-4.237031	3.491554	4.238722
C	2.803306	1.367018	1.903826
C	3.979847	0.627322	1.968073
H	4.790906	0.818924	1.259022
C	4.105002	-0.346192	2.942478
H	5.019482	-0.942673	3.017155
C	3.055946	-0.555255	3.822546
H	3.123795	-1.319368	4.602913
C	1.911264	0.222136	3.702792
C	2.564436	2.415727	0.920460
C	3.541493	2.743726	-0.120716
H	3.868886	1.829929	-0.646793
H	3.171013	3.448761	-0.877305
H	4.450742	3.184753	0.330989
C	-0.243364	4.435193	0.599614
C	-0.578795	5.536398	-0.404158
C	0.754772	0.093220	4.584922
C	0.713844	-0.883019	5.674863
H	0.819564	-1.908423	5.273950
H	-0.207775	-0.852468	6.271613
H	1.565417	-0.730081	6.362963
C	-2.156162	1.969584	4.481832
C	-3.407336	1.995470	5.354976

Fe^{3+} H_2dapsox LS LDA

Fe	0.347860	2.183715	2.343987
O	-1.002490	3.383552	1.436784
O	-0.008654	5.740096	-0.959866
O	-1.518665	3.517281	4.696696
O	-3.923083	1.105610	5.526965
O	-0.286362	0.823116	1.125300
H	0.289786	0.270605	0.552510
H	-1.131002	0.994350	0.652618
O	0.592134	3.535940	3.530064
H	1.442517	3.611999	4.016417
H	-0.480240	3.571769	4.214737
N	1.836916	1.221019	2.719010
N	1.498668	2.964072	1.109061
N	0.931643	3.938806	0.392662
H	1.310692	4.621994	-0.319500
N	-2.162449	5.531827	-0.199331
H	-2.799186	5.033293	0.421863
H	-2.528322	6.285070	-0.790876
N	-0.376108	1.102587	3.844115
N	-1.576150	1.173132	4.449051
H	-3.298900	0.448000	5.098920
N	-3.888056	3.311830	5.961866
H	-4.791814	3.277432	6.451470
H	-3.381117	4.201497	5.888078
C	2.952986	1.486375	2.005264
C	4.099434	0.734505	2.227483
H	5.015405	0.939401	1.664421
C	4.055748	-0.281951	3.171401
H	4.948830	-0.885218	3.360920
C	2.884237	-0.545361	3.872613
H	2.847228	-1.350710	4.612583
C	1.763407	0.238016	3.624131
C	2.745648	2.559422	1.046680
C	3.768363	3.103387	0.158704
H	4.472877	2.320762	-0.164826
H	3.346170	3.577614	-0.740678
H	4.369922	3.869170	0.689114
C	-0.375871	4.100046	0.619620
C	-0.880420	5.230288	-0.265472
C	0.460388	0.182028	4.271400
C	0.153672	-0.758076	5.345520
H	-0.909008	-1.044893	5.324065
H	0.331843	-0.290372	6.333932
H	0.779830	-1.659603	5.292086
C	-2.019305	2.345402	4.792120
C	-3.350655	2.251837	5.460014

Fe^{3+} H_2dapsox Isomer II LDA

Fe	-0.059390	2.169138	2.553329
O	-1.118357	3.518500	1.270730
O	0.149868	5.976082	-0.871887
O	-2.058000	2.079257	3.168728
O	-2.204403	3.578893	5.497856
O	-0.578069	0.845838	1.050204
H	-0.497736	-0.131983	1.054893
H	-1.395504	1.072378	0.553863
O	-0.085647	3.506208	4.053956
H	0.608180	4.137954	4.337161
H	-0.939842	3.633694	4.660371
N	1.820627	1.161711	2.792736
N	1.404404	3.116263	1.288574
N	0.924840	4.107146	0.541323
H	1.410928	4.783807	-0.098148
N	-2.073813	5.742728	-0.355201
H	-2.766300	5.220220	0.182506
H	-2.379535	6.528168	-0.938718
N	-0.232800	0.640991	4.108412
N	-1.358905	0.760827	4.835397
H	-1.394050	0.434190	5.811826
N	-4.118537	2.365727	5.795342
H	-4.543115	3.061440	6.421549
H	-4.677136	1.549890	5.533437
C	2.867445	1.539533	2.051645
C	4.092830	0.890395	2.140885
H	4.938517	1.219248	1.529170
C	4.223245	-0.173030	3.018148
H	5.176577	-0.703315	3.106879
C	3.135501	-0.553197	3.788247
H	3.217194	-1.383404	4.496154
C	1.941008	0.142172	3.651317
C	2.614198	2.666120	1.160556
C	3.626333	3.166672	0.230894
H	4.050040	2.334520	-0.359539
H	3.249422	3.917448	-0.476724
H	4.472176	3.617755	0.784395
C	-0.396591	4.265401	0.584192
C	-0.792517	5.439438	-0.301723
C	0.750550	-0.121624	4.457354
C	0.750933	-1.085153	5.561024
H	1.182992	-2.046248	5.231805
H	-0.252511	-1.305558	5.953316
H	1.387891	-0.729841	6.393704
C	-2.207473	1.682460	4.335126
C	-2.933519	2.595561	5.293400

Fe^{3+} Hdapsox Isomer III LDA

Fe	0.028783	2.375938	2.622405
O	-0.678036	4.213449	1.855415
O	-1.357263	3.594164	-0.811662
O	-2.003352	2.422657	3.194252
O	-1.956874	3.435457	5.817993
O	-0.653903	1.729903	0.821115
H	-1.265700	0.965200	0.769751
H	-0.989440	2.436139	0.119851
O	0.197230	3.361835	4.393546
H	0.695557	4.204900	4.450871
H	-0.649665	3.464660	5.003595
N	1.803277	1.164492	2.749709
N	1.595970	3.264660	1.418911
N	1.157121	4.224064	0.583537
H	1.642486	4.402826	-0.306926
N	-1.367581	5.876874	-0.935154
H	-1.081515	6.766941	-0.520430
H	-2.019175	5.897939	-1.729777
N	-0.353715	0.672003	3.903843
N	-1.488178	0.780309	4.619456
H	-1.573989	0.314229	5.533681
N	-4.080655	2.587036	5.786271
H	-4.420386	3.222396	6.519466
H	-4.754734	1.961246	5.339100
C	2.917619	1.545549	2.119595
C	4.088249	0.800469	2.199039
H	4.993832	1.132257	1.682655
C	4.086340	-0.369571	2.939459
H	4.993094	-0.977442	3.016667
C	2.923982	-0.760097	3.583548
H	2.896955	-1.680196	4.174778
C	1.793676	0.040659	3.471618
C	2.781923	2.756270	1.317338
C	3.848091	3.260038	0.448863

H	3.936255	2.644508	-0.467692
H	3.700671	4.310426	0.155950
H	4.825382	3.201760	0.955464
C	-0.142125	4.537486	0.787309
C	-1.021599	4.724633	-0.425313
C	0.538936	-0.227989	4.165948
C	0.372332	-1.337880	5.107060
H	0.850181	-2.253375	4.721359
H	-0.683893	-1.583022	5.297553
H	0.865051	-1.113704	6.073848
C	-2.222005	1.863265	4.277358
C	-2.838990	2.675974	5.389050

Fe^{3+} H_2dapsox Isomer V LDA

Fe	0.031513	2.375130	2.622166
O	-0.988538	3.732276	1.331417
O	0.345257	5.843491	-1.122343
O	-1.748576	2.911976	3.699020
O	-3.461886	1.049079	6.119167
O	-0.950151	1.066836	1.384635
H	-1.035532	0.090348	1.419188
H	-1.614933	1.412612	0.750259
O	0.729551	3.874074	3.835165
H	1.627995	4.249546	3.957355
H	0.099327	4.390698	4.382395
N	1.815011	1.169520	2.768757
N	1.465823	3.025462	1.143916
N	1.021650	4.001648	0.358048
H	1.512335	4.579257	-0.372341
N	-1.864688	5.839339	-0.507792
H	-2.572943	5.435052	0.104807
H	-2.130376	6.590780	-1.153209
N	-0.210980	0.919493	4.189446
N	-1.360550	1.017721	4.850511
H	-1.790860	0.397821	5.584183
N	-4.220063	3.042265	5.276977
H	-5.073111	3.050641	5.846601
H	-4.036040	3.821080	4.643951
C	2.848769	1.404733	1.953673
C	4.015356	0.651677	2.023963
H	4.854559	0.864861	1.354991
C	4.093189	-0.374676	2.950383
H	4.997142	-0.987754	3.022884
C	3.013670	-0.617971	3.784143
H	3.050871	-1.426948	4.519448
C	1.883837	0.184087	3.671761
C	2.634735	2.481509	0.993399
C	3.630530	2.860485	-0.009589
H	4.133368	1.971722	-0.424334
H	3.206539	3.424881	-0.853009
H	4.423285	3.485147	0.448233
C	-0.261700	4.319537	0.504337
C	-0.608688	5.441210	-0.466903
C	0.700723	0.052553	4.513288
C	0.570515	-0.924267	5.595771
H	0.051734	-1.836421	5.238676
H	-0.010638	-0.528369	6.444999
H	1.547861	-1.243484	5.983822
C	-2.110901	2.075743	4.550635
C	-3.376949	2.036932	5.398769

Fe^{3+} H_2dapsox Isomer VII LDA

Fe	10.548191	6.474851	1.942586
O	9.229736	5.551869	3.463202
O	9.615539	2.403558	4.961080
O	10.770906	10.751167	3.444190
O	8.932770	7.804810	2.416533
O	11.422758	7.288122	3.472722
N	11.933881	5.986825	0.397087
N	11.131964	4.438647	2.167651
N	10.563529	3.774926	3.169912
N	8.027163	3.916606	5.621063
H	7.644677	3.310015	6.354189
H	7.614474	4.837668	5.478790
N	11.261504	8.317679	1.015497
N	10.974410	9.497282	1.578647
N	11.746545	8.910434	5.011975
H	11.659709	9.922094	5.200487
H	12.080998	8.267241	5.737211
C	12.420427	4.742396	0.307888
C	13.272485	4.376253	-0.726386
H	13.676624	3.361943	-0.786286
C	13.596924	5.322276	-1.685086
H	14.252191	5.056741	-2.520793
C	13.104959	6.612620	-1.567746
H	13.376828	7.375792	-2.302069
C	12.285020	6.924668	-0.487573
C	11.971159	3.849663	1.366535
C	12.381725	2.453482	1.519902
H	12.929836	2.311233	2.471917
H	13.035499	2.106489	0.710790
H	11.502464	1.782155	1.553772
C	9.575314	4.401709	3.801496
C	9.034437	3.479485	4.890477
C	11.857646	8.275029	-0.138289
C	12.197045	9.473792	-0.911490
H	12.681107	9.243683	-1.868201
H	11.298229	10.075262	-1.144472
H	12.887596	10.123182	-0.338130
C	10.981737	9.678553	2.936688
C	11.399842	8.500141	3.828194
O	9.154759	5.973813	0.433797
H	10.940861	10.361585	1.014018
H	10.742123	2.806978	3.549748
H	8.358320	8.261085	1.763303
H	8.352213	7.353559	3.071504
H	9.412709	5.562490	-0.419278
H	8.252212	5.648936	0.643033

Fe^{3+} H_2dapsox Isomer VIII LDA

Fe	11.193977	6.473749	2.198092
O	8.317075	3.055192	3.457887
O	9.290889	6.003468	1.788807
O	12.722516	10.659491	3.495339
O	10.076447	8.047126	3.231786
O	12.734653	7.137124	3.295800
N	12.171732	5.918850	0.379922
N	11.226023	4.275973	2.022808
N	10.454283	3.555448	2.884539
N	7.279949	4.998049	2.037029
H	6.759006	5.736285	1.552720
H	6.786232	4.183214	2.432761
N	11.833867	8.286782	1.134796
N	11.795663	9.470385	1.803983
N	13.935036	8.595243	4.539909
H	14.098782	9.594345	4.741570
H	14.440035	7.869381	5.058122
C	12.461923	4.638165	0.135505
C	13.120908	4.246252	-1.021760

H	13.367828	3.193919	-1.189637
C	13.438544	5.206263	-1.967709
H	13.941392	4.924031	-2.898020
C	13.114489	6.528789	-1.718185
H	13.354257	7.309674	-2.445737
C	12.499793	6.853040	-0.516313
C	11.924748	3.689780	1.105353
C	12.088681	2.246082	0.916182
H	11.694603	1.624783	1.731769
H	13.157010	1.994981	0.792780
H	11.583861	1.925686	-0.015470
C	9.092180	3.794769	2.912552
C	8.573064	5.048430	2.188206
C	12.289024	8.226818	-0.075443
C	12.704958	9.357427	-0.909323
H	13.788473	9.291020	-1.123268
H	12.192933	9.321225	-1.887774
H	12.519888	10.347381	-0.471881
C	12.502557	9.594744	2.979759
C	13.062974	8.311557	3.615038
O	10.689828	5.820134	4.221337
H	11.140624	6.358701	4.907835
H	10.863946	4.872869	4.434324
H	9.237066	7.707165	3.612094
H	9.863810	8.888128	2.767252
H	10.712968	2.579060	3.101372
H	11.691188	10.350833	1.275468

Fe^{3+} H_2dapsox Isomer IX LDA

Fe	10.509196	6.614325	2.191549
O	9.882543	5.775316	4.168097
O	9.332276	2.426430	5.016665
O	9.999928	11.260043	3.033278
O	9.118835	7.865635	2.894375
O	8.855767	6.164796	1.037337
O	12.047158	7.040220	3.479489
N	11.738612	6.103489	0.532488
N	10.814383	4.454298	2.173304
N	10.288749	3.789211	3.196528
N	8.823000	4.195812	6.383947
H	8.453527	3.614046	7.143121
H	8.837364	5.209692	6.494783
N	11.192224	8.501834	1.232594
N	10.989505	9.729536	1.724509
N	8.159504	9.652583	3.906952
H	8.245133	10.672088	4.050835
H	7.386941	9.124717	4.322624
C	11.970619	4.815592	0.243075
C	12.680827	4.437305	-0.888020
H	12.862625	3.379329	-1.099461
C	13.158096	5.423381	-1.734650
H	13.717446	5.157037	-2.636931
C	12.926258	6.750755	-1.422491
H	13.302420	7.540601	-2.077130
C	12.209501	7.064042	-0.270473
C	11.455578	3.861297	1.215297
C	11.695211	2.421532	1.094050
H	11.240378	1.820061	1.892378
H	12.782140	2.215897	1.100591
H	11.313689	2.041154	0.129216
C	9.829164	4.533356	4.199744
C	9.279871	3.619006	5.291027
C	11.933058	8.422022	0.160278
C	12.454879	9.610818	-0.528097
H	12.984777	9.369512	-1.456600
H	11.638736	10.311244	-0.787683
H	13.179409	10.161167	0.105605
C	10.070703	10.114118	2.658983
C	9.076130	9.092408	3.172078
H	11.989181	6.703272	4.399976
H	12.952089	7.384208	3.321448
H	8.699331	5.515738	0.319818
H	8.044924	6.703840	1.162426
H	11.543592	10.515148	1.345509
H	10.192303	2.756668	3.356358

Fe^{3+} H_2dapsox Isomer X LDA

Fe	10.602419	6.718794	2.208560
O	9.411815	3.132018	5.101417
O	9.006924	6.119333	3.307115
O	9.324024	11.267306	2.615064
O	10.501732	8.138222	3.678568
O	8.975276	6.644831	0.883354
O	12.413877	6.633750	3.268546
N	11.764171	6.208529	0.527980
N	10.962336	4.525447	2.289485
N	10.614249	3.725952	3.300667
N	7.797041	5.159376	4.970145
H	7.745069	4.330452	5.584389
H	7.097739	5.904078	5.030244
N	10.919313	8.573536	1.044507
N	10.325098	9.744389	1.302297
N	9.739135	9.948275	4.818292
H	9.384656	10.911341	4.702753
H	9.842620	9.535280	5.749392
C	12.144364	4.941569	0.341142
C	12.889697	4.572277	-0.776580
H	13.186733	3.533645	-0.933161
C	13.240896	5.542552	-1.698612
H	13.823305	5.275746	-2.585286
C	12.845757	6.852063	-1.488460
H	13.114883	7.629498	-2.208537
C	12.100189	7.159057	-0.357800
C	11.724944	4.003022	1.366817
C	12.124226	2.588892	1.384693
H	12.732241	2.349066	2.280170
H	12.733353	2.304518	0.518896
H	11.238377	1.925746	1.396457
C	9.641719	3.939918	4.233199
C	8.790166	5.191202	4.127258
C	11.610780	8.493042	-0.055489
C	11.854124	9.653380	-0.927021
H	12.659734	9.475049	-1.649314
H	10.955240	9.921350	-1.517914
H	12.141525	10.539985	-0.333275
C	9.845695	10.184501	2.501494
C	10.052725	9.311829	3.726389
H	13.292510	6.294828	2.992507
H	12.549312	7.388842	3.882107
H	8.160219	6.219157	1.226517
H	8.928172	6.671742	-0.095964
H	11.078341	2.805998	3.391821
H	10.231936	10.436368	0.539743

Fe^{3+} H_2dapsox Isomer XI LDA

Fe	10.451931	6.548246	2.162630
O	9.079524	5.578666	3.641871
O	9.620815	2.482632	5.194513
O	9.953735	11.393573	2.823662

N	9.161674	8.137543	3.301838
O	8.745996	6.364682	1.003207
O	11.696895	6.834092	3.694602
N	11.743103	6.114450	0.567627
N	10.916006	4.465360	2.260106
N	10.381662	3.793053	3.277352
N	8.047385	3.980184	5.920630
H	7.744780	3.397469	6.709583
H	7.578682	4.872028	5.763169
N	10.935229	8.542088	1.058053
N	10.488464	9.781286	1.318361
O	10.857618	9.034505	4.524800
C	12.178100	4.851796	0.406156
C	13.023608	4.493647	-0.632587
H	13.361695	3.458392	-0.738706
C	13.426246	5.468463	-1.531395
H	14.089420	5.216276	-2.365209
C	12.977470	6.763443	-1.361134
H	13.289794	7.543080	-2.059611
C	12.132223	7.067639	-0.292648
C	11.701011	3.898332	1.394567
C	12.080775	2.485578	1.386031
H	11.452626	1.859083	2.035094
H	13.133484	2.362007	1.708370
H	12.017223	2.069990	0.365884
C	9.447419	4.430323	3.969946
C	9.003124	3.539120	5.130242
C	11.655087	8.410587	-0.028542
C	11.990699	9.560120	-0.882325
H	12.612974	9.295342	-1.743868
H	11.083605	10.045292	-1.292926
H	12.547620	10.325355	-0.305581
C	10.148468	10.237653	2.586368
C	10.067922	9.126053	3.604768
H	12.649938	6.608167	3.761902
H	11.499943	7.656211	4.284414
H	8.383212	8.398977	2.678003
H	8.863842	7.549669	4.097379
H	8.680564	6.507332	0.033253
H	8.062099	5.703145	1.248780
H	10.653032	10.532165	0.626385
H	10.610152	2.843226	3.675026

Fe^{3+} H_2dapsox Isomer XII LDA

Fe	10.674065	6.668748	2.149739
O	8.881152	3.170882	4.787075
O	8.133283	5.949071	4.401924
O	10.191602	11.312086	2.951308
N	9.057108	8.063089	2.890077
O	9.005700	6.015635	1.170662
O	12.462465	7.231654	2.984144
N	11.764511	6.128819	0.496978
N	10.960653	4.478371	2.303584
N	10.421512	3.655533	3.213565
N	10.392602	6.241144	4.344068
H	13.080510	6.536174	3.302503
H	11.243808	5.746866	4.642052
N	11.026485	8.524662	1.028753
N	10.679380	9.776132	1.369124
O	10.145159	8.966934	4.678606
C	12.176580	4.869795	0.370279
C	12.958183	4.476997	-0.710481
H	13.294426	3.441748	-0.794465
C	13.292327	5.416508	-1.665373
H	13.902784	5.134352	-2.524842
C	12.850475	6.718278	-1.523636
H	13.104144	7.477909	-2.263579
C	12.084240	7.050355	-0.412229
C	11.734868	3.948668	1.394335
C	12.129107	2.542398	1.312886
H	11.807670	1.913364	2.150127
H	13.228429	2.479535	1.260080
H	11.738019	2.101622	0.380492
C	9.484968	4.000550	4.137986
C	9.252903	5.477801	4.338743
C	11.622623	8.387850	-0.129430
C	11.841178	9.517564	-1.030120
H	12.292866	9.212565	-1.978539
H	10.883294	10.019498	-1.253440
H	12.510143	10.261967	-0.560095
C	10.250023	10.151383	2.606268
C	9.800184	9.031575	3.513992
H	13.005526	7.827310	2.420430
H	10.293981	7.188799	4.792686
H	8.547494	8.381076	2.054657
H	8.460775	7.472677	3.526566
H	8.542779	6.604273	0.532626
H	9.102463	5.150745	0.711902
H	10.593372	2.645015	3.110925
H	10.943078	10.541098	0.729103

Fe^{2+} dapsox Isomer I HS LDA

Fe	-1.992248	4.087351	11.170977
N	-2.833780	5.937373	10.992525
N	-2.639591	4.266239	9.162828
N	-2.457915	3.269009	8.285770
N	-1.283053	-0.024195	8.849213
N	-1.833450	5.013967	13.079147
N	-1.285827	4.380801	14.124687
N	0.365577	1.253446	14.273262
O	-1.885898	2.100905	10.193588
O	-1.888316	0.935909	6.870323
O	-0.640434	2.858384	12.509959
O	-0.084205	2.695010	15.983068
O	0.041343	4.404255	10.666039
O	-3.602469	2.867486	11.852521
H	-3.214368	2.203545	11.200305
C	-3.330136	6.345614	9.807466
C	-3.900645	7.602663	9.652639
C	-3.960613	8.455261	10.743463
C	-3.447730	8.032289	11.960584
C	-2.887669	6.765599	12.054878
C	-3.215146	5.367219	8.762714
C	-3.699902	5.583275	7.389697
C	-2.043608	2.200103	8.918067
C	-1.734088	0.983010	8.077806
C	-2.312072	6.215400	13.251180
C	-2.267057	6.933028	14.535546
H	-3.265212	7.306391	14.815372
H	-1.594354	7.805709	14.480371
H	-1.892936	6.245717	15.307938
C	-0.723185	3.266339	13.727947
C	-0.120221	2.391346	14.803864
H	-4.404221	9.448839	10.645657
H	-4.290919	7.899131	8.675532
H	0.265680	1.132338	13.264377
H	-3.475295	8.674790	12.844538
H	0.799505	0.562554	14.878199
H	-3.448390	4.700805	6.784336
H	0.330779	5.291151	10.955882

H	-1.018653	-0.905739	8.419556
H	-1.188121	0.162822	9.848515
H	-4.791953	5.736564	7.372230
H	0.204004	3.775568	11.442797
H	-3.237448	6.479884	6.945269
H	-4.447888	3.174639	11.471544

Fe^{2+} dapsox IS LDA

Fe	-2.177396	4.252982	10.948545
N	-2.966877	5.896193	10.939468
N	-2.675094	4.360560	9.165902
N	-2.429048	3.315223	8.356362
N	-1.206268	0.146386	9.390515
N	-1.820795	4.751613	12.817923
N	-1.335627	4.010238	13.811796
N	0.939207	1.405241	14.465970
O	-2.130204	2.352195	10.410831
O	-1.717483	0.812797	7.268694
O	0.246882	2.884865	12.490033
O	-0.596546	2.360663	15.853355
O	-0.219228	4.266151	10.529339
O	-4.076215	3.249267	11.841986
H	-3.717678	2.484850	11.323828
C	-3.391666	6.413330	9.751359
C	-3.862539	7.724788	9.698972
C	-3.854173	8.485956	10.853041
C	-3.352590	7.958730	12.043743
C	-2.902396	6.649091	12.063481
C	-3.239762	5.472539	8.704090
C	-3.626384	5.661316	7.298679
C	-2.095259	2.304017	9.109403
C	-1.657269	1.017385	8.467822
C	-2.285614	5.945471	13.146660
C	-2.167303	6.486922	14.506736
H	-3.024228	7.132128	14.751270
H	-1.246777	7.086442	14.621938
H	-2.093080	5.644431	15.212921
C	-0.412717	3.115171	13.558680
C	-0.051209	2.264243	14.768235
H	-4.216025	9.516666	10.827540
H	-4.211230	8.133632	8.747380
H	1.319608	1.451458	13.519639
H	-3.288464	8.566340	12.949393
H	1.300930	0.784663	15.183726
H	-3.241787	4.819436	6.705262
H	0.157239	5.158412	10.655996
H	-0.835776	-0.748844	9.084270
H	-1.168375	0.449739	10.364792
H	-4.723222	5.695693	7.182579
H	0.062973	3.678750	11.409020
H	-3.222930	6.606417	6.899951
H	-4.804569	3.607070	11.297377

Fe^{2+} dapsox LS LDA

Fe	-2.254628	4.232855	10.955056
N	-2.817417	5.934903	10.927512
N	-2.677495	4.295362	9.189528
N	-2.492812	3.205458	8.424415
N	-1.211339	0.069530	9.506869
N	-1.945197	4.665838	12.824251
N	-1.443186	3.914747	13.813571
N	1.079859	1.505048	14.304060
O	-1.829942	2.375067	10.477083
O	-1.899923	0.665213	7.413751
O	0.313758	3.142829	12.481681
O	-0.555009	2.180185	15.741828
O	-0.396123	4.531309	10.617973
O	-4.034849	3.556403	11.432563
H	-4.694067	3.969169	10.832215
C	-3.264330	6.421273	9.738253
C	-3.764451	7.715254	9.678940
C	-3.818212	8.470467	10.848488
C	-3.392051	7.941393	12.056872
C	-2.889590	6.639371	12.075266
C	-3.157701	5.429354	8.704830
C	-3.523667	5.623338	7.295331
C	-2.030455	2.255067	9.215251
C	-1.714619	0.915763	8.591403
C	-2.373870	5.874345	13.172678
C	-2.273295	6.380542	14.548952
H	-3.082058	7.091968	14.772487
H	-1.312686	6.899074	14.715764
H	-2.290671	5.526318	15.245321
C	-0.406521	3.170278	13.539516
C	0.013611	2.241319	14.665234
H	-4.206604	9.491133	10.812852
H	-4.112412	8.117530	8.724605
H	1.464301	1.669483	13.372498
H	-3.436450	8.523096	12.980552
H	1.469181	0.833119	14.958576
H	-3.369524	4.677217	6.756110
H	-0.184041	5.463561	10.824969
H	-0.949718	-0.871235	9.227177
H	-1.107654	0.417771	10.462300
H	-4.576715	5.935280	7.189850
H	-0.016952	3.914221	11.484291
H	-2.903376	6.407038	6.827679
H	-4.231751	3.894228	12.334629

Fe^{2+} dapsox Isomer II LDA

Fe	-1.922892	3.939714	11.236595
N	-2.840503	5.940460	11.011175
N	-2.614178	4.244053	9.163587
N	-2.475535	3.245829	8.291733
N	-1.058837	0.034402	8.867300
N	-1.814578	4.975118	13.087014
N	-1.237658	4.349634	14.113745
N	-0.028635	2.907423	15.938281
O	-1.649475	2.185988	10.160616
O	-1.958390	0.855478	6.934244
O	-0.944344	2.713384	12.533885
O	0.310911	1.189225	14.479734
O	-0.111351	4.849947	10.524511
O	-3.915874	3.229157	11.678108
H	-4.234548	2.876004	10.820725
C	-3.301466	6.341223	9.823632
C	-3.857092	7.610108	9.655421
C	-3.921142	8.448234	10.762343
C	-3.434568	8.033079	11.983596
C	-2.876610	6.747198	12.078060
C	-3.177911	5.355845	8.774116
C	-3.667178	5.594546	7.405896
C	-1.942928	2.209945	8.927460
C	-1.664094	0.966081	8.112714
C	-2.302133	6.183924	13.263419
C	-2.267293	6.917935	14.540894
H	-3.284751	7.168363	14.887413
H	-1.718012	7.870150	14.442364
H	-1.773338	6.296293	15.299459

C	-0.810445	3.155959	13.702779
C	-0.114677	2.299956	14.737592
H	-4.359182	9.445407	10.662356
H	-4.231974	7.920407	8.678053
H	-0.437123	3.840182	16.022279
H	-3.471735	8.678492	12.864152
H	0.413474	2.419115	16.711912
H	-3.449207	4.709186	6.791884
H	-0.330494	5.104911	9.602696
H	-0.801445	-0.856846	8.453727
H	-0.874955	0.268493	9.846224
H	-4.754343	5.784441	7.400031
H	-0.013073	5.688007	11.021385
H	-3.186614	6.482661	6.961179
H	-4.446742	4.034275	11.850055

Fe^{2+} dapsox Isomer III LDA

Fe	-1.981428	4.078063	11.174099
N	-2.830450	5.929362	10.995001
N	-2.587381	4.286279	9.140006
N	-2.408364	3.274266	8.282355
N	-1.846627	1.166344	6.806589
N	-1.877790	5.001146	13.106469
N	-1.322138	4.349373	14.133514
N	-0.233881	2.844262	15.989763
O	-1.899213	2.123434	10.208481
O	-1.734942	-0.161106	8.655288
O	-0.651400	2.894988	12.478760
O	0.735276	1.501870	14.424292
O	0.046130	4.366907	10.585839
O	-3.557450	2.851452	11.929169
H	-3.161138	2.133303	11.346959
C	-3.276531	6.360976	9.797112
C	-3.851306	7.616599	9.643415
C	-3.979998	8.441473	10.749189
C	-3.524095	7.993701	11.980176
C	-2.946518	6.734898	12.070875
C	-3.124772	5.403480	8.738022
C	-3.565721	5.660409	7.355857
C	-2.049878	2.189142	8.953655
C	-1.856838	0.930630	8.133208
C	-2.413371	6.174684	13.282929
C	-2.466228	6.873473	14.578930
H	-3.507310	7.094909	14.866304
H	-1.926967	7.834341	14.537492
H	-2.005798	6.237498	15.346652
C	-0.706466	3.262291	13.687190
C	0.013637	2.431671	14.731064
H	-4.434922	9.430068	10.653378
H	-4.198823	7.931424	8.655951
H	-0.815414	3.675501	16.107435
H	-3.606790	8.613111	12.877134
H	0.228866	2.375167	16.763602
H	-3.382159	4.763649	6.749206
H	0.371640	5.230476	10.907226
H	-1.772185	0.380617	6.166474
H	-2.032797	2.120973	6.495614
H	-4.639825	5.906779	7.320525
H	0.257264	3.701457	11.311836
H	-3.020537	6.512364	6.916876
H	-4.407174	3.095236	11.513670

Fe^{2+} dapsox Isomer V LDA

Fe	-2.066741	4.032176	10.956015
N	-2.856856	5.879212	10.932839
N	-2.702390	4.339885	9.020852
N	-2.560006	3.350792	8.126896
N	-1.528410	0.008306	8.722090
N	-1.808789	4.783145	12.991674
N	-1.355766	4.126756	14.056894
N	1.037783	1.715313	14.977934
O	-2.172424	2.144618	10.050874
O	-2.036370	0.983532	6.724577
O	0.440247	3.132497	12.923906
O	-0.648723	2.617700	16.217492
O	-0.106588	4.116421	10.788541
O	-3.807332	2.997077	11.760932
H	-3.588394	2.314198	11.065343
C	-3.326647	6.388973	9.772030
C	-3.819752	7.688910	9.705247
C	-3.821030	8.464121	10.848664
C	-3.327580	7.934069	12.035874
C	-2.845665	6.633420	12.048886
C	-3.264075	5.471039	8.676153
C	-3.779055	5.750730	7.325935
C	-2.239548	2.251878	8.759983
C	-1.927872	1.026951	7.937345
C	-2.287217	5.980564	13.206033
C	-2.247157	6.598939	14.540655
H	-3.060511	7.323499	14.683590
H	-1.287507	7.115909	14.713423
H	-2.298782	5.790924	15.290055
C	-0.338637	3.321050	13.926314
C	-0.017291	2.525304	15.179243
H	-4.201429	9.488052	10.820932
H	-4.193538	8.074357	8.753083
H	1.478951	1.740183	14.057886
H	-3.308956	8.527166	12.952871
H	1.359306	1.116468	15.732486
H	-3.484800	4.927620	6.658645
H	0.247300	5.018421	10.675361
H	-1.245005	-0.867261	8.291609
H	-1.443123	0.183054	9.723897
H	-4.879563	5.828484	7.324186
H	0.204015	3.715269	11.802198
H	-3.382900	6.703112	6.938413
H	-4.605351	3.465123	11.445997

Fe^{2+} dapsox Isomer VI LDA

Fe	0.083935	0.422382	-0.097652
O	2.065533	0.575105	0.424770
O	-2.143954	0.484671	0.025091
O	-0.061296	2.143172	1.064712
O	-0.054300	4.128992	-1.802614
O	1.566240	0.153844	2.793134
O	-0.596613	-1.438869	5.052987
N	-0.123584	4.405123	0.788758
N	-0.044738	1.793023	-1.582880
N	-0.018316	1.690339	-2.911656
N	0.059487	-0.986107	-1.563440
N	-0.036633	-1.282378	1.027609
N	-0.144277	-1.382777	2.354065
N	1.131166	0.026012	5.314647
C	-0.079754	3.159785	0.354128
C	-0.058668	3.086759	-1.158668
C	0.047165	0.535801	-3.498978
C	0.069472	0.633828	-4.987278
C	0.071411	-0.795367	-2.908365
C	0.081804	-1.889449	-3.776401

C	0.048845	-3.180741	-3.285096
C	-0.016902	-3.367083	-1.921195
C	-0.018058	-2.261689	-1.078908
C	-0.076664	-2.404792	0.344213
C	-0.161802	-3.701796	1.040673
C	0.599193	-0.616399	3.110616
C	0.290636	-0.738361	4.594830
H	-0.130038	4.627298	1.780365
H	-0.115449	5.105534	0.036184
H	0.057585	1.698222	-5.251701
H	0.973231	0.172286	-5.417283
H	-0.804830	0.144983	-5.448171
H	0.113076	-1.712815	-4.851828
H	0.063714	-4.035168	-3.966014
H	-0.057659	-4.368412	-1.488289
H	-0.733565	-3.549207	1.972158
H	-0.626464	-4.482517	0.424260
H	1.829469	0.556128	4.789744
H	1.054963	0.042345	6.327029
H	0.835056	-4.055637	1.356116
H	-2.435326	-0.448693	0.091572
H	-2.347330	0.763171	-0.892373
H	2.555927	-0.197345	0.083127
H	1.905210	0.373263	1.483193

Fe^{2+} dapsox Isomer VII LDA

Fe	10.589924	6.447587	1.782227
O	9.074861	5.377489	3.202693
O	9.689884	2.838309	5.580876
O	10.734619	10.592871	3.647046
O	8.850705	7.693423	2.093641
O	11.332884	7.137673	3.535447
N	11.884723	6.017007	0.326578
N	11.237957	4.504983	2.173153
N	10.770507	3.811599	3.214957
N	8.071661	4.433944	5.418518
H	7.592778	4.121895	6.258343
H	7.719116	5.184877	4.825960
N	11.339077	8.308100	1.137361
N	11.032670	9.488225	1.680735
N	11.528964	8.714062	5.142221
H	11.352473	9.721553	5.282212
H	11.697603	8.033629	5.879362
C	12.358862	4.761427	0.196872
C	13.204908	4.427953	-0.853602
H	13.576231	3.405205	-0.953153
C	13.577007	5.417437	-1.751247
H	14.235080	5.177537	-2.589967
C	13.150824	6.722262	-1.553870
H	13.476510	7.526408	-2.217829
C	12.322660	7.007919	-0.474140
C	11.923282	3.881437	1.246142
C	12.205184	2.438039	1.308047
H	12.304515	2.142282	2.364577
H	13.113186	2.176608	0.747058
H	11.369167	1.844961	0.898591
C	9.708025	4.374879	3.724720
C	9.174745	3.779921	5.004196
C	11.941988	8.316471	-0.027257
C	12.295640	9.567135	-0.716866
H	12.568443	9.395150	-1.766484
H	11.448016	10.267765	-0.653075
H	13.135991	10.070073	-0.208397
C	10.995232	9.554462	3.015113
C	11.316689	8.332228	3.893590
O	9.010305	5.468191	0.634849
H	9.143271	8.632625	2.188804
H	8.626722	7.332498	2.981147
H	9.410526	4.666594	0.240792
H	8.711297	5.195306	1.558237

Fe^{2+} dapsox Isomer VIII LDA

Fe	11.247059	6.445170	2.111226
O	8.370525	3.186438	3.708369
O	9.165579	5.955949	1.704253
O	12.433262	10.637724	3.649198
O	9.945073	8.010197	2.905845
O	12.893866	7.174412	3.327533
N	12.179955	5.915232	0.372864
N	11.136508	4.290587	1.959967
N	10.451850	3.528560	2.831099
N	7.228922	4.951426	2.326014
H	6.630185	5.694096	1.974779
H	6.929103	4.172999	2.942231
N	11.947254	8.272403	1.181525
N	11.848903	9.477151	1.769914
N	13.760157	8.767558	4.689145
H	13.639477	9.781449	4.866198
H	14.205171	8.106043	5.319985
C	12.371540	4.617698	0.066461
C	13.016952	4.227320	-1.099531
H	13.155907	3.163384	-1.306103
C	13.455814	5.196398	-1.985645
H	13.958319	4.913602	-2.913777
C	13.246830	6.529942	-1.676810
H	13.579730	7.327652	-2.345398
C	12.616451	6.858588	-0.483903
C	11.778916	3.699997	0.996568
C	11.808935	2.237399	0.819058
H	11.526634	1.761600	1.770122
H	12.804758	1.895932	0.497869
H	11.081418	1.910735	0.056432
C	9.163041	3.817465	2.990348
C	8.545669	5.016337	2.249402
C	12.452866	8.204818	-0.014100
C	12.910910	9.383729	-0.771001
H	14.010682	9.471735	-0.750176
H	12.602919	9.321444	-1.826300
H	12.493408	10.286901	-0.301806
C	12.393030	9.593210	2.979395
C	13.045545	8.373067	3.650720
O	11.016073	5.754278	4.171857
H	11.932371	6.035923	4.404621
H	10.986131	4.758088	4.123489
H	9.158206	7.647126	2.434111
H	10.229958	8.856415	2.461933

Fe^{2+} dapsox Isomer IX LDA

Fe	10.555273	6.597959	2.089693
O	9.855257	5.752107	4.165573
O	9.254216	2.513619	5.412217
O	10.220450	10.971993	3.466795
O	8.942532	7.823562	2.583604
O	8.805858	6.019255	0.885838
O	11.798376	7.205549	3.718818
N	11.697665	6.129688	0.496957
N	10.930635	4.503136	2.233777
N	10.425609	3.729640	3.204514
N	8.704139	4.592883	6.172183

H	8.258071	4.242740	7.014610
H	8.795504	5.586645	5.956286
N	11.206265	8.490592	1.278640
N	11.100267	9.697255	1.806882
N	8.279549	9.489475	3.969125
H	8.619383	10.424945	4.270225
H	7.448168	9.002463	4.293842
C	11.992003	4.841287	0.232733
C	12.700363	4.475448	-0.902886
H	12.925058	3.421308	-1.083076
C	13.109485	5.467421	-1.782391
H	13.663602	5.208204	-2.687833
C	12.823117	6.790150	-1.497152
H	13.145883	7.589940	-2.166898
C	12.124837	7.106393	-0.331385
C	11.524721	3.918587	1.228961
C	11.699730	2.460381	1.122008
H	11.148829	1.978857	1.942329
H	12.765207	2.184374	1.199189
H	11.334224	2.087229	0.151931
C	9.888119	4.467589	4.143067
C	9.253611	3.726605	5.299539
C	11.841122	8.430086	0.123928
C	12.303157	9.652235	-0.553065
H	13.054429	9.443382	-1.325524
H	11.462155	10.199845	-1.010759
H	12.712659	10.335218	0.210582
C	10.247661	9.922392	2.798619
C	9.110014	8.953626	3.099815
H	12.696411	6.828628	3.655185
H	11.227129	6.566961	4.260791
H	9.033331	6.231513	-0.041153
H	8.321590	6.802140	1.248087

Fe^{2+} dapsox Isomer X LDA

Fe	10.508993	6.643102	2.094123
O	9.799863	3.831686	5.538621
O	8.741252	5.493060	2.635735
O	10.271669	11.284401	3.172104
O	9.666606	7.835413	3.447346
O	8.774342	7.112880	0.764999
O	12.302409	7.131978	3.367472
N	11.597292	6.167263	0.494387
N	11.182529	4.669733	2.487762
N	11.020289	3.994087	3.615729
N	7.745013	4.933606	4.606555
H	8.009133	4.448153	5.485818
H	6.844124	5.348625	4.386282
N	11.137644	8.605990	1.179358
N	10.914500	9.860729	1.548760
N	9.373659	9.627826	4.782370
H	9.520443	10.654311	4.752918
H	8.958854	9.089132	5.538084
C	12.049716	4.901485	0.361734
C	12.726786	4.507828	-0.792127
H	13.051354	3.470834	-0.901723
C	12.979632	5.445365	-1.775759
H	13.507005	5.155471	-2.688023
C	12.595681	6.765742	-1.582916
H	12.833102	7.541051	-2.314841
C	11.921367	7.106121	-0.416345
C	11.792811	4.063243	1.489899
C	12.184581	2.645738	1.568067
H	12.370415	2.393766	2.624748
H	13.074266	2.431855	0.958895
H	11.368380	1.984687	1.227683
C	9.965083	4.251900	4.378955
C	8.766266	4.972359	3.772953
C	11.574735	8.448986	-0.053159
C	11.764204	9.575016	-0.987367
H	12.834532	9.819828	-1.104659
H	11.369365	9.335310	-1.986965
H	11.260859	10.460950	-0.576812
C	10.373782	10.126373	2.731428
C	9.783820	9.055005	3.666945
H	12.802332	6.290873	3.300110
H	12.682322	7.722841	2.680062
H	8.258445	6.457692	1.303768
H	8.961777	6.678963	-0.091175

Fe^{2+} dapsox Isomer XI LDA

Fe	10.586527	6.565181	2.082164
O	9.102234	5.561254	3.396847
O	9.248856	2.798731	5.556159
O	10.142741	11.048870	3.313356
N	8.730631	8.102674	2.868944
O	8.748450	6.112059	0.940818
O	11.752295	6.863527	3.748238
N	11.746550	6.108481	0.492220
N	11.059059	4.528698	2.262552
N	10.600874	3.823195	3.312843
N	8.431784	4.902516	5.873843
H	8.142728	4.691360	6.826228
H	8.461280	5.865480	5.537142
N	11.074603	8.506502	1.193787
N	10.842446	9.750948	1.586220
O	10.023610	8.430664	4.688483
C	12.185504	4.849906	0.312535
C	12.966376	4.504829	-0.787558
H	13.316763	3.476093	-0.905927
C	13.274072	5.488801	-1.706787
H	13.873223	5.249880	-2.589476
C	12.835697	6.788967	-1.501763
H	13.087063	7.578204	-2.211624
C	12.086258	7.088686	-0.365294
C	11.764826	3.937929	1.338312
C	12.094272	2.502013	1.342295
H	11.707546	2.048858	2.266125
H	13.185033	2.351330	1.288263
H	11.651833	1.983487	0.475554
C	9.612887	4.471139	3.874122
C	9.087421	3.946839	5.183017
C	11.674301	8.405999	0.022427
C	11.989628	9.615000	-0.753314
H	12.510172	9.391443	-1.692684
H	11.067554	10.180766	-0.966184
H	12.598865	10.297838	-0.136554
C	10.272058	9.944831	2.794118
C	9.675029	8.775175	3.549001
H	12.006326	6.038347	4.208398
H	11.204674	7.450736	4.380500
H	8.394105	8.434042	1.963194
H	8.260704	7.316042	3.336838
H	8.990240	5.454501	0.258147
H	8.566580	5.590101	1.781910

Fe^{2+} dapsox Isomer XII LDA

Fe	10.690545	6.670337	2.150252
O	8.934897	3.257776	4.879887

O	8.210050	5.970143	4.418936
O	10.040142	11.269041	2.969004
N	9.002873	8.019634	2.836426
O	8.892937	6.017171	1.046897
O	12.620089	7.239820	3.079954
N	11.757527	6.138537	0.530019
N	10.926617	4.442927	2.318799
N	10.383767	3.561321	3.174571
N	10.460063	6.272178	4.345581
H	13.285450	6.576028	2.792777
H	11.349036	5.807991	4.560087
N	11.057850	8.567407	1.068294
N	10.800399	9.849052	1.384552
O	10.023773	8.945205	4.639667
C	12.150319	4.864164	0.380821
C	12.903900	4.466654	-0.718673
H	13.218848	3.425714	-0.814477
C	13.223141	5.404406	-1.683610
H	13.801211	5.114243	-2.563725
C	12.806805	6.713295	-1.526264
H	13.051911	7.467533	-2.274981
C	12.080825	7.063044	-0.390506
C	11.702839	3.940067	1.390312
C	12.059254	2.514540	1.300244
H	11.638979	1.968584	2.152598
H	13.154133	2.389318	1.280406
H	11.672489	2.074683	0.365385
C	9.567008	4.019001	4.118866
C	9.348102	5.493043	4.321747
C	11.665083	8.406735	-0.085396
C	11.958279	9.549030	-0.961896
H	12.441894	9.248202	-1.897501
H	11.029428	10.096716	-1.189299
H	12.603552	10.270688	-0.433330
C	10.213335	10.106267	2.550801
C	9.727401	8.994138	3.439101
H	12.865598	8.047454	2.575456
H	10.345259	7.236848	4.752013
H	8.568430	8.245710	1.935544
H	8.444258	7.388541	3.468793
H	9.078567	6.187904	0.096932
H	8.922286	5.036363	1.114366

Fe^{2+} Hdapsox Isomer I HS LDA

Fe	0.149241	2.256319	2.620156
O	-0.914534	3.969998	1.455892
O	0.350598	5.890234	-1.184273
O	-1.892041	2.552311	3.507879
O	-3.562380	1.335135	6.365107
O	-1.182551	1.182825	1.421361
H	-1.932128	1.516912	1.990961
H	-1.166416	0.208867	1.517507
O	0.351111	3.899572	3.910969
H	0.774627	3.702355	4.771694
H	-0.629112	3.911733	4.075334
N	1.865984	1.125320	2.723197
N	1.458419	2.932527	1.117650
N	1.050571	3.934268	0.336054
H	1.581932	4.389044	-0.428368
N	-1.706116	6.064104	-0.180348
H	-2.299382	5.666225	0.548182
H	-2.030784	6.834664	-0.762876
N	-0.088104	0.945190	4.273418
N	-1.194827	0.961481	5.030400
N	-4.172580	2.868048	4.788610
H	-5.074840	3.053301	5.221026
H	-3.878632	3.332572	3.930903
C	2.881478	1.326421	1.860554
C	4.049503	0.572830	1.921065
H	4.857408	0.752626	1.208226
C	4.170699	-0.399093	2.894953
H	5.077733	-1.003948	2.962327
C	3.129126	-0.592437	3.791190
H	3.192163	-1.345985	4.580305
C	1.989251	0.187586	3.680439
C	2.622953	2.378184	0.918977
C	3.539662	2.809808	-0.148230
H	4.457583	2.210686	-0.172788
H	3.058953	2.722171	-1.139155
H	3.835003	3.866091	-0.015356
C	-0.171803	4.416243	0.575070
C	-0.495027	5.551731	-0.366166
C	0.851683	0.088767	4.561846
C	0.774073	-0.871458	5.669602
H	0.795607	-1.908589	5.294351
H	-0.159193	-0.708507	6.225784
H	1.635448	-0.757705	6.348567
C	-2.059785	1.822746	4.566082
C	-3.346411	1.968329	5.351582

Fe^{2+} Hdapsox IS LDA

Fe	0.234445	2.056945	2.864142
O	-1.578918	3.484300	0.477511
O	0.341066	6.220125	-0.539986
O	-1.292567	2.919987	3.814750
O	-3.843848	1.404002	5.728114
O	-1.111004	1.254848	1.625229
H	-1.871527	0.835110	2.080214
H	-1.435398	2.090846	1.125896
O	1.089432	3.767332	4.170301
H	1.440920	4.611880	3.826838
H	0.153161	3.937062	4.435540
N	1.837426	1.184332	2.883641
N	1.125233	2.954437	1.347852
N	0.671415	4.023514	0.657977
H	1.266354	4.821619	0.333995
N	-1.904068	5.840635	-0.843324
H	-2.649030	5.165250	-0.662862
H	-2.084329	6.702834	-1.355609
N	-0.092047	0.842775	4.208933
N	-1.288033	0.865915	4.820978
N	-3.718569	3.463157	4.754157
H	-4.643976	3.740193	5.075309
H	-3.135978	4.085630	4.196943
C	2.761405	1.458720	1.934734
C	3.928772	0.719272	1.858271
H	4.668603	0.937966	1.084483
C	4.132871	-0.311884	2.771328
H	5.052695	-0.899542	2.730419
C	3.159723	-0.616162	3.704996
H	3.282907	-1.448066	4.403400
C	1.990726	0.138964	3.739421
C	2.339877	2.522401	1.068961
C	3.178487	3.056940	-0.012463
H	3.797517	2.257862	-0.446898
H	2.576853	3.501425	-0.819663
H	3.873832	3.829883	0.363093
C	-0.602025	4.218228	0.306870
C	-0.683779	5.555806	-0.414490
C	0.834984	-0.043284	4.544461

C	0.654149	-1.055817	5.589503
H	0.908073	-2.060646	5.214504
H	-0.388506	-1.046454	5.936333
H	1.309101	-0.850769	6.453841
C	-1.865845	2.002240	4.540696
C	-3.253138	2.246126	5.083298

Fe^{2+} Hdapsox LS LDA

Fe	0.409766	2.199351	2.436057
O	-0.945773	3.524341	1.657687
O	-0.315784	5.673783	-1.028634
O	-1.403295	3.432176	4.761454
O	-4.167695	1.292440	4.907446
O	-0.466749	0.921900	1.210150
H	0.002287	0.058588	1.214938
H	-1.345448	0.740762	1.620792
O	0.802022	3.476778	3.773024
H	0.975833	4.364700	3.400827
H	-0.264942	3.483779	4.313047
N	1.866924	1.206388	2.713701
N	1.476334	2.924744	1.137398
N	0.887059	3.872051	0.374788
H	1.286917	4.411429	-0.412166
N	-2.257953	5.471918	0.184199
H	-2.698860	4.973646	0.958907
H	-2.770273	6.180396	-0.340361
N	-0.270844	1.137573	3.867192
N	-1.526214	1.145231	4.328376
N	-3.852513	3.415746	5.684009
H	-4.797482	3.493314	6.052834
H	-3.164660	4.157430	5.809538
C	2.965276	1.449622	1.952569
C	4.113697	0.698200	2.151166
H	5.004226	0.887415	1.546973
C	4.106935	-0.288270	3.130049
H	5.004956	-0.886668	3.298935
C	2.974108	-0.517158	3.897283
H	2.963196	-1.283492	4.676111
C	1.841261	0.256911	3.669688
C	2.711010	2.492552	0.990367
C	3.672988	2.982686	-0.006859
H	4.370391	2.182390	-0.296035
H	3.178898	3.332441	-0.927378
H	4.278998	3.816283	0.390626
C	-0.380276	4.117574	0.717903
C	-1.002866	5.185077	-0.141926
C	0.561398	0.224074	4.326516
C	0.196002	-0.709763	5.396009
H	0.745908	-1.658110	5.310970
H	-0.891759	-0.886063	5.366264
H	0.417539	-0.277806	6.388033
C	-2.010380	2.303917	4.689309
C	-3.466786	2.267359	5.105919

Fe^{2+} Hdapsox Isomer II LDA

Fe	-2.051887	4.060927	11.240430
N	-2.869598	5.940668	10.997878
N	-2.651861	4.242808	9.235500
N	-2.410441	3.222915	8.405974
N	-1.111144	-0.051192	8.408027
N	-1.781818	5.097742	13.095951
N	-1.174087	4.477680	14.117799
N	0.081769	3.005022	15.953213
O	-1.636701	2.023728	10.155722
O	-1.959110	1.296418	6.749359
O	-1.131454	2.715350	12.638477
O	0.248218	1.270959	14.478350
O	0.004490	4.134269	10.749385
O	-3.602835	2.883304	11.992306
H	-2.958329	2.237034	12.386964
C	-3.366942	6.321368	9.806972
C	-3.914539	7.591307	9.620232
C	-3.940436	8.469385	10.680919
C	-3.414925	8.072433	11.906854
C	-2.882383	6.802210	12.028898
C	-3.244159	5.321843	8.789334
C	-3.697658	5.490403	7.398001
C	-1.880250	2.124389	8.948499
C	-1.645724	1.057530	7.909228
C	-2.275872	6.288043	13.241764
C	-2.233568	7.062819	14.488084
H	-3.253951	7.283764	14.844217
H	-1.730530	8.031549	14.330858
H	-1.698825	6.495418	15.259807
C	-0.864420	3.244344	13.769767
C	-0.116072	2.392857	14.775359
H	-4.361330	9.470106	10.559089
H	-4.306208	7.881437	8.642551
H	-0.268277	3.954848	16.078167
H	-3.411147	8.748015	12.765663
H	0.579980	2.512363	16.691460
H	-4.127046	4.558564	6.993411
H	0.497190	4.915639	11.073259
H	-0.902507	-0.840287	7.797897
H	-0.895033	-0.085831	9.405966
H	-4.474174	6.263123	7.321132
H	0.209942	3.391619	11.376242
H	-2.865316	5.791458	6.736093
H	-4.193014	2.385600	11.393038
H	-2.561382	3.201907	7.381686

Fe^{2+} Hdapsox Isomer III LDA

Fe	0.081628	2.238063	2.550662
O	-0.935402	3.586069	1.233186
O	-1.971208	5.531452	-0.382824
O	-1.810298	2.782927	3.623464
O	-3.543323	3.386180	5.804722
O	-1.059621	1.134378	1.203262
H	-1.746945	0.461453	1.367995
H	-1.481878	1.968276	0.845973
O	0.478434	4.003652	3.701784
H	0.916052	4.670474	3.130155
H	-0.452710	4.314032	3.806130
N	1.837700	1.142295	2.773996
N	1.513722	3.055073	1.180167
N	1.149074	4.079600	0.399444
N	0.145594	6.075794	-1.038560
H	1.125982	5.800845	-0.978921
H	-0.169577	6.817915	-1.659846
N	-0.194608	0.870529	4.131545
N	-1.347186	0.947041	4.821713
H	-1.505304	0.393409	5.673349
N	-3.942360	1.136023	5.871396
H	-4.767366	1.298865	6.454856
H	-3.973300	0.310581	5.272033
C	2.898219	1.423658	2.003965
C	4.071511	0.695969	2.094664
H	4.920915	0.950664	1.456441
C	4.143770	-0.353415	3.006513

H	5.058893	-0.944121	3.093179
C	3.055940	-0.637211	3.801244
H	3.086184	-1.449676	4.531511
C	1.904530	0.141824	3.665240
C	2.695925	2.533229	1.089354
C	3.735267	2.977725	0.153207
H	4.011045	2.162243	-0.536862
H	3.367572	3.830745	-0.430661
H	4.652549	3.267864	0.692366
C	-0.159681	4.265531	0.494373
C	-0.768531	5.362294	-0.359295
C	0.720259	-0.010161	4.455405
C	0.617595	-1.025325	5.521013
H	0.880124	-2.021986	5.129313
H	-0.388100	-1.115651	5.958183
H	1.319296	-0.806545	6.344644
C	-2.123342	2.011478	4.534380
C	-3.305841	2.257032	5.444299

Fe^{2+} Hdapsox Isomer V LDA

Fe	0.025241	2.164519	2.824966
O	-1.344309	3.798695	-0.079943
O	1.002872	6.276764	-0.832810
O	-1.894042	2.589971	4.020704
O	-3.417985	0.967382	6.757176
O	-1.468055	1.896250	1.556819
H	-2.223369	2.072099	2.170469
H	-1.471245	2.619870	0.815030
O	0.136349	3.942410	3.783588
H	0.351681	4.853639	3.506690
H	-0.802419	3.863401	4.140273
N	1.765762	1.128119	2.761740
N	1.176367	2.983514	1.172135
N	0.900838	4.087508	0.438341
H	1.622663	4.798383	0.169521
N	-1.202621	6.131591	-1.454036
H	-2.033257	5.540483	-1.385980
H	-1.204943	6.985866	-2.009579
N	-0.110746	0.807008	4.407795
N	-1.160690	0.766645	5.234082
N	-4.093181	2.738124	5.489872
H	-4.959527	2.859176	6.009804
H	-3.854305	3.336166	4.701836
C	2.713337	1.406007	1.853112
C	3.902149	0.673324	1.806920
H	4.664864	0.904804	1.060849
C	4.097276	-0.341808	2.716260
H	5.019872	-0.926771	2.699240
C	3.112457	-0.613903	3.660165
H	3.240828	-1.403868	4.404054
C	1.954739	0.140849	3.653570
C	2.386691	2.498895	0.987212
C	3.319168	3.046927	-0.013537
H	4.185851	2.393059	-0.164910
H	2.817460	3.186041	-0.986014
H	3.713403	4.033794	0.293690
C	-0.270626	4.413362	-0.102117
C	-0.096170	5.729639	-0.846576
C	0.867540	-0.027700	4.598349
C	0.896741	-1.025188	5.671086
H	1.107674	-2.029706	5.268785
H	-0.066908	-1.022937	6.198571
H	1.699266	-0.791305	6.392833
C	-2.019857	1.710129	4.964474
C	-3.252154	1.750663	5.844701

Fe^{2+} Hdapsox Isomer VI LDA

Fe	0.013814	0.455033	-0.145495
O	1.975434	0.924431	0.464144
O	-2.111642	0.326321	0.225131
O	-0.370033	2.173036	0.973295
O	0.285830	4.088193	-1.863088
O	1.444222	0.464252	2.928998
O	-0.402406	-1.849885	4.787223
N	0.015419	4.409000	0.722482
N	0.013781	1.771200	-1.626852
N	0.067191	1.649796	-2.947162
N	-0.028158	-0.997622	-1.559989
N	0.150942	-1.261390	1.008473
N	0.073342	-1.315230	2.351681
N	0.942795	-0.141810	5.525258
C	-0.093835	3.180192	0.281648
C	0.103888	3.074165	-1.214122
C	0.031994	0.491456	-3.526353
C	0.044308	0.565536	-5.013135
C	-0.002467	-0.827360	-2.907541
C	-0.004583	-1.935810	-3.756695
C	-0.026711	-3.219726	-3.250991
C	-0.043704	-3.387246	-1.884924
C	-0.046146	-2.269862	-1.060228
C	-0.053949	-2.390089	0.367562
C	-0.280539	-3.655126	1.092286
C	0.688905	-0.478209	3.188457
C	0.345901	-0.893655	4.610727
H	-0.104178	4.650638	1.704380
H	0.219135	5.102903	-0.010874
H	0.058469	1.624050	-5.299435
H	0.929982	0.073300	-5.446346
H	-0.849990	0.095908	-5.454299
H	0.007921	-1.773076	-4.834769
H	-0.026798	-4.082972	-3.920335
H	-0.043673	-4.388334	-1.449933
H	-1.265188	-3.652970	1.596332
H	-0.268444	-4.528293	0.431598
H	1.553116	0.611512	5.203676
H	0.813704	-0.334685	6.517156
H	0.484109	-3.806748	1.873354
H	-0.469561	-2.034675	2.881667
H	-2.611819	0.130569	-0.593990
H	-2.335357	1.248228	0.479007
H	2.661907	0.306998	0.143201
H	1.879999	0.758781	1.471047

Fe^{2+} Hdapsox Isomer VII LDA

Fe	10.644102	6.435955	1.845599
O	9.082138	5.318682	3.120911
O	9.703792	2.822689	5.546610
O	10.791078	10.695245	3.524804
O	8.947726	7.761309	2.489828
O	11.365423	7.219045	3.546384
N	11.906071	5.998831	0.324739
N	11.255327	4.482522	2.177506
N	10.791709	3.792906	3.221857
N	8.004555	4.328010	5.349609
H	7.519956	3.973920	6.171362
H	7.588578	5.041422	4.755639
N	11.376938	8.283258	1.080709
N	11.122778	9.451110	1.682650
N	11.274492	8.775014	5.190190

H	11.130837	9.776242	5.366956
H	11.423286	8.095430	5.934984
C	12.366667	4.740113	0.196544
C	13.174768	4.383029	-0.872143
H	13.532242	3.354771	-0.965229
C	13.523397	5.349835	-1.803595
H	14.153711	5.089160	-2.656826
C	13.103100	6.655297	-1.623467
H	13.407307	7.438867	-2.321057
C	12.310658	6.960177	-0.522633
C	11.953105	3.863109	1.263128
C	12.261981	2.430221	1.333997
H	12.284616	2.123381	2.391374
H	13.216375	2.193835	0.843276
H	11.473728	1.827795	0.849529
C	9.703843	4.327805	3.694648
C	9.146914	3.730665	4.963135
C	11.947288	8.284523	-0.095119
C	12.283143	9.522833	-0.817996
H	12.790924	9.318785	-1.768096
H	11.377765	10.110472	-1.055582
H	12.948950	10.164489	-0.212889
C	10.998575	9.601223	3.028291
C	11.224205	8.396529	3.928622
O	8.979087	5.809603	0.632456
H	11.113865	10.329856	1.145419
H	8.292035	7.796352	1.761991
H	8.681937	6.972883	3.045070
H	9.185003	5.177681	-0.086445
H	8.717269	5.274988	1.446952

Fe^{2+} Hdapsox Isomer VIII LDA

Fe	11.328449	6.434720	2.154081
O	8.368916	3.129502	3.634680
O	9.200467	5.987829	1.788225
O	12.469398	10.743934	3.559363
O	10.014700	7.994290	3.008089
O	12.847115	7.245978	3.401673
N	12.173387	5.917937	0.345832
N	11.147383	4.287841	1.960936
N	10.473872	3.538303	2.846327
N	7.248822	4.940047	2.261465
H	6.656721	5.679470	1.887600
H	6.901880	4.125587	2.798095
N	11.998399	8.270244	1.132065
N	11.974307	9.470311	1.761966
N	13.545154	8.808109	4.896490
H	13.531210	9.815523	5.094363
H	14.000339	8.135493	5.510888
C	12.340763	4.617886	0.040473
C	12.936457	4.214078	-1.144905
H	13.058064	3.147218	-1.347165
C	13.345428	5.168938	-2.060887
H	13.809751	4.871639	-3.004021
C	13.152947	6.502587	-1.761354
H	13.461420	7.285502	-2.458071
C	12.578973	6.843753	-0.541504
C	11.766921	3.697068	0.986801
C	11.790891	2.238146	0.803353
H	11.492781	1.754547	1.744996
H	12.789370	1.892062	0.495432
H	11.075227	1.922216	0.024710
C	9.164074	3.785058	2.960145
C	8.558897	5.008145	2.245291
C	12.457519	8.198792	-0.083996
C	12.924486	9.331175	-0.907731
H	14.025824	9.324260	-0.981546
H	12.530183	9.251656	-1.932348
H	12.633756	10.318471	-0.522818
C	12.422545	9.642703	3.037172
C	12.942583	8.426955	3.785105
O	10.981238	5.725279	4.154208
H	11.829042	5.931306	4.600517
H	10.888000	4.723827	4.088463
H	9.252234	7.414291	2.729089
H	9.940713	8.806923	2.466046
H	11.907062	10.340917	1.215426

Fe^{2+} Hdapsox Isomer IX LDA

Fe	10.550331	6.567077	2.094354
O	9.922663	5.774933	4.091248
O	9.088479	2.567553	5.281324
O	10.184099	11.073657	3.339879
O	8.969794	7.850284	2.669674
O	8.748574	5.860660	1.173909
O	11.846627	7.255769	3.654702
N	11.726760	6.135328	0.491472
N	10.911364	4.485601	2.180233
N	10.362278	3.725892	3.136647
N	8.752608	4.643584	6.164316
H	8.319020	4.285136	7.012066
H	8.934787	5.636597	6.028655
N	11.175597	8.469257	1.217883
N	11.006123	9.672763	1.787210
N	8.301095	9.481204	4.102362
H	8.519425	10.441389	4.398541
H	7.498010	8.960923	4.451161
C	12.018915	4.848115	0.217370
C	12.740343	4.490126	-0.911075
H	12.961238	3.435649	-1.095179
C	13.175810	5.479379	-1.777339
H	13.743232	5.220874	-2.674127
C	12.895399	6.800181	-1.483038
H	13.242445	7.599133	-2.141489
C	12.172133	7.100899	-0.333315
C	11.538955	3.906928	1.194347
C	11.735354	2.454411	1.091447
H	11.154940	1.955707	1.880305
H	12.799545	2.194192	1.225031
H	11.429985	2.077254	0.102548
C	9.873292	4.488120	4.084344
C	9.198592	3.776426	5.237865
C	11.880278	8.433312	0.118744
C	12.383367	9.653113	-0.539030
H	12.840676	9.436662	-1.511304
H	11.568018	10.378963	-0.701944
H	13.161135	10.151099	0.071071
C	10.164198	9.977212	2.800867
C	9.100924	8.973564	3.188070
H	12.762325	6.915749	3.619309
H	11.318033	6.633497	4.247088
H	8.609036	4.898811	1.302991
H	8.088064	6.326002	1.735447
H	11.625754	10.449423	1.513765

Fe^{2+} Hdapsox Isomer X LDA

Fe	10.650172	6.713168	2.138854
O	9.512450	3.220772	5.171736
O	8.949188	6.133388	3.296917

O	8.976506	10.959765	2.590404
O	10.681129	8.115912	3.716685
O	8.798616	7.060220	0.990529
O	12.498177	6.524980	3.325882
N	11.740504	6.192337	0.524366
N	10.872568	4.533796	2.213716
N	10.550923	3.741438	3.248974
N	7.949733	5.273747	5.145160
H	7.975011	4.467472	5.782427
H	7.274431	6.031120	5.232564
N	10.950071	8.562995	1.067057
N	10.242180	9.675249	1.220930
N	9.669645	9.868881	4.738051
H	9.158742	10.735089	4.480925
H	9.828293	9.532904	5.685966
C	12.087415	4.912692	0.294080
C	12.886280	4.560654	-0.789590
H	13.141973	3.515407	-0.973369
C	13.356529	5.554821	-1.627227
H	13.993127	5.303059	-2.478649
C	13.009866	6.870987	-1.376745
H	13.365807	7.682069	-2.016325
C	12.183833	7.164228	-0.297281
C	11.608176	3.986553	1.280619
C	11.969796	2.556291	1.297507
H	12.663775	2.322594	2.127557
H	12.473305	2.250770	0.373330
H	11.074607	1.921003	1.415394
C	9.679338	4.005450	4.248217
C	8.840628	5.258611	4.174465
C	11.698381	8.482044	-0.008321
C	11.934311	9.623293	-0.907118
H	12.954804	10.024726	-0.780551
H	11.819591	9.336585	-1.963685
H	11.221988	10.422631	-0.656248
C	9.722764	9.989514	2.407686
C	10.081397	9.217279	3.676498
H	13.300236	6.698038	2.793395
H	12.301723	7.350732	3.834007
H	8.122186	6.930042	1.690865
H	8.760717	8.012030	0.737336
H	11.028992	2.833955	3.351327

Fe^{2+} Hdapsox Isomer XI LDA

Fe	10.627419	6.467170	2.147709
O	9.265606	5.595403	3.516806
O	9.093059	2.565094	5.288019
O	9.953506	11.225590	3.020781
N	8.765643	8.141205	3.175106
O	8.742678	6.276239	1.062750
O	11.928176	6.989540	3.611971
N	11.769276	6.084730	0.515342
N	11.064376	4.459846	2.259211
N	10.555074	3.719738	3.254735
N	8.379603	4.641498	5.891879
H	7.984302	4.301766	6.767069
H	8.442875	5.640110	5.709664
N	11.047525	8.491449	1.131302
N	10.679643	9.730523	1.500074
O	10.403090	8.702169	4.643715
C	12.193625	4.818828	0.318901
C	12.973325	4.478995	-0.783473
H	13.293918	3.442633	-0.916961
C	13.320226	5.461198	-1.685705
H	13.924864	5.221281	-2.563492
C	12.901004	6.766081	-1.462182
H	13.179816	7.556590	-2.160998
C	12.133699	7.051513	-0.343867
C	11.757663	3.881433	1.313557
C	12.036329	2.439923	1.257392
H	11.626910	1.954816	2.154353
H	13.121060	2.250081	1.200684
H	11.580151	1.979813	0.364401
C	9.646837	4.406471	3.888221
C	9.017246	3.761998	5.097667
C	11.695365	8.388432	0.008648
C	12.004579	9.569857	-0.820967
H	12.513978	9.307009	-1.753933
H	11.083198	10.114653	-1.095344
H	12.663226	10.272545	-0.277214
C	10.125193	10.070014	2.711114
C	9.763353	8.909834	3.611434
H	12.429480	6.295516	4.082523
H	11.484152	7.615385	4.279005
H	8.253856	8.355554	2.316020
H	8.530097	7.280171	3.697247
H	8.788388	5.718995	0.258776
H	8.438295	5.680696	1.797649
H	10.977150	10.538438	0.933718

Fe^{2+} Hdapsox Isomer XII LDA

Fe	10.670332	6.687961	2.166464
O	8.909986	3.188416	4.830070
O	8.152941	5.935835	4.423805
O	10.065945	11.273431	2.963587
N	8.994797	8.053076	2.872990
O	8.977057	6.059158	1.028385
O	12.551634	7.212205	3.027077
N	11.772764	6.124515	0.510361
N	10.973609	4.468637	2.318384
N	10.444591	3.644103	3.244415
N	10.408637	6.251958	4.408058
H	13.223026	6.497185	2.985686
H	11.295325	5.789834	4.633630
N	11.044679	8.563065	1.056614
N	10.770167	9.844652	1.358319
O	10.127892	8.927878	4.635673
C	12.158082	4.856721	0.360982
C	12.913882	4.456191	-0.731476
H	13.227874	3.416314	-0.837838
C	13.249081	5.407409	-1.680736
H	13.840623	5.123976	-2.553938
C	12.833759	6.713593	-1.522809
H	13.092733	7.471278	-2.263254
C	12.087481	7.057132	-0.394991
C	11.703932	3.930695	1.386649
C	12.063278	2.510000	1.265826
H	11.692338	1.861858	2.068452
H	13.161263	2.411021	1.248703
H	11.692063	2.107569	0.309071
C	9.525686	4.009116	4.166411
C	9.295590	5.486287	4.362869
C	11.647487	8.400847	-0.096674
C	11.913724	9.534347	-0.994155
H	12.372502	9.223364	-1.938881
H	10.976085	10.073067	-1.204828
H	12.571602	10.266274	-0.496026
C	10.229407	10.112062	2.545738
C	9.770026	9.003871	3.456124
H	12.931041	7.944632	2.493033

H	10.300015	7.234158	4.786207
H	8.534907	8.311907	1.994700
H	8.421226	7.448718	3.510736
H	8.881615	6.534624	0.174846
H	9.054933	5.112451	0.778966
H	10.593450	2.630259	3.142467

Fe^{2+} H_2dapsox Isomer I HS LDA

Fe	0.068941	2.334419	2.629245
O	-0.982682	3.904361	1.370337
O	0.361075	5.841583	-1.221113
O	-1.877646	2.826554	3.669905
O	-3.454394	1.033036	6.233735
O	-1.126009	1.134459	1.447971
H	-0.860770	0.348709	0.928579
H	-1.806926	1.622086	0.938442
O	0.642481	4.001826	3.717028
H	1.340050	4.026354	4.402928
H	-0.130918	4.499086	4.058592
N	1.801779	1.169289	2.759608
N	1.428727	2.951378	1.074546
N	1.010772	3.951952	0.301666
H	1.523420	4.458290	-0.451877
N	-1.729638	6.076614	-0.305151
H	-2.376103	5.715138	0.395485
H	-2.007693	6.847741	-0.914714
N	-0.158970	0.959372	4.257420
N	-1.315846	1.025551	4.914988
H	-1.674590	0.409903	5.675713
N	-4.320540	2.846070	5.125778
H	-5.197320	2.860179	5.649705
H	-4.148856	3.532294	4.391594
C	2.825478	1.362856	1.910690
C	3.989125	0.610868	1.973544
H	4.802604	0.800486	1.268042
C	4.101645	-0.376685	2.938254
H	5.007647	-0.983319	3.009506
C	3.047793	-0.580175	3.810671
H	3.101818	-1.350341	4.584894
C	1.912479	0.211437	3.695896
C	2.601356	2.416184	0.940424
C	3.619424	2.792157	-0.050567
H	3.903375	1.917598	-0.660427
H	3.297964	3.584818	-0.739197
H	4.537957	3.138899	0.453948
C	-0.229132	4.393310	0.514691
C	-0.527526	5.535470	-0.436757
C	0.757630	0.090921	4.559237
C	0.684995	-0.909763	5.633548
H	0.717095	-1.930792	5.214985
H	-0.218289	-0.830393	6.253136
H	1.554645	-0.814854	6.305649
C	-2.148363	2.002716	4.557575
C	-3.407311	1.925723	5.397455

Fe^{2+} H_2dapsox IS LDA

Fe	0.102323	2.326612	2.634737
O	-1.059364	3.831567	1.347126
O	0.328445	5.837764	-1.171786
O	-1.842688	2.926767	3.687130
O	-3.461661	1.061388	6.175740
O	-0.801466	1.198935	1.351079
H	-1.189071	0.358344	1.677464
H	-1.535915	1.756781	0.999799
O	0.679985	3.671968	3.896760
H	1.348474	4.324146	3.595538
H	-0.143252	4.164686	4.127682
N	1.818359	1.167006	2.763219
N	1.409423	2.997630	1.178872
N	0.979138	3.990492	0.393777
H	1.498051	4.508103	-0.349224
N	-1.831874	5.948995	-0.407187
H	-2.504632	5.555040	0.249851
H	-2.111307	6.701587	-1.039828
N	-0.187879	0.965899	4.164625
N	-1.343840	1.048588	4.831126
H	-1.713489	0.420041	5.578174
N	-4.270755	2.968485	5.188380
H	-5.136907	2.988930	5.730635
H	-4.079344	3.695107	4.499890
C	2.836401	1.383041	1.925699
C	3.997132	0.622118	1.975599
H	4.820269	0.819813	1.283798
C	4.085857	-0.390741	2.916866
H	4.984674	-1.009501	2.976558
C	3.026354	-0.613609	3.780180
H	3.069389	-1.408993	4.529345
C	1.901765	0.195522	3.676222
C	2.581057	2.458998	0.990975
C	3.555795	2.835350	-0.040720
H	3.741936	1.980007	-0.714387
H	3.251634	3.686079	-0.665266
H	4.525703	3.089282	0.420594
C	-0.291236	4.361088	0.526345
C	-0.594116	5.481732	-0.449673
C	0.722197	0.099768	4.509416
C	0.628738	-0.866778	5.612033
H	0.695774	-1.899458	5.227028
H	-0.291644	-0.789517	6.205890
H	1.479230	-0.732788	6.302724
C	-2.138075	2.074639	4.541282
C	-3.390901	2.000175	5.393485

Fe^{2+} H_2dapsox LS LDA

Fe	0.379041	2.213872	2.392509
O	-0.968377	3.488838	1.529253
O	-0.090828	5.735840	-1.014144
O	-1.618206	3.568701	4.595069
O	-3.785201	0.957312	5.428648
O	-0.322751	0.961674	1.067404
H	-0.333326	0.013965	1.323388
H	-1.247888	1.206886	0.842050
O	0.721243	3.550314	3.712307
H	1.049294	4.415908	3.391394
H	-0.241845	3.675478	4.129494
N	1.827218	1.208717	2.717508
N	1.499766	2.951737	1.140023
N	0.940000	3.923544	0.391350
H	1.352736	4.506441	-0.366624
N	-2.159472	5.558415	-0.034497
H	-2.711132	5.076353	0.675013
H	-2.584089	6.300428	-0.594925
N	-0.312137	1.150462	3.854468
N	-1.529962	1.264198	4.439640
H	-2.175245	0.478314	4.722638
N	-4.111640	3.203557	5.773948
H	-5.017585	3.099078	6.233927
H	-3.680832	4.125336	5.688714

C	2.930812	1.423282	1.960482
C	4.058652	0.642354	2.148936
H	4.950702	0.813918	1.540011
C	4.032232	-0.357908	3.113776
H	4.913673	-0.984237	3.270337
C	2.893068	-0.566033	3.875005
H	2.858629	-1.353787	4.632219
C	1.785944	0.246409	3.656928
C	2.718900	2.488878	1.003638
C	3.723039	2.939772	0.037043
H	4.058110	2.094961	-0.589971
H	3.359801	3.729494	-0.635348
H	4.618285	3.323913	0.557072
C	-0.347494	4.139324	0.654729
C	-0.886375	5.245664	-0.225029
C	0.512534	0.241003	4.336477
C	0.208585	-0.659833	5.451974
H	-0.139178	-1.645399	5.088740
H	-0.568624	-0.251712	6.115658
H	1.113184	-0.846362	6.050949
C	-2.089085	2.435038	4.745602
C	-3.449140	2.136526	5.365178

Fe^{2+} H_2dapsox Isomer II LDA

Fe	-0.001793	2.152651	2.528505
O	-1.103586	3.642542	1.354598
O	0.135944	5.992422	-0.921500
O	-2.185359	1.913822	3.119505
O	-2.319138	3.626203	5.438958
O	-0.751744	0.756737	1.181843
H	-1.726108	0.857029	1.130449
H	-0.418491	0.544419	0.287218
O	-0.120034	3.553187	4.022922
H	0.631626	3.986595	4.470012
H	-0.967951	3.699974	4.583692
N	1.823725	1.154508	2.762024
N	1.403418	3.055816	1.244552
N	0.942628	4.071445	0.511658
H	1.458104	4.693832	-0.143055
N	-2.034814	5.824210	-0.189050
H	-2.665259	5.311184	0.427718
H	-2.382128	6.602781	-0.751128
N	-0.191939	0.692052	4.132164
N	-1.305821	0.823874	4.879408
H	-1.274927	0.644758	5.891629
N	-4.133998	2.292481	5.776736
H	-4.603077	2.987878	6.365249
H	-4.635469	1.437829	5.532987
C	2.878841	1.512209	2.011158
C	4.105848	0.863354	2.115822
H	4.950340	1.188330	1.502119
C	4.239087	-0.180241	3.008658
H	5.191644	-0.705927	3.110369
C	3.148128	-0.545716	3.785804
H	3.229146	-1.359866	4.510622
C	1.958502	0.146436	3.641369
C	2.624928	2.619492	1.122830
C	3.646632	3.157156	0.211532
H	4.143148	2.340882	-0.338704
H	3.240770	3.852508	-0.536693
H	4.433914	3.690929	0.773856
C	-0.364015	4.318198	0.625264
C	-0.754978	5.486486	-0.251228
C	0.780496	-0.088062	4.463754
C	0.756655	-1.044167	5.579486
H	1.307674	-1.961166	5.321327
H	-0.269670	-1.340257	5.845178
H	1.247568	-0.623448	6.476188
C	-2.223367	1.653559	4.324865
C	-2.958298	2.583631	5.258786

Fe^{2+} H_2dapsox Isomer III LDA

Fe	0.109348	2.318363	2.631010
O	-0.820077	3.966225	1.540767
O	-1.633483	4.566903	-1.166144
O	-1.887067	2.605374	3.483686
O	-2.945614	3.318447	6.101507
O	-1.039050	1.277629	1.237283
H	-0.722076	0.702332	0.512744
H	-1.718644	1.881641	0.861471
O	0.459387	3.869061	3.980864
H	1.045230	3.856437	4.764145
H	-0.395625	4.270676	4.255561
N	1.831570	1.156661	2.760017
N	1.522103	3.048847	1.192398
N	1.104215	4.046999	0.395215
H	1.640726	4.335252	-0.432365
N	-0.435105	6.469680	-0.741359
H	0.107983	6.992717	-0.054211
H	-0.900529	6.994319	-1.487682
N	-0.180733	0.850830	4.172347
N	-1.334292	0.922009	4.856971
H	-1.482971	0.382651	5.718790
N	-4.328807	1.572198	5.572431
H	-5.060876	1.878469	6.219642
H	-4.560064	0.849488	4.890840
C	2.896694	1.419469	1.980808
C	4.057095	0.660600	2.037700
H	4.902278	0.899487	1.387285
C	4.124663	-0.403105	2.919949
H	5.025896	-1.017331	2.982398
C	3.030443	-0.674774	3.722853
H	3.053365	-1.503992	4.434585
C	1.901506	0.124704	3.620800
C	2.706163	2.533941	1.078248
C	3.737568	2.984652	0.130363
H	3.714191	2.385463	-0.798085
H	3.626461	4.045568	-0.143105
H	4.743658	2.872465	0.560176
C	-0.176538	4.431571	0.594881
C	-0.835667	5.215968	-0.517329
C	0.713881	-0.050204	4.429607
C	0.582185	-1.114480	5.436882
H	1.055740	-2.044195	5.088834
H	-0.466501	-1.358343	5.662642
H	1.081339	-0.833106	6.381256
C	-2.159137	1.923357	4.477826
C	-3.237852	2.328746	5.455415

Fe^{2+} H_2dapsox Isomer V LDA

Fe	0.174059	2.410016	2.410938
O	-0.866517	3.770894	1.113863
O	0.494694	5.805322	-1.393028
O	-2.029607	3.354491	4.638127
O	-3.502789	0.537397	6.084854
O	-0.991521	1.024593	1.347385
H	-0.587023	0.290712	0.840741
H	-1.686287	1.414952	0.776976
O	0.268376	3.861902	3.775672

H	0.629663	4.768719	3.756266
H	-0.669744	3.826150	4.211112
N	1.788375	1.191935	2.661584
N	1.582405	3.005063	1.018812
N	1.183836	3.982434	0.200439
H	1.723155	4.500062	-0.525598
N	-1.668274	5.884279	-0.628615
H	-2.333866	5.495814	0.039484
H	-1.957203	6.633158	-1.261144
N	-0.287484	1.134802	4.147233
N	-1.448695	1.118896	4.812990
H	-1.896662	0.282193	5.276836
N	-4.291718	2.695104	6.096797
H	-5.124665	2.493042	6.652096
H	-4.082226	3.652072	5.808456
C	2.885537	1.385026	1.907104
C	4.033990	0.621184	2.088773
H	4.913482	0.795730	1.463029
C	4.039317	-0.349878	3.068621
H	4.926809	-0.966225	3.232384
C	2.907853	-0.532015	3.853187
H	2.900557	-1.290563	4.638904
C	1.795147	0.263508	3.631914
C	2.750164	2.432436	0.925292
C	3.810149	2.775176	-0.032910
H	4.191876	1.870195	-0.533272
H	3.479973	3.468629	-0.819032
H	4.667247	3.241195	0.485354
C	-0.096303	4.329763	0.306759
C	-0.421235	5.438717	-0.669060
C	0.574214	0.199282	4.420696
C	0.338248	-0.823661	5.449423
H	-0.331478	-1.617680	5.068378
H	-0.143070	-0.387964	6.340962
H	1.265228	-1.313263	5.770783
C	-2.226408	2.190087	5.000515
C	-3.441203	1.729831	5.797796

Fe^{2+} H_2dapsox Isomer VII LDA

Fe	10.584707	6.484053	1.856087
O	9.162249	5.513620	3.521280
O	9.677215	2.395985	5.042903
O	10.790180	10.770397	3.422118
O	8.943243	7.826911	2.481189
O	11.380442	7.296476	3.505111
N	11.918824	5.988261	0.376149
N	11.169550	4.486961	2.183958
N	10.616289	3.818220	3.199115
N	8.098724	3.939045	5.659423
H	7.710347	3.365867	6.410681
H	7.710966	4.862045	5.470270
N	11.347010	8.305777	1.031428
N	11.082193	9.489527	1.596111
N	11.441441	8.902922	5.101619
H	11.330708	9.911781	5.265659
H	11.669754	8.253787	5.855101
C	12.383381	4.729617	0.271295
C	13.210933	4.349078	-0.775741
H	13.587730	3.325705	-0.843035
C	13.554989	5.290356	-1.732167
H	14.193647	5.012765	-2.574332
C	13.109836	6.593315	-1.593451
H	13.404534	7.358175	-2.315902
C	12.310275	6.923170	-0.505350
C	11.940162	3.862868	1.337640
C	12.284757	2.440159	1.463734
H	12.855909	2.253752	2.391397
H	12.895691	2.081590	0.627002
H	11.375226	1.814485	1.507689
C	9.602046	4.397682	3.839239
C	9.107072	3.473791	4.936653
C	11.935818	8.267482	-0.130015
C	12.294261	9.477622	-0.885265
H	12.792888	9.247107	-1.834017
H	11.401378	10.081192	-1.130374
H	12.978146	10.117099	-0.297088
C	10.998878	9.673822	2.945725
C	11.283759	8.488853	3.865072
O	9.127515	5.964596	0.436175
H	11.098907	10.355301	1.036516
H	10.849757	2.862095	3.545680
H	8.249008	8.292958	1.973447
H	8.510872	7.228806	3.135142
H	9.328619	5.432998	-0.361684
H	8.188951	5.808819	0.664548

Fe^{2+} H_2dapsox Isomer VIII LDA

Fe	10.876387	6.251249	1.826679
O	8.262106	2.748935	3.588476
O	9.089780	6.075481	2.809817
O	11.967854	10.760837	3.847236
O	9.556653	7.391264	0.644178
O	13.497690	7.607785	4.147832
N	12.092675	5.865523	0.281132
N	10.525584	4.193733	1.334556
N	9.737634	3.340758	2.009365
N	7.667282	5.139313	4.311127
H	7.318708	6.028277	4.673603
H	7.308238	4.231640	4.643398
N	12.154418	7.983182	1.653171
N	11.879572	9.184062	2.259464
N	13.719877	9.536395	5.308246
H	13.394122	10.509022	5.370588
H	14.372628	9.135677	5.983825
C	12.100164	4.644315	-0.285934
C	12.953409	4.341067	-1.336383
H	12.939696	3.348710	-1.792324
C	13.830833	5.308267	-1.798102
H	14.514606	5.086906	-2.621063
C	13.837199	6.551752	-1.196750
H	14.532930	7.325041	-1.530271
C	12.955708	6.804734	-0.152030
C	11.187419	3.705133	0.320066
C	11.042097	2.309094	-0.121630
H	11.443874	1.604890	0.632356
H	11.578629	2.108730	-1.055916
H	9.980457	2.054154	-0.290703
C	8.857968	3.630894	3.001061
C	8.565912	5.080530	3.360331
C	12.880531	8.053075	0.566005
C	13.532380	9.284815	0.101030
H	13.879335	9.895314	0.949331
H	14.383122	9.076124	-0.559924
H	12.828280	9.911713	-0.478622
C	12.281446	9.646530	3.474938
C	13.219189	8.803877	4.340811
O	11.786472	5.987327	3.547796
H	8.635373	7.319096	0.975133
H	9.525275	7.343402	-0.333452
H	12.574282	6.679550	3.761415
H	11.305978	5.813182	4.381577

H	11.390278	9.897463	1.702834
H	9.823098	2.330174	1.821042

Fe^{2+} H_2dapsox Isomer IX LDA

Fe	10.547716	6.671213	2.065217
O	9.854489	5.729967	4.422255
O	9.366164	2.312315	4.992427
O	10.087154	11.248235	3.045567
O	9.099945	7.884064	2.850352
O	8.754479	6.028840	1.170440
O	11.810002	7.174504	3.623054
N	11.710846	6.133968	0.496785
N	10.893561	4.527555	2.245684
N	10.354624	3.840469	3.251543
N	8.688857	4.051585	6.334599
H	8.275333	3.465355	7.061111
H	8.692042	5.067259	6.430546
N	11.178149	8.509344	1.150167
N	10.991620	9.737986	1.658290
N	8.287727	9.667681	3.992478
H	8.434378	10.675126	4.151820
H	7.527874	9.151697	4.437237
C	11.977861	4.836721	0.255667
C	12.711693	4.437303	-0.851029
H	12.918149	3.377197	-1.019574
C	13.187971	5.399346	-1.725736
H	13.765661	5.110303	-2.607005
C	12.935309	6.731863	-1.461117
H	13.314334	7.507692	-2.129769
C	12.197040	7.074304	-0.333643
C	11.471454	3.917790	1.254284
C	11.647743	2.462061	1.127216
H	11.011079	1.876038	1.804333
H	12.696472	2.183807	1.337804
H	11.428134	2.128620	0.101040
C	9.841525	4.498414	4.293446
C	9.257098	3.499743	5.273043
C	11.920628	8.427188	0.078004
C	12.467827	9.615808	-0.596088
H	12.983355	9.365882	-1.530060
H	11.669824	10.339681	-0.839408
H	13.210335	10.132632	0.042390
C	10.125619	10.104617	2.636961
C	9.131689	9.090739	3.174785
H	11.332497	6.657544	4.330389
H	12.765089	6.965818	3.662268
H	8.573994	5.825469	0.230855
H	8.024638	6.588976	1.511685
H	11.566945	10.517360	1.304961
H	10.260737	2.803082	3.344158

Fe^{2+} H_2dapsox Isomer X LDA

Fe	10.633867	6.702121	2.148198
O	9.534024	3.136671	5.139782
O	8.960403	6.089627	3.331922
O	9.296624	11.258533	2.541533
O	10.475208	8.169330	3.711537
O	8.855233	6.852805	0.978534
O	12.306777	6.545280	3.461453
N	11.757363	6.207765	0.520559
N	10.918120	4.515214	2.229441
N	10.609184	3.716552	3.261442
N	7.898075	5.136959	5.098793
H	7.912902	4.313147	5.716670
H	7.190786	5.866993	5.186253
N	11.003261	8.575807	1.064350
N	10.406136	9.753138	1.303995
N	9.569748	9.967962	4.764591
H	9.202909	10.915366	4.596820
H	9.613734	9.562476	5.699860
C	12.107799	4.926119	0.294647
C	12.859598	4.563006	-0.815862
H	13.120522	3.517251	-0.989642
C	13.277401	5.539596	-1.700316
H	13.876091	5.276061	-2.575478
C	12.923629	6.853877	-1.462307
H	13.244331	7.642178	-2.146257
C	12.152860	7.160007	-0.347725
C	11.667065	3.989405	1.300297
C	12.070967	2.571835	1.321090
H	12.760774	2.361746	2.161319
H	12.596793	2.270802	0.408303
H	11.193996	1.909678	1.432045
C	9.700916	3.942011	4.244414
C	8.828694	5.180419	4.175242
C	11.682606	8.490180	-0.045873
C	11.888439	9.646602	-0.936097
H	12.612126	9.439608	-1.732304
H	10.947542	9.943419	-1.438751
H	12.257993	10.520696	-0.371533
C	9.845663	10.176508	2.465429
C	9.988994	9.317867	3.705090
H	13.232029	6.543246	3.143228
H	12.191307	7.314083	4.064814
H	8.147621	6.456721	1.534215
H	8.773288	6.487205	0.074579
H	11.097471	2.813286	3.359650
H	10.334426	10.442275	0.540010

Fe^{2+} H_2dapsox Isomer XI LDA

Fe	10.511793	6.583823	2.127220
O	8.935048	5.518758	3.653853
O	9.621293	2.455571	5.222718
O	9.893699	11.363080	2.821780
N	9.182942	8.130693	3.334928
O	8.668838	6.417086	1.102831
O	11.707365	6.775822	3.753106
N	11.731847	6.126849	0.550568
N	10.902774	4.512721	2.256682
N	10.380841	3.828709	3.278143
N	8.012272	3.950855	5.879174
H	7.693784	3.389265	6.671824
H	7.565374	4.845181	5.681873
N	10.985746	8.548705	1.050376
N	10.533062	9.787581	1.324784
O	10.899383	9.038090	4.518078
C	12.176903	4.862034	0.406164
C	13.039561	4.497942	-0.620170
H	13.387683	3.465337	-0.703191
C	13.449610	5.459296	-1.520918
H	14.130152	5.203805	-2.336847
C	12.990314	6.756934	-1.371689
H	13.313648	7.533123	-2.067832
C	12.135565	7.066387	-0.321767
C	11.695557	3.935175	1.400871
C	12.082188	2.517636	1.433505
H	11.369745	1.896383	1.996070
H	13.079659	2.391709	1.893548

H	12.144734	2.102080	0.416557
C	9.403627	4.407385	3.966796
C	8.998408	3.504366	5.117337
C	11.653260	8.407577	-0.058864
C	11.924860	9.544741	-0.956089
H	12.498383	9.259342	-1.844201
H	10.985384	10.000324	-1.321238
H	12.498840	10.332196	-0.432254
C	10.150287	10.213462	2.578296
C	10.092390	9.106193	3.603446
H	12.669577	6.599838	3.748836
H	11.532918	7.619202	4.303476
H	8.409915	8.350339	2.693997
H	8.943353	7.478467	4.097370
H	8.615917	6.084541	0.182016
H	8.133516	5.808144	1.660628
H	10.676194	10.544065	0.638568
H	10.671468	2.901765	3.665586

Fe^{2+} H_2dapsox Isomer XII LDA

Fe	10.674654	6.672563	2.168886
O	8.926216	3.194218	4.837445
O	8.157710	5.941325	4.404304
O	10.106253	11.308163	2.929975
N	9.000652	8.065128	2.893565
O	8.971645	6.054215	1.083091
O	12.544451	7.182453	3.025856
N	11.775201	6.127470	0.497107
N	10.974486	4.464787	2.309561
N	10.453503	3.644679	3.241548
N	10.412107	6.256978	4.400876
H	13.207631	6.458151	3.032552
H	11.293167	5.790996	4.643151
N	11.028021	8.530775	1.023006
N	10.673502	9.787062	1.361484
O	10.104231	8.982028	4.661882
C	12.155052	4.859791	0.349611
C	12.923050	4.460700	-0.737480
H	13.232382	3.419922	-0.842407
C	13.278574	5.409381	-1.678066
H	13.879710	5.125251	-2.543357
C	12.868156	6.720236	-1.518939
H	13.140353	7.479326	-2.252664
C	12.111435	7.052855	-0.402949
C	11.693063	3.929053	1.369410
C	12.035032	2.507152	1.232714
H	11.606076	1.845910	1.994051
H	13.130647	2.388006	1.271084
H	11.707946	2.138333	0.247199
C	9.532849	4.011978	4.164729
C	9.296893	5.489698	4.354461
C	11.662114	8.402179	-0.106547
C	11.938132	9.542065	-0.990567
H	12.448754	9.240608	-1.910111
H	10.999620	10.047965	-1.276168
H	12.579865	10.284113	-0.482018
C	10.199101	10.144299	2.579805
C	9.751931	9.023866	3.487274
H	12.984558	7.918571	2.547560
H	10.304163	7.220615	4.809721
H	8.530950	8.316910	2.017819
H	8.435137	7.445743	3.529597
H	8.784863	6.549282	0.256116
H	9.030449	5.113786	0.805936
H	10.606909	2.631407	3.145510
H	10.953089	10.561178	0.740060

Mn^{2+} dapsox Isomer I HS LDA

Mn	-1.935096	3.990885	11.159838
N	-2.860221	5.949475	11.004174
N	-2.577556	4.290477	9.115190
N	-2.461040	3.272182	8.261164
N	-1.297398	-0.017290	8.907610
N	-1.867994	4.994002	13.132067
N	-1.294424	4.347223	14.145921
N	-0.206863	2.818441	15.981005
O	-2.026414	2.096401	10.199377
O	-1.883977	0.895089	6.897212
O	-0.560185	2.937698	12.468188
O	0.544291	1.339152	14.417727
O	0.183154	4.595675	10.657742
O	-3.847945	2.938699	11.812677
H	-3.502890	2.263328	11.162126
C	-3.278328	6.369025	9.801891
C	-3.805595	7.648722	9.640206
C	-3.911242	8.467291	10.748617
C	-3.478213	8.018654	11.987193
C	-2.930824	6.741776	12.077934
C	-3.182243	5.383754	8.748492
C	-3.741910	5.592846	7.402328
C	-2.108181	2.190420	8.917660
C	-1.756856	0.963342	8.109858
C	-2.378737	6.177312	13.293149
C	-2.381558	6.916429	14.570975
H	-3.409569	7.159376	14.883675
H	-1.833743	7.869904	14.483364
H	-1.904171	6.298348	15.341676
C	-0.670348	3.263101	13.684650
C	-0.042924	2.361017	14.726012
H	-4.336152	9.469577	10.649635
H	-4.136476	7.981123	8.652858
H	-0.759144	3.670663	16.098136
H	-3.559963	8.644754	12.879284
H	0.135721	2.263643	16.760618
H	-3.449437	4.743431	6.767032
H	0.370008	5.495574	10.993826
H	-0.965343	-0.883297	8.492359
H	-1.206235	0.185587	9.904158
H	-4.842750	5.657279	7.424583
H	0.392405	3.974635	11.410346
H	-3.369372	6.532675	6.960349
H	-4.608504	3.365123	11.370370

Mn^{2+} dapsox IS LDA

Mn	-2.092372	4.217447	10.920098
N	-2.870992	5.905554	10.910584
N	-2.742008	4.337955	9.135959
N	-2.555978	3.289435	8.308657
N	-1.240915	0.110183	9.178804
N	-1.859366	4.759218	12.867597
N	-1.395749	4.024981	13.878325
N	0.941234	1.501891	14.627740
O	-2.004937	2.322373	10.312285
O	-1.963396	0.802606	7.128897
O	0.334892	3.017247	12.654179
O	-0.696079	2.384311	15.945657
O	-0.135202	4.315616	10.681119
O	-3.951328	3.049077	11.853550

H	-3.556200	2.339678	11.285242
C	-3.361665	6.414707	9.731535
C	-3.860289	7.716337	9.692100
C	-3.854440	8.483508	10.837672
C	-3.345192	7.952236	12.028243
C	-2.857598	6.662819	12.044744
C	-3.278984	5.478471	8.690048
C	-3.714184	5.666815	7.297782
C	-2.127811	2.281278	9.009371
C	-1.774150	0.997793	8.316471
C	-2.285422	5.972181	13.156598
C	-2.170380	6.520182	14.513695
H	-2.906024	7.316230	14.692518
H	-1.161332	6.927919	14.697476
H	-2.299279	5.692556	15.231774
C	-0.413848	3.191014	13.685114
C	-0.089515	2.326317	14.890824
H	-4.244580	9.503417	10.818625
H	-4.250074	8.105159	8.747628
H	1.367410	1.562928	13.702571
H	-3.322172	8.545423	12.945369
H	1.263044	0.859717	15.345753
H	-3.510898	4.744877	6.734351
H	0.219359	5.223786	10.727769
H	-0.932301	-0.792726	8.829840
H	-1.110626	0.396148	10.149771
H	-4.792612	5.889672	7.241282
H	0.157366	3.740618	11.630227
H	-3.177182	6.502140	6.819068
H	-4.694363	3.407321	11.329383

Mn^{2+} dapsox LS LDA

Mn	0.283634	2.173281	2.873777
O	-1.311639	3.217522	0.395440
O	-0.143579	6.470827	-0.204612
O	-1.386473	2.913260	3.593658
O	-3.796946	1.730057	5.881600
O	-0.834239	1.164027	1.635799
H	-0.266499	0.574131	1.099849
H	-1.065280	2.034708	0.997751
O	0.956382	3.743845	3.928491
H	0.040282	3.995139	4.224871
H	1.208219	4.410144	3.245449
N	1.804303	1.119138	2.814502
N	1.218502	2.959816	1.383721
N	0.811033	4.115072	0.813188
N	-2.137883	5.434884	-0.598191
H	-2.616504	4.536169	-0.516563
H	-2.555057	6.250833	-1.036210
N	-0.052993	0.972429	4.277225
N	-1.246512	1.039745	4.916305
N	-3.803932	3.442778	4.376797
H	-4.757827	3.710529	4.603034
H	-3.286869	3.866218	3.605825
C	2.761531	1.362772	1.881057
C	3.907847	0.575862	1.821825
H	4.664872	0.788399	1.063193
C	4.059722	-0.461191	2.729872
H	4.955394	-1.085928	2.699031
C	3.073597	-0.710209	3.676403
H	3.167198	-1.524974	4.398301
C	1.940644	0.092924	3.706016
C	2.406831	2.473840	1.065947
C	3.252098	3.052638	0.012467
H	3.212079	2.451061	-0.912514
H	2.885276	4.063081	-0.226338
H	4.305163	3.095771	0.332269
C	-0.435190	4.147657	0.406425
C	-0.866642	5.490455	-0.162179
C	0.808637	0.007936	4.560257
C	0.591010	-1.008768	5.597324
H	0.722557	-2.024553	5.188518
H	-0.427653	-0.903428	5.997146
H	1.309855	-0.893062	6.426876
C	-1.881896	2.083324	4.478608
C	-3.260537	2.379927	5.003149

Mn^{2+} dapsox Isomer II LDA

Mn	-1.935096	3.990885	11.159838
N	-2.860221	5.949475	11.004174
N	-2.577556	4.290477	9.115190
N	-2.461040	3.272182	8.261164
N	-1.297398	-0.017290	8.907610
N	-1.867994	4.994002	13.132067
N	-1.294424	4.347223	14.145921
N	-0.206863	2.818441	15.981005
O	-2.026414	2.096401	10.199377
O	-1.883977	0.895089	6.897212
O	-0.560185	2.937698	12.468188
O	0.544291	1.339152	14.417727
O	0.183154	4.595675	10.657742
O	-3.847945	2.938699	11.812677
H	-3.502890	2.263328	11.162126
C	-3.278328	6.369025	9.801891
C	-3.805595	7.648722	9.640206
C	-3.911242	8.467291	10.748617
C	-3.478213	8.018654	11.987193
C	-2.930824	6.741776	12.077934
C	-3.182243	5.383754	8.748492
C	-3.741910	5.592846	7.402328
C	-2.108181	2.190420	8.917660
C	-1.756856	0.963342	8.109858
C	-2.378737	6.177312	13.293149
C	-2.381558	6.916429	14.570975
H	-3.409569	7.159376	14.883675
H	-1.833743	7.869904	14.483364
H	-1.904171	6.298348	15.341676
C	-0.670348	3.263101	13.684650
C	-0.042924	2.361017	14.726012
H	-4.336152	9.469577	10.649635
H	-4.136476	7.981123	8.652858
H	-0.759144	3.670663	16.098136
H	-3.559963	8.644754	12.879284
H	0.135721	2.263643	16.760618
H	-3.449437	4.743431	6.767032
H	0.370008	5.495574	10.993826
H	-0.965343	-0.883297	8.492359
H	-1.206235	0.185587	9.904158
H	-4.842750	5.657279	7.424583
H	0.392405	3.974635	11.410346
H	-3.369372	6.532675	6.960349
H	-4.608504	3.365123	11.370370

Mn^{2+} dapsox Isomer III LDA

Mn	-1.933419	3.956119	11.186151
N	-2.836213	5.941762	10.995311
N	-2.520608	4.295995	9.095520
N	-2.386207	3.276416	8.248345
N	-1.868834	1.154320	6.786270

N	-1.937354	4.956663	13.150556
N	-1.339232	4.333985	14.165802
N	-0.231363	2.818776	16.003977
O	-2.100629	2.073689	10.195622
O	-1.729043	-0.174122	8.632377
O	-0.526308	2.976232	12.484766
O	0.868504	1.593532	14.428180
O	0.183663	4.568424	10.623528
O	-3.834479	2.912068	11.880252
H	-3.527793	2.215233	11.235521
C	-3.219952	6.373575	9.790595
C	-3.784810	7.637597	9.631076
C	-3.970629	8.425284	10.754227
C	-3.579271	7.960945	11.998764
C	-2.989750	6.701316	12.083275
C	-3.059760	5.414822	8.715383
C	-3.535490	5.684497	7.346557
C	-2.131244	2.163678	8.933215
C	-1.885158	0.914943	8.112607
C	-2.460304	6.134758	13.308406
C	-2.474981	6.874419	14.583499
H	-3.506385	7.110360	14.894335
H	-1.932594	7.831100	14.500322
H	-1.996234	6.258434	15.356863
C	-0.645708	3.295181	13.702553
C	0.083211	2.467912	14.741572
H	-4.426448	9.414605	10.658407
H	-4.080361	7.984681	8.637770
H	-0.889891	3.588863	16.131215
H	-3.719533	8.562405	12.900506
H	0.193978	2.316238	16.778171
H	-3.294739	4.822433	6.709784
H	0.364664	5.465129	10.966569
H	-1.667635	0.387629	6.150302
H	-2.005595	2.117400	6.475540
H	-4.626171	5.849073	7.324362
H	0.413954	3.945892	11.370447
H	-3.061246	6.589040	6.931813
H	-4.615418	3.331589	11.469965

Mn^{2+} dapsox Isomer V LDA

Mn	-2.028545	4.025252	10.997024
N	-2.948901	5.894211	10.963417
N	-2.712629	4.322791	9.016188
N	-2.604158	3.308538	8.159567
N	-1.339461	0.045281	8.757941
N	-1.796000	4.846450	13.029113
N	-1.307490	4.240263	14.110038
N	0.885259	1.561994	14.802652
O	-2.051515	2.153420	10.086374
O	-2.008678	0.957096	6.776335
O	0.126324	2.950341	12.791811
O	-0.512909	2.666512	16.226998
O	0.022741	4.319648	10.757108
O	-3.876443	2.901143	11.746215
H	-3.581492	2.232035	11.073507
C	-3.355821	6.382089	9.778425
C	-3.750429	7.709475	9.657244
C	-3.707916	8.517079	10.781650
C	-3.261958	8.005339	11.990891
C	-2.861838	6.673615	12.050145
C	-3.346409	5.417603	8.700496
C	-3.973352	5.650855	7.389405
C	-2.186971	2.239386	8.801284
C	-1.842780	1.024088	7.981479
C	-2.306843	6.035824	13.223684
C	-2.291045	6.677302	14.549046
H	-3.073749	7.441077	14.650886
H	-1.312711	7.142681	14.759208
H	-2.409610	5.885999	15.308036
C	-0.439884	3.279280	13.885119
C	-0.043580	2.482788	15.118103
H	-4.014174	9.564094	10.713627
H	-4.079639	8.096249	8.689499
H	1.174205	1.518896	13.823956
H	-3.214624	8.631049	12.884940
H	1.238853	0.936069	15.519437
H	-3.740148	4.800132	6.732467
H	0.317183	5.241177	10.885437
H	-1.019878	-0.816696	8.325809
H	-1.218447	0.243031	9.751740
H	-5.068534	5.750064	7.474859
H	0.193315	3.796115	11.670041
H	-3.597496	6.580904	6.932186
H	-4.670804	3.328988	11.371648

Mn^{2+} dapsox Isomer VI LDA

Mn	0.183103	0.420647	-0.163311
O	2.242793	0.436241	0.330004
O	-2.126394	0.295713	0.357189
O	-0.064780	1.954739	1.053254
O	-0.468399	4.089852	-1.682518
O	1.814351	-0.121038	2.712582
O	-0.761507	-0.900836	4.964499
N	-0.394966	4.213696	0.954768
N	0.020635	1.791399	-1.557452
N	0.155521	1.709063	-2.865726
N	-0.081168	-0.952258	-1.590875
N	0.066133	-1.269785	0.987591
N	-0.192801	-1.244090	2.306942
N	1.300076	0.041467	5.227970
C	-0.232669	3.024937	0.409092
C	-0.245107	3.044477	-1.075298
C	0.192510	0.568949	-3.495541
C	0.386176	0.698686	-4.968058
C	0.097504	-0.754253	-2.930143
C	0.185452	-1.855779	-3.783953
C	0.075541	-3.145285	-3.301775
C	-0.085241	-3.335231	-1.937358
C	-0.131524	-2.235991	-1.103299
C	-0.216469	-2.363502	0.320633
C	-0.583276	-3.608594	1.017825
C	0.691307	-0.609414	3.047425
C	0.305885	-0.516133	4.516227
H	-0.442321	4.345862	1.961165
H	-0.533958	4.963988	0.265722
H	0.438302	1.767740	-5.208180
H	1.315958	0.215330	-5.310638
H	-0.449644	0.255069	-5.533345
H	0.321553	-1.679495	-4.851807
H	0.127866	-3.998555	-3.981918
H	-0.153282	-4.335337	-1.503096
H	-1.109201	-3.335680	1.948346
H	-1.206119	-4.266979	0.397556
H	2.126688	0.334824	4.703349
H	1.191278	0.179609	6.227996
H	0.315003	-4.168157	1.331535
H	-2.034262	-0.106979	1.252863
H	-2.422515	-0.435306	-0.223038
H	2.768502	-0.255689	-0.114557

H	2.130921	0.137264	1.348355

Mn^{2+} dapsox Isomer VII LDA

Mn	10.847607	6.642898	2.006272
O	8.591996	4.830804	3.151523
O	9.785123	2.475469	5.492873
O	10.648522	10.935474	3.252817
O	9.044974	7.329237	2.912667
O	11.719496	7.588705	3.560657
N	11.941287	6.037304	0.347568
N	11.110702	4.491823	2.217160
N	10.647796	3.742335	3.216595
N	7.831580	3.639400	5.328197
H	7.440949	3.228679	6.171023
H	7.329609	4.314696	4.751618
N	11.466968	8.465154	1.018871
N	11.215810	9.686731	1.448042
N	11.288995	9.276741	5.003820
H	10.958174	10.259215	4.983201
H	11.442270	8.705161	5.830883
C	12.271715	4.748582	0.215610
C	13.053325	4.323973	-0.854764
H	13.321089	3.270843	-0.961836
C	13.480063	5.271116	-1.772981
H	14.084546	4.962986	-2.630325
C	13.162178	6.605750	-1.599853
H	13.507090	7.365276	-2.304824
C	12.395579	6.976704	-0.493843
C	11.746292	3.881935	1.250980
C	11.915379	2.419757	1.235959
H	11.895831	2.059976	2.278317
H	12.848435	2.121518	0.737612
H	11.079260	1.921289	0.715769
C	9.462319	4.024893	3.670364
C	9.065509	3.280488	4.927419
C	12.085861	8.334626	-0.130290
C	12.516810	9.497636	-0.923258
H	12.531373	9.279928	-2.000914
H	11.836913	10.336238	-0.704798
H	13.527045	9.831106	-0.626635
C	11.027171	9.862981	2.757360
C	11.385819	8.774911	3.789683
O	8.946794	5.829889	0.788581
H	8.472428	7.516125	2.136415
H	8.755120	6.387518	3.197923
H	9.235211	5.250923	0.057595
H	8.757266	5.229780	1.593893

Mn^{2+} dapsox Isomer VIII LDA

Mn	11.244682	6.442635	2.109953
O	8.445695	3.159581	3.821893
O	9.041715	5.964363	1.786215
O	12.324970	10.701525	3.620783
O	9.929648	8.077152	2.808537
O	12.879607	7.234146	3.479081
N	12.234330	5.886518	0.278672
N	11.034250	4.223144	1.812634
N	10.391792	3.426804	2.675309
N	7.193238	5.005204	2.684381
H	6.572216	5.768990	2.430033
H	6.961364	4.216280	3.316014
N	12.130369	8.286077	1.169829
N	12.024540	9.506800	1.708279
N	13.503052	8.892565	4.894576
H	13.339821	9.909308	5.013875
H	13.878444	8.262594	5.598904
C	12.358956	4.595696	-0.039254
C	12.995327	4.201651	-1.214044
H	13.089470	3.139670	-1.451944
C	13.477096	5.178295	-2.066706
H	13.970551	4.896471	-3.000757
C	13.332589	6.513028	-1.733362
H	13.709265	7.307176	-2.381964
C	12.709685	6.836547	-0.530222
C	11.735968	3.662701	0.874991
C	11.831740	2.203266	0.691249
H	11.475625	1.715443	1.611100
H	12.864419	1.894566	0.465789
H	11.191950	1.859284	-0.139652
C	9.159664	3.790651	3.024603
C	8.484202	5.034965	2.407698
C	12.591572	8.193107	-0.040135
C	13.043494	9.351993	-0.830972
H	14.145047	9.400995	-0.877138
H	12.670000	9.301095	-1.865849
H	12.684985	10.268117	-0.338042
C	12.379114	9.635402	2.984963
C	12.952227	8.444143	3.781309
O	11.063177	5.650856	4.168217
H	11.955403	6.006897	4.407324
H	11.108508	4.664353	4.100101
H	9.142097	7.668247	2.370451
H	10.197176	8.892577	2.315431

Mn^{2+} dapsox Isomer IX LDA

Mn	10.545184	6.599235	2.203437
O	10.001683	5.675022	4.257571
O	9.148019	2.443442	5.358489
O	10.042136	11.115971	3.232970
O	8.935367	7.814999	2.722599
O	8.836733	6.357808	0.608628
O	12.057771	7.028640	3.775001
N	11.753289	6.111626	0.514727
N	10.832050	4.437395	2.194143
N	10.357640	3.660069	3.171635
N	8.785009	4.521587	6.226631
H	8.307723	4.169082	7.050808
H	8.948091	5.514465	6.053220
N	11.176310	8.533207	1.257743
N	10.982151	9.771716	1.675693
N	8.299155	9.541277	4.037981
H	8.584254	10.521591	4.230799
H	7.537501	9.024555	4.470067
C	11.985469	4.825626	0.235141
C	12.675439	4.453922	-0.913885
H	12.853690	3.398002	-1.129928
C	13.116939	5.455030	-1.764577
H	13.662021	5.195931	-2.676390
C	12.871000	6.780752	-1.465161
H	13.217594	7.576507	-2.126899
C	12.169407	7.092943	-0.294832
C	11.494777	3.883959	1.221555
C	11.748572	2.436659	1.127337
H	11.195964	1.932377	1.933330
H	12.823178	2.210822	1.235425
H	11.429205	2.042262	0.148883
C	9.918244	4.397479	4.167656
C	9.247761	3.656426	5.304158
C	11.846370	8.431045	0.128755

C	12.285522	9.633014	-0.600942
H	13.047483	9.412916	-1.359122
H	11.434633	10.140749	-1.085787
H	12.669249	10.361293	0.133631
C	10.124129	10.012738	2.664736
C	9.077050	8.995587	3.125517
H	12.903323	6.569348	3.610672
H	11.473345	6.395089	4.299845
H	9.229246	6.749763	-0.197038
H	8.437957	7.116208	1.101099

Mn^{2+} dapsox Isomer X LDA

Mn	10.523485	6.739035	2.196422
O	9.720916	3.414667	5.397442
O	8.748460	5.760708	2.967384
O	9.733193	11.389538	2.800549
O	10.088262	8.006914	3.691855
O	8.801639	6.800571	0.687602
O	12.585350	6.789305	3.315064
N	11.743419	6.209805	0.558565
N	11.077518	4.520903	2.426703
N	10.841229	3.706950	3.446846
N	7.877438	5.026778	4.929326
H	8.126231	4.353192	5.680294
H	7.074800	5.650160	4.904377
N	11.032392	8.682262	1.117975
N	10.722230	9.936954	1.398229
N	9.257428	9.853352	4.681470
H	9.132620	10.862458	4.476911
H	9.016046	9.364711	5.539570
C	12.060021	4.923477	0.347516
C	12.694675	4.528291	-0.829752
H	12.945540	3.477499	-0.987833
C	12.994543	5.491510	-1.778132
H	13.487449	5.204818	-2.711221
C	12.676083	6.815521	-1.544205
H	12.912661	7.594672	-2.271728
C	12.043244	7.156069	-0.344695
C	11.713648	4.002850	1.400715
C	12.062812	2.571556	1.324546
H	11.977147	2.143998	2.335517
H	13.077539	2.419718	0.926096
H	11.362992	2.021001	0.671583
C	9.880097	4.003883	4.313443
C	8.791664	5.028660	3.979735
C	11.701442	8.509101	-0.002786
C	12.078020	9.624559	-0.894787
H	13.173334	9.710820	-0.993356
H	11.668595	9.479715	-1.908554
H	11.678823	10.554984	-0.467071
C	10.109215	10.232345	2.542054
C	9.834254	9.226978	3.671094
H	12.718378	5.817020	3.262493
H	13.156343	7.158111	2.609867
H	8.316535	6.182331	1.287430
H	9.051712	6.287007	-0.105320

Mn^{2+} dapsox Isomer XI LDA

Mn	10.668536	6.601992	2.239357
O	9.975945	5.719941	4.166023
O	8.924216	2.548118	5.269574
O	9.713172	11.148293	2.950492
N	8.882653	7.840987	2.778672
O	8.881007	6.108222	0.566944
O	12.065187	7.124335	3.807938
N	11.830206	6.113861	0.553893
N	10.728894	4.441751	2.114825
N	10.213435	3.687707	3.093656
N	8.746730	4.634535	6.178601
H	8.278336	4.300325	7.016130
H	8.983644	5.617943	6.035783
N	11.100589	8.553308	1.191276
N	10.781015	9.796375	1.492008
O	9.600156	8.855040	4.674919
C	12.034926	4.821491	0.253312
C	12.713402	4.447870	-0.898205
H	12.873939	3.391924	-1.126274
C	13.171020	5.453858	-1.739760
H	13.717903	5.195693	-2.650667
C	12.927226	6.776923	-1.440598
H	13.277400	7.569902	-2.103316
C	12.217417	7.101416	-0.273763
C	11.504612	3.885305	1.222244
C	11.821449	2.448463	1.209176
H	11.189533	1.940071	1.951911
H	12.879759	2.268896	1.464202
H	11.652991	2.015722	0.209662
C	9.813988	4.445703	4.088025
C	9.116166	3.750848	5.232983
C	11.854032	8.431482	0.108861
C	12.269679	9.629553	-0.642607
H	12.980490	9.402416	-1.446731
H	11.390351	10.145358	-1.064561
H	12.711133	10.360526	0.054340
C	10.022971	10.018043	2.598563
C	9.491064	8.882497	3.467835
H	12.961272	6.737438	3.786029
H	11.515093	6.577162	4.435825
H	8.488657	8.029338	1.850776
H	8.316672	7.231500	3.382309
H	9.450157	6.266995	-0.215289
H	9.044479	5.164684	0.791332

Mn^{2+} dapsox Isomer XII LDA

Mn	10.661832	6.678349	2.186558
O	9.113305	3.220682	5.027306
O	8.211591	5.884942	4.358423
O	9.863214	11.304566	2.853813
N	8.915978	8.075127	2.884517
O	8.885009	6.080880	0.956491
O	12.669480	7.152161	3.081617
N	11.771134	6.133799	0.505493
N	10.873326	4.404269	2.299539
N	10.397400	3.516817	3.192756
N	10.441760	6.266715	4.468097
H	13.310575	6.446085	2.848137
H	11.349955	5.844156	4.682478
N	11.105474	8.612171	1.080800
N	10.790025	9.893799	1.350792
O	10.111551	8.985277	4.579495
C	12.085887	4.847820	0.331729
C	12.835873	4.445095	-0.770087
H	13.090672	3.392811	-0.908683
C	13.243925	5.405490	-1.677204
H	13.833103	5.116142	-2.550890
C	12.909030	6.733005	-1.481335
H	13.232209	7.494992	-2.191375
C	12.158150	7.077874	-0.359581
C	11.601620	3.911345	1.330114

C	11.932851	2.481895	1.198294
H	11.453146	1.912937	2.002944
H	13.024433	2.331593	1.245519
H	11.601207	2.091023	0.222425
C	9.649865	3.976786	4.190705
C	9.370654	5.449089	4.372120
C	11.759788	8.437778	-0.041069
C	12.088664	9.572277	-0.918571
H	12.648723	9.270818	-1.809988
H	11.164314	10.086560	-1.229063
H	12.668436	10.324276	-0.358474
C	10.136551	10.144897	2.482383
C	9.700887	9.038284	3.412173
H	12.977263	7.935268	2.573676
H	10.295180	7.250528	4.813330
H	8.451829	8.267281	1.992056
H	8.417100	7.416838	3.537219
H	9.005105	6.406198	0.037955
H	8.946731	5.103428	0.876824

Mn^{2+} Hdapsox Isomer I HS LDA

Mn	0.070255	2.314287	2.733087
O	-1.090293	3.876283	1.232155
O	0.333994	5.820022	-1.309627
O	-1.635394	2.877090	3.928880
O	-3.805246	1.082422	6.043066
O	-1.321523	1.188478	1.479343
H	-1.869521	0.558261	1.993668
H	-1.915282	1.925267	1.211341
O	0.554614	4.131786	3.854099
H	-0.334383	4.005173	4.292648
H	1.232101	4.115413	4.558299
N	1.904454	1.218539	2.830362
N	1.401283	2.954458	1.077124
N	0.979072	3.933617	0.284645
N	-1.795758	5.958652	-0.463665
H	-2.425462	5.568966	0.238596
H	-2.090298	6.724841	-1.067671
N	-0.178107	0.826515	4.214321
N	-1.307482	0.816939	4.923981
N	-4.026628	3.097053	4.993859
H	-4.949511	3.273189	5.383964
H	-3.552155	3.771711	4.395712
C	2.874534	1.421823	1.935179
C	4.000533	0.612816	1.891739
H	4.790153	0.795113	1.158744
C	4.090438	-0.439378	2.790858
H	4.965501	-1.093983	2.780717
C	3.063529	-0.666631	3.688085
H	3.106348	-1.494641	4.400095
C	1.958255	0.179802	3.674108
C	2.619492	2.515586	1.009855
C	3.641257	3.009864	0.070268
H	3.626101	2.426987	-0.868636
H	3.489456	4.068277	-0.193762
H	4.650027	2.921430	0.498389
C	-0.286998	4.349108	0.422315
C	-0.563949	5.472398	-0.551642
C	0.806022	0.036154	4.541045
C	0.755057	-0.909180	5.663637
H	1.029315	-1.925631	5.336665
H	-0.262595	-0.916042	6.079677
H	1.461492	-0.623499	6.461721
C	-2.014137	1.897091	4.678835
C	-3.377820	1.966606	5.327190
H	1.517847	4.432871	-0.450735

Mn^{2+} Hdapsox IS LDA

Mn	0.397676	2.353765	2.426581
O	-0.762212	3.551285	1.336121
O	-0.075649	5.985698	-1.124304
O	-2.005942	3.451840	4.339205
O	-3.594395	0.698387	5.800705
O	-1.125587	1.020833	1.382566
H	-0.756841	0.372679	0.749925
H	-1.411869	1.801496	0.848989
O	0.402888	3.989657	3.716369
H	0.987497	3.942469	4.497699
H	-0.568648	3.909868	4.046030
N	1.853338	1.211441	2.692842
N	1.581109	2.922136	1.038624
N	1.206880	3.928689	0.231416
N	-1.940867	5.580099	0.126199
H	-2.323592	5.032843	0.895535
H	-2.454880	6.357620	-0.282976
N	-0.217861	1.194939	4.037772
N	-1.410002	1.231936	4.654552
H	-1.868129	0.401146	5.100251
N	-4.345947	2.859727	5.607000
H	-5.231028	2.699737	6.085681
H	-4.090042	3.785254	5.259581
C	2.954034	1.345402	1.885128
C	4.050246	0.519324	2.048065
H	4.913747	0.642694	1.389724
C	4.035240	-0.457147	3.036067
H	4.894462	-1.116947	3.171607
C	2.921289	-0.588003	3.846862
H	2.889415	-1.349982	4.629264
C	1.832522	0.255219	3.667565
C	2.780546	2.376266	0.925188
C	3.742149	2.806193	-0.091170
H	3.478293	2.378953	-1.075080
H	3.690473	3.898923	-0.213605
H	4.765393	2.497553	0.160183
C	-0.038008	4.218278	0.478470
C	-0.673681	5.364202	-0.269658
C	0.628636	0.254563	4.420988
C	0.319194	-0.680739	5.513764
H	-0.517371	-1.352061	5.245432
H	0.016704	-0.135164	6.424525
H	1.178000	-1.315303	5.763051
C	-2.211248	2.293722	4.729969
C	-3.482383	1.867491	5.442096

Mn^{2+} Hdapsox LS LDA

Mn	0.328787	2.246578	2.393069
O	-0.859530	3.416312	1.391876
O	-0.262775	5.969468	-0.971663
O	-1.749370	3.544075	4.461932
O	-3.714071	0.892534	5.621760
O	-0.516569	0.929750	1.157678
H	0.128407	0.518226	0.542208
H	-1.031667	1.590039	0.624973
O	0.604135	3.817890	3.542371
H	1.290021	3.689980	4.227938
H	-0.317450	3.817677	4.016263
N	1.831349	1.194088	2.707636
N	1.519574	2.930226	1.119238
N	1.113558	3.969211	0.357286

N	-2.109157	5.462869	0.269342
H	-2.481131	4.864329	1.004680
H	-2.660781	6.217083	-0.134621
N	-0.237459	1.177764	3.946812
N	-1.446690	1.254106	4.546698
H	-1.985522	0.430909	4.899030
N	-4.213936	3.132656	5.568680
H	-5.131986	3.035572	6.000815
H	-3.843448	4.048893	5.311428
C	2.930885	1.364726	1.915077
C	4.045427	0.558019	2.076926
H	4.914999	0.712043	1.433574
C	4.033585	-0.430762	3.053862
H	4.906348	-1.073035	3.190590
C	2.919679	-0.598847	3.855186
H	2.897010	-1.366013	4.632325
C	1.814931	0.229609	3.666460
C	2.732719	2.429363	0.984231
C	3.714629	2.923129	0.014396
H	3.711749	2.309426	-0.903949
H	3.456334	3.950713	-0.280248
H	4.732975	2.891547	0.430493
C	-0.148856	4.170621	0.585679
C	-0.835202	5.305409	-0.132382
C	0.588944	0.236729	4.386160
C	0.256377	-0.667378	5.496812
H	-0.539269	-1.383609	5.220761
H	-0.103366	-0.103645	6.374858
H	1.130575	-1.255866	5.802674
C	-2.115660	2.390605	4.728203
C	-3.456984	2.063285	5.361818

Mn^{2+} Hdapsox Isomer II LDA

Mn	-1.984567	4.097266	11.362539
N	-2.740636	6.012784	10.998244
N	-2.688142	4.184766	9.244242
N	-2.449565	3.152420	8.439392
N	-1.297136	-0.160856	8.330176
N	-1.929624	5.086286	13.207464
N	-1.327310	4.455444	14.215669
N	-0.148580	2.887927	16.029100
O	-1.950475	1.756764	10.179369
O	-1.901711	1.353364	6.707265
O	-0.747746	2.984903	12.542563
O	0.472550	1.417818	14.399507
O	0.041651	4.107321	10.400118
O	-3.606677	2.792104	11.920468
H	-3.266726	2.051960	11.349680
C	-3.267638	6.333151	9.809433
C	-3.934478	7.535141	9.618765
C	-4.073596	8.393797	10.698465
C	-3.566418	8.032840	11.934718
C	-2.910041	6.813934	12.064561
C	-3.098362	5.325771	8.775605
C	-3.414747	5.621109	7.366084
C	-2.051202	1.989870	8.971593
C	-1.733869	1.004309	7.871103
C	-2.335919	6.320043	13.299467
C	-2.220484	7.142015	14.512029
H	-3.211335	7.492949	14.845932
H	-1.599946	8.036181	14.334736
H	-1.765369	6.544156	15.312710
C	-0.767855	3.340155	13.766511
C	-0.078735	2.437934	14.765629
H	-4.592892	9.347567	10.576070
H	-4.343121	7.792675	8.638400
H	-0.642081	3.760374	16.216061
H	-3.668091	8.689848	12.802195
H	0.278268	2.339286	16.772419
H	-3.198914	4.790144	6.680783
H	0.598744	4.910322	10.392159
H	-1.035026	-0.906064	7.686668
H	-1.198844	-0.277201	9.340825
H	-4.487153	5.858904	7.258794
H	0.361201	3.549204	11.157299
H	-2.854503	6.502463	7.013744
H	-4.543432	2.942727	11.687958
H	-2.454740	3.147334	7.398457

Mn^{2+} Hdapsox Isomer III LDA

Mn	-1.947866	4.054838	11.290993
N	-2.782510	5.997116	10.997204
N	-2.590149	4.294179	9.150458
N	-2.363951	3.262866	8.333851
N	-1.344976	1.094919	6.817789
N	-1.978492	5.007533	13.189658
N	-1.356005	4.388465	14.190071
N	-0.133888	2.854272	15.993489
O	-1.807248	2.028393	10.141271
O	-2.499798	-0.121878	8.369173
O	-0.628760	3.014006	12.494838
O	0.780376	1.580746	14.333518
O	0.128250	4.220305	10.393176
O	-3.552675	2.740291	11.953172
H	-3.340052	1.873738	11.543971
C	-3.259870	6.380695	9.809041
C	-3.949498	7.574481	9.651673
C	-4.160422	8.366931	10.771432
C	-3.692518	7.949471	12.003871
C	-3.007203	6.740187	12.091716
C	-3.036392	5.431758	8.727754
C	-3.363469	5.771027	7.329331
C	-1.984543	2.099401	8.929911
C	-1.934952	0.888824	8.019308
C	-2.454769	6.211376	13.321331
C	-2.418062	6.987616	14.570748
H	-3.433499	7.288803	14.877741
H	-1.825900	7.910551	14.454215
H	-1.969968	6.375414	15.364039
C	-0.695317	3.338471	13.721520
C	0.068001	2.488694	14.714933
H	-4.700808	9.311476	10.679509
H	-4.321470	7.876546	8.671055
H	-0.736634	3.654851	16.184116
H	-3.845635	8.553398	12.900364
H	0.339576	2.345104	16.735018
H	-2.956181	5.054421	6.600428
H	0.620048	5.052935	10.524646
H	-1.268154	0.269800	6.218092
H	-0.590717	1.781793	6.739123
H	-4.457049	5.809335	7.182472
H	0.401304	3.625860	11.147036
H	-2.964988	6.762998	7.066027
H	-4.524679	2.821867	12.013716
H	-2.587007	3.290456	7.331460

Mn^{2+} Hdapsox Isomer V LDA

Mn	0.249302	2.547898	2.387740
O	-0.718553	3.707312	0.939572

O	0.356417	5.895854	-1.598626
O	-2.145345	3.328275	4.788376
O	-3.472442	0.427185	6.212454
O	-1.263475	1.284822	1.406387
H	-0.962108	0.517854	0.879997
H	-1.399743	2.037997	0.768300
O	0.019417	4.095907	3.727589
H	0.716772	4.335725	4.367139
H	-0.838953	3.865195	4.245951
N	1.798299	1.164739	2.662813
N	1.692737	3.036478	0.967490
N	1.394681	3.951730	0.049196
N	-1.629981	5.734638	-0.487789
H	-2.121927	5.261319	0.268095
H	-2.055828	6.496335	-1.010791
N	-0.275620	1.189691	4.217059
N	-1.435927	1.120310	4.883499
H	-1.814271	0.251505	5.332002
N	-4.345997	2.549702	6.183827
H	-5.176726	2.320899	6.727793
H	-4.169090	3.503001	5.862405
C	2.915961	1.362900	1.938452
C	4.058250	0.605125	2.171578
H	4.945777	0.759433	1.552804
C	4.040857	-0.339769	3.179708
H	4.930032	-0.940324	3.386824
C	2.890146	-0.522161	3.930288
H	2.866570	-1.256956	4.737452
C	1.775701	0.256678	3.646848
C	2.805915	2.361110	0.898746
C	3.819946	2.565784	-0.143301
H	3.863272	1.705379	-0.833367
H	3.559608	3.462840	-0.723600
H	4.824255	2.683267	0.294653
C	0.125435	4.277529	0.143426
C	-0.356682	5.394134	-0.752231
C	0.528877	0.176541	4.384968
C	0.204356	-0.953019	5.277003
H	-0.703970	-1.478887	4.929060
H	0.003571	-0.607355	6.306502
H	1.005756	-1.699331	5.312127
C	-2.265330	2.141008	5.106896
C	-3.451325	1.614631	5.901910

Mn^{2+} Hdapsox Isomer VI LDA

Mn	0.068877	0.437158	-0.169737
O	2.059161	0.930913	0.437653
O	-2.182692	0.161459	0.106563
O	-0.374851	2.021422	0.971802
O	0.085237	4.109299	-1.780463
O	1.624918	0.411762	2.887881
O	-0.422246	-1.693287	4.791586
N	-0.169595	4.293476	0.840822
N	0.050834	1.767710	-1.603343
N	0.157685	1.646515	-2.915674
N	-0.084810	-0.984765	-1.583737
N	0.206863	-1.235948	1.004568
N	0.103634	-1.250513	2.344212
N	1.057708	-0.087542	5.498648
C	-0.185081	3.088856	0.330896
C	0.012778	3.065249	-1.158947
C	0.145782	0.506351	-3.523693
C	0.249209	0.596748	-5.004290
C	0.045857	-0.820080	-2.919636
C	0.052749	-1.927168	-3.762837
C	-0.061736	-3.207046	-3.240540
C	-0.158784	-3.368566	-1.879269
C	-0.155347	-2.247895	-1.051730
C	-0.180419	-2.339798	0.368628
C	-0.575122	-3.547818	1.113961
C	0.789042	-0.459552	3.170259
C	0.406580	-0.808545	4.593448
H	-0.296376	4.472709	1.835242
H	-0.026997	5.041102	0.146743
H	0.306642	1.656129	-5.281918
H	1.145374	0.082920	-5.387435
H	-0.629090	0.152352	-5.500157
H	0.129264	-1.775063	-4.839494
H	-0.059918	-4.075842	-3.903072
H	-0.208899	-4.366706	-1.439570
H	-1.537192	-3.396992	1.639475
H	-0.712316	-4.414009	0.456727
H	1.736428	0.600425	5.168449
H	0.900158	-0.244341	6.492466
H	0.176535	-3.810442	1.879370
H	-0.504317	-1.910882	2.879219
H	-2.624629	0.026227	-0.756452
H	-2.558584	0.984966	0.479647
H	2.812206	0.440407	0.055737
H	2.007692	0.702011	1.441206

Mn^{2+} Hdapsox Isomer VII LDA

Mn	10.752110	6.432068	2.018979
O	9.173836	5.330923	3.271682
O	9.588502	2.514245	5.360707
O	10.688117	10.872224	3.340540
O	8.949785	7.787136	2.446325
O	11.434995	7.438788	3.668939
N	11.964169	5.981535	0.328918
N	11.208727	4.358336	2.133593
N	10.691387	3.608594	3.105639
N	8.080912	4.222158	5.429444
H	7.608419	3.851788	6.250898
H	7.752324	5.060812	4.956663
N	11.496096	8.348093	1.093235
N	11.191823	9.539408	1.610309
N	11.078529	9.097527	5.165394
H	10.867713	10.098630	5.252920
H	11.205757	8.483911	5.969260
C	12.363430	4.713229	0.172659
C	13.166412	4.352382	-0.907485
H	13.477635	3.312649	-1.033480
C	13.552690	5.327808	-1.805361
H	14.177869	5.067455	-2.663226
C	13.164428	6.644479	-1.605388
H	13.487214	7.428826	-2.293045
C	12.376801	6.940215	-0.501778
C	11.881450	3.784310	1.175818
C	12.115608	2.335321	1.112514
H	11.938903	1.905288	2.110211
H	13.137311	2.105683	0.774386
H	11.417533	1.843554	0.412593
C	9.691539	4.217657	3.690011
C	9.123181	3.544287	4.914794
C	12.001846	8.290154	-0.098160
C	12.251719	9.488433	-0.918860
H	12.702069	9.244724	-1.887851
H	11.309569	10.026818	-1.129681
H	12.926411	10.190332	-0.396724
C	10.974474	9.760524	2.934575

C	11.184374	8.626503	3.938847
O	8.839259	5.808334	0.768605
H	11.140398	10.381507	1.017966
H	8.429030	7.545713	1.644427
H	8.661891	7.115107	3.115069
H	8.870182	5.144183	0.052871
H	8.706710	5.314444	1.637038

Mn^{2+} Hdapsox Isomer VIII LDA

Mn	11.232225	6.389839	2.086417
O	8.470676	3.098081	3.808287
O	9.055516	6.045114	2.009786
O	12.453018	10.816673	3.513581
O	10.021389	8.148520	2.838888
O	12.813710	7.317012	3.576610
N	12.218045	5.894385	0.231664
N	10.992287	4.207221	1.750026
N	10.380470	3.398084	2.617608
N	7.195816	5.001630	2.767920
H	6.567642	5.770973	2.543441
H	6.931061	4.161441	3.312982
N	12.284254	8.282605	1.126598
N	12.277885	9.489258	1.713282
N	13.086976	8.931519	5.154087
H	13.030929	9.945538	5.303855
H	13.370348	8.284904	5.888350
C	12.337961	4.597050	-0.078653
C	12.973014	4.195972	-1.255503
H	13.065538	3.130682	-1.479272
C	13.449971	5.153536	-2.123193
H	13.941279	4.860693	-3.054496
C	13.300591	6.494825	-1.804017
H	13.682452	7.274702	-2.466142
C	12.691835	6.822506	-0.602187
C	11.729296	3.656122	0.830233
C	11.875013	2.201362	0.663468
H	11.499716	1.705096	1.570193
H	12.923541	1.918746	0.481096
H	11.277694	1.835253	-0.189580
C	9.161914	3.761551	3.029601
C	8.483101	5.048395	2.521583
C	12.614805	8.194422	-0.118543
C	12.990523	9.329617	-0.985131
H	14.081628	9.499279	-0.957354
H	12.710699	9.133211	-2.029623
H	12.504365	10.275970	-0.700171
C	12.465129	9.691927	3.044979
C	12.790689	8.499118	3.942965
O	11.130864	5.576338	4.088524
H	11.995989	5.893935	4.437632
H	11.123234	4.584747	4.042460
H	9.229267	7.556074	2.674961
H	9.883021	8.943323	2.286492
H	12.322252	10.350934	1.147362

Mn^{2+} Hdapsox Isomer IX LDA

Mn	10.490887	6.513895	2.200534
O	9.987937	5.681660	4.151146
O	9.192925	2.458679	5.323602
O	10.041213	11.216817	3.110053
O	8.974198	7.888530	2.766698
O	8.751326	6.176919	0.873179
O	11.878529	7.283060	3.757441
N	11.793432	6.115859	0.526049
N	10.818056	4.404836	2.146869
N	10.359718	3.641537	3.135226
N	8.829990	4.526634	6.214916
H	8.378854	4.159178	7.049101
H	8.957855	5.525100	6.061211
N	11.146160	8.523170	1.176738
N	10.926958	9.747538	1.670524
N	8.342473	9.572389	4.148597
H	8.522299	10.557017	4.378062
H	7.610093	9.023930	4.596532
C	11.983468	4.824444	0.211960
C	12.647732	4.463756	-0.958734
H	12.808818	3.406990	-1.186090
C	13.099597	5.456642	-1.804156
H	13.620844	5.197943	-2.729286
C	12.893740	6.786295	-1.471507
H	13.248535	7.580628	-2.130885
C	12.227683	7.081654	-0.288227
C	11.501285	3.863210	1.180376
C	11.779550	2.423184	1.083421
H	11.236286	1.904140	1.886151
H	12.857227	2.212824	1.191379
H	11.465554	2.022623	0.105422
C	9.915335	4.395302	4.116023
C	9.276207	3.670005	5.278119
C	11.954853	8.438355	0.165113
C	12.567779	9.626504	-0.462203
H	13.191464	9.367966	-1.324895
H	11.798778	10.342613	-0.801628
H	13.226016	10.156232	0.251849
C	10.068811	10.079204	2.668832
C	9.088639	9.048899	3.195268
H	12.819735	7.021307	3.735249
H	11.401612	6.617048	4.337817
H	8.767433	6.059787	-0.096565
H	8.164115	6.934916	1.075505
H	11.504510	10.541012	1.352701

Mn^{2+} Hdapsox Isomer X LDA

Mn	10.587265	6.762039	2.184250
O	9.415033	3.118659	5.110461
O	8.863660	6.059313	3.266688
O	9.192974	11.126067	2.657708
O	10.646087	8.119665	3.749052
O	8.804451	6.844415	0.818301
O	12.609537	6.568025	3.339298
N	11.785104	6.200970	0.545912
N	10.907937	4.493599	2.258892
N	10.555252	3.683044	3.266610
N	7.857629	5.164362	5.094958
H	7.885705	4.353177	5.725198
H	7.178667	5.917810	5.188734
N	10.899928	8.611777	1.033427
N	10.342884	9.792362	1.242604
N	9.752788	9.931646	4.768917
H	9.311416	10.836954	4.513353
H	9.859953	9.561751	5.711402
C	12.154502	4.932295	0.347841
C	12.887133	4.559226	-0.770946
H	13.178837	3.520503	-0.935289
C	13.234892	5.539226	-1.689318
H	13.813690	5.274989	-2.578038
C	12.843516	6.843832	-1.480371
H	13.109869	7.633507	-2.186565
C	12.093944	7.156790	-0.342114

C	11.731308	4.002223	1.382723
C	12.214637	2.608521	1.445182
H	12.828185	2.441813	2.350810
H	12.846562	2.350040	0.588528
H	11.372970	1.893850	1.470141
C	9.612229	3.919471	4.209594
C	8.753870	5.171244	4.127448
C	11.619693	8.485810	-0.060443
C	11.892044	9.610874	-0.971832
H	12.946685	9.931167	-0.910682
H	11.690770	9.342135	-2.020924
H	11.260878	10.461535	-0.676804
C	9.848383	10.098128	2.442978
C	10.135519	9.268374	3.703566
H	13.364411	6.807416	2.765496
H	12.375452	7.386102	3.838395
H	8.058120	6.691969	1.435490
H	8.677447	7.737341	0.433637
H	11.047015	2.785729	3.396529

Mn^{2+} Hdapsox Isomer XI LDA

Mn	10.570096	6.526925	2.209225
O	9.849115	5.706925	4.082320
O	8.936003	2.492144	5.182335
O	9.849915	11.260825	2.910883
N	8.895821	7.932555	2.914316
O	8.771292	6.140011	0.781602
O	11.959112	7.190529	3.728989
N	11.830330	6.117135	0.533727
N	10.803841	4.413978	2.136611
N	10.295906	3.659141	3.111642
N	8.715603	4.537095	6.169321
H	8.257305	4.156376	6.994268
H	8.926570	5.530199	6.088539
N	11.059668	8.531285	1.100175
N	10.692494	9.762512	1.474056
O	9.750567	9.016205	4.728939
C	12.092563	4.826056	0.274757
C	12.817591	4.458092	-0.855486
H	13.039687	3.404246	-1.040364
C	13.240416	5.444351	-1.724513
H	13.806103	5.181271	-2.621961
C	12.940515	6.771354	-1.459076
H	13.265069	7.556088	-2.144683
C	12.223702	7.078020	-0.308243
C	11.590275	3.875289	1.247215
C	11.944417	2.449442	1.232104
H	11.340051	1.925216	1.986536
H	13.011092	2.299097	1.472154
H	11.770495	2.003693	0.239183
C	9.790567	4.418690	4.059078
C	9.103776	3.695819	5.194413
C	11.846767	8.434322	0.070262
C	12.329042	9.624303	-0.659066
H	13.020556	9.370274	-1.469630
H	11.491914	10.193553	-1.103012
H	12.870394	10.306147	0.022664
C	10.019726	10.098329	2.633241
C	9.532534	8.981475	3.543474
H	12.898717	6.923482	3.765872
H	11.485859	6.710416	4.455437
H	8.381584	8.114274	2.044706
H	8.426406	7.293334	3.572557
H	9.056723	6.154844	-0.155779
H	8.500880	5.210506	0.945554
H	11.047405	10.583858	0.961583

Mn^{2+} Hdapsox Isomer XII LDA

Mn	10.665670	6.714354	2.174835
O	8.980296	3.168518	4.900129
O	8.163367	5.895309	4.409853
O	9.946165	11.302552	2.892834
N	8.923480	8.105322	2.904012
O	8.895725	6.040458	1.040828
O	12.627940	7.160047	3.106823
N	11.775004	6.119062	0.500677
N	10.934080	4.414985	2.289526
N	10.419013	3.595404	3.221855
N	10.409419	6.240279	4.461285
H	13.296656	6.457797	2.953155
H	11.305649	5.792792	4.682044
N	11.098855	8.606281	1.071286
N	10.790787	9.888202	1.343534
O	10.190153	8.944427	4.585408
C	12.133660	4.845982	0.335267
C	12.895137	4.447879	-0.753423
H	13.187688	3.403821	-0.878300
C	13.267712	5.409527	-1.677906
H	13.865106	5.128667	-2.548006
C	12.884211	6.723218	-1.499299
H	13.177319	7.485600	-2.221925
C	12.128098	7.063597	-0.377595
C	11.662113	3.901153	1.346203
C	12.021819	2.482494	1.207121
H	11.590505	1.818201	1.964766
H	13.117965	2.374656	1.257975
H	11.709276	2.109586	0.218900
C	9.555788	3.980001	4.190468
C	9.313515	5.461103	4.382913
C	11.703300	8.418686	-0.077142
C	11.961452	9.538403	-0.994425
H	12.434805	9.220555	-1.929234
H	11.015460	10.055132	-1.224471
H	12.597252	10.292877	-0.501730
C	10.186490	10.144229	2.502976
C	9.752390	9.035667	3.432357
H	12.979069	7.938607	2.620598
H	10.295821	7.231260	4.811122
H	8.429021	8.354193	2.041914
H	8.398812	7.478077	3.559165
H	8.764453	6.554100	0.214683
H	9.038689	5.119743	0.730002
H	10.559074	2.578916	3.128500

Mn^{2+} H_2dapsox Isomer I HS LDA

Mn	-0.02185	2.38957	2.60199
O	-0.92208	4.08080	1.35920
O	0.48635	5.85022	-1.31308
O	-2.02898	2.68298	3.62209
O	-3.38210	0.99959	6.37580
O	-1.21628	1.06790	1.38275
H	-2.07889	1.38689	1.04811
H	-0.91310	0.36497	0.77356
O	0.50634	3.92694	4.02303
H	1.39794	4.22824	4.29031
H	-0.10121	4.68559	4.13917
N	1.83057	1.15030	2.74434
N	1.45049	2.97340	1.03045
N	1.05242	3.96239	0.23872

H	1.56462	4.43036	-0.54181
N	-1.58715	6.20409	-0.39648
H	-2.24499	5.88849	0.31600
H	-1.83564	6.96837	-1.02677
N	-0.16274	0.93120	4.28916
N	-1.30081	0.99626	4.96660
H	-1.60915	0.43818	5.79353
N	-4.36851	2.70710	5.20195
H	-5.22150	2.72242	5.76334
H	-4.25618	3.34635	4.41543
C	2.82895	1.34388	1.88234
C	4.00450	0.60732	1.95338
H	4.81554	0.78229	1.24192
C	4.12808	-0.34946	2.94584
H	5.04149	-0.94481	3.02587
C	3.08683	-0.54630	3.83538
H	3.16036	-1.29637	4.62700
C	1.94248	0.23106	3.70273
C	2.59066	2.38558	0.87933
C	3.58568	2.69807	-0.15674
H	4.01353	1.77591	-0.58033
H	3.17115	3.28123	-0.99140
H	4.42650	3.27377	0.27120
C	-0.16204	4.48151	0.46981
C	-0.41132	5.60689	-0.51606
C	0.78420	0.11043	4.59315
C	0.77538	-0.86133	5.69595
H	0.90701	-1.88634	5.30830
H	-0.14877	-0.84674	6.28913
H	1.61722	-0.67152	6.38405
C	-2.19737	1.91143	4.57503
C	-3.40918	1.83722	5.48288

Mn^{2+} H_2dapsox IS LDA

Mn	0.195230	2.105447	2.830075
O	-0.816074	5.006032	1.798200
O	0.185470	5.274354	-1.536428
O	-1.872339	2.391490	3.305463
O	-3.375370	1.267018	6.265722
O	-0.926038	1.154693	1.176086
H	-1.892678	1.156696	1.336570
H	-0.703810	0.284283	0.787046
O	0.211550	3.902453	3.800840
H	1.061564	4.311065	4.061495
H	-0.227815	4.492744	3.063077
N	1.762035	1.096060	2.806617
N	1.199343	2.947542	1.262992
N	0.696454	3.877107	0.435580
H	0.960562	4.007392	-0.585275
N	-1.402344	6.520466	-0.439048
H	-1.861628	6.662942	0.461661
H	-1.624701	7.122422	-1.234026
N	-0.052764	0.914977	4.316220
N	-1.207305	1.065742	4.991399
H	-1.486855	0.634569	5.895496
N	-4.285195	2.773238	4.789527
H	-5.157011	2.889578	5.309763
H	-4.125794	3.307945	3.936069
C	2.735944	1.376421	1.896732
C	3.918895	0.661645	1.890141
H	4.685203	0.894554	1.145284
C	4.120593	-0.348308	2.825945
H	5.051460	-0.919873	2.825555
C	3.137885	-0.615595	3.759116
H	3.277252	-1.393263	4.515485
C	1.958479	0.119088	3.745647
C	2.385306	2.436553	1.001713
C	3.275536	2.876528	-0.080087
H	3.466384	2.051854	-0.788380
H	2.894979	3.735797	-0.647646
H	4.254555	3.168412	0.337514
C	-0.241703	4.781615	0.726650
C	-0.487343	5.576014	-0.552562
C	0.864725	0.015024	4.639582
C	0.749461	-0.912093	5.770202
H	1.285996	-1.849674	5.565070
H	-0.297815	-1.178091	5.986103
H	1.184520	-0.478365	6.689368
C	-2.102179	1.855659	4.413041
C	-3.352197	1.954031	5.253761

Mn^{2+} H_2dapsox LS LDA

Mn	0.295999	2.200821	2.361140
O	-0.947315	3.420546	1.343007
O	0.078165	5.886175	-0.929820
O	-1.727696	3.570487	4.520407
O	-3.675591	0.881095	5.607761
O	-0.560455	0.794474	1.274033
H	-0.055849	-0.004653	1.011811
H	-1.054224	1.111061	0.487317
O	0.541057	3.783043	3.483044
H	1.263374	3.730041	4.142597
H	-0.372781	3.784211	4.007724
N	1.803880	1.180517	2.681509
N	1.510335	2.920773	1.118764
N	1.016828	3.945683	0.393013
H	1.516831	4.595794	-0.244933
N	-2.048704	5.631138	-0.103173
H	-2.645509	5.097839	0.528700
H	-2.436537	6.419757	-0.625166
N	-0.255859	1.179123	3.964472
N	-1.462587	1.272021	4.561358
H	-2.058662	0.467566	4.900355
N	-4.165407	3.116866	5.787490
H	-5.060605	2.979353	6.259794
H	-3.815611	4.059610	5.611314
C	2.923891	1.387408	1.926247
C	4.057188	0.614414	2.126326
H	4.951701	0.800604	1.525980
C	4.044999	-0.373969	3.098826
H	4.933041	-0.987589	3.266719
C	2.913651	-0.561699	3.876635
H	2.898442	-1.311460	4.671827
C	1.795807	0.232372	3.653728
C	2.735734	2.453847	0.989524
C	3.740104	2.973939	0.055553
H	4.456264	2.187452	-0.224666
H	3.287814	3.350545	-0.876102
H	4.323223	3.797466	0.507686
C	-0.276218	4.161648	0.579051
C	-0.763209	5.335127	-0.234963
C	0.566635	0.239730	4.390663
C	0.262992	-0.662971	5.505830
H	-0.311616	-1.545155	5.165805
H	-0.338442	-0.158059	6.279507
H	1.182831	-1.039226	5.974784
C	-2.105358	2.420899	4.778778
C	-3.429905	2.073629	5.447474

Mn^{2+} H_2dapsox Isomer II LDA

Mn	-2.022215	3.914444	11.289228
N	-2.802536	5.977117	10.985494
N	-2.571599	4.234546	9.159575
N	-2.377885	3.179346	8.376208
N	-1.308630	-0.176773	8.386010
N	-2.080219	5.058775	13.228921
N	-1.437312	4.442940	14.236956
N	0.325270	2.123157	15.704724
O	-1.661524	1.983420	10.169676
O	-2.068056	1.269859	6.771297
O	-1.740290	2.513070	13.108490
O	1.069744	2.782664	13.656119
O	0.064006	3.955646	11.558147
O	-3.966434	3.084311	11.764606
H	-3.782198	2.335891	12.372337
C	-3.198485	6.358161	9.771671
C	-3.717370	7.625634	9.537463
C	-3.828836	8.503796	10.600598
C	-3.423848	8.099064	11.860228
C	-2.913864	6.816245	12.015658
C	-3.050325	5.350745	8.719975
C	-3.441965	5.638467	7.332798
C	-1.911227	2.065382	8.964444
C	-1.759675	0.977887	7.920832
C	-2.427886	6.296843	13.296919
C	-2.327607	7.154874	14.487101
H	-3.259795	7.725479	14.627556
H	-1.516875	7.897127	14.377788
H	-2.161223	6.582473	15.411106
C	-1.150857	3.137494	13.992078
C	0.178574	2.637101	14.499334
H	-4.232355	9.508046	10.446950
H	-4.028153	7.921571	8.532172
H	-0.470571	1.959154	16.321740
H	-3.501458	8.775808	12.714910
H	1.244662	1.767415	15.983427
H	-3.324471	4.782645	6.654709
H	0.725198	4.136821	10.863085
H	-1.172868	-0.964230	7.750297
H	-1.084744	-0.268427	9.377338
H	-4.498108	5.955360	7.288990
H	0.539068	3.441288	12.311401
H	-2.843374	6.472506	6.927192
H	-4.688226	2.806554	11.166218
H	-2.535775	3.077996	7.349885
H	-0.897443	4.989225	14.922059

Mn^{2+} Hdapsox Isomer III LDA

Mn	-1.962309	3.975629	11.200652
N	-2.856146	5.974928	10.997659
N	-2.585739	4.329896	9.081609
N	-2.393578	3.296806	8.255822
N	-1.440245	0.900580	6.793598
N	-1.942830	5.030200	13.171613
N	-1.352583	4.361205	14.166557
N	-0.281662	2.322116	16.063703
O	-1.585111	2.137015	10.013495
O	-2.742727	0.029244	8.460784
O	-0.918016	2.704311	12.699202
O	1.341354	2.528308	14.464026
O	0.146228	4.210031	10.707639
O	-3.558542	2.624276	11.794867
H	-3.274957	1.721864	11.525210
C	-3.275775	6.398690	9.805152
C	-3.844905	7.654509	9.639012
C	-3.973437	8.476080	10.744872
C	-3.533664	8.029944	11.978742
C	-2.974336	6.761820	12.067533
C	-3.107162	5.445380	8.702663
C	-3.533957	5.788739	7.336856
C	-1.917638	2.157620	8.829739
C	-2.031684	0.896223	7.998282
C	-2.454412	6.203311	13.320642
C	-2.518386	6.974183	14.572616
H	-3.541486	7.347953	14.743302
H	-1.858673	7.858441	14.521834
H	-2.236213	6.395021	15.463252
C	-0.783875	3.171026	13.829289
C	0.188708	2.593659	14.837425
H	-4.418165	9.469574	10.644582
H	-4.185881	7.985549	8.654806
H	-1.275909	2.155374	16.223107
H	-3.622104	8.662840	12.865380
H	0.375740	1.912119	16.734147
H	-3.210380	5.062429	6.577827
H	0.719933	4.997873	10.792421
H	-1.502051	0.038126	6.243853
H	-0.659087	1.525688	6.591704
H	-4.633836	5.870196	7.279392
H	0.621664	3.467048	11.142833
H	-3.124588	6.768166	7.039390
H	-4.518390	2.681451	11.614965
H	-2.743656	3.295530	7.288284
H	-1.185043	4.786523	15.088278

Mn^{2+} H_2dapsox Isomer V LDA

Mn	0.138850	2.465182	2.432238
O	-0.859616	3.901274	0.814380
O	0.860291	5.816018	-1.557736
O	-2.241851	3.184075	4.735698
O	-3.338647	0.251062	6.274445
O	-1.646581	1.632413	1.723365
H	-1.852454	0.712555	1.460046
H	-1.926081	2.239251	0.998395
O	-0.183699	4.063755	3.623998
H	0.470271	4.453672	4.236869
H	-1.033474	3.790155	4.163529
N	1.828535	1.198010	2.700353
N	1.607914	2.981144	0.910291
N	1.279473	3.947374	0.058108
H	1.881847	4.463378	-0.622872
N	-1.343758	6.061957	-0.963335
H	-2.080728	5.725965	-0.343350
H	-1.524014	6.842158	-1.597650
N	-0.259261	1.107014	4.239767
N	-1.396024	1.027402	4.942263
H	-1.749159	0.172660	5.458392
N	-4.376907	2.298659	6.246613
H	-5.172805	2.010745	6.818171
H	-4.298629	3.262018	5.916694
C	2.897119	1.369248	1.913405
C	4.052161	0.619914	2.086040
H	4.917985	0.776842	1.437993
C	4.083837	-0.325869	3.094562
H	4.980031	-0.930725	3.255963
C	2.972056	-0.502054	3.897778
H	2.986539	-1.244202	4.698279
C	1.847672	0.285735	3.677214
C	2.755639	2.386810	0.872350

C	3.825812	2.671245	-0.092297
H	4.318416	1.743407	-0.420909
H	3.457740	3.183944	-0.992979
H	4.606266	3.307391	0.364368
C	0.010975	4.379994	0.077775
C	-0.138698	5.517234	-0.914387
C	0.634263	0.195489	4.487130
C	0.439060	-0.835907	5.519268
H	-0.391296	-1.514966	5.248529
H	0.170621	-0.372867	6.485671
H	1.323342	-1.462223	5.675787
C	-2.284876	2.012023	5.116792
C	-3.422991	1.434444	5.953976

Mn^{2+} H_2dapsox Isomer VII LDA

Mn	10.603886	6.512451	1.977585
O	9.203117	5.450095	3.659234
O	9.612912	2.201649	4.907866
O	10.784967	10.925046	3.277831
O	8.902115	7.814519	2.523193
O	11.390865	7.465025	3.609681
N	11.945293	5.967049	0.357554
N	11.089233	4.387068	2.130375
N	10.534306	3.692518	3.119535
N	8.153198	3.774025	5.713691
H	7.773123	3.170273	6.444890
H	7.811702	4.728656	5.610450
N	11.430188	8.358501	1.030988
N	11.133418	9.558851	1.532434
N	11.414821	9.180583	5.082315
H	11.292181	10.196330	5.179806
H	11.625495	8.580782	5.880856
C	12.371249	4.705128	0.246467
C	13.217449	4.320043	-0.785070
H	13.566326	3.288627	-0.871448
C	13.612265	5.273716	-1.707650
H	14.268670	4.996327	-2.536654
C	13.191507	6.583787	-1.563326
H	13.524162	7.350569	-2.266395
C	12.365564	6.906044	-0.491752
C	11.874566	3.801125	1.281997
C	12.221758	2.374550	1.367815
H	12.822199	2.174327	2.274521
H	12.802393	2.023488	0.507033
H	11.313100	1.749757	1.434668
C	9.588989	4.291935	3.856234
C	9.098284	3.313160	4.908588
C	11.978592	8.271495	-0.139689
C	12.291898	9.446714	-0.968698
H	12.726816	9.178120	-1.938240
H	11.384716	10.041193	-1.181248
H	13.009189	10.110172	-0.450933
C	11.014552	9.805964	2.871589
C	11.286254	8.678607	3.875877
O	9.033460	6.002887	0.432628
H	11.143508	10.402961	0.938749
H	10.725322	2.707523	3.411629
H	8.201319	8.082110	1.893854
H	8.481676	7.237388	3.201847
H	9.319565	5.620935	-0.422791
H	8.211844	5.527593	0.673716

Mn^{2+} H_2dapsox Isomer VIII LDA

Mn	11.235915	6.448544	2.129974
O	8.314137	2.791601	3.497421
O	8.970546	5.964633	2.141487
O	12.776935	10.908089	3.415427
O	9.970771	8.105443	2.708021
O	12.636068	7.409899	3.695831
N	12.236606	5.888661	0.284009
N	10.945389	4.162784	1.679428
N	10.235614	3.351382	2.480733
N	7.067952	4.973588	2.890622
H	6.471130	5.785793	2.731138
H	6.696049	4.103049	3.292429
N	12.298430	8.309212	1.152256
N	12.281996	9.529021	1.714997
N	13.395111	9.038800	5.086580
H	13.519501	10.056397	5.172003
H	13.659425	8.402692	5.839855
C	12.416070	4.600521	-0.027499
C	13.058922	4.207128	-1.194055
H	13.196826	3.147012	-1.418643
C	13.479205	5.176173	-2.084548
H	13.968204	4.894790	-3.020868
C	13.272180	6.506073	-1.773120
H	13.604731	7.295810	-2.450800
C	12.668845	6.827084	-0.563963
C	11.804469	3.632564	0.873437
C	12.087935	2.188882	0.770504
H	12.080914	1.685744	1.752007
H	13.080850	2.004310	0.338827
H	11.343310	1.680150	0.131113
C	8.966545	3.627665	2.909312
C	8.348317	4.990524	2.604271
C	12.560298	8.207642	-0.108478
C	12.838824	9.324826	-1.030145
H	13.927076	9.490126	-1.129451
H	12.446214	9.108735	-2.034947
H	12.390061	10.280663	-0.719484
C	12.631502	9.772759	3.014457
C	12.879572	8.601634	3.962018
O	11.110360	5.561133	4.099604
H	11.822351	6.135942	4.493969
H	11.295884	4.630713	4.338327
H	9.118924	7.605171	2.576563
H	9.896255	8.965801	2.248293
H	10.471569	2.346796	2.534391
H	12.341968	10.370295	1.118323

Mn^{2+} H_2dapsox Isomer IX LDA

Mn	10.539520	6.663853	2.176472
O	9.857161	5.656089	4.365375
O	9.354905	2.239393	4.936377
O	10.054503	11.356864	2.885619
O	9.080639	7.981634	2.894235
O	8.627951	6.004603	1.345165
O	11.828793	7.272607	3.778618
N	11.746331	6.117172	0.478105
N	10.895798	4.454211	2.215254
N	10.355501	3.758138	3.207314
N	8.677493	3.966804	6.288358
H	8.255742	3.370641	7.001760
H	8.666492	4.981025	6.390941
N	11.193424	8.558812	1.124729
N	10.949454	9.801724	1.554359
N	8.378873	9.798209	4.058136
H	8.531298	10.809127	4.175242
H	7.650957	9.296182	4.566842

C	11.997525	4.828000	0.231930
C	12.739062	4.429701	-0.872274
H	12.929856	3.370101	-1.060426
C	13.237564	5.402157	-1.719806
H	13.826410	5.121233	-2.596953
C	12.993032	6.734911	-1.444507
H	13.391278	7.510397	-2.101469
C	12.234772	7.065061	-0.325979
C	11.468541	3.877690	1.211067
C	11.634056	2.428140	1.020650
H	11.115596	1.820181	1.774187
H	12.703980	2.156351	1.057018
H	11.261569	2.119468	0.029686
C	9.840345	4.425574	4.247843
C	9.248607	3.425458	5.223848
C	11.931677	8.439262	0.062691
C	12.439740	9.608105	-0.677502
H	12.977572	9.333444	-1.591187
H	11.610859	10.276732	-0.972648
H	13.144607	10.198800	-0.061511
C	10.102990	10.190549	2.548615
C	9.150614	9.191699	3.187384
H	12.802913	7.237695	3.856302
H	11.437231	6.732292	4.507608
H	8.366261	5.682391	0.459946
H	7.966956	6.671664	1.629484
H	11.461050	10.593614	1.134291
H	10.251515	2.721562	3.301113

Mn^{2+} H_2dapsox Isomer X LDA

Mn	10.599943	6.731318	2.231985
O	9.446166	2.930519	5.019578
O	8.934859	5.992778	3.375058
O	9.459319	11.398489	2.497376
O	10.422659	8.245437	3.711445
O	8.748968	7.021262	1.074406
O	12.333553	6.568968	3.591984
N	11.799048	6.209416	0.522166
N	10.963388	4.445317	2.258692
N	10.609472	3.601513	3.232582
N	7.892944	4.980715	5.119836
H	7.899403	4.129727	5.698885
H	7.205758	5.722788	5.252605
N	11.024711	8.648938	1.011594
N	10.513024	9.856542	1.269058
N	9.470939	10.056530	4.693067
H	9.148608	11.016686	4.509642
H	9.430546	9.637380	5.622136
C	12.164938	4.937380	0.326715
C	12.836818	4.545052	-0.826134
H	13.108844	3.499767	-0.984717
C	13.126803	5.492955	-1.787484
H	13.636841	5.205759	-2.710773
C	12.762792	6.807798	-1.570492
H	12.984662	7.571638	-2.318364
C	12.099915	7.138024	-0.393575
C	11.791957	3.989884	1.370269
C	12.317311	2.610876	1.402165
H	12.756596	2.370681	2.388121
H	13.114496	2.447312	0.668179
H	11.519989	1.871611	1.202974
C	9.657795	3.789442	4.186172
C	8.805204	5.049355	4.178052
C	11.674428	8.502796	-0.101023
C	11.956618	9.605420	-1.041147
H	12.892409	9.431048	-1.589551
H	11.156926	9.717882	-1.796689
H	12.080124	10.571736	-0.525456
C	9.942856	10.285457	2.427513
C	9.968103	9.405021	3.667436
H	13.279924	6.487423	3.359245
H	12.242252	7.356214	4.171915
H	8.072197	6.560087	1.617027
H	8.544231	6.851961	0.133522
H	11.060010	2.674826	3.293586
H	10.497133	10.572780	0.526805

Mn^{2+} H_2dapsox Isomer XI LDA

Mn	10.523211	6.585527	2.196967
O	9.146142	5.570840	3.788791
O	9.601364	2.388518	5.185285
O	9.774359	11.373673	2.726457
N	8.856112	8.243415	3.232333
O	8.675009	6.393751	1.013683
O	11.702923	6.898719	3.875792
N	11.776165	6.094932	0.524564
N	10.888865	4.413456	2.213835
N	10.368393	3.745115	3.237410
N	8.300036	4.051536	6.074477
H	8.013287	3.505311	6.889392
H	7.980535	5.013597	5.973310
N	11.065850	8.573813	1.069691
N	10.701224	9.830352	1.363271
O	10.551691	9.037051	4.518078
C	12.131074	4.817759	0.329671
C	12.922047	4.436686	-0.742910
H	13.204221	3.389977	-0.881296
C	13.342263	5.410763	-1.631456
H	13.959501	5.143000	-2.493145
C	12.981637	6.726727	-1.418018
H	13.316388	7.500327	-2.111046
C	12.195345	7.048067	-0.313429
C	11.641813	3.859970	1.323856
C	12.005131	2.437760	1.268806
H	11.450520	1.821476	1.989735
H	13.084011	2.300843	1.461987
H	11.807669	2.026785	0.264775
C	9.514856	4.409302	4.024151
C	9.119430	3.514647	5.184600
C	11.801695	8.417496	0.006954
C	12.238645	9.570292	-0.803721
H	12.885705	9.289748	-1.640855
H	11.376511	10.113414	-1.233972
H	12.809669	10.286838	-0.183403
C	10.065085	10.223568	2.521641
C	9.822774	9.128433	3.535962
H	12.678377	6.971198	3.848722
H	11.355969	7.716133	4.381175
H	8.183276	8.451203	2.487375
H	8.558640	7.578760	3.959589
H	8.706065	6.374246	0.034047
H	8.054002	5.683568	1.280266
H	10.966782	10.606107	0.737390
H	10.572676	2.776665	3.577330

Mn^{2+} H_2dapsox Isomer XII LDA

Mn	10.663264	6.684194	2.183086
O	9.000721	3.173169	4.909521
O	8.167938	5.899635	4.380200

O	9.995513	11.341614	2.869839
N	8.927864	8.116161	2.914101
O	8.896832	6.047359	1.074357
O	12.618706	7.137620	3.082732
N	11.778301	6.124646	0.488297
N	10.936213	4.417627	2.284626
N	10.428799	3.598791	3.220701
N	10.411721	6.247921	4.465021
H	13.266828	6.406169	2.986130
H	11.301592	5.801171	4.712577
N	11.088023	8.576949	1.037516
N	10.719280	9.831487	1.358173
O	10.149066	9.001248	4.614912
C	12.130147	4.850758	0.325290
C	12.895946	4.452824	-0.763234
H	13.182073	3.406899	-0.887681
C	13.285339	5.409269	-1.681450
H	13.887719	5.125269	-2.546538
C	12.909491	6.727919	-1.502029
H	13.214257	7.491634	-2.218355
C	12.146606	7.059025	-0.389821
C	11.656597	3.904554	1.334304
C	12.008765	2.486356	1.188434
H	11.558023	1.818129	1.931002
H	13.103330	2.370041	1.257563
H	11.710685	2.125995	0.191104
C	9.566170	3.981983	4.191813
C	9.315452	5.463437	4.375151
C	11.716540	8.421028	-0.090719
C	11.990138	9.548469	-0.990172
H	12.493442	9.240161	-1.911159
H	11.047728	10.050276	-1.271296
H	12.630595	10.297689	-0.490849
C	10.157705	10.178440	2.542082
C	9.727208	9.055461	3.462976
H	13.047887	7.899546	2.635889
H	10.285776	7.217946	4.848082
H	8.426245	8.365506	2.055177
H	8.407444	7.474971	3.564090
H	8.707440	6.558178	0.257536
H	9.004588	5.122601	0.760969
H	10.577871	2.583359	3.130525
H	11.000821	10.608643	0.742083

Co^{2+} dapsox Isomer I HS LDA

Co	0.138586	2.255360	2.623171
O	-1.012627	3.542087	1.235259
O	-0.110662	6.150591	-0.948153
O	-1.632970	2.904112	3.677602
O	-3.767160	1.488692	6.091021
O	-1.021864	0.998192	1.340702
H	-0.408987	0.578037	0.706322
H	-1.270618	1.879431	0.933522
O	0.681512	3.956252	3.796554
H	-0.293745	3.962028	4.017055
H	0.821395	4.685318	3.157502
N	1.828260	1.118824	2.746338
N	1.429070	2.977689	1.175152
N	1.083310	4.028162	0.412626
N	-2.096380	5.534494	-0.006324
H	-2.522097	4.839338	0.609456
H	-2.624374	6.273065	-0.462073
N	-0.167595	0.944036	4.186226
N	-1.305369	0.973750	4.888379
N	-3.929584	3.353062	4.786097
H	-4.840244	3.614858	5.152010
H	-3.452576	3.875076	4.049658
C	2.863602	1.375633	1.939915
C	4.037867	0.631031	2.011419
H	4.872586	0.866153	1.346531
C	4.114295	-0.395587	2.938211
H	5.022548	-0.998866	3.014477
C	3.038703	-0.650958	3.772883
H	3.070278	-1.448343	4.519441
C	1.899601	0.141028	3.657049
C	2.622528	2.471795	1.037539
C	3.623355	2.964220	0.078762
H	3.857672	2.197269	-0.679263
H	3.226807	3.856485	-0.425827
H	4.567826	3.212322	0.591018
C	-0.204926	4.241792	0.524271
C	-0.775449	5.419190	-0.236657
C	0.721072	0.036811	4.475630
C	0.558558	-0.969693	5.535364
H	0.749631	-1.984835	5.150210
H	-0.464311	-0.903927	5.932699
H	1.270850	-0.791795	6.359561
C	-1.996247	2.031226	4.547705
C	-3.325306	2.238232	5.239519

Co^{2+} dapsox LS LDA

Co	0.323923	2.050687	2.862617
O	-1.388033	3.261440	0.445846
O	-0.134513	6.491849	-0.095785
O	-1.399131	2.882402	3.476096
O	-3.726355	1.841445	5.897817
O	-0.906466	1.090088	1.554486
H	-0.370838	0.538305	0.951913
H	-1.134025	1.981276	1.014484
O	0.891920	3.937870	3.968298
H	-0.096164	3.987715	4.055612
H	1.087320	4.521643	3.200953
N	1.837170	1.097718	2.825188
N	1.173930	2.952512	1.394035
N	0.772450	4.076918	0.796983
N	-2.139078	5.508291	-0.567959
H	-2.641784	4.621384	-0.499395
H	-2.536462	6.347129	-0.980206
N	-0.047766	0.966608	4.275434
N	-1.215090	1.093109	4.923469
N	-3.817568	3.400819	4.233852
H	-4.759186	3.697196	4.473761
H	-3.300663	3.784936	3.440951
C	2.765077	1.368161	1.891571
C	3.920313	0.594572	1.826732
H	4.679073	0.809230	1.070365
C	4.077454	-0.442545	2.735670
H	4.978882	-1.059260	2.701609
C	3.099889	-0.707606	3.687956
H	3.210653	-1.522922	4.406958
C	1.962830	0.087960	3.718016
C	2.366918	2.479809	1.078431
C	3.203943	3.065794	0.022504
H	3.116663	2.500680	-0.921856
H	2.859169	4.093267	-0.173270
H	4.265339	3.063213	0.315222
C	-0.491430	4.158817	0.442589
C	-0.879831	5.526527	-0.098841
C	0.819431	0.020331	4.578924

C	0.616572	-0.958020	5.654015
H	0.748347	-1.987927	5.282883
H	-0.397395	-0.839669	6.061805
H	1.345303	-0.805544	6.468953
C	-1.858088	2.112229	4.410701
C	-3.235412	2.418574	4.945030

Co^{2+} dapsox Isomer II LDA

Co	-2.000394	4.099914	11.181855
N	-2.828545	5.959011	10.999878
N	-2.619516	4.273306	9.205565
N	-2.424711	3.267416	8.344676
N	-1.181614	0.019281	9.038951
N	-1.853181	4.986737	13.054847
N	-1.296747	4.309688	14.067217
N	-0.174251	2.757032	15.870986
O	-1.914796	2.152192	10.287819
O	-1.877548	0.849152	7.029689
O	-0.712216	2.866042	12.381075
O	0.509353	1.279937	14.275736
O	0.005968	4.462363	10.535195
O	-3.734295	3.016784	11.844742
H	-3.325448	2.297358	11.279428
C	-3.293886	6.366332	9.811819
C	-3.862855	7.627635	9.653256
C	-3.959071	8.455484	10.760460
C	-3.485088	8.022233	11.987917
C	-2.910025	6.756631	12.072893
C	-3.153964	5.379263	8.773820
C	-3.575792	5.602422	7.382239
C	-2.037259	2.207446	9.013546
C	-1.696600	0.960533	8.229498
C	-2.351024	6.171585	13.262808
C	-2.347370	6.865441	14.561645
H	-3.375199	7.086344	14.895705
H	-1.812952	7.828521	14.495317
H	-1.853408	6.231115	15.310198
C	-0.731639	3.208336	13.596015
C	-0.061150	2.302547	14.609942
H	-4.408918	9.447158	10.665064
H	-4.225065	7.938376	8.671445
H	-0.704333	3.618123	16.015266
H	-3.550086	8.650516	12.879290
H	0.207532	2.204469	16.634409
H	-3.352288	4.699628	6.797309
H	0.291397	5.311009	10.923834
H	-0.866909	-0.862382	8.643297
H	-1.053054	0.259244	10.024990
H	-4.658545	5.815874	7.324602
H	0.232106	3.769782	11.221019
H	-3.050699	6.465643	6.943259
H	-4.484789	3.356031	11.320008

Co^{2+} dapsox Isomer III LDA

Co	-2.002069	4.080043	11.190145
N	-2.841833	5.944198	11.002787
N	-2.607106	4.266616	9.197268
N	-2.417387	3.257929	8.341348
N	-1.966721	1.138635	6.865673
N	-1.900302	4.977853	13.075882
N	-1.332761	4.326944	14.095526
N	-0.169968	2.843404	15.924033
O	-1.788328	2.149014	10.249254
O	-1.498497	-0.132114	8.697725
O	-0.753878	2.850123	12.437767
O	0.695381	1.451202	14.341751
O	0.019660	4.420137	10.585985
O	-3.624017	2.864604	11.864241
H	-3.141436	2.130789	11.385727
C	-3.280103	6.360857	9.808317
C	-3.839293	7.625454	9.640482
C	-3.952689	8.453075	10.744798
C	-3.505762	8.013190	11.979421
C	-2.942089	6.742845	12.072895
C	-3.120334	5.383739	8.766483
C	-3.514712	5.641054	7.371595
C	-1.995206	2.191501	9.006198
C	-1.786567	0.931856	8.184770
C	-2.402014	6.163713	13.272208
C	-2.400476	6.870788	14.563635
H	-3.429339	7.063301	14.912100
H	-1.898120	7.849075	14.477436
H	-1.877224	6.259454	15.310557
C	-0.749114	3.226891	13.641268
C	0.006759	2.399984	14.664122
H	-4.391935	9.448745	10.642587
H	-4.178906	7.940992	8.651059
H	-0.746441	3.675533	16.057717
H	-3.581085	8.639622	12.871507
H	0.300808	2.364446	16.687024
H	-3.294925	4.753711	6.763741
H	0.334244	5.218216	11.054580
H	-1.861174	0.358272	6.223098
H	-2.232573	2.078562	6.567194
H	-4.591687	5.869705	7.299980
H	0.225071	3.665917	11.209966
H	-2.970399	6.507916	6.960596
H	-4.395731	3.061678	11.297591

Co^{2+} dapsox Isomer V LDA

Co	-2.000441	4.093599	11.185861
N	-2.832632	5.957192	10.997905
N	-2.624071	4.263968	9.213034
N	-2.443691	3.261412	8.344300
N	-1.271975	-0.028935	8.930802
N	-1.858274	4.993132	13.051260
N	-1.304660	4.349027	14.086057
N	0.390469	1.239876	14.142694
O	-1.848318	2.122182	10.254186
O	-1.931478	0.901297	6.954923
O	-0.711574	2.852113	12.440733
O	-0.013092	2.657263	15.884145
O	0.022715	4.474003	10.613251
O	-3.675891	2.937881	11.836901
H	-3.244098	2.243991	11.256003
C	-3.299628	6.360571	9.810311
C	-3.864675	7.622477	9.645580
C	-3.949612	8.460153	10.745161
C	-3.470610	8.033299	11.972474
C	-2.906165	6.763628	12.063477
C	-3.159786	5.369978	8.777350
C	-3.582163	5.592427	7.386112
C	-2.027897	2.198915	8.985443
C	-1.744737	0.965273	8.156525
C	-2.346512	6.184867	13.254927
C	-2.330167	6.874261	14.554112
H	-3.346771	7.187142	14.845235
H	-1.709298	7.785627	14.512225
H	-1.918648	6.193458	15.312509

C	-0.747415	3.243004	13.662979
C	-0.090012	2.364520	14.704653
H	-4.392965	9.454178	10.644740
H	-4.230693	7.927520	8.662233
H	0.243292	1.122532	13.139121
H	-3.523491	8.667165	12.860956
H	0.850604	0.545235	14.723655
H	-3.312522	4.710991	6.787519
H	0.275064	5.335179	11.000951
H	-1.025172	-0.919564	8.509333
H	-1.156211	0.171678	9.925251
H	-4.671979	5.753695	7.323027
H	0.204703	3.799833	11.332857
H	-3.096559	6.489741	6.967398
H	-4.453285	3.246146	11.330695

Co^{2+} dapsox Isomer VI LDA

Co	0.085145	0.322109	-0.248623
O	2.130993	0.398551	0.166420
O	-2.082377	0.322581	0.294546
O	-0.022659	1.674280	1.128422
O	-0.300884	4.047015	-1.414705
O	1.778574	-0.070129	2.603247
O	-0.881096	-0.551972	4.845401
N	-0.213380	3.949418	1.262189
N	0.002018	1.707850	-1.454746
N	0.084273	1.704307	-2.756663
N	0.008786	-0.964396	-1.574634
N	0.023874	-1.201550	0.917212
N	-0.270206	-1.104699	2.222978
N	1.218573	0.307153	5.090497
C	-0.129111	2.811403	0.592616
C	-0.161946	2.955663	-0.867553
C	0.124422	0.588224	-3.450175
C	0.235687	0.787178	-4.919969
C	0.093235	-0.738660	-2.923957
C	0.157087	-1.827514	-3.797246
C	0.124635	-3.126185	-3.331532
C	0.038227	-3.342939	-1.961201
C	-0.010846	-2.263279	-1.106295
C	-0.090980	-2.362244	0.310629
C	-0.306119	-3.603564	1.070984
C	0.627387	-0.470799	2.949394
C	0.213938	-0.254786	4.396965
H	-0.224278	3.974378	2.277677
H	-0.304987	4.782503	0.672270
H	0.259382	1.865755	-5.118699
H	1.150888	0.331421	-5.332048
H	-0.623226	0.352989	-5.457802
H	0.221359	-1.628917	-4.868343
H	0.167010	-3.966562	-4.027623
H	0.015252	-4.352279	-1.543528
H	-0.981347	-3.384834	1.915440
H	-0.720463	-4.405376	0.446126
H	2.072286	0.512510	4.566547
H	1.099872	0.511599	6.077941
H	0.635218	-3.961040	1.522801
H	-1.910895	0.040172	1.229259
H	-2.452844	-0.471686	-0.142644
H	2.533576	-0.393874	-0.241516
H	2.040168	0.165453	1.199255

Co^{2+} dapsox Isomer VII LDA

Co	10.709273	6.605594	1.757734
O	8.585912	4.923424	3.067985
O	9.902079	2.971551	5.697952
O	10.660639	10.608352	3.527029
O	9.042894	7.429119	2.756402
O	11.616491	7.220448	3.457510
N	11.902460	6.055803	0.311130
N	11.160361	4.651995	2.218305
N	10.718907	4.008569	3.291830
N	7.836591	3.854216	5.307759
H	7.457048	3.515423	6.186847
H	7.297194	4.411027	4.645153
N	11.405729	8.355853	1.055363
N	11.120990	9.523895	1.588497
N	11.501137	8.800331	5.067282
H	11.200319	9.780881	5.188699
H	11.695092	8.142164	5.817324
C	12.296800	4.778656	0.221305
C	13.109642	4.363557	-0.827552
H	13.429143	3.322010	-0.900660
C	13.514526	5.309662	-1.760528
H	14.143557	5.008285	-2.601631
C	13.158916	6.638774	-1.609056
H	13.508005	7.399408	-2.310716
C	12.361708	7.002422	-0.523475
C	11.813758	3.969286	1.312154
C	12.048039	2.523258	1.437965
H	12.131781	2.276348	2.510490
H	12.952668	2.210844	0.897026
H	11.198094	1.935015	1.050294
C	9.504113	4.244610	3.686564
C	9.126546	3.610669	5.007501
C	12.018471	8.327236	-0.108639
C	12.412837	9.558315	-0.808599
H	12.715845	9.362781	-1.846026
H	11.577277	10.277053	-0.787648
H	13.246949	10.055892	-0.282794
C	10.995633	9.584453	2.920111
C	11.402021	8.394939	3.812991
O	9.047748	5.771274	0.717359
H	8.409954	7.688650	2.055542
H	8.722865	6.511476	3.071222
H	9.397357	5.132723	0.062888
H	8.790962	5.233594	1.565971

Co^{2+} dapsox Isomer VIII LDA

Co	11.253124	6.438189	2.105743
O	8.370795	3.249083	3.689864
O	9.212456	5.960659	1.613338
O	12.433780	10.588215	3.651555
O	9.930391	7.951925	2.998053
O	12.930660	7.126848	3.276347
N	12.183906	5.913774	0.379311
N	11.178618	4.324605	1.997705
N	10.472849	3.580244	2.860530
N	7.264655	5.002358	2.267487
H	6.676348	5.733416	1.876070
H	6.949109	4.242166	2.897347
N	11.867974	8.240686	1.187155
N	11.775538	9.431453	1.796140
N	13.796081	8.719832	4.638167
H	13.663807	9.730821	4.826419
H	14.271883	8.059066	5.246825
C	12.395713	4.622362	0.092716
C	13.038989	4.231057	-1.076804
H	13.199660	3.168780	-1.275278

C	13.443078	5.203644	-1.974177
H	13.941903	4.922506	-2.905195
C	13.208994	6.535731	-1.681306
H	13.517365	7.332934	-2.361836
C	12.584403	6.859037	-0.481268
C	11.811297	3.716414	1.040254
C	11.826012	2.253278	0.870041
H	11.526432	1.783762	1.818820
H	12.824684	1.902266	0.566747
H	11.109565	1.929164	0.095815
C	9.178700	3.866887	2.979446
C	8.581972	5.049410	2.192434
C	12.395720	8.197803	0.000867
C	12.863654	9.385519	-0.734720
H	13.964855	9.455951	-0.730660
H	12.539928	9.345547	-1.787141
H	12.462981	10.286310	-0.247374
C	12.374464	9.547361	2.978857
C	13.064512	8.323817	3.612372
O	10.962578	5.828153	4.188519
H	11.894122	6.104590	4.365378
H	10.950374	4.833529	4.146104
H	9.196718	7.565488	2.461384
H	10.210461	8.797358	2.552109

Co^{2+} dapsox Isomer IX LDA

Co	10.585214	6.601224	2.064220
O	9.812938	5.804623	4.198097
O	9.234117	2.545720	5.394523
O	10.219855	10.916779	3.503948
O	8.985237	7.762840	2.605450
O	8.846979	5.997236	0.848900
O	11.851070	7.150060	3.683196
N	11.685884	6.141789	0.468937
N	10.931685	4.561917	2.247922
N	10.425721	3.798180	3.223521
N	8.677906	4.610367	6.188599
H	8.221277	4.245772	7.019172
H	8.763592	5.607214	5.983880
N	11.194121	8.466894	1.274966
N	11.094753	9.658560	1.827904
N	8.255126	9.428779	3.955098
H	8.574047	10.363260	4.274144
H	7.432847	8.924044	4.275756
C	11.983072	4.856212	0.231276
C	12.693749	4.479585	-0.901620
H	12.926284	3.425756	-1.071741
C	13.096616	5.468361	-1.788258
H	13.651965	5.201427	-2.691130
C	12.812007	6.793099	-1.519821
H	13.139530	7.587716	-2.193377
C	12.108616	7.113756	-0.354542
C	11.517440	3.954868	1.251600
C	11.691640	2.496059	1.165300
H	11.170646	2.026748	2.011642
H	12.760862	2.225147	1.205834
H	11.292318	2.105659	0.214932
C	9.868330	4.526864	4.160146
C	9.231682	3.760284	5.303792
C	11.823014	8.431942	0.117029
C	12.286357	9.662540	-0.543399
H	13.042041	9.460529	-1.314004
H	11.447486	10.211773	-1.003569
H	12.692245	10.339098	0.227751
C	10.249765	9.874156	2.829276
C	9.118807	8.895826	3.115479
H	12.681174	6.639724	3.621200
H	11.198907	6.574499	4.207454
H	9.070779	6.320277	-0.046341
H	8.354308	6.735370	1.284378

Co^{2+} dapsox Isomer X LDA

Co	10.490702	6.684346	2.001333
O	10.045821	4.129742	5.643404
O	8.799094	5.467724	2.655399
O	10.740591	11.054825	3.499148
O	9.200313	7.931656	3.044888
O	8.811393	6.973711	0.579473
O	11.768319	7.093453	3.707667
N	11.533621	6.151475	0.427127
N	11.225009	4.801670	2.457250
N	11.225116	4.310410	3.695757
N	7.820143	4.778325	4.589281
H	8.097591	4.385057	5.502489
H	6.883075	5.072718	4.329084
N	11.172535	8.536486	1.194623
N	11.138342	9.763193	1.686636
N	9.237892	9.462980	4.707362
H	9.659504	10.386347	4.913151
H	8.614990	8.932094	5.311414
C	11.967070	4.890397	0.301769
C	12.630680	4.478052	-0.850158
H	12.963984	3.442410	-0.949510
C	12.880559	5.414451	-1.840120
H	13.408793	5.118797	-2.750435
C	12.508678	6.736053	-1.654950
H	12.759959	7.505300	-2.388953
C	11.844311	7.086214	-0.480696
C	11.770533	4.111540	1.493216
C	12.227024	2.722080	1.659664
H	12.452021	2.553013	2.725264
H	13.113348	2.508286	1.044150
H	11.436565	2.005604	1.377044
C	10.133571	4.446332	4.446673
C	8.856528	4.957527	3.782717
C	11.555994	8.428765	-0.065757
C	11.855261	9.595401	-0.916664
H	12.938675	9.813523	-0.917755
H	11.550979	9.421283	-1.960234
H	11.350722	10.483335	-0.512724
C	10.585256	9.990861	2.876031
C	9.623018	8.999763	3.535034
H	11.911960	6.172068	4.056278
H	12.620484	7.369223	3.314798
H	9.133287	7.784652	0.131413
H	8.297851	7.304435	1.352979

Co^{2+} dapsox Isomer XI LDA

Co	10.576274	6.572127	2.108579
O	9.848159	5.815552	4.068591
O	8.927346	2.669149	5.324827
O	9.890688	11.041855	3.178128
N	8.931300	7.785282	2.743462
O	8.940937	6.077915	0.630641
O	11.984528	7.153484	3.574246
N	11.774698	6.125848	0.534208
N	10.841316	4.514896	2.182682
N	10.292521	3.759101	3.147314
N	8.723447	4.782953	6.161977

H	8.262311	4.468771	7.011484
H	8.934881	5.767782	5.985657
N	11.043438	8.495799	1.182037
N	10.768043	9.723799	1.563563
O	9.649359	8.636188	4.729816
C	12.087100	4.842601	0.290473
C	12.844936	4.473468	-0.811399
H	13.090716	3.422540	-0.978609
C	13.268989	5.472897	-1.678830
H	13.868036	5.217525	-2.556938
C	12.933057	6.786424	-1.434587
H	13.257610	7.581341	-2.108180
C	12.168262	7.104513	-0.300870
C	11.561127	3.923305	1.267701
C	11.821383	2.475323	1.242301
H	11.180466	1.985294	1.989023
H	12.874689	2.261336	1.493448
H	11.634729	2.052633	0.242087
C	9.793402	4.537075	4.076627
C	9.104800	3.871919	5.248613
C	11.771670	8.418025	0.080300
C	12.197273	9.639573	-0.624948
H	12.880920	9.427113	-1.456808
H	11.323934	10.198131	-1.001055
H	12.681289	10.322939	0.092547
C	10.106782	9.923148	2.731669
C	9.557467	8.751712	3.527206
H	12.765130	6.569847	3.499997
H	11.406749	6.749214	4.277084
H	8.517886	8.090236	1.856852
H	8.371769	7.123414	3.296023
H	9.492830	6.197494	-0.172336
H	8.929401	5.106915	0.773029

Co^{2+} dapsox Isomer XII LDA

Co	10.686428	6.670492	2.149171
O	9.020677	3.276278	4.966932
O	8.239348	5.968263	4.446092
O	9.948932	11.258336	2.943988
N	9.009746	7.979459	2.811084
O	8.963432	6.049458	0.996924
O	12.610082	7.178069	3.018592
N	11.752604	6.141248	0.534210
N	10.909041	4.450382	2.323708
N	10.397963	3.571915	3.199888
N	10.481235	6.298063	4.319012
H	13.251695	6.519520	2.673262
H	11.386293	5.857040	4.508000
N	11.063370	8.569286	1.082121
N	10.784784	9.847150	1.387944
O	9.977784	8.942542	4.623642
C	12.103791	4.860112	0.365681
C	12.854091	4.458693	-0.735853
H	13.131924	3.409394	-0.851349
C	13.224939	5.407259	-1.669612
H	13.809282	5.117461	-2.545863
C	12.853844	6.726145	-1.488880
H	13.141126	7.488966	-2.213378
C	12.114063	7.072719	-0.360866
C	11.634912	3.934594	1.364769
C	11.943400	2.499860	1.241042
H	11.450399	1.940126	2.043805
H	13.032412	2.333430	1.295357
H	11.611409	2.112252	0.263916
C	9.611191	4.029691	4.166774
C	9.380299	5.504047	4.340094
C	11.712561	8.419949	-0.045930
C	12.048858	9.569060	-0.900251
H	12.606706	9.277227	-1.796590
H	11.129335	10.096931	-1.201760
H	12.637503	10.303592	-0.326578
C	10.165340	10.099669	2.537046
C	9.698478	8.976688	3.419242
H	12.855855	8.011518	2.558990
H	10.355568	7.263786	4.720192
H	8.577650	8.188216	1.906189
H	8.453992	7.349918	3.446799
H	9.148551	6.306363	0.067122
H	9.020891	5.068260	0.988026

Co^{2+} Hdapsox Isomer I HS LDA

Co	0.179931	2.341844	2.599787
O	-0.871062	3.699390	1.404402
O	-0.065549	5.988905	-1.140981
O	-1.828463	3.011912	3.712091
O	-3.572189	1.095110	6.066305
O	-1.066618	1.154977	1.376020
H	-0.571220	0.679484	0.678968
H	-1.361817	2.012876	0.962022
O	0.716520	4.028056	3.720653
H	1.198422	3.883546	4.558536
H	-0.192287	4.311115	3.969417
N	1.836126	1.145186	2.757665
N	1.479274	2.951344	1.108938
N	1.125551	3.949372	0.297693
N	-1.963320	5.689320	0.088327
H	-2.386723	5.129485	0.826885
H	-2.472136	6.426380	-0.394169
N	-0.155905	1.031871	4.192651
N	-1.338658	1.093626	4.808816
H	-1.727260	0.412778	5.487642
N	-4.275492	3.016032	5.021519
H	-5.183408	3.052749	5.483310
H	-4.008157	3.716624	4.329342
C	2.863946	1.335449	1.920684
C	4.015537	0.559540	2.008016
H	4.839229	0.736060	1.311824
C	4.088244	-0.424722	2.977658
H	4.981778	-1.047869	3.063291
C	3.021187	-0.615841	3.839919
H	3.049035	-1.387706	4.612728
C	1.903752	0.198382	3.699785
C	2.640942	2.385774	0.957849
C	3.621794	2.760466	-0.068218
H	3.866045	1.900046	-0.714149
H	3.212596	3.574229	-0.682574
H	4.565396	3.095029	0.395559
C	-0.115741	4.281153	0.536808
C	-0.697785	5.418700	-0.275556
C	0.714383	0.123019	4.518190
C	0.557302	-0.889686	5.575201
H	0.439357	-1.896939	5.138850
H	-0.298403	-0.704653	6.240004
H	1.459753	-0.919385	6.207488
C	-2.134337	2.121069	4.511554
C	-3.428002	2.029722	5.288499

Co^{2+} Hdapsox LS LDA

Co	0.474085	2.261020	2.452968

O	-0.859692	3.419282	1.561122
O	-0.444646	5.750506	-1.041873
O	-1.716523	3.625387	4.478466
O	-3.783283	0.956651	5.382566
O	-0.674498	0.866236	1.154474
H	-0.183143	0.583704	0.356127
H	-1.179905	1.673833	0.883174
O	0.711132	3.927931	3.633053
H	1.348685	3.827324	4.366537
H	-0.223482	3.916050	4.042731
N	1.884847	1.193249	2.742956
N	1.521985	2.907660	1.122317
N	1.040570	3.873122	0.333659
N	-2.179114	5.377334	0.394915
H	-2.482888	4.834541	1.202243
H	-2.768780	6.091442	-0.026682
N	-0.227470	1.227806	3.924093
N	-1.451389	1.323535	4.483950
H	-2.044567	0.506342	4.757504
N	-4.222384	3.208830	5.471426
H	-5.159171	3.112931	5.860773
H	-3.809139	4.127597	5.303044
C	2.967665	1.373360	1.950972
C	4.074085	0.555101	2.119087
H	4.955008	0.696490	1.487807
C	4.032494	-0.443081	3.086067
H	4.895994	-1.097857	3.223831
C	2.903239	-0.621861	3.869931
H	2.859196	-1.413546	4.621422
C	1.820547	0.229077	3.675869
C	2.740862	2.424909	0.994491
C	3.698358	2.887507	-0.012852
H	3.992176	2.062348	-0.684267
H	3.243915	3.691220	-0.608946
H	4.620148	3.264649	0.461268
C	-0.210776	4.089069	0.656307
C	-0.946997	5.171644	-0.100284
C	0.554544	0.261187	4.359305
C	0.176438	-0.676687	5.424529
H	-0.460965	-1.490720	5.032135
H	-0.390317	-0.169082	6.222230
H	1.063861	-1.145189	5.871383
C	-2.108403	2.472426	4.668094
C	-3.486796	2.135793	5.219294

Co^{2+} Hdapsox Isomer II LDA

Co	-2.045804	4.073872	11.255526
N	-2.867765	5.941883	11.006010
N	-2.653441	4.228307	9.267160
N	-2.407161	3.203921	8.446722
N	-1.073085	-0.057770	8.463446
N	-1.783008	5.088783	13.065586
N	-1.166059	4.465806	14.080125
N	0.082831	2.947687	15.889045
O	-1.640079	2.020015	10.205523
O	-1.911123	1.287758	6.798140
O	-1.166255	2.730919	12.583920
O	0.221107	1.235105	14.386371
O	-0.019690	4.249692	10.704533
O	-3.684685	3.002439	12.006970
H	-3.060797	2.364562	12.440943
C	-3.366119	6.314920	9.820424
C	-3.917871	7.574892	9.623268
C	-3.947268	8.459967	10.686613
C	-3.423262	8.073237	11.907276
C	-2.881248	6.799145	12.033332
C	-3.234409	5.295151	8.807339
C	-3.670639	5.450410	7.409725
C	-1.870874	2.111445	8.999363
C	-1.611795	1.046133	7.960831
C	-2.269642	6.280754	13.233732
C	-2.215231	7.046104	14.486175
H	-3.232400	7.273645	14.847984
H	-1.702335	8.011124	14.336372
H	-1.684073	6.468810	15.252998
C	-0.872449	3.235451	13.718460
C	-0.127985	2.356254	14.702650
H	-4.374294	9.457740	10.560346
H	-4.310730	7.859850	8.644808
H	-0.259633	3.897415	16.034292
H	-3.422172	8.749605	12.765625
H	0.574097	2.435289	16.618555
H	-4.160999	4.535851	7.035317
H	0.420342	5.006658	11.142908
H	-0.847427	-0.842222	7.853075
H	-0.873443	-0.096273	9.464797
H	-4.387271	6.274599	7.300397
H	0.229757	3.456271	11.240874
H	-2.813317	5.667613	6.746756
H	-4.169051	2.482531	11.335398
H	-2.543727	3.180633	7.420371

Co^{2+} Hdapsox Isomer III LDA

Co	0.117891	2.255570	2.557686
O	-0.929327	3.527160	1.270733
O	-2.016943	5.534234	-0.239443
O	-1.874991	2.693986	3.481764
O	-3.508187	3.460817	5.716361
O	-0.876712	1.017797	1.160602
H	-1.617947	0.481808	1.503993
H	-1.287253	1.855198	0.803579
O	0.441824	3.944890	3.770807
H	1.031600	4.575153	3.305879
H	-0.458242	4.342836	3.724442
N	1.830487	1.136449	2.749618
N	1.498560	3.047355	1.209845
N	1.129045	4.078604	0.439437
N	0.072895	6.065569	-0.984833
H	1.057534	5.802741	-0.949696
H	-0.260534	6.832251	-1.565268
N	-0.169297	0.919293	4.158519
N	-1.322248	1.006053	4.846859
H	-1.452594	0.518785	5.742213
N	-3.976927	1.226330	5.838730
H	-4.802345	1.417263	6.412838
H	-3.999237	0.371876	5.281324
C	2.885797	1.410793	1.974228
C	4.063676	0.675240	2.067066
H	4.907664	0.922731	1.418530
C	4.141228	-0.354268	2.986490
H	5.054998	-0.946519	3.076581
C	3.052442	-0.621774	3.799653
H	3.088088	-1.417192	4.547921
C	1.910491	0.154628	3.653808
C	2.676206	2.516393	1.073124
C	3.691126	2.955985	0.106467
H	3.918852	2.150555	-0.612538
H	3.324290	3.830315	-0.445592
H	4.635485	3.213719	0.614460
C	-0.176317	4.245980	0.542266

C	-0.816403	5.353952	-0.271807
C	0.719899	0.025043	4.462529
C	0.603887	-0.992970	5.521091
H	0.956479	-1.968826	5.151118
H	-0.425368	-1.139820	5.880350
H	1.234855	-0.730955	6.388595
C	-2.140586	2.015477	4.469987
C	-3.310186	2.315191	5.385111

Co^{2+} Hdapsox Isomer V LDA

Co	-2.188187	4.023506	10.936087
N	-2.932942	5.839254	10.962167
N	-2.546153	4.405894	9.015308
N	-2.337620	3.416039	8.153445
N	-1.893429	-0.052431	8.817721
N	-1.732218	4.762047	12.890803
N	-1.204517	4.057582	13.905091
N	1.162701	1.808848	15.160858
O	-2.395711	2.213225	10.101601
O	-1.702753	1.067935	6.841469
O	0.507668	2.972555	12.785644
O	-0.571448	2.978056	16.108235
O	-0.200055	3.921610	10.519873
O	-3.922816	3.191482	11.831495
H	-3.903856	2.449094	11.174161
C	-3.289175	6.398841	9.789127
C	-3.767959	7.703607	9.745683
C	-3.835816	8.432145	10.919132
C	-3.405016	7.864524	12.109211
C	-2.940706	6.555974	12.096229
C	-3.136858	5.515848	8.663734
C	-3.610712	5.804005	7.303569
C	-2.221543	2.295238	8.819701
C	-1.906732	1.041942	8.038415
C	-2.367189	5.856611	13.222458
C	-2.442327	6.345194	14.609218
H	-2.857702	7.358279	14.664901
H	-1.444397	6.350150	15.080773
H	-3.091453	5.696507	15.225899
C	-0.160763	3.230262	13.787127
C	0.131110	2.640470	15.160308
H	-4.206026	9.460127	10.906649
H	-4.080176	8.134085	8.790484
H	1.653378	1.642058	14.280276
H	-3.410471	8.444321	13.034840
H	1.463941	1.362319	16.025903
H	-3.227941	5.034998	6.616953
H	0.254503	4.715959	10.181594
H	-1.670646	-0.952718	8.398801
H	-2.018524	0.051785	9.823350
H	-4.713009	5.795150	7.253087
H	0.226624	3.631418	11.397174
H	-3.275576	6.798897	6.968865
H	-4.738266	3.702591	11.655274
H	-1.525693	4.106202	14.899846

Co^{2+} Hdapsox Isomer VI LDA

Co	0.003218	0.362656	-0.248346
O	2.002656	0.769829	0.245925
O	-2.134482	0.168334	0.067989
O	-0.320209	1.826208	1.071771
O	0.146915	4.056743	-1.565807
O	1.658101	0.415481	2.760869
O	-0.598250	-1.355162	4.762611
N	-0.023074	4.091926	1.083465
N	-0.001785	1.713362	-1.524661
N	0.080881	1.661064	-2.837208
N	-0.036663	-0.986590	-1.567236
N	0.140350	-1.169954	0.952087
N	-0.002197	-1.123478	2.290610
N	1.050439	0.116425	5.387175
C	-0.106151	2.922462	0.496384
C	0.038763	2.988188	-0.998165
C	0.084453	0.533147	-3.483077
C	0.139991	0.668712	-4.959794
C	0.061113	-0.801013	-2.906086
C	0.113897	-1.898511	-3.760443
C	0.071095	-3.189170	-3.253856
C	-0.012133	-3.370574	-1.893240
C	-0.062338	-2.261760	-1.053915
C	-0.115824	-2.333550	0.359934
C	-0.410483	-3.553655	1.129573
C	0.739955	-0.349081	3.082801
C	0.319880	-0.577668	4.522104
H	-0.108465	4.204759	2.091910
H	0.131259	4.884838	0.447509
H	0.139845	1.735728	-5.212705
H	1.047302	0.205462	-5.380097
H	-0.728764	0.191833	-5.442287
H	0.165884	-1.730467	-4.836681
H	0.108155	-4.048052	-3.927765
H	-0.024436	-4.374396	-1.462376
H	-1.436745	-3.534831	1.541505
H	-0.337334	-4.455045	0.508864
H	1.804793	0.697630	5.017620
H	0.893392	0.021038	6.388840
H	0.282157	-3.665005	1.981308
H	-0.678916	-1.700123	2.836192
H	-2.627858	0.198779	-0.777510
H	-2.339354	1.003736	0.539986
H	2.604800	0.087860	-0.112461
H	1.958568	0.607583	1.262100

Co^{2+} Hdapsox Isomer VII LDA

Co	10.638631	6.440209	1.793464
O	9.059289	5.341395	3.070279
O	9.808550	3.059436	5.660478
O	10.752357	10.574231	3.623481
O	8.963520	7.748013	2.312781
O	11.323289	7.093793	3.577631
N	11.871191	5.999620	0.287407
N	11.259104	4.534625	2.166407
N	10.825398	3.892520	3.248869
N	7.999831	4.404529	5.329405
H	7.527077	4.070427	6.166840
H	7.540788	5.039112	4.679302
N	11.405187	8.253419	1.115718
N	11.167914	9.401849	1.755467
N	11.200484	8.615039	5.244914
H	11.060661	9.610991	5.447158
H	11.337526	7.915324	5.973725
C	12.336053	4.746864	0.172029
C	13.145099	4.389891	-0.900649
H	13.508224	3.363042	-0.990941
C	13.490707	5.359050	-1.827276
H	14.122194	5.100234	-2.680676
C	13.079032	6.669162	-1.641712
H	13.400126	7.458002	-2.325605
C	12.283713	6.965104	-0.541980

C	11.942112	3.888861	1.262125
C	12.286674	2.464772	1.362405
H	12.190881	2.147757	2.412056
H	13.309170	2.275356	1.001892
H	11.602055	1.838655	0.764269
C	9.722366	4.415286	3.696793
C	9.190943	3.872164	5.001901
C	11.947083	8.287530	-0.068126
C	12.294562	9.538937	-0.761698
H	12.773543	9.350063	-1.730072
H	11.397235	10.153093	-0.959624
H	12.989777	10.147111	-0.155096
C	10.982167	9.499915	3.099296
C	11.178988	8.262194	3.973657
O	8.997634	5.745407	0.577385
H	11.164042	10.297216	1.246391
H	8.378825	7.658962	1.528608
H	8.680505	7.003515	2.918450
H	9.244065	5.090325	-0.106591
H	8.761511	5.233407	1.414233

Co^{2+} Hdapsox Isomer VIII LDA

Co	11.227525	6.447069	2.083120
O	8.385078	3.098335	3.641583
O	9.164249	5.942168	1.707802
O	12.512871	10.616762	3.584441
O	9.995292	7.947681	2.970311
O	12.816570	7.124765	3.325407
N	12.195640	5.911676	0.369664
N	11.198249	4.293166	1.952570
N	10.415546	3.543013	2.770148
N	7.215581	5.116361	2.531107
H	6.639868	5.859242	2.138166
H	6.821205	4.350150	3.089349
N	11.885127	8.248426	1.172271
N	11.771413	9.433158	1.778698
N	13.796341	8.703577	4.620139
H	13.761485	9.726459	4.779052
H	14.273237	8.039304	5.226712
C	12.458607	4.628444	0.087826
C	13.138321	4.244595	-1.059088
H	13.336009	3.188458	-1.254821
C	13.534429	5.222249	-1.955577
H	14.057076	4.950346	-2.875710
C	13.264304	6.545020	-1.666628
H	13.573249	7.348557	-2.339609
C	12.604592	6.862031	-0.482958
C	11.866720	3.696062	1.015685
C	11.932103	2.239977	0.792967
H	11.712814	1.640878	1.688831
H	12.935177	1.949248	0.448002
H	11.215147	1.935784	0.009685
C	9.104149	3.836618	2.993415
C	8.522472	5.089445	2.344818
C	12.404618	8.204835	-0.015750
C	12.857384	9.389122	-0.761430
H	13.958831	9.459861	-0.771392
H	12.519962	9.346583	-1.809306
H	12.464152	10.293468	-0.275361
C	12.406810	9.567679	2.948666
C	13.039955	8.327233	3.614696
O	10.792272	5.824785	4.190593
H	11.526019	6.451263	4.418640
H	11.167763	4.937489	4.371435
H	9.166442	7.676718	2.515394
H	10.296786	8.812954	2.558711
H	10.667180	2.563743	2.964330

Co^{2+} Hdapsox Isomer IX LDA

Co	10.581125	6.558128	2.091628
O	9.901401	5.814626	4.076865
O	9.166730	2.618425	5.349689
O	10.159418	11.027909	3.369609
O	8.992824	7.783741	2.739455
O	8.857176	5.989591	0.970360
O	11.921388	7.194451	3.617748
N	11.745973	6.126722	0.494078
N	10.895268	4.508448	2.180144
N	10.361438	3.760599	3.150805
N	8.718865	4.706489	6.151613
H	8.276331	4.360558	6.999906
H	8.851010	5.701144	5.974741
N	11.136716	8.428392	1.230557
N	10.988365	9.621102	1.829177
N	8.214801	9.459852	4.059734
H	8.406623	10.428804	4.342485
H	7.411899	8.933005	4.399198
C	12.007959	4.842297	0.215032
C	12.707724	4.482271	-0.930352
H	12.914197	3.427582	-1.128590
C	13.135748	5.476281	-1.792292
H	13.688164	5.218627	-2.699097
C	12.867161	6.799922	-1.494219
H	13.206913	7.598894	-2.156251
C	12.162788	7.093221	-0.330621
C	11.515286	3.913152	1.200680
C	11.696210	2.458944	1.099300
H	11.151380	1.967194	1.917093
H	12.764252	2.190531	1.173515
H	11.334996	2.080894	0.128595
C	9.871555	4.531123	4.090372
C	9.217849	3.828620	5.264597
C	11.861686	8.419989	0.147529
C	12.386063	9.647309	-0.478679
H	12.821974	9.443922	-1.464102
H	11.587536	10.397473	-0.611609
H	13.187208	10.107765	0.130451
C	10.139926	9.930768	2.836369
C	9.072110	8.928035	3.211924
H	12.793496	6.754565	3.575883
H	11.343987	6.620942	4.210406
H	8.649076	5.045899	1.134954
H	8.202093	6.506493	1.492036
H	11.622679	10.391432	1.571983

Co^{2+} Hdapsox Isomer X LDA

Co	10.701415	6.729222	2.116060
O	9.230674	3.155091	4.966757
O	9.099802	6.348083	3.521747
O	8.784662	10.765664	2.624009
O	10.890920	8.171816	3.643634
O	8.832714	6.814466	1.041462
O	12.527789	6.365452	3.335321
N	11.833334	6.240457	0.562314
N	10.799757	4.572760	2.164498
N	10.373209	3.755798	3.141351
N	7.963943	5.378914	5.229907
H	7.877044	4.500762	5.756152
H	7.420861	6.212598	5.448432

N	10.861841	8.509924	1.033891
N	10.063033	9.551352	1.191656
N	9.905408	9.906363	4.725932
H	9.285775	10.708887	4.518125
H	10.220440	9.637968	5.655885
C	12.173571	4.963749	0.344755
C	12.978717	4.607461	-0.727911
H	13.247010	3.564291	-0.904731
C	13.423353	5.603529	-1.586282
H	14.062610	5.348215	-2.434881
C	13.034218	6.910055	-1.378044
H	13.346572	7.710698	-2.052594
C	12.209792	7.205143	-0.290624
C	11.626817	4.037373	1.311669
C	12.008198	2.612222	1.356806
H	12.588613	2.380766	2.269788
H	12.636586	2.331419	0.504147
H	11.119848	1.955727	1.340585
C	9.508940	4.017896	4.148466
C	8.851154	5.380333	4.253989
C	11.633968	8.489417	-0.027025
C	11.791383	9.639453	-0.931387
H	12.753518	10.153411	-0.762157
H	11.760011	9.330811	-1.987697
H	10.985777	10.361281	-0.729285
C	9.612172	9.875226	2.405636
C	10.208303	9.218817	3.648264
H	13.299517	6.579857	2.773815
H	12.323602	7.194732	3.837255
H	8.225838	6.731135	1.810068
H	8.738737	7.747564	0.736520
H	10.754825	2.799055	3.188558

Co^{2+} Hdapsox Isomer XI LDA

Co	10.542012	6.546622	2.093058
O	9.757521	5.813897	3.979466
O	9.002700	2.645193	5.288524
O	10.046040	11.107611	3.179239
N	8.908330	7.847232	2.776418
O	8.852261	6.025983	0.794700
O	11.912730	7.194676	3.545957
N	11.769207	6.126562	0.514979
N	10.868468	4.504661	2.183585
N	10.335611	3.756404	3.153973
N	8.708715	4.734493	6.158130
H	8.272659	4.387075	7.010125
H	8.877868	5.730490	6.018045
N	11.029979	8.467028	1.120527
N	10.693354	9.686475	1.565770
O	9.645725	8.717976	4.756870
C	12.103825	4.844773	0.292660
C	12.883709	4.479338	-0.798132
H	13.146533	3.429193	-0.947228
C	13.311397	5.463026	-1.670706
H	13.925012	5.203122	-2.536814
C	12.962902	6.780928	-1.436527
H	13.298272	7.570094	-2.111963
C	12.184185	7.084355	-0.322925
C	11.593357	3.918875	1.272245
C	11.876652	2.477989	1.247879
H	11.272861	1.977012	2.017250
H	12.942633	2.285021	1.461176
H	11.661519	2.043047	0.258298
C	9.777544	4.532830	4.048877
C	9.123083	3.852604	5.234696
C	11.784147	8.419793	0.060869
C	12.238979	9.632446	-0.646167
H	12.878165	9.395534	-1.504305
H	11.385950	10.225168	-1.022790
H	12.831706	10.283734	0.023116
C	10.108198	9.969596	2.783255
C	9.525968	8.805692	3.560038
H	12.749936	6.688700	3.536918
H	11.383980	6.835209	4.304477
H	8.453469	8.142846	1.905611
H	8.386970	7.158624	3.338395
H	9.194563	5.936070	-0.119433
H	8.579515	5.117764	1.048026
H	11.092548	10.517494	1.103889

Co^{2+} Hdapsox Isomer XII LDA

Co	10.687084	6.688496	2.144937
O	8.918022	3.225426	4.856470
O	8.182534	5.965641	4.443261
O	10.066045	11.252283	2.992344
N	9.034053	7.997368	2.818632
O	8.970021	6.047835	1.032156
O	12.552187	7.214013	3.047818
N	11.758384	6.131790	0.530703
N	10.962499	4.467800	2.316119
N	10.432489	3.648396	3.241998
N	10.437633	6.274875	4.340719
H	13.219731	6.530843	2.818878
H	11.327851	5.813246	4.556669
N	11.055220	8.560806	1.071588
N	10.795027	9.836043	1.387178
O	10.033075	8.915673	4.641046
C	12.145243	4.862676	0.370425
C	12.893837	4.461369	-0.725679
H	13.202556	3.419586	-0.829498
C	13.228693	5.407349	-1.678811
H	13.815181	5.122046	-2.554633
C	12.815828	6.712729	-1.514501
H	13.072119	7.473467	-2.252702
C	12.078079	7.058268	-0.382849
C	11.695050	3.932247	1.388167
C	12.049694	2.510850	1.265863
H	11.664473	1.860965	2.059942
H	13.147109	2.406738	1.260571
H	11.686648	2.115730	0.303254
C	9.530592	4.030454	4.171169
C	9.319897	5.510675	4.345233
C	11.651479	8.400369	-0.084717
C	11.921223	9.537669	-0.975485
H	12.367697	9.228273	-1.926636
H	10.986926	10.087133	-1.172884
H	12.591864	10.258155	-0.477873
C	10.228751	10.095963	2.563951
C	9.748612	8.973712	3.441546
H	12.849437	8.012112	2.557083
H	10.329331	7.247963	4.738831
H	8.591629	8.250953	1.929535
H	8.446371	7.392527	3.442611
H	9.009511	6.452104	0.137914
H	9.073667	5.086025	0.860676
H	10.583475	2.634090	3.148473

Co^{2+} H_2dapsox Isomer I HS LDA

Co	0.082513	2.327627	2.624727
O	-1.002523	3.808435	1.392446
O	0.295571	5.874677	-1.118592
O	-1.801747	2.869926	3.636932
O	-3.475670	1.104080	6.154451
O	-1.102735	1.047114	1.485378
H	-0.702613	0.361706	0.912615
H	-1.673104	1.597055	0.907348
O	0.734301	3.980996	3.709541
H	1.428301	3.893618	4.394303
H	-0.048003	4.373309	4.152310
N	1.816787	1.159390	2.759227
N	1.414712	2.945118	1.112710
N	0.992135	3.957635	0.358106
H	1.515106	4.498374	-0.361791
N	-1.826188	5.985359	-0.250046
H	-2.469498	5.580436	0.429323
H	-2.124801	6.763692	-0.840666
N	-0.155969	0.967585	4.219842
N	-1.323188	1.037672	4.855646
H	-1.699125	0.418256	5.603702
N	-4.272847	2.955822	5.058703
H	-5.155202	2.989360	5.572644
H	-4.074935	3.644293	4.333423
C	2.833713	1.365116	1.916229
C	4.002459	0.618424	1.982106
H	4.820058	0.813906	1.283293
C	4.107130	-0.370864	2.944074
H	5.014213	-0.976149	3.017681
C	3.050240	-0.585707	3.811247
H	3.100629	-1.361041	4.580266
C	1.915719	0.205360	3.690187
C	2.589835	2.426224	0.955501
C	3.591044	2.819239	-0.044842
H	3.969951	1.929369	-0.574942
H	3.207695	3.513253	-0.805496
H	4.461542	3.295167	0.440923
C	-0.263716	4.352224	0.557545
C	-0.596182	5.506564	-0.366452
C	0.741585	0.091768	4.537528
C	0.647999	-0.911862	5.605900
H	0.701717	-1.931170	5.184932
H	-0.271172	-0.843338	6.203190
H	1.500700	-0.810046	6.299360
C	-2.119867	2.046116	4.507766
C	-3.392016	2.004037	5.329735

Co^{2+} H_2dapsox LS LDA

Co	0.415111	2.209359	2.426234
O	-0.972639	3.465065	1.513828
O	-0.014515	5.771723	-0.939458
O	-1.777081	3.618090	4.434086
O	-3.655062	0.874167	5.500558
O	-0.704755	0.790483	1.244501
H	-0.275062	0.144342	0.647225
H	-1.386651	1.248466	0.710156
O	0.595622	3.912348	3.546292
H	1.251696	3.894437	4.272046
H	-0.339889	3.903059	3.979365
N	1.862809	1.177608	2.714869
N	1.496602	2.878275	1.109268
N	0.953003	3.876598	0.398314
H	1.395533	4.497642	-0.310780
N	-2.071876	5.661951	0.075706
H	-2.628608	5.182429	0.782980
H	-2.470215	6.445195	-0.445933
N	-0.233935	1.216440	3.927049
N	-1.453448	1.317856	4.479329
H	-2.047262	0.513928	4.834373
N	-4.223965	3.094622	5.640144
H	-5.116375	2.937175	6.111155
H	-3.893245	4.044422	5.463567
C	2.947050	1.368534	1.930081
C	4.074283	0.585573	2.115048
H	4.960978	0.741169	1.494183
C	4.053504	-0.394514	3.099555
H	4.932366	-1.025493	3.254227
C	2.926640	-0.577718	3.886808
H	2.902361	-1.351956	4.658092
C	1.824182	0.241481	3.676713
C	2.716942	2.426024	0.968838
C	3.701748	2.923332	0.004249
H	4.353081	2.106393	-0.342793
H	3.232817	3.372506	-0.884663
H	4.356606	3.686149	0.464818
C	-0.326518	4.132879	0.681843
C	-0.819273	5.295943	-0.149951
C	0.562472	0.270556	4.378038
C	0.211892	-0.640615	5.470431
H	-0.404799	-1.483044	5.103013
H	-0.368613	-0.127812	6.254547
H	1.110481	-1.075061	5.930611
C	-2.124289	2.461712	4.674917
C	-3.449894	2.073226	5.325063

Co^{2+} H_2dapsox Isomer II LDA

Co	0.014466	2.115878	2.566182
O	-1.112216	3.634701	1.474702
O	0.045342	5.947664	-0.878845
O	-2.130100	1.892406	3.073892
O	-2.345262	3.653186	5.379676
O	-0.590292	0.915445	0.980238
H	-0.258854	-0.003161	0.918769
H	-1.567868	0.856041	1.040602
O	0.003980	3.522695	4.114814
H	0.444696	4.384825	3.989437
H	-0.881335	3.707839	4.577564
N	1.825633	1.116376	2.741541
N	1.393674	3.061295	1.296252
N	0.905045	4.067762	0.573185
H	1.393533	4.667298	-0.122144
N	-2.108559	5.770909	-0.102844
H	-2.725231	5.256629	0.526339
H	-2.475307	6.531787	-0.676851
N	-0.150515	0.761523	4.138322
N	-1.261706	0.913828	4.889266
H	-1.213514	0.800275	5.909729
N	-4.205589	2.350547	5.588349
H	-4.711462	3.056649	6.131506
H	-4.692706	1.495125	5.320518
C	2.865702	1.475634	1.982011
C	4.090982	0.829380	2.071632
H	4.928576	1.148999	1.445978
C	4.234595	-0.206744	2.978789
H	5.188664	-0.732100	3.070481
C	3.165949	-0.551710	3.787943
H	3.262209	-1.342406	4.536503
C	1.970597	0.141049	3.646865
C	2.587496	2.600003	1.105889
C	3.572950	3.116138	0.146437

H	4.096566	2.288056	-0.356804
H	3.127581	3.746746	-0.636430
H	4.342481	3.716081	0.666031
C	-0.402758	4.300260	0.712424
C	-0.826702	5.446430	-0.181465
C	0.800158	-0.041725	4.487334
C	0.757161	-0.961507	5.631496
H	1.324760	-1.880248	5.420847
H	-0.273743	-1.256714	5.880796
H	1.217369	-0.504071	6.526970
C	-2.197295	1.683970	4.289028
C	-2.988160	2.622846	5.164814

Co^{2+} H_2dapsox Isomer III LDA

Co	0.118710	2.309739	2.631184
O	-0.794667	3.971338	1.640284
O	-1.897016	4.769233	-0.875016
O	-1.860975	2.588206	3.393294
O	-3.214264	3.503431	5.748008
O	-0.836325	1.339137	1.045535
H	-1.005705	0.376340	1.026819
H	-1.701481	1.783646	0.905115
O	0.475994	3.674049	4.176420
H	1.297138	4.196951	4.267666
H	-0.271655	4.311586	4.193297
N	1.841728	1.148340	2.761786
N	1.504177	3.030280	1.204359
N	1.058755	4.007120	0.396890
H	1.543784	4.248067	-0.476883
N	-0.270707	6.377181	-0.794782
H	0.410060	6.845439	-0.196174
H	-0.744233	6.947698	-1.501734
N	-0.181168	0.863002	4.142975
N	-1.329780	0.966227	4.831811
H	-1.459493	0.495906	5.736571
N	-4.151367	1.415736	5.697721
H	-4.918599	1.697295	6.315260
H	-4.283299	0.571558	5.140225
C	2.882035	1.389371	1.956957
C	4.043693	0.631311	2.010428
H	4.875651	0.850484	1.336261
C	4.125262	-0.400160	2.928930
H	5.027700	-1.013131	2.994430
C	3.048967	-0.646071	3.763313
H	3.081992	-1.452686	4.500178
C	1.917717	0.150780	3.649194
C	2.664629	2.488560	1.033219
C	3.667906	2.868591	0.027636
H	3.746987	2.096268	-0.758264
H	3.464089	3.832580	-0.460270
H	4.663376	2.951956	0.493920
C	-0.200735	4.417801	0.655961
C	-0.892119	5.254255	-0.402963
C	0.727637	0.004125	4.468088
C	0.641301	-0.998681	5.539888
H	0.963627	-1.984466	5.165734
H	-0.372259	-1.128711	5.945453
H	1.315035	-0.738459	6.375632
C	-2.149734	1.952035	4.409803
C	-3.275951	2.364801	5.336522

Co^{2+} H_2dapsox Isomer V LDA

Co	0.178859	2.259281	2.338442
O	-0.922778	3.480550	0.993516
O	0.413717	6.008486	-1.025900
O	-1.945390	3.459706	4.558334
O	-3.490386	0.691391	6.017044
O	-0.949894	0.866362	1.369291
H	-0.657887	-0.037352	1.131645
H	-1.440660	1.234273	0.604117
O	0.264819	3.962233	3.433213
H	1.007377	4.083294	4.058000
H	-0.597803	3.865083	3.988099
N	1.793564	1.134643	2.638191
N	1.593821	3.019304	1.095493
N	1.166744	4.040533	0.353559
H	1.710158	4.718985	-0.221222
N	-1.803206	5.753655	-0.485072
H	-2.474295	5.203799	0.050958
H	-2.119265	6.561933	-1.024350
N	-0.246990	1.175380	4.116222
N	-1.412253	1.212382	4.772590
H	-1.897127	0.397493	5.242769
N	-4.242460	2.861654	5.990224
H	-5.093214	2.677139	6.524131
H	-4.018199	3.810387	5.685959
C	2.906002	1.378374	1.928773
C	4.065276	0.646522	2.137204
H	4.964474	0.855668	1.551464
C	4.061829	-0.340167	3.109329
H	4.961092	-0.933517	3.293752
C	2.924213	-0.546985	3.870730
H	2.921452	-1.291716	4.670215
C	1.795808	0.226086	3.620409
C	2.761015	2.469675	0.978194
C	3.806667	2.876916	0.032689
H	4.400831	2.012229	-0.298110
H	3.386259	3.357827	-0.864184
H	4.506991	3.592317	0.501817
C	-0.153453	4.237649	0.372613
C	-0.515058	5.446429	-0.461442
C	0.572947	0.201740	4.404299
C	0.307294	-0.796567	5.449327
H	-0.343190	-1.607632	5.070914
H	-0.201118	-0.344949	6.317584
H	1.230734	-1.269838	5.807750
C	-2.167800	2.307595	4.932594
C	-3.403184	1.880093	5.717313

Co^{2+} H_2dapsox Isomer VII LDA

Co	10.589658	6.513154	1.780188
O	8.970911	5.453987	3.425396
O	9.886035	2.588867	5.221468
O	10.818542	10.669993	3.518102
O	8.972923	7.775117	2.299476
O	11.303862	7.171163	3.536584
N	11.893209	6.003881	0.330584
N	11.130719	4.555251	2.168661
N	10.627299	3.923590	3.232476
N	8.122559	3.973589	5.703958
H	7.806352	3.433181	6.511478
H	7.613414	4.809589	5.418443
N	11.377148	8.293582	1.050060
N	11.121229	9.454462	1.655856
N	11.384857	8.750152	5.151287
H	11.296899	9.757391	5.336259
H	11.585234	8.078708	5.893232
C	12.342116	4.744688	0.245394
C	13.172736	4.351444	-0.793509

H	13.539932	3.324090	-0.855958
C	13.537574	5.292816	-1.744324
H	14.177755	5.005446	-2.582441
C	13.123773	6.605760	-1.605055
H	13.450936	7.369653	-2.314529
C	12.313895	6.941957	-0.524743
C	11.895291	3.905318	1.341541
C	12.261296	2.493652	1.517829
H	12.894067	2.359140	2.415222
H	12.823228	2.097478	0.663279
H	11.362798	1.865229	1.655721
C	9.554159	4.442061	3.832151
C	9.181826	3.570028	5.019394
C	11.964179	8.286558	-0.110879
C	12.354571	9.509144	-0.828169
H	12.849511	9.290742	-1.782114
H	11.478672	10.142924	-1.057892
H	13.053605	10.113514	-0.220677
C	11.005877	9.585885	3.010295
C	11.238187	8.362167	3.904959
O	9.078235	5.937684	0.373925
H	11.153103	10.341604	1.131160
H	10.966754	3.038972	3.672789
H	8.341081	7.850881	1.551914
H	8.574622	7.119425	2.927915
H	9.380291	5.662138	-0.517519
H	8.495422	5.217810	0.696700

Co^{2+} H_2dapsox Isomer VIII LDA

Co	11.237929	6.445542	2.117961
O	8.357807	3.023251	3.540957
O	9.161372	5.976148	1.787600
O	12.641418	10.712141	3.493175
O	10.053132	7.961843	3.075221
O	12.819520	7.191371	3.380442
N	12.179178	5.916927	0.371307
N	11.188104	4.290625	1.965134
N	10.429624	3.550916	2.818817
N	7.188095	5.004074	2.339931
H	6.615194	5.738516	1.921961
H	6.763190	4.197530	2.815270
N	11.899936	8.260083	1.143560
N	11.850790	9.453213	1.797114
N	13.755438	8.740689	4.749216
H	13.818140	9.749853	4.936862
H	14.230154	8.056661	5.339919
C	12.430998	4.631620	0.093298
C	13.079956	4.238856	-1.069177
H	13.272917	3.179888	-1.257941
C	13.453325	5.201425	-1.988200
H	13.955791	4.919798	-2.916938
C	13.181038	6.527299	-1.708692
H	13.468866	7.318236	-2.405923
C	12.556845	6.849538	-0.511807
C	11.863174	3.693077	1.037993
C	11.972661	2.240475	0.830017
H	11.685968	1.634707	1.701026
H	13.007500	1.967016	0.571365
H	11.333332	1.923685	-0.014003
C	9.082327	3.788402	2.947104
C	8.500409	5.045368	2.293194
C	12.379494	8.212124	-0.056061
C	12.834742	9.349180	-0.871211
H	13.930360	9.307658	-1.005269
H	12.387244	9.301209	-1.877561
H	12.598340	10.336256	-0.451559
C	12.489498	9.617412	3.002287
C	13.030561	8.375468	3.716457
O	10.824411	5.835415	4.143093
H	11.588394	6.342780	4.510642
H	11.016568	4.887055	4.317424
H	9.196812	7.508889	2.882961
H	10.030151	8.813045	2.583636
H	10.691584	2.570540	3.003827
H	11.783413	10.323529	1.248761

Co^{2+} H_2dapsox Isomer IX LDA

Co	10.573025	6.624502	2.091323
O	9.747840	5.810078	4.174532
O	9.544649	2.440023	5.105218
O	10.142400	11.198799	3.135824
O	9.093952	7.868500	2.790306
O	8.891327	6.286289	0.852215
O	12.094098	6.890848	3.489298
N	11.714820	6.120955	0.466127
N	10.849685	4.537245	2.164361
N	10.359282	3.863836	3.201673
N	8.741234	4.219037	6.310310
H	8.388103	3.652023	7.083085
H	8.631928	5.232373	6.323919
N	11.213536	8.469941	1.209330
N	11.065722	9.689386	1.755924
N	8.201374	9.648649	3.878351
H	8.345939	10.649369	4.071962
H	7.401840	9.135188	4.250225
C	11.943959	4.832215	0.188112
C	12.640673	4.445963	-0.947872
H	12.829323	3.388717	-1.149276
C	13.101951	5.425576	-1.810547
H	13.654256	5.151034	-2.712845
C	12.867611	6.754244	-1.513762
H	13.237920	7.540965	-2.174389
C	12.167402	7.071909	-0.354074
C	11.432751	3.913369	1.189919
C	11.599872	2.454592	1.112312
H	10.759233	1.910698	1.571923
H	12.524976	2.138264	1.629084
H	11.677076	2.113101	0.070702
C	9.818491	4.577890	4.194940
C	9.338876	3.633340	5.283567
C	11.907637	8.418889	0.108658
C	12.421881	9.620551	-0.569944
H	12.875723	9.385960	-1.539609
H	11.612580	10.350433	-0.749542
H	13.205945	10.124940	0.027247
C	10.162437	10.066247	2.696504
C	9.109314	9.067446	3.131704
H	11.658529	10.462740	1.417934
H	10.386736	2.836269	3.375110
H	12.940702	7.365585	3.380949
H	11.819914	6.957088	4.425431
H	8.535997	5.385165	0.715523
H	8.193864	6.796780	1.319969

Co^{2+} H_2dapsox Isomer X LDA

Co	10.653727	6.684085	2.115706
O	9.540863	3.304002	5.192593
O	8.928997	6.148887	3.234281
O	9.261732	11.159388	2.628404

O	10.460762	8.063625	3.751335
O	8.924222	6.831924	0.844683
O	12.379693	6.550917	3.381313
N	11.771006	6.198964	0.506048
N	10.917315	4.560538	2.229686
N	10.606854	3.798935	3.285460
N	7.866694	5.267616	5.038277
H	7.889899	4.474263	5.694308
H	7.148135	5.990285	5.087298
N	11.007220	8.533661	1.103343
N	10.379073	9.687087	1.363371
N	9.596533	9.860844	4.840215
H	9.232337	10.811527	4.687444
H	9.661218	9.449269	5.771598
C	12.115186	4.922114	0.293488
C	12.863635	4.555458	-0.818838
H	13.133782	3.511336	-0.990178
C	13.263519	5.536386	-1.707670
H	13.855108	5.273050	-2.588295
C	12.908338	6.852647	-1.476015
H	13.216463	7.638421	-2.168943
C	12.148677	7.155473	-0.352040
C	11.667020	4.005955	1.321563
C	12.072234	2.590459	1.372691
H	12.788538	2.402799	2.195812
H	12.568767	2.267263	0.450362
H	11.199906	1.930785	1.526186
C	9.696736	4.064061	4.258226
C	8.803791	5.281833	4.120249
C	11.659903	8.478283	-0.021875
C	11.820058	9.641433	-0.911954
H	12.544358	9.453279	-1.713175
H	10.866972	9.909152	-1.407851
H	12.170747	10.526262	-0.352137
C	9.825136	10.087305	2.537496
C	9.989783	9.216405	3.766895
H	13.257115	6.757861	3.000261
H	12.154746	7.287665	3.995930
H	8.257693	6.481703	1.480014
H	8.886149	6.255483	0.054536
H	11.108816	2.908749	3.425878
H	10.276601	10.381073	0.606853

Co^{2+} H_2dapsox Isomer XI LDA

Co	10.492253	6.593840	2.107090
O	8.883879	5.512210	3.637810
O	9.652665	2.495491	5.252794
O	9.899587	11.326360	2.864413
N	9.256459	8.043103	3.276891
O	8.699340	6.453922	1.042639
O	11.767728	6.718580	3.729163
N	11.724170	6.139202	0.549651
N	10.899165	4.551135	2.276529
N	10.397760	3.877773	3.313204
N	7.979659	3.936816	5.869759
H	7.665080	3.368042	6.658985
H	7.501758	4.811184	5.655301
N	10.991566	8.544987	1.056117
N	10.522324	9.774937	1.332379
O	10.897823	8.993663	4.535552
C	12.170354	4.878403	0.418148
C	13.031208	4.504098	-0.601716
H	13.386194	3.472974	-0.672721
C	13.435357	5.460773	-1.515492
H	14.113681	5.197250	-2.331121
C	12.978971	6.756253	-1.376920
H	13.298933	7.528550	-2.079197
C	12.125649	7.073706	-0.322972
C	11.689333	3.963714	1.434302
C	12.082911	2.549570	1.487839
H	11.366406	1.931507	2.048794
H	13.076406	2.433942	1.959214
H	12.158742	2.125200	0.475300
C	9.388558	4.428803	3.976919
C	8.994539	3.520434	5.130223
C	11.642984	8.413381	-0.061356
C	11.899131	9.551034	-0.963764
H	12.481985	9.268770	-1.847297
H	10.955344	9.990194	-1.337614
H	12.459525	10.349615	-0.442519
C	10.160498	10.183765	2.597817
C	10.125061	9.053404	3.597652
H	12.733631	6.687885	3.572993
H	11.595276	7.549972	4.278324
H	8.483856	8.262680	2.632964
H	8.992489	7.398733	4.040147
H	8.694220	6.219092	0.090974
H	8.176213	5.763569	1.507397
H	10.639519	10.532884	0.642617
H	10.718161	2.968614	3.717986

Co^{2+} H_2dapsox Isomer XII LDA

Co	10.687625	6.664914	2.148051
O	8.900153	3.232658	4.843933
O	8.197311	5.983204	4.460035
O	10.093598	11.281669	2.966278
N	9.024538	8.015452	2.860768
O	8.979116	6.095640	1.036079
O	12.559376	7.164480	3.021626
N	11.765231	6.132482	0.519650
N	10.948450	4.470743	2.301799
N	10.403688	3.650258	3.217264
N	10.453464	6.273752	4.329740
H	13.207859	6.441832	2.872393
H	11.335859	5.801657	4.556909
N	11.037406	8.526775	1.043059
N	10.688805	9.782720	1.385823
O	10.058081	8.950185	4.663163
C	12.158221	4.866875	0.370799
C	12.926745	4.470102	-0.715776
H	13.240961	3.429333	-0.813814
C	13.272595	5.412735	-1.663949
H	13.873833	5.128773	-2.529745
C	12.849021	6.719034	-1.508781
H	13.112181	7.480628	-2.243813
C	12.094656	7.052102	-0.392106
C	11.696981	3.937272	1.384976
C	12.063467	2.519803	1.271735
H	11.693903	1.874668	2.076882
H	13.162138	2.429147	1.258434
H	11.696990	2.112952	0.314988
C	9.517879	4.034099	4.162382
C	9.325525	5.516216	4.349968
C	11.645895	8.397626	-0.099157
C	11.897824	9.535114	-0.991448
H	12.358688	9.228159	-1.935320
H	10.953407	10.054295	-1.229671
H	12.572398	10.266381	-0.510935
C	10.195416	10.124215	2.598789
C	9.742991	8.986675	3.478442

H	12.940694	7.928658	2.536019
H	10.358273	7.231166	4.755328
H	8.558700	8.263464	1.980839
H	8.450937	7.403102	3.495710
H	9.028531	6.466998	0.127750
H	9.001795	5.123817	0.894774
H	10.539116	2.634926	3.110015
H	10.976034	10.558409	0.770306

Zn^{2+} dapsox Isomer I LDA

Zn	0.213910	2.234185	2.625168
O	-0.826252	4.526870	1.050284
O	0.663401	5.776270	-1.881675
O	-2.286155	2.711776	4.160594
O	-3.579203	0.512972	6.580111
O	-1.559794	2.120850	1.714969
H	-2.082552	2.289722	2.565838
H	-1.469164	3.040098	1.293497
O	-0.124922	3.988420	3.513478
H	-0.392216	4.437426	2.644561
H	-0.998618	3.666406	3.922692
N	1.847511	1.125659	2.753037
N	1.415874	2.967086	0.954819
N	1.192100	3.902283	0.026183
N	-1.285586	6.263783	-0.805132
H	-1.851170	6.017207	0.007863
H	-1.562037	6.968635	-1.482220
N	-0.226379	0.926762	4.318695
N	-1.294822	0.809957	5.113285
N	-4.324059	2.494605	5.732508
H	-5.183102	2.481707	6.274332
H	-4.095794	3.232299	5.065275
C	2.826298	1.344124	1.882350
C	4.007115	0.610814	1.968781
H	4.815442	0.787564	1.256030
C	4.123906	-0.330049	2.977536
H	5.042709	-0.915639	3.069784
C	3.087675	-0.532147	3.873293
H	3.167369	-1.264358	4.679245
C	1.929695	0.228668	3.729713
C	2.574707	2.371735	0.885450
C	3.596194	2.695941	-0.124311
H	3.895143	1.795404	-0.685713
H	3.182655	3.448596	-0.810715
H	4.504976	3.100373	0.353501
C	0.080149	4.588865	0.147171
C	-0.126437	5.602894	-0.970505
C	0.765357	0.124760	4.594723
C	0.733773	-0.835541	5.709412
H	1.181573	-1.799578	5.425278
H	-0.312178	-0.963198	6.026435
H	1.296545	-0.446113	6.575777
C	-2.242836	1.702374	4.948756
C	-3.447209	1.481985	5.853571

Zn^{2+} dapsox Isomer II LDA

Zn	0.219366	2.234445	2.646548
O	-0.828011	4.521758	1.074672
O	0.608529	5.771805	-1.880937
O	-2.290414	2.598768	4.055157
O	-4.463315	2.196869	5.650752
O	-1.498842	2.058651	1.654768
H	-2.061100	2.192570	2.487934
H	-1.439640	2.988461	1.255579
O	-0.157192	3.980311	3.525027
H	-0.410266	4.427687	2.647663
H	-1.040533	3.659410	3.903340
N	1.852076	1.127495	2.760323
N	1.422159	2.991718	0.976859
N	1.193393	3.923612	0.046333
N	-1.289674	6.299239	-0.733942
H	-1.839583	6.053219	0.090175
H	-1.580484	7.004491	-1.404552
N	-0.200664	0.912347	4.365910
N	-1.263434	0.821346	5.169651
N	-3.300507	0.599513	6.785455
H	-4.064584	0.408960	7.428265
H	-2.412703	0.094981	6.798974
C	2.825120	1.351449	1.882033
C	4.004671	0.613838	1.950689
H	4.805941	0.796752	1.231709
C	4.127034	-0.340042	2.945351
H	5.044705	-0.929417	3.022925
C	3.096763	-0.551466	3.845523
H	3.182279	-1.296015	4.639385
C	1.939792	0.214534	3.722262
C	2.572231	2.382512	0.890544
C	3.580098	2.691948	-0.137243
H	3.872394	1.783855	-0.689839
H	3.154602	3.433662	-0.828354
H	4.494416	3.106693	0.320466
C	0.074450	4.599944	0.171361
C	-0.150667	5.616566	-0.940544
C	0.787062	0.095779	4.600242
C	0.781193	-0.905083	5.682085
H	1.195780	-1.865825	5.341431
H	-0.250353	-1.045247	6.030829
H	1.387602	-0.564528	6.539486
C	-2.242980	1.688211	4.921159
C	-3.463125	1.526854	5.823493

Zn^{2+} dapsox Isomer III LDA

Zn	0.225266	2.239059	2.636902
O	-0.791549	4.497775	1.079222
O	-1.166902	6.333086	-0.898788
O	-2.295557	2.598700	4.037868
O	-4.469729	2.207691	5.639137
O	-1.487254	2.048332	1.645211
H	-2.053714	2.184380	2.476494
H	-1.441210	2.975513	1.242046
O	-0.147288	3.973949	3.529841
H	-0.397311	4.431391	2.657311
H	-1.035510	3.660750	3.901468
N	1.853283	1.124789	2.757475
N	1.461127	2.993029	0.960452
N	1.220135	3.925362	0.036370
N	0.771121	5.639101	-1.875123
H	1.550070	4.988233	-1.764857
H	0.684183	6.284130	-2.655956
N	-0.207291	0.917495	4.360763
N	-1.269178	0.830131	5.164291
N	-3.301195	0.624729	6.787839
H	-4.059719	0.448043	7.441110
H	-2.409975	0.126854	6.809795
C	2.835262	1.339146	1.886220
C	4.010371	0.594939	1.965884
H	4.818625	0.768702	1.252664

C	4.121964	-0.355916	2.964515
H	5.035737	-0.950241	3.050107
C	3.085189	-0.556743	3.858245
H	3.160496	-1.298178	4.655908
C	1.932521	0.214525	3.724664
C	2.601751	2.367348	0.887795
C	3.636848	2.648180	-0.123612
H	3.890328	1.739668	-0.694489
H	3.266053	3.419749	-0.809465
H	4.565290	3.007515	0.351407
C	0.078795	4.597242	0.178631
C	-0.180834	5.622488	-0.923491
C	0.778600	0.099341	4.598721
C	0.766984	-0.899742	5.682652
H	1.183275	-1.861589	5.347472
H	-0.267025	-1.039070	6.024512
H	1.366687	-0.556960	6.543896
C	-2.249590	1.696390	4.910411
C	-3.467562	1.543121	5.817416

Zn^{2+} dapsox Isomer V LDA

Zn	-2.006033	4.112801	11.087396
N	-2.858311	5.985501	10.961841
N	-2.720638	4.258136	9.100008
N	-2.559926	3.264928	8.230615
N	-1.245411	0.001957	8.670955
N	-1.767831	4.961340	13.064758
N	-1.240202	4.358224	14.125872
N	0.463666	1.304062	14.644059
O	-1.841740	2.063433	10.091692
O	-2.004111	0.986714	6.754958
O	-0.359479	2.743109	12.687222
O	-0.275019	2.808633	16.193858
O	0.019247	4.260869	10.756404
O	-3.537860	2.820811	11.800658
H	-3.114266	2.178764	11.148406
C	-3.373104	6.363332	9.797679
C	-3.945152	7.626100	9.668328
C	-3.961502	8.452485	10.782111
C	-3.421257	8.029146	11.985361
C	-2.858628	6.753548	12.043047
C	-3.288174	5.366697	8.735535
C	-3.801168	5.615598	7.378937
C	-2.076522	2.194807	8.844229
C	-1.778056	1.006289	7.951672
C	-2.244005	6.165786	13.223000
C	-2.192629	6.893409	14.502584
H	-3.189346	7.272215	14.782623
H	-1.516646	7.763699	14.443481
H	-1.819227	6.205843	15.276016
C	-0.613619	3.231884	13.833171
C	-0.133425	2.442201	15.040478
H	-4.406140	9.448902	10.709595
H	-4.366073	7.947644	8.712571
H	0.501643	1.137111	13.636668
H	-3.429880	8.669951	12.870233
H	0.825530	0.653749	15.334608
H	-3.564615	4.742885	6.752496
H	0.326856	5.133258	11.071346
H	-0.968284	-0.858831	8.208752
H	-1.097042	0.176871	9.666530
H	-4.893270	5.771730	7.384690
H	0.085543	3.625614	11.578009
H	-3.344922	6.519744	6.942555
H	-4.388635	3.086047	11.399369

Zn^{2+} dapsox Isomer VI LDA

Zn	0.163435	0.436583	-0.095663
O	2.153007	0.542661	0.393880
O	-2.141953	0.484951	-0.058161
O	-0.080239	2.118742	1.103304
O	-0.153716	4.141816	-1.759325
O	1.608129	0.107594	2.779422
O	-0.576272	-1.403976	5.070661
N	-0.231560	4.372169	0.819808
N	-0.027459	1.807485	-1.579145
N	0.027602	1.694946	-2.902665
N	0.016241	-1.013995	-1.597366
N	-0.002838	-1.304475	1.056978
N	-0.100776	-1.425088	2.372950
N	1.087891	0.139902	5.297371
C	-0.133577	3.128577	0.384463
C	-0.100859	3.083606	-1.139825
C	0.070677	0.540319	-3.495197
C	0.119973	0.637901	-4.982976
C	0.050676	-0.805162	-2.923048
C	0.049625	-1.903625	-3.796732
C	0.001968	-3.184499	-3.290334
C	-0.059451	-3.375494	-1.924560
C	-0.056952	-2.258345	-1.094049
C	-0.112722	-2.396325	0.349310
C	-0.265699	-3.707112	1.008393
C	0.636150	-0.632391	3.118262
C	0.296989	-0.693964	4.600595
H	-0.262063	4.589880	1.811767
H	-0.256014	5.071085	0.065727
H	0.135293	1.702310	-5.247153
H	1.018277	0.155276	-5.402187
H	-0.759189	0.169626	-5.457126
H	0.088400	-1.736020	-4.873416
H	0.011024	-4.043363	-3.967008
H	-0.096551	-4.377193	-1.492798
H	-0.739654	-3.532250	1.989807
H	-0.854450	-4.414237	0.408291
H	1.778020	0.668980	4.760321
H	0.971652	0.223579	6.302597
H	0.715541	-4.166979	1.221045
H	-2.456653	-0.440912	-0.075360
H	-2.214304	0.805649	-0.981658
H	2.678347	-0.188073	0.018180
H	1.997013	0.314164	1.420066

Zn^{2+} dapsox Isomer VII LDA

Zn	10.837735	6.660040	1.938337
O	8.539281	4.799170	3.094748
O	9.726768	2.567628	5.553775
O	10.569421	10.823405	3.323983
O	9.154975	7.277395	3.002009
O	11.857755	7.531205	3.466123
N	11.980731	6.053619	0.382158
N	11.078090	4.526238	2.253940
N	10.624567	3.782086	3.262985
N	7.708801	3.578877	5.225348
H	7.294939	3.179458	6.062497
H	7.211056	4.220438	4.606714
N	11.360501	8.463906	0.983954
N	11.108175	9.672296	1.443914
N	11.537893	9.196156	4.956917
H	11.149172	10.155002	4.994767

H	11.795538	8.618862	5.753488
C	12.293041	4.770426	0.269592
C	13.023132	4.322620	-0.826534
H	13.282895	3.267643	-0.933586
C	13.409875	5.261334	-1.774540
H	13.982152	4.940293	-2.649349
C	13.087184	6.596459	-1.622892
H	13.402407	7.340479	-2.357695
C	12.352083	6.982633	-0.497694
C	11.793575	3.925548	1.347372
C	12.061941	2.479419	1.401019
H	12.044390	2.167716	2.459043
H	13.021074	2.223266	0.929944
H	11.267001	1.903569	0.896031
C	9.412127	4.034328	3.662185
C	8.988649	3.300680	4.918958
C	12.003940	8.340724	-0.149053
C	12.448860	9.505695	-0.932255
H	12.482897	9.290251	-2.010237
H	11.765153	10.344805	-0.727245
H	13.454595	9.838381	-0.619151
C	10.977938	9.795044	2.767172
C	11.502291	8.697559	3.736958
O	8.997319	5.885592	0.779801
H	8.562823	7.607241	2.293194
H	8.802779	6.336605	3.201340
H	9.270364	5.319442	0.033014
H	8.781468	5.265472	1.561793

Zn^{2+} dapsox Isomer VIII LDA

Zn	11.269606	6.432886	2.079805
O	8.456429	3.286687	3.919274
O	9.022678	5.884399	1.613910
O	12.199870	10.635166	3.703971
O	9.904063	7.919849	2.767606
O	13.064721	7.239588	3.379019
N	12.224643	5.889968	0.295859
N	11.043086	4.243637	1.855289
N	10.393233	3.480324	2.737300
N	7.191176	5.041701	2.658489
H	6.561291	5.769201	2.330293
H	6.970445	4.312033	3.361149
N	12.086098	8.283478	1.188486
N	11.955068	9.486667	1.753108
N	13.488884	8.861555	4.910444
H	13.238068	9.854767	5.072590
H	13.932719	8.237328	5.578728
C	12.343658	4.601276	-0.012238
C	12.983382	4.205418	-1.184926
H	13.077029	3.143697	-1.423690
C	13.469413	5.183473	-2.033794
H	13.966954	4.900875	-2.965701
C	13.324062	6.519352	-1.704625
H	13.702656	7.312063	-2.353678
C	12.695598	6.842911	-0.504033
C	11.709524	3.673968	0.903379
C	11.758162	2.215261	0.698319
H	11.371099	1.726076	1.605054
H	12.784333	1.874122	0.488853
H	11.125121	1.906070	-0.151025
C	9.160321	3.854819	3.068908
C	8.473831	5.035182	2.344552
C	12.571698	8.199243	-0.008220
C	13.046389	9.359757	-0.783021
H	14.148616	9.392766	-0.824814
H	12.676537	9.326823	-1.820234
H	12.696770	10.275874	-0.283420
C	12.323830	9.602203	3.026469
C	13.005870	8.425855	3.761273
O	11.183614	5.759270	4.102463
H	12.114204	6.066204	4.262729
H	11.166018	4.769894	4.062040
H	9.164592	7.505440	2.250011
H	10.178516	8.763347	2.326799

Zn^{2+} dapsox Isomer IX LDA

Zn	10.699351	6.752765	2.079738
O	10.366731	5.374402	4.946868
O	8.654581	2.314570	4.901478
O	9.847575	11.195753	2.931455
O	9.118648	7.737839	2.910004
O	8.885316	6.415836	0.680945
O	11.722584	7.055037	3.781957
N	11.806600	6.179392	0.514232
N	10.779663	4.599391	2.321219
N	10.199229	3.806031	3.213616
N	8.902660	3.936609	6.486405
H	8.342746	3.445614	7.176524
H	9.350991	4.837795	6.659914
N	11.114424	8.615513	1.068207
N	10.832308	9.863055	1.410342
N	8.508425	9.516819	4.141956
H	8.684077	10.539299	4.195258
H	7.900040	8.960304	4.738420
C	12.000470	4.877514	0.336450
C	12.695245	4.428241	-0.785361
H	12.874004	3.361569	-0.935681
C	13.137985	5.371365	-1.699297
H	13.681130	5.046611	-2.591285
C	12.889580	6.719006	-1.504970
H	13.218964	7.462912	-2.232875
C	12.197008	7.108745	-0.356490
C	11.440781	4.011854	1.357845
C	11.596697	2.548801	1.281470
H	10.886581	2.090169	1.987602
H	12.615680	2.236933	1.570240
H	11.414958	2.181618	0.258978
C	9.961045	4.294020	4.407200
C	9.101434	3.385364	5.274901
C	11.837764	8.469433	-0.017324
C	12.277672	9.629079	-0.811753
H	13.133979	9.391833	-1.456863
H	11.458873	10.020819	-1.439742
H	12.528547	10.448365	-0.118144
C	10.036800	10.061988	2.463101
C	9.205022	8.961607	3.175457
H	12.655891	6.780155	3.710825
H	11.201843	6.285441	4.332695
H	9.122700	7.000677	-0.066768
H	8.438245	7.011908	1.328732

Zn^{2+} dapsox Isomer X LDA

Zn	10.714799	6.881611	2.044982
O	10.045003	4.175241	5.628148
O	8.106001	4.832629	2.764240
O	9.994622	11.291165	3.019472
O	9.842318	7.795753	3.530691
O	8.858509	6.589221	1.133115
O	12.424478	6.696329	3.490967

N	11.752745	6.263098	0.444885
N	10.909655	4.714571	2.341775
N	10.887269	4.116414	3.527269
N	7.693795	4.755452	4.991735
H	8.195838	4.544843	5.871127
H	6.695723	4.918986	4.892334
N	11.183964	8.715893	1.099597
N	10.894484	9.951572	1.467201
N	9.248279	9.631927	4.669031
H	9.262680	10.665210	4.571764
H	8.882284	9.087182	5.445999
C	11.942621	4.958786	0.257765
C	12.554305	4.520676	-0.918437
H	12.716932	3.455629	-1.096513
C	12.952218	5.473930	-1.842721
H	13.447438	5.155054	-2.764299
C	12.734935	6.824054	-1.618271
H	13.054129	7.580809	-2.338264
C	12.099944	7.200923	-0.433951
C	11.553661	4.115022	1.369840
C	11.982567	2.708941	1.471241
H	12.112812	2.473462	2.541874
H	12.913615	2.515127	0.919088
H	11.205845	2.023183	1.090367
C	9.915705	4.347528	4.405144
C	8.487235	4.690637	3.933510
C	11.791358	8.562807	-0.054935
C	12.146326	9.692672	-0.932236
H	13.235527	9.743191	-1.099756
H	11.666085	9.598600	-1.920783
H	11.809452	10.621547	-0.449415
C	10.262275	10.144098	2.626862
C	9.783640	9.041077	3.620362
H	12.168378	5.826527	3.891514
H	13.195988	6.486337	2.928029
H	8.527960	5.821518	1.728566
H	9.005294	6.196574	0.250957

Zn^{2+} dapsox Isomer XI LDA

Zn	10.778475	6.802951	2.117796
O	10.182702	5.419657	4.781844
O	8.363573	2.414504	4.746884
O	9.066628	10.969449	2.516712
N	9.309904	7.746216	3.295095
O	8.802786	6.312486	0.910514
O	12.014749	6.739591	3.723078
N	11.829967	6.183360	0.534906
N	10.715763	4.581261	2.252715
N	10.068833	3.791306	3.112069
N	8.689439	4.006803	6.347954
H	8.101753	3.539055	7.032028
H	9.178376	4.882376	6.540148
N	11.041835	8.620319	1.037894
N	10.519979	9.815315	1.218163
O	10.403934	9.294151	4.560754
C	12.085160	4.887560	0.375037
C	12.868547	4.455538	-0.687832
H	13.087996	3.395065	-0.824799
C	13.350889	5.416933	-1.569151
H	13.972344	5.109909	-2.415030
C	13.048125	6.751723	-1.398675
H	13.420634	7.502339	-2.097851
C	12.250488	7.132834	-0.309724
C	11.473957	4.003830	1.359059
C	11.689953	2.547215	1.331766
H	10.897724	2.069307	1.929789
H	12.657803	2.279937	1.790568
H	11.692683	2.156046	0.303379
C	9.777331	4.316901	4.277782
C	8.864473	3.455974	5.134633
C	11.802415	8.469974	-0.030480
C	12.098786	9.623408	-0.896801
H	12.728920	9.360654	-1.755596
H	11.156504	10.075669	-1.250885
H	12.588035	10.418719	-0.310158
C	9.783119	9.990845	2.346506
C	9.866683	9.017465	3.516774
H	12.825161	6.227102	3.542944
H	11.357546	6.112644	4.256827
H	8.498957	7.705232	2.663718
H	9.217392	7.176156	4.155751
H	9.060180	6.511212	-0.012564
H	8.933873	5.344607	1.016822

Zn^{2+} dapsox Isomer XII LDA

Zn	10.832617	6.631984	2.154536
O	9.105075	3.291913	5.021141
O	8.163367	5.887848	4.260605
O	9.814752	11.322970	2.816064
N	8.504808	8.368062	3.040218
O	8.937740	6.232810	1.259635
O	12.774402	7.091223	3.097995
N	11.818941	6.082987	0.522317
N	10.922514	4.361313	2.292031
N	10.426034	3.506242	3.201706
N	10.386141	6.347924	4.217908
H	13.444865	6.516947	2.667779
H	11.288596	5.945537	4.500061
N	11.063177	8.557213	1.143984
N	10.769534	9.846850	1.405626
O	10.099491	8.939786	4.542274
C	12.111724	4.799563	0.322525
C	12.819095	4.417020	-0.812796
H	13.069120	3.367841	-0.981552
C	13.186835	5.397592	-1.717717
H	13.741454	5.124915	-2.618690
C	12.850889	6.722007	-1.495088
H	13.133823	7.490935	-2.214366
C	12.147959	7.046626	-0.336462
C	11.634770	3.856794	1.323612
C	11.936242	2.423367	1.173969
H	11.489725	1.862250	2.003737
H	13.025213	2.251844	1.156991
H	11.539990	2.038441	0.219453
C	9.644454	4.009440	4.154462
C	9.325074	5.486922	4.237389
C	11.733607	8.392982	0.025704
C	12.064159	9.542899	-0.830712
H	12.608345	9.252130	-1.735144
H	11.142654	10.077091	-1.114352
H	12.662484	10.274620	-0.262880
C	10.060571	10.141525	2.490490
C	9.538679	9.090165	3.432055
H	13.018278	7.999187	2.815122
H	10.221897	7.334337	4.595283
H	8.131199	8.477437	2.096405
H	8.164916	7.563456	3.616315
H	8.950393	6.611927	0.353602
H	8.956578	5.259870	1.115881

Zn^{2+} Hdapsox Isomer I LDA

Zn	0.123093	2.197935	2.741636
O	-1.022999	4.559984	0.867781
O	1.047986	5.767234	-1.683234
O	-2.347203	2.581243	4.110219
O	-3.421826	0.522437	6.751948
O	-1.569389	2.027872	1.707313
H	-2.131355	2.162101	2.551706
H	-1.592468	2.909898	1.245259
O	-0.315032	3.992474	3.480603
H	-0.619201	4.474756	2.667857
H	-1.177136	3.623701	3.904708
N	1.822728	1.176972	2.727297
N	1.397572	3.040342	0.982077
N	1.102992	4.021332	0.129222
H	1.732862	4.382862	-0.627813
N	-1.093116	6.409912	-1.159774
H	-1.868947	6.232910	-0.519679
H	-1.168463	7.110797	-1.896356
N	-0.209148	0.925347	4.360803
N	-1.253210	0.804782	5.178724
N	-4.364551	2.355589	5.776509
H	-5.195087	2.320255	6.362842
H	-4.241832	3.064396	5.055558
C	2.793385	1.389592	1.846249
C	3.965914	0.651149	1.887713
H	4.765521	0.828573	1.165679
C	4.099342	-0.315881	2.874621
H	5.013419	-0.912500	2.933512
C	3.079565	-0.522428	3.780287
H	3.161184	-1.276358	4.566625
C	1.923878	0.253968	3.684346
C	2.538400	2.442207	0.860948
C	3.565989	2.740491	-0.153761
H	3.915102	1.808159	-0.625080
H	3.227688	3.403630	-0.961493
H	4.444766	3.210874	0.321176
C	-0.047764	4.693718	0.118300
C	0.017496	5.704054	-1.019522
C	0.793717	0.118761	4.585792
C	0.808906	-0.872344	5.669803
H	1.016070	-1.883142	5.281125
H	-0.166748	-0.859183	6.175669
H	1.596760	-0.636349	6.406124
C	-2.245420	1.643047	4.983519
C	-3.405182	1.431746	5.944871

Zn^{2+} Hdapsox Isomer II LDA

Zn	0.110769	2.164017	2.777014
O	-1.063636	4.491651	0.844822
O	1.044541	5.855972	-1.590369
O	-2.242582	2.516991	4.064478
O	-4.418851	2.186864	5.636945
O	-1.525296	1.948495	1.665362
H	-2.128067	2.073844	2.473138
H	-1.548618	2.833749	1.204746
O	-0.275445	3.994392	3.460105
H	-0.595743	4.456352	2.641601
H	-1.134030	3.647055	3.897130
N	1.831037	1.165970	2.737073
N	1.354457	3.011078	0.982068
N	1.077849	4.001076	0.131309
H	1.732100	4.383328	-0.592337
N	-1.107290	6.458789	-1.061599
H	-1.891739	6.243486	-0.443779
H	-1.169043	7.212038	-1.745936
N	-0.159556	0.901080	4.430448
N	-1.206346	0.803152	5.247159
N	-3.313288	0.585556	6.825494
H	-4.093275	0.426058	7.459548
H	-2.440750	0.063030	6.892914
C	2.778930	1.370181	1.824278
C	3.946713	0.622353	1.839005
H	4.727677	0.780199	1.093833
C	4.104593	-0.338742	2.827478
H	5.015928	-0.941444	2.860588
C	3.115174	-0.529349	3.767708
H	3.220278	-1.276431	4.557610
C	1.959453	0.249940	3.698279
C	2.499774	2.423130	0.847094
C	3.461758	2.799218	-0.205706
H	4.353209	2.163397	-0.215355
H	2.993491	2.731297	-1.203894
H	3.801239	3.842211	-0.071666
C	-0.076283	4.672918	0.122915
C	0.003504	5.747101	-0.950437
C	0.860776	0.116906	4.638760
C	0.934580	-0.863831	5.732496
H	1.039270	-1.889208	5.339456
H	0.018848	-0.804862	6.332946
H	1.804318	-0.669979	6.382334
C	-2.203976	1.640571	4.971993
C	-3.439008	1.502498	5.852111

Zn^{2+} Hdapsox Isomer III LDA

Zn	0.113206	2.162425	2.811668
O	-0.897507	4.540159	0.950941
O	-0.399252	6.894851	-0.576831
O	-2.224536	2.508121	4.029892
O	-4.452504	2.170028	5.530821
O	-1.478212	2.011231	1.632156
H	-2.108946	2.108652	2.420698
H	-1.468357	2.923754	1.225991
O	-0.202224	3.987937	3.527444
H	-0.465511	4.493720	2.712868
H	-1.085271	3.686331	3.932303
N	1.847004	1.175026	2.764970
N	1.392566	2.993515	0.954742
N	1.106838	3.930404	0.037258
H	1.801196	4.178934	-0.683063
N	0.305598	5.436787	-2.191727
H	0.157188	4.481070	-2.519762
H	0.207634	6.171326	-2.898711
N	-0.171143	0.879602	4.426633
N	-1.236784	0.769025	5.213704
N	-3.394886	0.538697	6.721946
H	-4.194666	0.375617	7.329947
H	-2.528194	0.009417	6.808348
C	2.813489	1.383634	1.871930
C	3.993048	0.655723	1.922506
H	4.790099	0.818625	1.195966
C	4.144965	-0.295343	2.921283
H	5.065288	-0.882154	2.980614
C	3.135306	-0.497171	3.835777
H	3.229803	-1.240306	4.630675
C	1.969563	0.264035	3.734583
C	2.540563	2.406799	0.860707
C	3.517768	2.745330	-0.194669
H	4.441635	2.162230	-0.123113

H	3.094985	2.557686	-1.198408
H	3.803289	3.811748	-0.137863
C	-0.027127	4.673592	0.097035
C	-0.092755	5.785577	-0.941960
C	0.855098	0.108028	4.651122
C	0.917685	-0.878604	5.740277
H	1.045075	-1.900326	5.344496
H	-0.012779	-0.834270	6.319185
H	1.768665	-0.676814	6.412174
C	-2.223157	1.618518	4.921960
C	-3.484737	1.474415	5.762378

Zn^{2+} Hdapsox Isomer V LDA

Zn	0.090221	2.227545	2.729117
O	-1.201677	3.977718	-0.005105
O	1.240319	6.023827	-1.430587
O	-1.978017	3.036320	5.054254
O	-3.712691	0.222303	6.190940
O	-1.488128	2.043255	1.587781
H	-1.717942	1.186643	1.181994
H	-1.417681	2.773830	0.863099
O	-0.271991	3.903637	3.584436
H	0.457873	4.332586	4.068567
H	-1.041696	3.512105	4.341163
N	1.795259	1.204828	2.744900
N	1.352397	2.997057	0.924017
N	1.117249	4.019417	0.094243
H	1.853560	4.616364	-0.354403
N	-1.043510	6.168183	-1.614062
H	-1.918279	5.735227	-1.312412
H	-1.042102	6.979930	-2.230342
N	-0.267959	0.936628	4.329908
N	-1.336925	0.781847	5.086365
N	-4.176404	2.452799	6.328928
H	-5.073843	2.308000	6.784818
H	-3.843417	3.381891	6.075278
C	2.783710	1.425304	1.880385
C	3.963481	0.702325	1.950609
H	4.779144	0.883925	1.248977
C	4.088864	-0.256935	2.947257
H	5.011065	-0.837677	3.031190
C	3.054861	-0.474886	3.830243
H	3.143264	-1.216585	4.626358
C	1.883294	0.278120	3.707358
C	2.538441	2.476100	0.893953
C	3.589535	2.898366	-0.050566
H	4.293136	2.082645	-0.260823
H	3.164194	3.225722	-1.012374
H	4.180374	3.736728	0.361451
C	-0.093798	4.443900	-0.276348
C	0.096548	5.652769	-1.183118
C	0.743997	0.142684	4.585685
C	0.689078	-0.815440	5.697285
H	-0.347340	-1.189546	5.772220
H	0.885642	-0.315075	6.661682
H	1.395578	-1.647324	5.584684
C	-2.143055	1.795587	5.297001
C	-3.430711	1.389968	5.994227

Zn^{2+} Hdapsox Isomer VI LDA

Zn	0.001001	0.418435	-0.144166
O	1.963322	0.932578	0.338633
O	-2.168812	0.247316	-0.013199
O	-0.427226	2.068545	0.924877
O	0.299624	4.176250	-1.782109
O	1.424007	0.586747	2.851399
O	-0.320171	-1.761987	4.730347
N	-0.217563	4.335921	0.891861
N	0.065990	1.854653	-1.657028
N	0.244742	1.615827	-2.855784
N	0.017949	-1.012471	-1.564739
N	0.085245	-1.217579	1.067525
N	0.157241	-1.302033	2.360093
N	1.112951	-0.162556	5.542779
C	-0.194931	3.152546	0.318766
C	0.094698	3.173858	-1.123309
C	0.206023	0.418362	-3.526153
C	0.286515	0.572182	-4.984288
C	0.084512	-0.852658	-2.907489
C	0.013990	-1.984282	-3.768593
C	-0.175078	-3.244090	-3.237376
C	-0.269511	-3.398732	-1.876127
C	-0.144761	-2.267476	-1.028168
C	-0.149550	-2.393514	0.370299
C	-0.336339	-3.644072	1.111821
C	0.758303	-0.394841	3.187079
C	0.482480	-0.826273	4.596263
H	-0.407871	4.437701	1.888951
H	-0.026634	5.157359	0.310203
H	0.371346	1.632595	-5.252978
H	1.159946	0.035769	-5.401101
H	-0.602926	0.151531	-5.489493
H	0.095397	-1.843187	-4.846408
H	-0.245731	-4.111616	-3.899164
H	-0.421286	-4.387404	-1.441897
H	-1.269458	-3.629443	1.709822
H	-0.395158	-4.520881	0.458788
H	1.765978	0.579791	5.283338
H	0.971412	-0.403159	6.525873
H	0.497629	-3.822246	1.817389
H	-0.236348	-2.092334	2.942314
H	-2.801340	-0.029143	-0.706003
H	-2.569567	1.005205	0.459683
H	2.744722	0.429522	0.034580
H	1.911481	0.854088	1.348368

Zn^{2+} Hdapsox Isomer VII LDA

Zn	10.726647	6.529258	1.855948
O	8.632356	4.976559	3.140143
O	9.896311	2.841226	5.633340
O	10.773365	10.805815	3.426180
O	9.042338	7.469161	2.683041
O	11.594984	7.364812	3.520018
N	11.963556	6.058825	0.313569
N	11.076873	4.510031	2.178729
N	10.628379	3.794459	3.199027
N	7.858021	3.838970	5.385168
H	7.491546	3.465365	6.257238
H	7.289374	4.410691	4.762455
N	11.450186	8.417533	1.010959
N	11.174544	9.585509	1.589213
N	11.344087	8.945159	5.113735
H	11.121206	9.933953	5.273341
H	11.528311	8.289391	5.872551
C	12.314535	4.779542	0.220481
C	13.108456	4.364540	-0.850650
H	13.395653	3.315794	-0.953432
C	13.519479	5.307293	-1.773183
H	14.138417	5.002857	-2.621321

C	13.167549	6.643523	-1.623836
H	13.515851	7.393644	-2.336754
C	12.380923	6.988414	-0.535241
C	11.814982	3.916285	1.279565
C	12.113333	2.479835	1.350278
H	12.142760	2.186957	2.413748
H	13.058894	2.223650	0.853036
H	11.308775	1.877825	0.892319
C	9.471492	4.164663	3.684557
C	9.108660	3.525783	5.008409
C	12.026466	8.358462	-0.141725
C	12.398991	9.553350	-0.918659
H	12.917555	9.301995	-1.851316
H	11.506205	10.144099	-1.191558
H	13.063549	10.209252	-0.327848
C	11.034884	9.723175	2.939254
C	11.338892	8.528092	3.864278
O	8.936619	5.792386	0.736314
H	11.164305	10.468064	1.055695
H	8.432558	7.528424	1.913495
H	8.754427	6.594628	3.121951
H	9.051539	5.157667	0.002787
H	8.719034	5.252769	1.586003

Zn^{2+} Hdapsox Isomer VIII LDA

Zn	11.279373	6.531771	2.090007
O	8.325591	3.035670	3.665115
O	9.042820	5.960194	1.818159
O	12.343354	10.683250	3.615634
O	9.972875	7.995041	2.954125
O	12.837478	7.218726	3.467164
N	12.234714	5.855447	0.342350
N	10.988223	4.125173	1.735901
N	10.237212	3.359490	2.531563
N	7.176198	5.180191	2.844768
H	6.602064	5.979040	2.580215
H	6.810721	4.396196	3.397629
N	12.017273	8.291410	1.168662
N	11.911513	9.501892	1.718994
N	13.727808	8.878676	4.717151
H	13.642391	9.900699	4.852549
H	14.208184	8.246371	5.354625
C	12.455065	4.576405	0.040314
C	13.139446	4.201109	-1.105164
H	13.309431	3.146198	-1.329807
C	13.562673	5.192165	-1.977569
H	14.087554	4.927486	-2.899109
C	13.313166	6.511573	-1.672232
H	13.639350	7.319659	-2.330812
C	12.653730	6.821404	-0.481549
C	11.833278	3.595745	0.926255
C	12.083070	2.147713	0.777657
H	11.959675	1.597340	1.724131
H	13.105756	1.952489	0.427232
H	11.385882	1.704839	0.044394
C	9.010222	3.758549	2.965961
C	8.441978	5.101868	2.477408
C	12.481571	8.187930	-0.036017
C	12.916565	9.339694	-0.841140
H	14.017118	9.413017	-0.878666
H	12.551673	9.269300	-1.877663
H	12.536439	10.257514	-0.368434
C	12.361486	9.631712	2.970415
C	13.009804	8.440424	3.709445
O	10.964896	5.662956	4.062059
H	11.659948	6.306137	4.376987
H	11.364323	4.781476	4.205243
H	9.157047	7.657924	2.514459
H	10.227179	8.851833	2.519548
H	10.435305	2.354020	2.663084

Zn^{2+} Hdapsox Isomer IX LDA

Zn	10.563275	6.658158	2.017780
O	10.232553	5.518014	4.826265
O	8.841943	2.310009	4.953773
O	10.006980	11.226905	3.001763
O	9.053399	7.838687	2.821675
O	8.783751	6.197901	0.864651
O	11.579527	7.189298	3.669319
N	11.756815	6.188935	0.461790
N	10.792547	4.589878	2.298602
N	10.282464	3.805486	3.229488
N	8.909562	4.007103	6.476607
H	8.413431	3.477756	7.188976
H	9.279509	4.940669	6.650285
N	11.114327	8.596292	1.014683
N	10.850331	9.810684	1.495304
N	8.545241	9.521705	4.239201
H	8.710090	10.516620	4.433401
H	7.911059	8.944126	4.790155
C	11.983275	4.884064	0.305243
C	12.734680	4.446849	-0.790684
H	12.933785	3.381129	-0.925317
C	13.218351	5.382458	-1.680611
H	13.802882	5.058622	-2.545779
C	12.975485	6.737031	-1.481841
H	13.367457	7.478999	-2.180019
C	12.226088	7.107312	-0.375672
C	11.453240	4.006927	1.326302
C	11.658411	2.551354	1.269893
H	10.988412	2.078473	2.004560
H	12.694926	2.278205	1.534124
H	11.457847	2.155550	0.261729
C	9.958981	4.358890	4.380586
C	9.177339	3.428229	5.294471
C	11.911969	8.487821	0.002182
C	12.507648	9.655076	-0.675389
H	13.083919	9.370709	-1.563281
H	11.732059	10.372939	-0.995384
H	13.202471	10.188716	-0.000040
C	10.068394	10.088139	2.573016
C	9.195544	9.006383	3.219123
H	12.525512	6.947436	3.664429
H	11.061137	6.419069	4.247451
H	8.774910	6.251411	-0.110409
H	8.137600	6.853967	1.200376
H	11.350963	10.636071	1.129789

Zn^{2+} Hdapsox Isomer X LDA

Zn	10.745416	6.942553	2.012906
O	9.903120	3.412868	5.418808
O	8.035256	5.237213	3.101085
O	9.744625	11.286606	2.816857
O	10.114415	7.865758	3.645327
O	8.859561	6.745791	1.286958
O	12.475748	6.726067	3.385665
N	11.794615	6.244978	0.469413
N	10.840386	4.591452	2.270121
N	10.615160	3.816683	3.344732

N	7.854341	4.978849	5.344013
H	8.252735	4.462429	6.135933
H	6.924054	5.392388	5.376150
N	11.171592	8.725635	1.055215
N	10.829484	9.955810	1.377687
N	9.130609	9.669886	4.554299
H	8.999326	10.685534	4.362812
H	8.812693	9.158461	5.375407
C	12.040517	4.952880	0.280274
C	12.677243	4.520235	-0.874878
H	12.873770	3.461975	-1.054002
C	13.047929	5.474513	-1.815309
H	13.550767	5.161203	-2.734087
C	12.790153	6.810500	-1.595356
H	13.088556	7.572890	-2.318650
C	12.137476	7.187247	-0.416502
C	11.622464	4.073160	1.370924
C	12.125972	2.688400	1.469525
H	12.797796	2.570756	2.342284
H	12.714191	2.395624	0.592656
H	11.295489	1.971828	1.592611
C	9.744241	4.015242	4.369511
C	8.473182	4.844130	4.180804
C	11.811072	8.552655	-0.081792
C	12.154264	9.662114	-0.986576
H	13.244834	9.745952	-1.128651
H	11.703303	9.520522	-1.983115
H	11.777006	10.597723	-0.550318
C	10.148193	10.159473	2.511051
C	9.802886	9.088682	3.593617
H	13.281048	7.163735	3.043822
H	12.105235	7.335300	4.062464
H	8.458968	6.052657	1.914655
H	8.806776	6.390806	0.378859
H	11.292226	3.068357	3.558811

Zn^{2+} Hdapsox Isomer XI LDA

Zn	10.760012	6.672805	2.119235
O	10.171265	5.521965	4.719665
O	8.278085	2.580250	4.634359
O	9.295040	11.108921	2.633203
N	9.277298	7.713913	3.240122
O	8.759190	6.159867	1.014740
O	11.977184	6.901996	3.711265
N	11.830627	6.191734	0.497915
N	10.812873	4.579786	2.270040
N	10.158974	3.810788	3.133015
N	8.660143	4.075816	6.317350
H	8.036555	3.607154	6.970571
H	9.181124	4.911115	6.581310
N	11.048798	8.585516	1.004569
N	10.525556	9.767824	1.320331
O	10.257145	9.229380	4.644473
C	12.126025	4.898817	0.364992
C	12.920319	4.481657	-0.703069
H	13.174195	3.425533	-0.819575
C	13.365042	5.429412	-1.604460
H	13.985461	5.124860	-2.451511
C	13.023625	6.766497	-1.448832
H	13.368733	7.512993	-2.166500
C	12.237748	7.120328	-0.360827
C	11.557037	4.005406	1.360687
C	11.781364	2.553017	1.317685
H	11.061420	2.065643	1.993065
H	12.797433	2.296760	1.665771
H	11.673804	2.154027	0.296976
C	9.801882	4.387649	4.262820
C	8.831558	3.563944	5.089442
C	11.770279	8.476439	-0.066027
C	12.077587	9.632679	-0.927871
H	12.749489	9.374050	-1.754169
H	11.158774	10.055274	-1.375041
H	12.563106	10.435408	-0.343652
C	9.808008	10.028319	2.472497
C	9.790176	8.966193	3.570353
H	12.883206	6.542657	3.665536
H	11.379742	6.246888	4.271945
H	8.478763	7.684505	2.589751
H	9.182982	7.088378	4.068968
H	8.757413	6.167668	0.036406
H	8.618442	5.220219	1.265244
H	10.630915	10.577874	0.690407

Zn^{2+} Hdapsox Isomer XII LDA

Zn	10.827363	6.703960	2.136168
O	8.956852	3.222018	4.887501
O	8.150686	5.898878	4.384046
O	9.817577	11.319666	2.808677
N	8.503960	8.410954	3.122976
O	8.943797	6.216987	1.352537
O	12.738286	7.041155	3.126086
N	11.822923	6.069347	0.529519
N	10.949038	4.347246	2.264693
N	10.416427	3.556107	3.203666
N	10.382295	6.299864	4.197228
H	13.435183	6.583268	2.606496
H	11.285648	5.868483	4.433561
N	11.049565	8.559505	1.125799
N	10.751072	9.846450	1.379490
O	10.246858	8.878640	4.493061
C	12.153157	4.795910	0.331465
C	12.876495	4.417953	-0.788467
H	13.152960	3.374110	-0.947155
C	13.230556	5.400453	-1.699567
H	13.802103	5.135255	-2.591699
C	12.856261	6.712690	-1.489021
H	13.127338	7.484749	-2.209451
C	12.133931	7.032832	-0.339400
C	11.684259	3.835963	1.334159
C	12.041737	2.417901	1.187989
H	11.700807	1.779772	2.012234
H	13.136552	2.314073	1.119403
H	11.622053	2.016337	0.250986
C	9.541734	3.991630	4.141137
C	9.293382	5.487144	4.259064
C	11.694469	8.377800	-0.005002
C	11.975815	9.513475	-0.895704
H	12.436004	9.206010	-1.840188
H	11.042928	10.062429	-1.101281
H	12.635859	10.237632	-0.388983
C	10.070345	10.141819	2.483301
C	9.594375	9.085003	3.443994
H	12.978279	7.991404	3.073658
H	10.272158	7.297560	4.582981
H	8.013344	8.609411	2.250361
H	8.149831	7.642263	3.729101
H	8.750633	6.771589	0.565849
H	9.018622	5.303735	0.995656
H	10.550692	2.535297	3.153212

Zn^{2+} H_2dapsox Isomer I LDA

Zn	0.167865	2.279327	2.631511
O	-0.956386	4.590609	0.894157
O	1.084063	5.588812	-1.770330
O	-2.501902	2.665789	4.155436
O	-3.067874	0.437960	6.795495
O	-1.565834	2.100697	1.687089
H	-2.190183	2.225810	2.459475
H	-1.580553	2.982124	1.208961
O	-0.292297	4.028188	3.452048
H	-0.556924	4.536855	2.632231
H	-1.159591	3.779157	3.887480
N	1.793926	1.153691	2.743416
N	1.416352	3.008098	0.966535
N	1.116678	3.962666	0.088389
N	-0.972695	6.441310	-1.207946
H	-1.746838	6.372877	-0.546470
H	-1.004314	7.123937	-1.967501
N	-0.234683	0.952989	4.345259
N	-1.320357	0.926835	5.116053
N	-4.463104	2.113034	6.069547
H	-5.200414	1.929901	6.753070
H	-4.569354	2.866465	5.388515
C	2.786987	1.365446	1.883229
C	3.962274	0.629125	1.964513
H	4.777547	0.804039	1.258175
C	4.080487	-0.324422	2.959655
H	4.998964	-0.911679	3.051110
C	3.032229	-0.534913	3.838381
H	3.110826	-1.283324	4.630463
C	1.881487	0.231356	3.700089
C	2.557719	2.403382	0.873240
C	3.601091	2.672499	-0.128463
H	3.855425	1.746519	-0.672336
H	3.333508	3.429333	-0.876921
H	4.525690	3.013458	0.370207
C	-0.009078	4.676300	0.097633
C	0.071998	5.645653	-1.076704
C	0.713895	0.101012	4.576893
C	0.695484	-0.922064	5.633758
H	1.154472	-1.857940	5.281336
H	-0.314485	-1.172936	5.987807
H	1.281864	-0.581870	6.507854
C	-2.357225	1.754568	4.984445
C	-3.368662	1.375629	6.060937
H	-1.514255	0.272313	5.926507
H	1.709752	4.290650	-0.727043

Zn^{2+} H_2dapsox Isomer II LDA

Zn	0.204031	2.294498	2.700075
O	-0.918946	4.673257	1.017525
O	1.004937	5.558422	-1.768584
O	-2.263792	2.675783	4.272494
O	-4.492281	1.163697	5.213660
O	-1.523456	2.165587	1.739276
H	-2.178337	2.234280	2.486514
H	-1.541376	3.073010	1.311195
O	-0.142614	4.047240	3.546435
H	-0.432380	4.578025	2.750415
H	-0.996494	3.799803	4.010412
N	1.818571	1.136223	2.733106
N	1.395428	3.024574	1.008787
N	1.096425	3.980197	0.130364
N	-1.034903	6.427581	-1.167043
H	-1.779334	6.393160	-0.469109
H	-1.097541	7.078998	-1.951960
N	-0.148824	0.954885	4.421312
N	-1.218063	0.898725	5.231879
N	-3.363180	1.196978	7.206189
H	-4.216287	0.965471	7.725855
H	-2.636722	1.693874	7.724561
C	2.772575	1.332658	1.822345
C	3.923387	0.554835	1.830330
H	4.710029	0.708784	1.089243
C	4.056626	-0.425216	2.796614
H	4.953124	-1.050778	2.822657
C	3.053198	-0.612693	3.730314
H	3.154144	-1.385646	4.494349
C	1.926694	0.197415	3.672129
C	2.514313	2.390538	0.841795
C	3.442887	2.708221	-0.253593
H	2.952836	2.562223	-1.234423
H	3.761345	3.765571	-0.202850
H	4.347148	2.090798	-0.247327
C	-0.014771	4.719763	0.171865
C	0.020292	5.645675	-1.039421
C	0.799108	0.091399	4.604100
C	0.746475	-0.930375	5.663406
H	1.640043	-1.562669	5.696286
H	-0.116949	-1.606373	5.514904
H	0.645216	-0.461213	6.659400
C	-2.261464	1.758182	5.092501
C	-3.505728	1.377526	5.880831
H	-1.298290	0.132154	5.915543
H	1.663811	4.266240	-0.717377

Zn^{2+} H_2dapsox Isomer III LDA

Zn	0.237736	2.292819	2.837518
O	-1.311818	4.147111	0.785528
O	0.796712	5.569134	-1.606126
O	-1.553019	3.007592	5.436716
O	-3.621971	1.512217	3.723142
O	-1.553961	1.998364	2.184109
H	-2.381571	1.809336	2.755734
H	-1.691480	2.816472	1.605871
O	0.398099	3.850911	4.043220
H	0.229056	4.760259	3.724998
H	-0.302250	3.634600	4.752089
N	1.874117	1.138070	2.831101
N	1.298670	2.967364	1.099270
N	0.920919	3.882940	0.210253
N	-1.422961	6.031157	-1.245630
H	-2.236789	5.788251	-0.678884
H	-1.499226	6.725032	-1.991066
N	-0.012684	0.931908	4.553911
N	-1.234024	0.771057	5.110028
N	-4.406991	1.787718	5.844869
H	-5.387116	1.761469	5.548251
H	-4.193654	1.995986	6.821128
C	2.838201	1.439618	1.964549
C	4.050728	0.762198	2.006178
H	4.849178	0.990817	1.297330
C	4.226633	-0.226614	2.959114
H	5.172383	-0.773102	3.009598
C	3.205301	-0.528699	3.843621
H	3.334373	-1.308916	4.597418
C	2.022390	0.191423	3.754308
C	2.493209	2.468981	0.980274
C	3.416322	2.891286	-0.083633

H	4.372978	2.358592	-0.056922
H	2.967648	2.721819	-1.079920
H	3.637091	3.972176	-0.007013
C	-0.315171	4.403231	0.115053
C	-0.274091	5.420413	-1.022689
C	0.849579	-0.026813	4.611702
C	0.674017	-1.255333	5.396295
H	1.635127	-1.637461	5.769608
H	0.242825	-2.062940	4.774611
H	0.013295	-1.087626	6.260864
C	-2.002352	1.877709	5.289737
C	-3.460136	1.686675	4.937489
H	-1.686984	-0.149741	5.043962
H	1.531347	4.319447	-0.534339

Zn^{2+} H_2dapsox Isomer V LDA

Zn	0.140456	2.293216	2.616379
O	-1.189488	3.990653	0.071557
O	1.283986	5.982747	-1.370566
O	-2.250579	3.061207	4.815252
O	-3.225642	0.195451	6.545967
O	-1.477846	2.019782	1.579047
H	-1.670405	1.181337	1.115834
H	-1.428078	2.796312	0.879237
O	-0.379788	3.975699	3.434069
H	0.247630	4.527238	3.941294
H	-1.159079	3.680183	4.066362
N	1.780524	1.187801	2.762143
N	1.395540	3.023169	0.968475
N	1.135320	4.028131	0.129218
H	1.845390	4.650080	-0.355397
N	-0.990798	6.183681	-1.609795
H	-1.890867	5.783894	-1.339304
H	-0.952014	6.985661	-2.241149
N	-0.261817	1.006300	4.343929
N	-1.366682	0.928512	5.087818
H	-1.685281	0.093376	5.657873
N	-4.329358	2.206048	6.430204
H	-5.102658	1.927395	7.036531
H	-4.296298	3.148198	6.037444
C	2.786790	1.415809	1.920393
C	3.956747	0.672575	2.004243
H	4.787795	0.860613	1.320596
C	4.047345	-0.312794	2.971561
H	4.957143	-0.913145	3.057746
C	2.985183	-0.538570	3.829903
H	3.050375	-1.314388	4.595241
C	1.845027	0.244375	3.701804
C	2.568289	2.471060	0.925053
C	3.626631	2.827468	-0.030655
H	4.147527	1.927671	-0.391686
H	3.240068	3.357075	-0.913335
H	4.390571	3.469018	0.445975
C	-0.084880	4.448033	-0.226622
C	0.122194	5.646283	-1.149996
C	0.666557	0.125718	4.564419
C	0.549882	-0.899199	5.612163
H	-0.208205	-1.657393	5.338013
H	0.223624	-0.446848	6.565574
H	1.488618	-1.433359	5.796334
C	-2.263415	1.910122	5.253269
C	-3.358230	1.354750	6.160229

Zn^{2+} H_2dapsox Isomer VII LDA

Zn	10.686153	6.619194	1.819107
O	8.586665	5.102582	3.326525
O	9.947718	2.497623	5.230124
O	10.871521	10.826512	3.393122
O	9.008592	7.676507	2.590952
O	11.473803	7.335232	3.528600
N	11.972587	6.040059	0.351451
N	11.041880	4.519895	2.189240
N	10.511684	3.853572	3.217602
N	7.933150	3.544243	5.567793
H	7.669160	2.978256	6.376173
H	7.291766	4.249691	5.203684
N	11.456623	8.424599	0.974921
N	11.208207	9.597809	1.549651
N	11.412507	8.974325	5.078370
H	11.278053	9.984071	5.221172
H	11.601613	8.336721	5.852739
C	12.360746	4.772701	0.294279
C	13.150648	4.325695	-0.757043
H	13.467137	3.282271	-0.825697
C	13.521365	5.239972	-1.731022
H	14.129808	4.914733	-2.579293
C	13.144243	6.568449	-1.622504
H	13.469962	7.298140	-2.367312
C	12.366973	6.948113	-0.534637
C	11.884345	3.930169	1.401034
C	12.313062	2.531770	1.548546
H	12.446716	2.243958	2.603952
H	13.263320	2.338220	1.034415
H	11.553992	1.848916	1.122314
C	9.343995	4.218165	3.752186
C	9.082658	3.322336	4.953819
C	12.022294	8.334237	-0.182926
C	12.401545	9.502020	-0.991793
H	12.904781	9.227591	-1.926333
H	11.513913	10.101001	-1.265326
H	13.085342	10.162136	-0.426410
C	11.083525	9.738499	2.905911
C	11.334095	8.535229	3.845297
O	8.917651	5.892500	0.748112
H	11.249713	10.481964	1.018865
H	8.345751	7.772380	1.871468
H	8.646649	6.947009	3.160428
H	8.918938	5.299588	-0.030652
H	8.582953	5.368042	1.529720
H	10.919817	3.034084	3.737680

Zn^{2+} H_2dapsox Isomer VIII LDA

Zn	11.284327	6.415475	2.029282
O	8.243330	2.681676	3.502486
O	8.713844	5.841843	2.076640
O	12.758132	11.024743	3.430728
O	9.983592	7.842443	2.528089
O	12.923767	7.551413	3.810320
N	12.209465	5.898237	0.324794
N	10.814239	4.144850	1.654241
N	10.110766	3.332537	2.453988
N	6.875398	4.829599	2.958482
H	6.251563	5.622487	2.804173
H	6.542630	3.960579	3.393475
N	12.406454	8.333221	1.235688
N	12.377299	9.552927	1.788287
N	13.499237	9.263171	5.196928
H	13.537744	10.287198	5.268656

H	13.801714	8.661250	5.963555
C	12.360671	4.606466	0.013618
C	13.012413	4.215358	-1.147812
H	13.133541	3.154433	-1.378358
C	13.454821	5.185823	-2.026365
H	13.946881	4.903095	-2.960972
C	13.268837	6.517787	-1.709077
H	13.621239	7.306882	-2.377288
C	12.667545	6.844570	-0.501160
C	11.724234	3.632765	0.894706
C	12.071693	2.200952	0.808141
H	11.948083	1.668757	1.765401
H	13.122474	2.065887	0.513999
H	11.444245	1.681036	0.061431
C	8.830499	3.552580	2.897951
C	8.137672	4.877867	2.599445
C	12.591759	8.226897	-0.037658
C	12.804066	9.334017	-0.990368
H	13.881366	9.491711	-1.178906
H	12.328693	9.111850	-1.958023
H	12.392132	10.297313	-0.652660
C	12.710817	9.864523	3.082709
C	13.051752	8.755393	4.071553
O	11.341411	5.727761	3.896782
H	12.059302	6.361083	4.242377
H	11.617492	4.807221	4.077106
H	9.140343	7.288557	2.410104
H	9.904197	8.664442	2.004957
H	10.384213	2.339206	2.537172
H	12.373121	10.387246	1.178536

Zn^{2+} H_2dapsox Isomer IX LDA

Zn	10.601687	6.798342	2.031762
O	10.032533	5.476232	4.956145
O	9.162942	2.104228	4.696461
O	9.975404	11.371533	2.780227
O	9.139175	7.947450	2.904639
O	8.801097	6.209800	1.051067
O	11.564812	7.110240	3.769751
N	11.762702	6.164158	0.505776
N	10.796639	4.587309	2.337441
N	10.228702	3.863337	3.300651
N	8.856455	3.498171	6.495376
H	8.441081	2.788150	7.100643
H	9.015148	4.445375	6.841561
N	11.188434	8.618882	1.026824
N	10.905760	9.855588	1.434159
N	8.459979	9.761998	4.070497
H	8.577786	10.780741	4.160095
H	7.797037	9.238218	4.643474
C	11.957934	4.859844	0.334049
C	12.680076	4.393207	-0.758102
H	12.842322	3.322763	-0.905010
C	13.190705	5.314804	-1.655461
H	13.759193	4.974633	-2.525375
C	12.982124	6.668091	-1.452094
H	13.380614	7.398773	-2.158979
C	12.250733	7.069136	-0.340960
C	11.387778	3.977004	1.359536
C	11.537605	2.518701	1.225748
H	11.229209	1.958828	2.119085
H	12.592093	2.260267	1.031741
H	10.954178	2.140731	0.367276
C	9.874191	4.341428	4.500322
C	9.241262	3.186750	5.270841
C	11.955319	8.465344	-0.006246
C	12.495438	9.604741	-0.766825
H	13.086735	9.295664	-1.635957
H	11.682506	10.256690	-1.135503
H	13.160422	10.223095	-0.134370
C	10.073737	10.205916	2.457507
C	9.197108	9.165914	3.166136
H	12.507495	6.865848	3.857001
H	11.017780	6.467092	4.362883
H	8.655784	6.129687	0.087552
H	8.113521	6.815190	1.402480
H	11.372073	10.662956	0.990659
H	9.976641	2.839727	3.254590

Zn^{2+} H_2dapsox Isomer X LDA

Zn	10.638475	6.723942	2.176468
O	9.589799	3.077290	5.195405
O	8.903681	5.983065	3.360646
O	9.493968	11.384893	2.559191
O	10.328498	8.158006	3.682519
O	8.826375	7.080206	1.144212
O	12.295088	6.580986	3.515929
N	11.749528	6.210475	0.507048
N	10.963589	4.461541	2.293869
N	10.683987	3.683022	3.342371
N	7.776808	4.914114	5.019037
H	7.811675	4.093520	5.638303
H	7.024308	5.600657	5.074829
N	11.083453	8.684564	1.030282
N	10.589692	9.887829	1.316315
N	9.371564	9.949160	4.684976
H	9.078374	10.923119	4.526802
H	9.259455	9.485657	5.586838
C	12.086892	4.933752	0.312092
C	12.782425	4.535664	-0.823868
H	13.050754	3.487246	-0.969952
C	13.121062	5.486844	-1.766573
H	13.659734	5.198966	-2.673341
C	12.777519	6.807240	-1.548483
H	13.043786	7.576732	-2.276042
C	12.089735	7.142494	-0.387297
C	11.713009	3.980903	1.355979
C	12.214424	2.595118	1.270399
H	11.835725	1.922218	2.051796
H	13.317054	2.564796	1.301286
H	11.908245	2.145995	0.310214
C	9.725845	3.874208	4.288258
C	8.767216	5.046513	4.166715
C	11.693269	8.519861	-0.097599
C	11.977246	9.581253	-1.084064
H	13.018624	9.507406	-1.435650
H	11.329444	9.490039	-1.973817
H	11.866979	10.600878	-0.687598
C	9.963230	10.268158	2.461357
C	9.904356	9.328673	3.658928
H	13.225467	6.632530	3.218899
H	12.130355	7.356372	4.097807
H	8.239307	6.615797	1.791385
H	8.642652	6.710874	0.257653
H	11.206053	2.803905	3.477021
H	10.606114	10.633676	0.603150

Zn^{2+} H_2dapsox Isomer XI LDA

Zn	10.693216	6.759124	2.086687

O	9.979482	5.552074	4.848255
O	8.876635	2.243614	4.592335
O	9.445965	11.226806	2.563345
N	9.220966	7.821405	3.156496
O	8.776117	6.395129	0.815710
O	11.849996	6.976988	3.739576
N	11.787242	6.160792	0.517349
N	10.766896	4.589490	2.305851
N	10.160935	3.882114	3.263118
N	8.629047	3.644116	6.396787
H	8.125690	2.969122	6.976260
H	8.852346	4.569815	6.765850
N	11.117518	8.609043	0.997933
N	10.641396	9.816547	1.287351
O	10.144470	9.315174	4.628134
C	12.031933	4.861810	0.368855
C	12.820048	4.405001	-0.677946
H	13.026842	3.339206	-0.802462
C	13.338494	5.336636	-1.563405
H	13.967575	5.008443	-2.395517
C	13.057869	6.681282	-1.399737
H	13.457120	7.415809	-2.102284
C	12.257923	7.073435	-0.330615
C	11.420729	3.976886	1.368203
C	11.603314	2.521589	1.261227
H	11.053510	1.943443	2.015564
H	12.673496	2.268728	1.374330
H	11.299001	2.160628	0.264224
C	9.777198	4.405630	4.433431
C	9.030448	3.308909	5.185464
C	11.848743	8.453377	-0.063153
C	12.208977	9.581533	-0.937963
H	12.876708	9.292592	-1.757394
H	11.310210	10.032539	-1.399845
H	12.720587	10.375780	-0.363416
C	9.906507	10.125281	2.419611
C	9.772733	9.072683	3.518382
H	12.802136	6.775820	3.827582
H	11.321269	6.411056	4.386578
H	8.435939	7.862175	2.487138
H	8.982865	7.286945	4.011388
H	8.781483	6.649598	-0.130337
H	8.263276	5.561026	0.852086
H	10.806596	10.613560	0.652517
H	9.850760	2.871023	3.223913

Zn^{2+} H_2dapsox Isomer XII LDA

Zn	10.887719	6.603564	2.177392
O	8.948769	3.226579	4.866223
O	8.148080	5.918665	4.379182
O	9.690048	11.351789	2.669805
N	8.413746	8.479389	3.226026
O	8.979066	6.348915	1.389950
O	12.742679	7.039670	3.137754
N	11.855997	6.079269	0.522582
N	10.953762	4.363001	2.251632
N	10.403450	3.575403	3.183605
N	10.387481	6.304476	4.224196
H	13.480787	6.580258	2.681280
H	11.274859	5.869915	4.512661
N	11.078878	8.531426	1.118865
N	10.710866	9.791713	1.416798
O	10.293700	8.907139	4.433579
C	12.151847	4.801356	0.309454
C	12.845944	4.420438	-0.830064
H	13.091861	3.371650	-1.006250
C	13.207370	5.400400	-1.736556
H	13.753754	5.130364	-2.642409
C	12.869048	6.722103	-1.504721
H	13.142203	7.494247	-2.224105
C	12.175339	7.036829	-0.343482
C	11.669517	3.843308	1.308521
C	11.983507	2.419187	1.144490
H	11.708779	1.797753	2.005244
H	13.063817	2.290827	0.974809
H	11.466831	2.019322	0.256013
C	9.533860	4.004950	4.131799
C	9.287444	5.499823	4.268973
C	11.741290	8.388371	0.004775
C	12.028791	9.531738	-0.872083
H	12.537951	9.236228	-1.793553
H	11.092357	10.044242	-1.155495
H	12.674084	10.266716	-0.357848
C	9.963114	10.176273	2.478311
C	9.542522	9.112507	3.460322
H	12.985294	7.989761	3.106617
H	10.277229	7.300018	4.595188
H	7.859932	8.687443	2.393721
H	8.114662	7.682563	3.828324
H	8.824103	6.950676	0.629761
H	8.920782	5.447232	1.002541
H	10.531008	2.554489	3.123343
H	11.019625	10.552943	0.794488

Ni^{2+} dapsox Isomer V LDA

Ni	-2.174208	4.165740	11.005864
N	-2.854758	5.946629	10.947694
N	-2.719576	4.281120	9.118116
N	-2.540269	3.246942	8.301116
N	-1.245085	0.020208	9.006388
N	-1.840977	4.783583	12.969635
N	-1.332295	4.127878	13.998478
N	0.918885	1.484773	14.613888
O	-1.954574	2.163470	10.274853
O	-1.941948	0.869860	7.006757
O	0.200409	2.987792	12.656535
O	-0.544568	2.488445	16.047614
O	-0.220359	4.383105	10.663879
O	-3.922121	3.148189	11.569944
H	-3.462527	2.373905	11.130372
C	-3.315254	6.392701	9.773724
C	-3.818134	7.684980	9.678583
C	-3.835109	8.469409	10.824996
C	-3.358430	7.976952	12.028814
C	-2.855283	6.675090	12.062271
C	-3.229759	5.409133	8.709037
C	-3.661051	5.663024	7.326229
C	-2.106059	2.213196	9.000553
C	-1.760534	0.970509	8.206906
C	-2.281727	5.999788	13.202245
C	-2.187511	6.637540	14.525804
H	-3.079853	7.245109	14.741271
H	-1.306168	7.299005	14.595505
H	-2.062361	5.846553	15.282433
C	-0.418654	3.217763	13.743007
C	-0.037841	2.369874	14.945304
H	-4.227102	9.488803	10.776038
H	-4.186511	8.063267	8.721762
H	1.236920	1.496186	13.643123
H	-3.365552	8.587316	12.934905

H	1.257524	0.823686	15.306215
H	-3.404478	4.788831	6.710114
H	0.049513	5.303131	10.851054
H	-0.914568	-0.848516	8.596102
H	-1.108953	0.257215	9.990720
H	-4.749536	5.834092	7.269734
H	0.037739	3.812411	11.537738
H	-3.168387	6.560728	6.917312
H	-4.626855	3.412823	10.944682

Ni^{2+} dapsox Isomer VI LDA

Ni	0.043226	0.334560	-0.185117
O	2.047587	0.460454	0.147176
O	-2.094272	0.375256	0.092267
O	-0.114083	1.835281	1.188150
O	-0.178193	4.112071	-1.474336
O	1.740318	-0.010244	2.589941
O	-0.716784	-0.840194	4.955688
N	-0.207273	4.112221	1.126385
N	-0.006523	1.769913	-1.476885
N	0.090432	1.718676	-2.787411
N	-0.024139	-1.007603	-1.583379
N	-0.008234	-1.275594	0.979600
N	-0.199214	-1.261747	2.294979
N	1.215646	0.369726	5.081896
C	-0.142675	2.916915	0.572124
C	-0.107660	3.007946	-0.942533
C	0.128647	0.590125	-3.434837
C	0.242120	0.740666	-4.913353
C	0.100761	-0.765034	-2.902220
C	0.211270	-1.847542	-3.787218
C	0.178147	-3.142799	-3.313897
C	0.044699	-3.367549	-1.955385
C	-0.044130	-2.272821	-1.107896
C	-0.145076	-2.397998	0.327476
C	-0.368795	-3.680505	1.018728
C	0.656084	-0.533195	2.984323
C	0.288832	-0.369477	4.449072
H	-0.239588	4.239990	2.133825
H	-0.231049	4.876178	0.436621
H	0.236340	1.813099	-5.144099
H	1.174457	0.301743	-5.306951
H	-0.598850	0.262047	-5.442480
H	0.314560	-1.652911	-4.855525
H	0.259448	-3.983075	-4.008328
H	0.020116	-4.377937	-1.540605
H	-0.860648	-3.465864	1.982187
H	-0.977647	-4.373244	0.420360
H	2.008420	0.680052	4.515012
H	1.122953	0.559611	6.074949
H	0.585225	-4.180784	1.259007
H	-2.082452	0.165860	1.054229
H	-2.421556	-0.438970	-0.342367
H	2.505164	-0.282507	-0.292241
H	1.986128	0.208389	1.173654

Ni^{2+} Hdapsox Isomer V LDA

Ni	0.349110	2.312999	2.428677
O	-0.883590	3.603323	1.328885
O	-0.076598	5.938827	-1.167190
O	-1.938075	3.425469	4.331920
O	-3.655493	0.792660	5.859976
O	-0.802278	1.069728	1.248475
H	-0.303856	0.666217	0.508487
H	-1.208784	1.906811	0.881541
O	0.521747	3.921770	3.634087
H	1.123565	3.804054	4.395552
H	-0.429099	3.854798	3.992512
N	1.860648	1.169933	2.739460
N	1.544515	2.956231	1.041225
N	1.140436	3.930139	0.241079
N	-1.946633	5.680680	0.116158
H	-2.350856	5.146683	0.884373
H	-2.435174	6.461924	-0.315255
N	-0.233358	1.171536	4.134033
N	-1.423007	1.208327	4.742499
H	-1.900061	0.401667	5.206334
N	-4.365220	2.945516	5.494010
H	-5.279654	2.823725	5.926788
H	-4.080563	3.842908	5.097519
C	2.909458	1.348607	1.924237
C	4.034721	0.543307	2.068656
H	4.890576	0.676469	1.401584
C	4.037511	-0.428055	3.056186
H	4.910127	-1.074384	3.179616
C	2.937559	-0.589937	3.886853
H	2.929307	-1.358302	4.663423
C	1.845358	0.247979	3.696863
C	2.713138	2.386600	0.930353
C	3.711940	2.746187	-0.083877
H	3.932243	1.893540	-0.748636
H	3.328852	3.580528	-0.688530
H	4.662947	3.045796	0.387592
C	-0.122339	4.220488	0.494356
C	-0.701656	5.381398	-0.287272
C	0.605506	0.231597	4.463500
C	0.374520	-0.775979	5.511876
H	0.058969	-1.739499	5.072167
H	-0.387994	-0.464053	6.241163
H	1.305561	-0.969577	6.066928
C	-2.199573	2.299791	4.758194
C	-3.509845	1.935566	5.437717

Ni^{2+} Hdapsox Isomer VI LDA

Ni	-0.013517	0.365092	-0.207072
O	1.956742	0.763469	0.180864
O	-2.114709	0.274248	-0.081503
O	-0.362641	1.895422	1.108273
O	0.204362	4.090606	-1.561271
O	1.626764	0.397023	2.722268
O	-0.498352	-1.429379	4.810180
N	-0.058345	4.157007	1.035602
N	-0.044344	1.757021	-1.527008
N	0.059495	1.663850	-2.832671
N	-0.010099	-1.020848	-1.564109
N	0.104876	-1.228919	0.985089
N	0.014337	-1.208827	2.326165
N	1.058186	0.161957	5.373257
C	-0.137198	2.967022	0.493483
C	0.039412	3.013531	-1.012892
C	0.099525	0.530825	-3.463113
C	0.175325	0.646959	-4.944589
C	0.081961	-0.812270	-2.888280
C	0.132516	-1.914293	-3.752829
C	0.085598	-3.198230	-3.253066
C	-0.010412	-3.388654	-1.887853

C	-0.057772	-2.275430	-1.062465
C	-0.137256	-2.361258	0.377387
C	-0.447290	-3.602039	1.107392
C	0.750533	-0.389706	3.084232
C	0.367315	-0.604026	4.539671
H	-0.156311	4.315451	2.036183
H	0.115417	4.910542	0.353087
H	0.171693	1.711929	-5.207085
H	1.092961	0.190375	-5.350201
H	-0.684107	0.164029	-5.438587
H	0.191421	-1.742905	-4.828589
H	0.122596	-4.055091	-3.930361
H	-0.036552	-4.394451	-1.463763
H	-1.486769	-3.586983	1.484316
H	-0.353711	-4.491179	0.472919
H	1.763973	0.786309	4.978838
H	0.905633	0.099223	6.378554
H	0.217649	-3.727072	1.978595
H	-0.617522	-1.809386	2.899700
H	-2.471396	0.562454	-0.948494
H	-2.194742	1.059367	0.508340
H	2.583392	0.135193	-0.228507
H	1.953486	0.583394	1.186276

[Fe(dapsox)Cl] HS LDA

Fe	1.187192	1.006334	2.320719
O	-0.209691	2.289530	2.950787
O	0.148443	4.065206	-0.032290
O	0.876449	1.731641	5.634321
O	-1.670263	2.106432	6.836761
N	-0.993681	4.361580	2.459462
N	0.938560	1.962386	0.685977
N	1.467935	1.730869	-0.500495
N	1.601610	-0.594931	1.298820
N	0.680704	-0.365221	3.731859
N	-0.041456	-0.251670	4.817418
N	-1.781988	-0.168004	6.906754
C	-0.320260	3.259247	2.170964
C	0.291735	3.179742	0.793382
C	2.015012	0.596844	-0.808588
C	2.576523	0.540504	-2.199700
C	2.044095	-0.615535	0.023143
C	2.476891	-1.819867	-0.548704
C	2.448309	-2.987924	0.202177
C	1.985443	-2.955347	1.503074
C	1.555005	-1.735475	2.049497
C	1.030029	-1.599221	3.376168
C	0.802659	-2.734194	4.311848
C	-0.007096	0.894667	5.575821
C	-1.250251	1.014616	6.489807
H	-1.394036	4.495655	3.376180
H	-1.021677	5.087876	1.757681
H	2.024063	-0.164188	-2.833803
H	3.631322	0.243340	-2.200817
H	2.494266	1.533362	-2.644997
H	2.820653	-1.839160	-1.575858
H	2.786771	-3.926902	-0.233517
H	1.956676	-3.861065	2.098129
H	1.339352	-3.636998	4.020108
H	-0.267436	-2.973541	4.378813
H	1.124500	-2.445192	5.318252
H	-1.527992	-1.003035	6.402113
H	-2.666748	-0.132641	7.391607
Cl	3.150301	1.768232	2.906789

[Fe(dapsox)Cl] IS LDA

Fe	1.190451	0.983319	2.342432
O	-0.227298	2.221610	3.007282
O	0.061266	4.047263	0.032691
O	0.976984	1.692519	5.646607
O	-1.589090	2.251752	6.734271
N	-1.052038	4.284510	2.545544
N	0.903989	1.948773	0.717549
N	1.445434	1.740951	-0.469119
N	1.610719	-0.603194	1.301664
N	0.708483	-0.392796	3.741042
N	-0.017757	-0.252034	4.820069
N	-1.910385	-0.006427	6.737247
C	-0.366032	3.197317	2.234569
C	0.231146	3.150653	0.844117
C	2.017653	0.620841	-0.786699
C	2.606424	0.602508	-2.168286
C	2.056138	-0.604661	0.027146
C	2.496905	-1.800997	-0.556600
C	2.463452	-2.978798	0.179514
C	1.991670	-2.964887	1.478143
C	1.563190	-1.750942	2.039880
C	1.040877	-1.627494	3.371135
C	0.808139	-2.781566	4.283299
C	0.045561	0.910239	5.559299
C	-1.242459	1.130110	6.395117
H	-1.438640	4.400491	3.470963
H	-1.097652	5.018993	1.853111
H	2.085290	-0.101549	-2.828324
H	3.667764	0.329847	-2.150985
H	2.511576	1.602262	-2.594805
H	2.849389	-1.809701	-1.580914
H	2.803959	-3.911343	-0.268359
H	1.954340	-3.880341	2.058067
H	1.443147	-3.635314	4.042306
H	-0.239238	-3.112465	4.244095
H	1.009969	-2.476967	5.314336
H	-1.685619	-0.854887	6.240392
H	-2.823405	0.094889	7.155611
Cl	3.168582	1.747508	2.881807

[Fe(dapsox)Cl] LS LDA

Fe	1.188002	0.983988	2.343705
O	-0.243794	2.212566	2.998639
O	0.039482	4.031332	0.018495
O	0.989403	1.705056	5.618915
O	-1.576568	2.258974	6.724120
N	-1.102054	4.257660	2.519423
N	0.910319	1.949536	0.718055
N	1.474673	1.751397	-0.459545
N	1.607340	-0.601939	1.300253
N	0.698151	-0.394706	3.736916
N	-0.011234	-0.251998	4.827146
N	-1.833268	-0.005464	6.827200
C	-0.393905	3.181408	2.219412
C	0.216610	3.139926	0.834822
C	2.058413	0.634970	-0.771035
C	2.680126	0.627706	-2.137839
C	2.076832	-0.596406	0.034688
C	2.519871	-1.790595	-0.551075
C	2.462597	-2.974533	0.174650
C	1.964294	-2.967501	1.463258

C	1.534209	-1.755806	2.027733
C	0.995618	-1.634270	3.352677
C	0.713881	-2.786096	4.253030
C	0.061917	0.915436	5.557213
C	-1.208348	1.133388	6.418772
H	-1.497058	4.371779	3.441250
H	-1.153588	4.988105	1.822825
H	2.174300	-0.069431	-2.816737
H	3.740369	0.352856	-2.096621
H	2.597407	1.631360	-2.557800
H	2.892207	-1.793623	-1.568150
H	2.806031	-3.905477	-0.273613
H	1.914087	-3.887842	2.034719
H	1.207560	-3.703239	3.931522
H	-0.366471	-2.978830	4.306680
H	1.043890	-2.548453	5.269748
H	-1.602740	-0.866908	6.356687
H	-2.735211	0.088572	7.270730
Cl	3.167446	1.745835	2.880883

$[Fe(Hdapsox)Cl]^+$ HS LDA

Fe	1.341062	1.235355	2.414793
O	-0.128389	2.620262	2.831857
O	-0.112491	3.805257	-0.457154
O	0.696651	1.838048	5.566889
O	-1.760484	-0.294241	6.917395
N	-1.277909	4.370379	1.943842
N	0.985395	1.997802	0.573668
N	1.627647	1.731072	-0.553678
N	1.575368	-0.570794	1.310377
N	0.512628	-0.350707	3.721346
N	-0.192209	-0.170411	4.853556
N	-1.020195	1.705627	7.759735
C	-0.435577	3.359408	1.866243
C	0.168842	3.107086	0.497928
C	2.201716	0.586894	-0.773712
C	2.918323	0.503456	-2.089252
C	2.104491	-0.617957	0.067190
C	2.502158	-1.854962	-0.479468
C	2.309090	-3.020868	0.231929
C	1.706043	-2.958296	1.482919
C	1.357390	-1.713716	2.002557
C	0.711438	-1.576869	3.317053
C	0.289061	-2.766954	4.111508
C	-0.065288	0.902620	5.696518
C	-1.051069	0.707493	6.871159
H	-1.723379	4.622065	2.813730
H	-1.444880	4.902508	1.098897
H	2.414475	-0.177950	-2.785427
H	3.954035	0.167312	-1.967694
H	2.925437	1.496594	-2.540788
H	2.943775	-1.888621	-1.469091
H	2.609481	-3.980043	-0.185916
H	1.518627	-3.872162	2.034937
H	0.918967	-3.633504	3.913725
H	-0.745783	-3.053143	3.876316
H	0.350115	-2.563839	5.184814
H	-0.371393	2.467772	7.635181
H	-1.611455	1.665529	8.576157
Cl	3.338672	1.801948	2.955739
H	-0.856590	-0.865888	5.193417

$[Fe(Hdapsox)Cl]^+$ IS LDA

Fe	1.180748	1.089836	2.257111
O	-0.205718	2.393207	2.832715
O	0.170230	4.010165	-0.239724
O	0.818565	1.875398	5.709704
O	-1.892045	-0.150929	6.680732
N	-1.136464	4.361409	2.168691
N	0.997457	1.974809	0.611407
N	1.576910	1.699331	-0.530976
N	1.584997	-0.567995	1.299491
N	0.600198	-0.270115	3.684278
N	-0.127679	-0.049377	4.800201
N	-1.049466	1.697525	7.745850
C	-0.374952	3.302101	1.983766
C	0.297533	3.182564	0.635958
C	2.145335	0.568444	-0.802753
C	2.784334	0.485320	-2.155754
C	2.105147	-0.624055	0.056558
C	2.542063	-1.856178	-0.462474
C	2.424831	-3.008027	0.292546
C	1.862484	-2.935552	1.561699
C	1.452578	-1.696553	2.046850
C	0.841722	-1.518882	3.363033
C	0.494587	-2.671545	4.239471
C	0.004120	0.980231	5.701500
C	-1.094774	0.780314	6.775141
H	-1.619095	4.518231	3.041393
H	-1.201354	5.031906	1.413356
H	2.261925	-0.222111	-2.810963
H	3.833908	0.178228	-2.086213
H	2.744222	1.470896	-2.621881
H	2.958488	-1.899694	-1.462603
H	2.762696	-3.963548	-0.104378
H	1.752694	-3.833513	2.159622
H	1.189258	-3.501152	4.104337
H	-0.514348	-3.048259	4.020053
H	0.525984	-2.381597	5.293349
H	-0.329046	2.403491	7.727684
H	-1.708372	1.656755	8.508441
Cl	3.121703	1.783153	2.908926
H	-0.873795	-0.692135	5.078164

$[Fe(Hdapsox)Cl]^+$ LS LDA

Fe	1.029911	0.986570	2.193236
O	-0.108854	2.434194	2.951471
O	0.079927	3.990809	-0.167772
O	1.037618	1.717912	5.759300
O	-2.003166	0.102451	6.492839
N	-1.044451	4.410018	2.322205
N	0.925150	1.941873	0.640255
N	1.534909	1.741520	-0.515789
N	1.607273	-0.544807	1.337458
N	0.629461	-0.278010	3.629499
N	-0.108237	-0.031701	4.743699
N	-1.027042	1.856407	7.604440
C	-0.324514	3.328572	2.101278
C	0.246990	3.170671	0.704490
C	2.148161	0.620022	-0.764806
C	2.841490	0.580790	-2.092254
C	2.137987	-0.572262	0.083290
C	2.629748	-1.780357	-0.433637
C	2.563670	-2.949809	0.303911
C	1.997502	-2.913125	1.569728
C	1.540758	-1.699340	2.075459
C	0.937537	-1.535372	3.376043
C	0.648521	-2.656164	4.309300

C	0.097624	0.958690	5.669598
C	-1.101971	0.924169	6.647089
H	-1.452983	4.592958	3.227426
H	-1.157610	5.069430	1.562963
H	2.364554	-0.124901	-2.782450
H	3.894680	0.298418	-1.985677
H	2.793344	1.575528	-2.537401
H	3.062618	-1.791253	-1.427635
H	2.944084	-3.883568	-0.104778
H	1.912855	-3.819542	2.160152
H	1.340955	-3.486828	4.168378
H	-0.369018	-3.045248	4.161224
H	0.727809	-2.318154	5.347027
H	-0.204833	2.438708	7.660888
H	-1.731302	1.894530	8.325497
Cl	2.937710	1.592650	2.868501
H	-0.960669	-0.564147	4.930486

$[Fe(dapsox)H_2O]^+$ HS LDA

Fe	1.176147	1.174389	2.365390
O	2.581622	1.637792	3.476822
O	-0.366996	2.487140	2.719549
O	-0.078941	3.796627	-0.528869
O	1.252498	1.438276	5.707139
O	-0.531059	1.876826	7.618153
N	-1.482347	4.227972	1.771012
N	1.020113	2.017975	0.554751
N	1.787523	1.805071	-0.514776
N	1.623523	-0.563072	1.258808
N	0.499305	-0.386731	3.652581
N	-0.188353	-0.209743	4.803971
N	-1.751808	0.048629	7.000271
C	-0.603031	3.248682	1.745238
C	0.147253	3.077197	0.427674
C	2.376612	0.669297	-0.733374
C	3.233204	0.648635	-1.965649
C	2.208625	-0.576022	0.042788
C	2.629781	-1.798307	-0.514730
C	2.419766	-2.979492	0.171803
C	1.787810	-2.946989	1.409241
C	1.399083	-1.714953	1.931388
C	0.742331	-1.602485	3.243461
C	0.409171	-2.812799	4.041309
C	0.185753	0.691398	5.668779
C	-0.743123	0.939546	6.871437
H	-2.021437	4.433795	2.599843
H	-1.585026	4.781339	0.928843
H	2.797187	0.018009	-2.749901
H	4.243404	0.280986	-1.754967
H	3.302761	1.664427	-2.357272
H	3.114755	-1.814395	-1.484198
H	2.744554	-3.927189	-0.254016
H	1.613957	-3.864809	1.960651
H	-0.085616	-3.568953	3.424758
H	-0.240476	-2.546271	4.874469
H	1.321137	-3.260695	4.456174
H	-1.939489	-0.623751	6.275014
H	-2.440416	0.218423	7.717220
H	1.819342	1.422128	4.867786
H	3.066857	2.469779	3.394187

$[Fe(dapsox)H_2O]^+$ IS LDA

Fe	1.006357	0.963564	2.237094
O	2.407735	1.640945	3.320488
O	-0.527127	2.158466	2.726052
O	0.284921	4.090512	-0.087308
O	1.175707	1.663530	5.449030
O	-0.789374	2.249871	7.181848
N	-1.279254	4.236052	2.181822
N	1.029484	1.982504	0.666790
N	1.719356	1.787150	-0.442216
N	1.591568	-0.602447	1.244803
N	0.548428	-0.408606	3.624081
N	-0.103361	-0.204451	4.780690
N	-1.503515	0.082612	7.120097
C	-0.543001	3.165275	1.971641
C	0.305932	3.176475	0.709725
C	2.296842	0.665814	-0.737986
C	3.041455	0.665725	-2.039213
C	2.210526	-0.581982	0.047137
C	2.733863	-1.774998	-0.479580
C	2.602245	-2.960185	0.224587
C	1.945245	-2.962617	1.447954
C	1.445095	-1.759507	1.943985
C	0.791420	-1.643035	3.243859
C	0.463710	-2.829883	4.075213
C	0.197129	0.831804	5.532370
C	-0.756725	1.130059	6.704073
H	-1.866837	4.317649	2.999948
H	-1.223914	4.987204	1.505310
H	2.591998	-0.025976	-2.761539
H	4.091588	0.383366	-1.904671
H	3.003188	1.669935	-2.463148
H	3.237011	-1.768402	-1.439517
H	3.013808	-3.883824	-0.178268
H	1.842720	-3.879741	2.018460
H	0.135443	-3.671592	3.460662
H	-0.324283	-2.573714	4.784420
H	1.338713	-3.149548	4.656598
H	-1.523357	-0.775827	6.595827
H	-2.207892	0.253799	7.821571
H	1.754169	1.620168	4.549403
H	2.807518	2.496975	3.116851

$[Fe(dapsox)H_2O]^+$ LS LDA

Fe	0.906028	0.964025	2.160819
O	2.355557	1.470085	3.114017
O	-0.296725	2.396317	2.822100
O	0.073559	3.949596	-0.296662
O	1.290354	1.413848	5.523560
O	-0.278165	1.818936	7.637156
N	-1.339717	4.268566	2.053079
N	0.990863	1.975353	0.623842
N	1.729872	1.807329	-0.465418
N	1.631481	-0.532615	1.328947
N	0.447772	-0.333415	3.554891
N	-0.287432	-0.108421	4.677933
N	-1.814278	0.305504	6.888132
C	-0.509493	3.254308	1.926650
C	0.217064	3.142351	0.595915
C	2.361199	0.689363	-0.683533
C	3.165240	0.675263	-1.948868
C	2.269209	-0.527175	0.126940
C	2.799722	-1.726279	-0.377564
C	2.671082	-2.910766	0.325741
C	1.997178	-2.903130	1.540573
C	1.486870	-1.703240	2.022639
C	0.776580	-1.574811	3.277001
C	0.484524	-2.725991	4.169578

C	0.168114	0.747150	5.545954
C	-0.668889	1.019507	6.807019
H	-1.858688	4.423949	2.905863
H	-1.437478	4.898587	1.266522
H	2.738074	-0.010960	-2.690016
H	4.204449	0.380335	-1.768120
H	3.156492	1.678795	-2.376629
H	3.314947	-1.716791	-1.331433
H	3.088622	-3.834893	-0.068669
H	1.876291	-3.816873	2.114157
H	0.174300	-3.606248	3.600683
H	-0.301590	-2.462683	4.878057
H	1.377158	-2.994080	4.750273
H	-2.116118	-0.285766	6.131598
H	-2.429449	0.484145	7.666726
H	1.747058	1.339327	4.627958
H	2.476336	2.422011	2.957669

$[Fe(Hdapsox)H_2O]^{2+}$ HS LDA

Fe	1.131288	1.231967	2.341468
O	2.553337	1.881307	3.627267
O	-0.427530	2.472993	2.522273
O	0.283527	3.868961	-0.625992
O	1.201539	1.540479	5.790881
O	-1.578430	-0.313627	6.908406
N	-1.502134	4.183443	1.475139
N	1.278374	2.132444	0.609883
N	2.169199	1.896014	-0.345661
N	1.548020	-0.521004	1.261134
N	0.499581	-0.373742	3.689464
N	-0.076284	-0.191106	4.898085
N	-0.442995	1.308941	8.074014
C	-0.572357	3.265073	1.542876
C	0.378257	3.161230	0.351624
C	2.644496	0.712895	-0.575922
C	3.703025	0.638129	-1.626572
C	2.163072	-0.541938	0.059225
C	2.347700	-1.758604	-0.618238
C	1.861306	-2.931649	-0.070698
C	1.239143	-2.894098	1.172126
C	1.114597	-1.672379	1.829041
C	0.521497	-1.577727	3.181077
C	0.021349	-2.795917	3.872475
C	0.282847	0.718866	5.831869
C	-0.687305	0.527372	7.026425
H	-2.180040	4.310540	2.216325
H	-1.538123	4.771726	0.649421
H	3.311414	0.193839	-2.550579
H	4.557097	0.036766	-1.296594
H	4.042999	1.646824	-1.867092
H	2.854756	-1.774342	-1.577295
H	1.974076	-3.876480	-0.599889
H	0.863485	-3.809766	1.616693
H	-0.942708	-3.112362	3.450052
H	-0.106760	-2.648244	4.945661
H	0.721897	-3.625887	3.745541
H	0.337338	1.948451	8.072497
H	-1.019472	1.228644	8.901181
H	2.133344	1.798793	4.549551
H	3.004855	2.736423	3.574993
H	-0.879745	-0.742637	5.241635

$[Fe(Hdapsox)H_2O]^{2+}$ IS LDA

Fe	1.030162	1.060283	2.225517
O	2.588734	1.701269	3.429754
O	-0.386301	2.345984	2.692847
O	0.379296	4.060394	-0.272326
O	1.150001	1.592976	5.631775
O	-1.702314	-0.143858	6.753024
N	-1.352668	4.253571	1.908423
N	1.198913	2.067854	0.685930
N	2.004669	1.862786	-0.331445
N	1.572967	-0.540569	1.249426
N	0.463958	-0.348675	3.587618
N	-0.161567	-0.116472	4.761986
N	-0.550817	1.490528	7.887625
C	-0.499726	3.263633	1.827878
C	0.397886	3.229114	0.599379
C	2.556246	0.727864	-0.615016
C	3.489548	0.722777	-1.781506
C	2.242036	-0.540444	0.081518
C	2.596372	-1.760451	-0.520566
C	2.220374	-2.955469	0.065537
C	1.519254	-2.935570	1.268026
C	1.225067	-1.709730	1.855079
C	0.564110	-1.585685	3.160730
C	0.066393	-2.767183	3.909425
C	0.205785	0.809381	5.683672
C	-0.793453	0.678835	6.861562
H	-1.999252	4.338196	2.682819
H	-1.368546	4.940393	1.161825
H	3.053453	0.192083	-2.637203
H	4.441479	0.241844	-1.530742
H	3.684375	1.750730	-2.090489
H	3.143614	-1.760182	-1.456943
H	2.469668	-3.903773	-0.407409
H	1.214217	-3.865872	1.735879
H	-0.936295	-3.049665	3.555565
H	0.004934	-2.572588	4.982482
H	0.717101	-3.632344	3.769243
H	0.245111	2.110793	7.878147
H	-1.140423	1.449305	8.708068
H	2.180138	1.737052	4.343407
H	3.066678	2.532152	3.293462
H	-0.983351	-0.646503	5.090694

$[Fe(Hdapsox)H_2O]^{2+}$ LS LDA

Fe	1.050062	1.044519	2.201612
O	2.531332	1.467923	3.481039
O	-0.127742	2.501785	2.853917
O	0.141290	3.911026	-0.340186
O	1.276747	1.340160	5.707985
O	-1.935474	0.132775	6.523544
N	-1.207466	4.355486	2.071666
N	1.144467	2.021372	0.676930
N	1.888099	1.855149	-0.391179
N	1.590118	-0.514231	1.280288
N	0.436496	-0.292644	3.496770
N	-0.255639	-0.020535	4.638596
N	-0.567773	1.402332	7.863597
C	-0.384459	3.342105	1.947922
C	0.306831	3.186318	0.602557
C	2.489564	0.721411	-0.645956
C	3.395646	0.738954	-1.828475
C	2.233601	-0.527107	0.082194
C	2.614481	-1.747102	-0.499469
C	2.314744	-2.947988	0.121649
C	1.641426	-2.924970	1.336599
C	1.302047	-1.698367	1.901344

C	0.624446	-1.557175	3.176542
C	0.197813	-2.716042	3.999558
C	0.193478	0.752009	5.648836
C	-0.892403	0.741723	6.753971
H	-1.709835	4.530927	2.933010
H	-1.347972	4.969057	1.276345
H	2.961618	0.178328	-2.667025
H	4.369719	0.295150	-1.595374
H	3.537920	1.768903	-2.159294
H	3.135784	-1.744616	-1.451009
H	2.601204	-3.893507	-0.334400
H	1.382904	-3.851236	1.841134
H	-0.685580	-3.197197	3.556535
H	-0.049770	-2.425364	5.021293
H	0.991278	-3.467442	4.047264
H	0.331605	1.849750	7.959606
H	-1.215154	1.413928	8.640351
H	2.115238	1.407898	4.417751
H	2.836878	2.385566	3.399670
H	-1.193873	-0.399341	4.827733

Fe^{3+} dapsox Isomer I HS OPBE

Fe	0.017162	2.352035	2.613495
O	-0.928489	3.693189	1.310954
O	-0.025123	6.128320	-1.087504
O	-1.712509	2.794830	3.666618
O	-3.720735	1.419213	6.231686
O	-0.966728	0.823354	1.257105
H	-0.410153	0.119744	0.896785
H	-1.313172	1.290678	0.483787
O	0.890382	3.962455	3.954814
H	0.150544	4.357791	4.437960
H	1.296217	4.701480	3.480103
N	1.821265	1.139305	2.752165
N	1.474938	3.049437	1.120094
N	1.123650	4.044903	0.299871
N	-2.076425	5.583115	-0.240515
H	-2.588651	5.014849	0.413674
H	-2.540182	6.323138	-0.744091
N	-0.216032	0.890841	4.236321
N	-1.326233	0.927824	4.972593
N	-4.039289	3.286102	4.955860
H	-4.930895	3.485281	5.381773
H	-3.709602	3.843338	4.185379
C	2.869016	1.410839	1.952165
C	4.041917	0.648836	2.019499
H	4.885178	0.871627	1.372673
C	4.103223	-0.404241	2.923800
H	5.002242	-1.015264	2.988465
C	3.019603	-0.672244	3.749679
H	3.058216	-1.486215	4.467476
C	1.879466	0.135582	3.647525
C	2.666966	2.517481	1.019061
C	3.704819	2.960693	0.051179
H	3.956025	2.154121	-0.648855
H	3.343822	3.817395	-0.517680
H	4.627898	3.239165	0.573724
C	-0.163478	4.309941	0.486987
C	-0.737863	5.446139	-0.372284
C	0.698521	-0.010020	4.494169
C	0.580208	-1.048532	5.550797
H	0.695414	-2.052369	5.124362
H	-0.392728	-0.977206	6.036772
H	1.362792	-0.921604	6.309195
C	-2.049080	1.970670	4.590429
C	-3.364254	2.184124	5.353097

Fe^{3+} dapsox IS OPBE

Fe	0.174513	2.056213	2.824291
O	-1.293129	3.233218	0.037880
O	-0.146289	6.553283	0.184784
O	-1.500989	2.716119	3.526161
O	-3.641689	1.790355	6.189481
O	-0.945177	0.967460	1.288522
H	-0.444098	0.334272	0.758306
H	-1.111100	1.755481	0.682033
O	1.154745	4.105624	4.055694
H	0.590482	4.417472	4.775559
H	1.147486	4.844072	3.429233
N	1.793689	1.076432	2.819808
N	1.177803	2.978862	1.305893
N	0.756810	4.099778	0.769461
N	-1.860615	5.672414	-1.046873
H	-2.376307	4.841093	-1.287380
H	-2.168229	6.573937	-1.376774
N	-0.086502	0.905119	4.345533
N	-1.211340	1.034079	5.061221
N	-3.916831	3.359503	4.550283
H	-4.830908	3.620090	4.887263
H	-3.567206	3.756907	3.693699
C	2.739387	1.380995	1.899853
C	3.902616	0.612404	1.843440
H	4.669109	0.831341	1.105849
C	4.067602	-0.437360	2.747216
H	4.971890	-1.042020	2.707162
C	3.096836	-0.710926	3.702748
H	3.227633	-1.514834	4.421201
C	1.942045	0.078292	3.725434
C	2.390887	2.514310	1.063781
C	3.287533	3.121064	0.047616
H	3.171270	2.625647	-0.925966
H	3.023766	4.173541	-0.088076
H	4.337058	3.046115	0.343299
C	-0.475623	4.160104	0.224530
C	-0.801689	5.602467	-0.216430
C	0.823180	-0.012858	4.632440
C	0.702261	-0.984627	5.744604
H	0.763496	-2.011528	5.364205
H	-0.246905	-0.853773	6.264150
H	1.522185	-0.846958	6.460668
C	-1.911264	2.020375	4.540473
C	-3.257663	2.369172	5.189883

Fe^{3+} dapsox LS OPBE

Fe	0.259624	2.179688	2.919657
O	-1.311372	3.163462	0.214231
O	-0.095945	6.437575	-0.313043
O	-1.385650	2.901508	3.644352
O	-3.672312	1.767128	6.092259
O	-0.849860	1.203598	1.634544
H	-0.314381	0.574501	1.129767
H	-1.049011	2.011071	0.953388
O	1.147218	3.556242	4.172595
H	0.397870	3.939379	4.658155
H	1.486650	4.294977	3.642723
N	1.795115	1.120081	2.807663
N	1.185218	3.036249	1.400850
N	0.726601	4.145381	0.830391
N	-2.032348	5.448589	-1.016880
H	-2.575219	4.601293	-1.057468

H	-2.333487	6.268472	-1.520009
N	-0.105190	0.906765	4.281472
N	-1.276403	0.997930	4.934378
N	-3.890220	3.438283	4.549944
H	-4.813852	3.679350	4.875713
H	-3.519857	3.883226	3.726239
C	2.755762	1.441353	1.914620
C	3.914453	0.662148	1.832304
H	4.686181	0.901926	1.106763
C	4.051526	-0.425100	2.687029
H	4.946866	-1.041834	2.635641
C	3.052586	-0.733077	3.609010
H	3.153834	-1.579738	4.281833
C	1.912651	0.068588	3.654823
C	2.395609	2.594681	1.113870
C	3.260845	3.211176	0.077639
H	3.193000	2.657124	-0.868353
H	2.937769	4.236816	-0.115197
H	4.309164	3.210509	0.390069
C	-0.491709	4.123434	0.281554
C	-0.842643	5.474561	-0.381052
C	0.754064	-0.059788	4.521249
C	0.560985	-1.127334	5.531438
H	0.622465	-2.116712	5.061771
H	-0.410013	-1.022996	6.015799
H	1.346098	-1.075718	6.296550
C	-1.889229	2.084197	4.519055
C	-3.254530	2.404847	5.143562

Fe^{3+} dapsox Isomer V OPBE

Fe	-1.930297	4.012441	10.880601
N	-2.826067	5.917888	10.898256
N	-2.772400	4.311320	8.947010
N	-2.729896	3.298767	8.079929
N	-1.487389	-0.053352	8.460047
N	-1.843910	4.777565	12.998034
N	-1.476593	4.023177	14.043660
N	1.156849	2.048348	15.387468
O	-1.851768	2.204291	9.918091
O	-2.667125	0.886814	6.745852
O	0.643880	3.466423	13.166437
O	-1.031279	2.231391	16.008879
O	-0.040667	4.259337	10.906808
O	-3.524756	2.787293	11.977323
H	-3.529641	1.881817	11.635976
C	-3.298775	6.409975	9.737184
C	-3.766981	7.725291	9.661629
C	-3.736504	8.508781	10.807879
C	-3.273149	7.975710	12.005929
C	-2.824211	6.651328	12.024003
C	-3.298064	5.462741	8.620779
C	-3.867295	5.778088	7.285578
C	-2.229782	2.234072	8.690252
C	-2.148884	0.952722	7.845873
C	-2.326568	5.969358	13.223353
C	-2.374032	6.595330	14.571292
H	-3.305189	7.149119	14.720090
H	-1.539781	7.296117	14.707444
H	-2.287246	5.823323	15.339135
C	-0.330885	3.402820	14.036951
C	-0.108956	2.497551	15.255513
H	-4.086543	9.539240	10.771677
H	-4.144512	8.125239	8.725278
H	1.873970	2.258602	14.713342
H	-3.257232	8.580307	12.907416
H	1.364447	1.431608	16.157867
H	-3.786668	4.910907	6.630031
H	0.272775	5.152565	10.708900
H	-1.344995	-0.911651	7.950280
H	-1.012212	0.092644	9.335560
H	-4.922979	6.063027	7.372468
H	0.369625	3.889430	12.235507
H	-3.335025	6.620007	6.825913
H	-3.410790	2.698104	12.935467

Fe^{3+} Hdapsox Isomer I HS OPBE

Fe	-0.000226	2.360191	2.678963
O	-0.993774	3.918066	1.394861
O	0.221627	5.878122	-1.268089
O	-1.721099	2.772978	3.712395
O	-3.890721	0.995921	5.799988
O	-1.007317	0.933842	1.276632
H	-1.027137	-0.006915	1.504404
H	-1.929591	1.155965	1.080416
O	0.887614	3.976151	3.955582
H	0.328679	4.263234	4.691410
H	1.778274	3.908859	4.327035
N	1.824866	1.163640	2.764403
N	1.426262	3.001764	1.072630
N	0.980770	3.986182	0.289720
N	-1.875079	6.028945	-0.334053
H	-2.505914	5.675100	0.368088
H	-2.179854	6.772875	-0.947370
N	-0.172385	0.918385	4.308890
N	-1.293581	0.924083	5.026091
N	-4.047539	3.195207	5.195007
H	-4.958487	3.307945	5.616937
H	-3.615735	3.976277	4.729373
C	2.827787	1.373908	1.892472
C	4.010123	0.635207	1.950694
H	4.819176	0.813324	1.248584
C	4.140923	-0.345176	2.931223
H	5.053969	-0.934832	2.996456
C	3.100723	-0.566983	3.820524
H	3.185004	-1.330240	4.588792
C	1.940003	0.212822	3.713353
C	2.580581	2.431757	0.896031
C	3.578184	2.752453	-0.159976
H	3.871814	1.840316	-0.691713
H	3.217194	3.458525	-0.908726
H	4.486260	3.175903	0.288494
C	-0.275903	4.411861	0.510515
C	-0.641297	5.539712	-0.466582
C	0.789041	0.075856	4.605739
C	0.734751	-0.903183	5.719113
H	0.882824	-1.924060	5.345524
H	-0.226348	-0.850090	6.229678
H	1.533011	-0.705920	6.446299
C	-2.057821	1.927764	4.615525
C	-3.438179	2.002513	5.278157
H	1.488270	4.450775	-0.464692

Fe^{3+} Hdapsox IS OPBE

Fe	0.111463	2.076717	2.891068
O	-1.521213	3.540383	0.362867
O	0.442682	6.283423	-0.647075
O	-1.537271	2.650957	3.644536
O	-3.522716	1.708383	6.414307
O	-0.941965	0.941007	1.278025
H	-1.641462	0.307333	1.490192
H	-1.379448	1.662998	0.784946
O	1.099256	3.982439	4.130931
H	0.462384	4.608093	4.503305

H	1.730191	3.844809	4.850931
N	1.770647	1.117329	2.823312
N	1.141213	3.032068	1.276900
N	0.710289	4.109892	0.606634
N	-1.775774	5.938636	-1.138127
H	-2.564417	5.316305	-1.046283
H	-1.869751	6.786687	-1.680595
N	-0.122335	0.816831	4.331766
N	-1.236009	0.896325	5.066763
N	-4.004638	3.188399	4.739656
H	-4.890067	3.447553	5.151976
H	-3.738577	3.582554	3.852232
C	2.731832	1.482769	1.947081
C	3.935054	0.781931	1.913808
H	4.729041	1.069436	1.231348
C	4.115989	-0.306006	2.770981
H	5.050989	-0.862961	2.743699
C	3.112583	-0.674934	3.653043
H	3.242450	-1.519055	4.324904
C	1.927772	0.070654	3.669481
C	2.372389	2.621617	1.093056
C	3.314948	3.245702	0.131025
H	4.102967	2.557853	-0.175981
H	2.794252	3.580041	-0.772146
H	3.801820	4.122901	0.582550
C	-0.575681	4.295032	0.182943
C	-0.601031	5.633971	-0.592160
C	0.791351	-0.118779	4.543510
C	0.662450	-1.196095	5.549292
H	0.699080	-2.175858	5.054746
H	-0.273499	-1.109497	6.100273
H	1.499006	-1.156245	6.258481
C	-1.940551	1.912317	4.638098
C	-3.260435	2.258958	5.363331
H	1.318486	4.883376	0.301481

Fe^{3+} Hdapsox LS OPBE

Fe	0.240127	2.136204	2.990940
O	-1.500983	3.297710	0.304521
O	0.201268	6.211878	-0.696434
O	-1.317298	2.947650	3.823742
O	-3.929459	1.413837	5.596148
O	-0.838781	1.191810	1.663342
H	-1.612221	0.730615	2.025564
H	-1.190049	1.957312	1.090382
O	1.251604	3.472433	4.173224
H	0.589913	3.949633	4.700012
H	1.860147	3.090163	4.824854
N	1.788056	1.154619	2.825749
N	1.124204	3.071590	1.354222
N	0.633408	4.116421	0.653003
N	-1.955569	5.633380	-1.239200
H	-2.686057	4.942966	-1.152816
H	-2.115732	6.457364	-1.803049
N	-0.139672	0.857790	4.271298
N	-1.322043	0.917734	4.903786
N	-3.619166	3.653616	5.246158
H	-4.525113	3.897483	5.622350
H	-3.040549	4.377383	4.852009
C	2.746192	1.530382	1.952630
C	3.936530	0.806449	1.892608
H	4.726901	1.082330	1.200806
C	4.098316	-0.296695	2.733914
H	5.024293	-0.867580	2.696259
C	3.086334	-0.680156	3.605233
H	3.204302	-1.548282	4.248383
C	1.909888	0.077606	3.641267
C	2.352737	2.674158	1.118118
C	3.248631	3.295166	0.111386
H	4.033048	2.612173	-0.215258
H	2.688997	3.614407	-0.773860
H	3.741239	4.183904	0.533504
C	-0.628724	4.154860	0.157731
C	-0.772053	5.462014	-0.653670
C	0.742423	-0.107956	4.488058
C	0.552810	-1.214628	5.451404
H	0.597297	-2.180705	4.932148
H	-0.407638	-1.129188	5.959719
H	1.353090	-1.211863	6.202608
C	-1.877814	2.079643	4.606233
C	-3.265271	2.358871	5.213192
H	1.188362	4.927454	0.345762

Fe^{3+} Hdapsox Isomer V OPBE

Fe	-0.062544	2.235959	2.929036
O	-1.374323	3.676238	-0.046677
O	0.833290	6.250624	-0.983311
O	-1.682943	2.679196	4.075401
O	-3.662620	0.850445	6.341678
O	-1.276437	1.563581	1.409375
H	-2.175786	1.298386	1.653702
H	-1.374024	2.336674	0.758289
O	0.772343	3.957262	4.060738
H	1.713956	4.093507	4.234856
H	0.322767	4.163912	4.892398
N	1.755242	1.156756	2.817222
N	1.181453	3.097607	1.189585
N	0.845783	4.164445	0.429939
H	1.510968	4.888771	0.114214
N	-1.354108	5.995003	-1.645852
H	-2.184941	5.426052	-1.582132
H	-1.357213	6.816094	-2.235471
N	-0.143108	0.759294	4.444373
N	-1.214089	0.736855	5.235107
N	-3.953362	3.012425	5.661009
H	-4.829303	3.109052	6.155507
H	-3.599435	3.786391	5.123126
C	2.707324	1.485061	1.926857
C	3.905358	0.766174	1.866687
H	4.689799	1.031599	1.166001
C	4.089146	-0.314703	2.722932
H	5.013757	-0.888526	2.685026
C	3.088753	-0.658946	3.620301
H	3.216123	-1.502615	4.292538
C	1.919833	0.110282	3.651248
C	2.389564	2.616651	1.038492
C	3.364647	3.148428	0.048795
H	4.144672	2.429399	-0.196050
H	2.862540	3.421909	-0.884862
H	3.862147	4.049430	0.436219
C	-0.363511	4.374818	-0.139011
C	-0.248030	5.663835	-0.984463
C	0.817152	-0.123301	4.587456
C	0.810337	-1.222102	5.580716
H	0.885239	-2.193271	5.073977
H	-0.103861	-1.202353	6.173195
H	1.673580	-1.141512	6.253852
C	-1.977826	1.782185	4.952664
C	-3.297269	1.845176	5.735461

Fe^{3+} H_2dapsox Isomer I HS OPBE

Fe	0.018629	2.377719	2.623515

O	-0.947606	3.866917	1.370266
O	0.303012	5.918301	-1.206944
O	-1.847975	2.797188	3.654101
O	-3.525311	1.078729	6.232891
O	-0.945339	0.960795	1.259590
H	-0.862062	-0.002587	1.220645
H	-1.701978	1.188191	0.699871
O	0.813295	3.911550	3.969130
H	1.729866	4.185536	4.114946
H	0.262842	4.547673	4.448291
N	1.820421	1.159464	2.759148
N	1.467798	3.016674	1.075455
N	1.029872	4.010395	0.297733
H	1.544490	4.494186	-0.444170
N	-1.840957	6.033392	-0.384599
H	-2.520537	5.660193	0.260224
H	-2.118188	6.783908	-1.007646
N	-0.196684	0.913473	4.269707
N	-1.350417	1.010408	4.935384
H	-1.683335	0.412377	5.697861
N	-4.350857	2.942191	5.169023
H	-5.206544	2.963967	5.712787
H	-4.198041	3.656794	4.474094
C	2.841049	1.369978	1.904553
C	4.008204	0.600442	1.963172
H	4.829473	0.774114	1.272975
C	4.104926	-0.403028	2.920813
H	5.001857	-1.018145	2.983469
C	3.047526	-0.613849	3.799077
H	3.113942	-1.394213	4.552519
C	1.909671	0.193420	3.695083
C	2.630775	2.449366	0.918712
C	3.655020	2.789255	-0.099785
H	3.908233	1.900354	-0.692049
H	3.350308	3.568812	-0.798956
H	4.579464	3.124905	0.389887
C	-0.233831	4.408167	0.499974
C	-0.602071	5.559852	-0.463367
C	0.739026	0.062674	4.585961
C	0.700198	-0.929626	5.688735
H	0.737101	-1.949907	5.282093
H	-0.184262	-0.858882	6.323068
H	1.576864	-0.809109	6.337678
C	-2.167414	2.006493	4.566725
C	-3.460571	1.986704	5.413104

Fe^{3+} H_2dapsox IS OPBE

Fe	0.039800	2.356431	2.624089
O	-0.888120	4.130468	1.410907
O	0.272051	5.805361	-1.442618
O	-2.058786	2.630730	3.608021
O	-3.431753	1.233155	6.516681
O	-0.918625	1.082671	1.220573
H	-1.882096	1.056482	1.125588
H	-0.608864	0.180881	1.051893
O	0.701558	3.825214	4.020024
H	1.643425	3.983294	4.178834
H	0.274093	4.692549	4.076189
N	1.815186	1.155366	2.756165
N	1.461326	3.003389	1.049484
N	1.048065	3.991821	0.240433
H	1.581886	4.370859	-0.539326
N	-1.690841	6.233465	-0.337488
H	-2.275649	6.000782	0.451112
H	-1.985169	6.964697	-0.974727
N	-0.183272	0.925163	4.308385
N	-1.323583	1.007896	5.011443
H	-1.535772	0.460123	5.844452
N	-4.502260	2.671973	5.085502
H	-5.354793	2.713552	5.634209
H	-4.445160	3.191039	4.221471
C	2.835297	1.362709	1.901080
C	4.010060	0.602967	1.967371
H	4.825453	0.770893	1.269084
C	4.120537	-0.384021	2.937157
H	5.025043	-0.986054	3.010624
C	3.064097	-0.594689	3.814969
H	3.141332	-1.361776	4.580963
C	1.915863	0.196397	3.698051
C	2.624485	2.432935	0.906870
C	3.657703	2.756542	-0.109839
H	3.902296	1.864131	-0.699779
H	3.373428	3.538412	-0.815222
H	4.584436	3.082181	0.381445
C	-0.163426	4.514437	0.486455
C	-0.539727	5.617206	-0.536996
C	0.749943	0.061089	4.594556
C	0.724098	-0.958408	5.673257
H	0.865350	-1.960443	5.246594
H	-0.198752	-0.983655	6.255062
H	1.549372	-0.789178	6.377926
C	-2.233005	1.905209	4.594795
C	-3.497123	1.917497	5.495489

Fe^{3+} H_2dapsox LS OPBE

Fe	0.377960	2.233358	2.373437
O	-1.007402	3.477595	1.364822
O	0.001299	5.727797	-1.160729
O	-1.496069	3.471876	4.928508
O	-4.059256	1.101501	5.528233
O	-0.306744	0.789593	1.072463
H	0.285886	0.346385	0.445831
H	-1.094417	1.035106	0.562184
O	0.594046	3.551591	3.593315
H	1.471082	3.655584	3.995680
H	-0.561990	3.512177	4.433337
N	1.853616	1.244954	2.742366
N	1.525314	3.006405	1.112893
N	0.965916	3.963713	0.355932
H	1.421355	4.554524	-0.349314
N	-2.159906	5.530321	-0.404215
H	-2.800271	5.073453	0.226287
H	-2.519582	6.233639	-1.039600
N	-0.394347	1.092940	3.885845
N	-1.620657	1.143702	4.471581
H	-3.517971	0.438369	5.048627
N	-3.906448	3.245289	6.153899
H	-4.817261	3.190360	6.604759
H	-3.395762	4.120075	6.187495
C	2.973458	1.503795	2.016408
C	4.110881	0.717338	2.221073
H	5.027889	0.904056	1.668207
C	4.048853	-0.321417	3.146769
H	4.926848	-0.942351	3.318403
C	2.870960	-0.582325	3.849716
H	2.829890	-1.403724	4.560756
C	1.758501	0.233803	3.627193
C	2.774057	2.586420	1.047991
C	3.804782	3.125183	0.132129
H	4.609378	2.407725	-0.037963
H	3.389680	3.394731	-0.845078
H	4.257058	4.030951	0.565750
C	-0.359175	4.149991	0.531445
C	-0.861894	5.241564	-0.440729
C	0.440860	0.157080	4.284082

C	0.157176	-0.851854	5.328202
H	-0.907100	-0.920445	5.550586
H	0.683557	-0.591884	6.258470
H	0.519787	-1.837327	5.017465
C	-2.034411	2.293190	4.912783
C	-3.393992	2.210843	5.557806

Fe^{3+} H_2dapsox Isomer V OPBE

Fe	-2.111037	3.896554	10.888332
N	-2.820174	5.873945	10.901562
N	-2.734474	4.338815	8.891695
N	-2.636891	3.321020	8.028724
N	-1.953593	-0.184289	7.820268
N	-1.823278	4.756935	13.045071
N	-1.319288	4.074273	14.104303
N	1.215536	2.266125	15.804715
O	-2.050518	2.021569	9.771606
O	-2.513221	1.467378	6.321246
O	0.683328	3.307195	13.212491
O	-0.799371	3.203471	16.387792
O	-0.133966	3.833157	10.937929
O	-3.748732	2.848687	11.786983
H	-4.453376	3.215964	12.340843
C	-3.215050	6.423236	9.732636
C	-3.713848	7.725645	9.675039
C	-3.824388	8.452731	10.856007
C	-3.409985	7.880084	12.052373
C	-2.888806	6.580254	12.044419
C	-3.121299	5.539297	8.553977
C	-3.464745	6.000839	7.189217
C	-2.293176	2.134591	8.549106
C	-2.255287	1.053781	7.445033
C	-2.361390	5.928615	13.263204
C	-2.437548	6.621660	14.574314
H	-3.483906	6.736991	14.889932
H	-2.014420	7.629841	14.490397
H	-1.894148	6.114007	15.370831
C	-0.125551	3.445657	14.135127
C	0.095933	2.931690	15.582557
H	-4.226830	9.465061	10.842510
H	-4.026736	8.166634	8.732505
H	1.896532	2.119169	15.072778
H	-3.486986	8.445474	12.976730
H	1.417581	1.925758	16.738467
H	-3.194410	5.296925	6.400672
H	0.377362	3.293605	10.314666
H	-1.930628	-0.914082	7.116115
H	-1.761208	-0.431873	8.779108
H	-4.545705	6.191124	7.115274
H	0.275355	3.660117	11.896853
H	-2.954750	6.947089	6.970924
H	-4.079524	2.000240	11.455671
H	-2.837228	3.333214	7.023476
H	-1.743561	4.067831	15.049247

Fe^{2+} dapsox Isomer I HS OPBE

Fe	0.098040	2.351092	2.597590
O	-0.699281	4.113779	1.631783
O	-0.053532	6.019132	-1.279457
O	-1.968625	2.534985	3.452064
O	-3.718078	1.388082	6.303442
O	-1.144339	0.996581	1.142215
H	-1.112445	1.430428	0.278797
H	-1.998636	1.267082	1.511431
O	0.746249	4.086914	4.139563
H	0.133522	3.972909	4.878720
H	0.308397	4.749050	3.583167
N	1.881680	1.132165	2.765100
N	1.426862	2.906825	1.027630
N	1.075203	3.875927	0.154642
N	-1.858258	5.932955	0.111293
H	-2.211779	5.565373	0.980312
H	-2.288684	6.729078	-0.329452
N	-0.138530	0.986087	4.313274
N	-1.259856	1.002614	5.054503
N	-4.299488	2.859898	4.657293
H	-5.174318	3.089359	5.098712
H	-3.971950	3.363067	3.848256
C	2.860663	1.297235	1.859017
C	4.032300	0.516009	1.923868
H	4.826891	0.645720	1.195160
C	4.145196	-0.421515	2.934985
H	5.041622	-1.036503	3.007349
C	3.117333	-0.583390	3.866158
H	3.200333	-1.317905	4.661127
C	1.978903	0.219466	3.743109
C	2.594078	2.317880	0.864662
C	3.567322	2.661104	-0.210084
H	3.805399	1.782430	-0.822715
H	3.145800	3.436069	-0.851241
H	4.509873	3.029513	0.214619
C	-0.053005	4.428627	0.567693
C	-0.625544	5.543772	-0.309713
C	0.813027	0.149594	4.630951
C	0.741715	-0.807940	5.768938
H	0.811771	-1.843671	5.413642
H	-0.204381	-0.676703	6.295196
H	1.569645	-0.645493	6.470178
C	-2.132567	1.845850	4.511756
C	-3.457332	1.989705	5.272418

Fe^{2+} dapsox IS OPBE

Fe	-2.159730	4.243528	10.928571
N	-2.923283	5.948974	10.900836
N	-2.702483	4.335089	9.118537
N	-2.495468	3.255835	8.306554
N	-1.308514	-0.001332	9.263005
N	-1.798323	4.823084	12.826189
N	-1.460335	3.973169	13.832861
N	1.110851	1.678312	14.737588
O	-2.026867	2.306312	10.373101
O	-1.913872	0.741025	7.175412
O	0.543847	3.330871	12.756194
O	-1.024386	1.852725	15.562755
O	-0.021214	4.381144	10.473090
O	-3.915333	3.023831	12.268484
H	-3.410406	2.961330	13.108262
C	-3.386504	6.432800	9.701720
C	-3.870853	7.748549	9.625222
C	-3.844232	8.545174	10.772319
C	-3.327511	8.046823	11.976670
C	-2.859802	6.726558	12.022366
C	-3.269437	5.451065	8.655709
C	-3.712246	5.638566	7.244069
C	-2.113477	2.248550	9.069676
C	-1.770768	0.927768	8.379625
C	-2.275277	6.019887	13.146671
C	-2.252770	6.546394	14.543622

H	-3.026843	7.307851	14.695352
H	-1.274878	6.993488	14.782590
H	-2.403642	5.714837	15.244864
C	-0.351511	3.248353	13.656450
C	-0.150677	2.188898	14.766125
H	-4.212612	9.570626	10.727310
H	-4.243587	8.135951	8.677769
H	1.708404	1.936272	13.957497
H	-3.275431	8.676487	12.863494
H	1.341433	0.904044	15.348788
H	-3.408441	4.773312	6.645570
H	0.258844	5.314019	10.445122
H	-0.975573	-0.888442	8.904118
H	-1.142536	0.268702	10.227277
H	-4.807377	5.739509	7.186848
H	0.293111	4.032769	11.389108
H	-3.271671	6.549943	6.812577
H	-3.663295	2.210394	11.786931

Fe^{2+} dapsox LS OPBE

Fe	-2.271668	4.240505	10.960118
N	-2.831028	5.943809	10.925298
N	-2.711209	4.279164	9.183374
N	-2.520100	3.191917	8.398054
N	-1.154456	0.015863	9.333400
N	-1.933045	4.702662	12.851458
N	-1.496606	3.900569	13.845389
N	1.205125	1.685189	14.506433
O	-1.923561	2.283142	10.456495
O	-1.995408	0.658806	7.310611
O	0.404528	3.312389	12.603254
O	-0.737315	1.972295	15.670598
O	-0.357465	4.561427	10.611207
O	-4.047580	3.377520	11.571178
H	-3.952692	3.356683	12.536171
C	-3.268677	6.424499	9.723427
C	-3.730405	7.740923	9.645628
C	-3.740840	8.522681	10.802542
C	-3.305145	8.004860	12.020098
C	-2.847003	6.681936	12.062191
C	-3.177190	5.418605	8.688325
C	-3.558129	5.623873	7.266475
C	-2.088792	2.214364	9.173931
C	-1.749147	0.891242	8.484242
C	-2.330883	5.924468	13.184099
C	-2.225650	6.461404	14.567783
H	-3.050149	7.143618	14.794197
H	-1.285210	7.012188	14.707554
H	-2.223993	5.632688	15.280937
C	-0.391530	3.222971	13.596905
C	-0.018329	2.232544	14.715318
H	-4.099040	9.549710	10.753190
H	-4.081878	8.142570	8.699027
H	1.694913	1.903543	13.652763
H	-3.315167	8.616154	12.918156
H	1.535592	0.970087	15.132738
H	-3.342298	4.722104	6.691510
H	-0.181819	5.498824	10.769058
H	-0.809607	-0.854820	8.963671
H	-0.917931	0.311303	10.267670
H	-4.628628	5.850619	7.174568
H	0.006486	4.064896	11.489655
H	-3.005121	6.464559	6.828243
H	-3.763193	2.484661	11.297042

Fe^{2+} dapsox Isomer V OPBE

Fe	-2.054739	4.022128	10.958318
N	-2.845642	5.921249	10.913261
N	-2.793513	4.292343	9.019536
N	-2.708844	3.278285	8.137097
N	-1.420943	-0.032455	8.623267
N	-1.827283	4.837157	13.018625
N	-1.466928	4.097082	14.079726
N	1.126725	1.912075	15.106803
O	-1.893259	2.171485	10.013930
O	-2.325983	0.889188	6.740189
O	0.483416	3.355562	12.995694
O	-0.997461	2.095182	15.932542
O	0.042113	4.463515	10.749490
O	-3.694511	2.710164	12.175404
H	-3.497226	1.833339	11.818086
C	-3.306516	6.409384	9.736789
C	-3.723967	7.742266	9.628367
C	-3.653278	8.560392	10.746801
C	-3.192307	8.041934	11.957121
C	-2.798537	6.703503	12.013533
C	-3.312835	5.441567	8.656171
C	-3.854678	5.728971	7.298703
C	-2.210783	2.226243	8.766736
C	-1.997277	0.972998	7.913574
C	-2.301058	6.041192	13.217103
C	-2.331972	6.694077	14.557462
H	-3.271839	7.230448	14.720804
H	-1.510739	7.415509	14.664070
H	-2.207224	5.932248	15.330162
C	-0.377612	3.353526	13.929036
C	-0.142397	2.390915	15.108289
H	-3.962013	9.602759	10.683100
H	-4.093930	8.127433	8.682146
H	1.691924	2.094545	14.290928
H	-3.135950	8.671695	12.840421
H	1.367205	1.170399	15.743955
H	-3.763114	4.840060	6.673345
H	0.187289	5.416447	10.796333
H	-1.122951	-0.856636	8.127219
H	-1.066319	0.163559	9.546222
H	-4.910742	6.021152	7.351159
H	0.304638	4.105076	11.673574
H	-3.307695	6.552069	6.822232
H	-3.374289	2.675468	13.089599

Fe^{2+} Hdapsox Isomer I HS OPBE

Fe	0.044708	2.269961	2.732658
O	-0.961946	4.206062	1.395372
O	0.403248	5.869949	-1.397597
O	-1.845509	2.529709	3.617385
O	-3.650893	1.202674	6.360879
O	-1.103974	1.001206	1.184142
H	-2.031281	1.085766	1.448850
H	-0.917760	0.057208	1.280355
O	0.758659	4.005955	4.062951
H	1.280487	3.684559	4.810955
H	-0.038957	4.370194	4.472872
N	1.845329	1.130440	2.766901
N	1.410256	2.969074	1.083838
N	1.013439	3.959766	0.277621
H	1.549467	4.329130	-0.505318
N	-1.634068	6.240093	-0.400809
H	-2.253503	5.957050	0.342535
H	-1.901498	6.978378	-1.033919
N	-0.109069	0.874408	4.348287
N	-1.219704	0.858749	5.102771
N	-4.220452	2.806796	4.839121

H	-5.120845	2.961654	5.263856
H	-3.933671	3.338035	4.033808
C	2.841001	1.336938	1.876070
C	4.019975	0.588866	1.907758
H	4.816189	0.759693	1.190812
C	4.170904	-0.391988	2.883436
H	5.081991	-0.985524	2.926998
C	3.149723	-0.604063	3.797128
H	3.246988	-1.364299	4.566747
C	1.990615	0.176988	3.718538
C	2.568904	2.399236	0.904192
C	3.511170	2.802095	-0.179612
H	4.428102	2.216013	-0.179938
H	3.044466	2.677464	-1.165647
H	3.796808	3.857061	-0.074189
C	-0.193132	4.534078	0.492697
C	-0.449441	5.634217	-0.546725
C	0.862668	0.039234	4.625877
C	0.832786	-0.947265	5.740924
H	0.926464	-1.972177	5.361365
H	-0.106817	-0.859970	6.286652
H	1.664023	-0.778833	6.436495
C	-2.060701	1.765975	4.629546
C	-3.392379	1.882342	5.382414

Fe^{2+} Hdapsox IS OPBE

Fe	0.424730	2.320417	2.386932
O	-0.820842	3.439866	1.305662
O	-0.247743	5.884603	-1.208351
O	-1.832852	3.542080	4.645520
O	-3.809117	0.792360	5.662058
O	-0.968808	0.711054	1.209125
H	-0.494545	0.177326	0.544196
H	-1.397789	1.422984	0.690581
O	0.614011	4.148727	3.652781
H	1.320601	4.164643	4.323951
H	-0.242345	4.052739	4.154591
N	1.859439	1.158445	2.657613
N	1.605845	2.993201	1.096485
N	1.189951	4.014930	0.296836
N	-2.064212	5.539792	0.157079
H	-2.438792	5.024724	0.945763
H	-2.602413	6.279202	-0.281586
N	-0.231566	1.214164	4.045602
N	-1.470044	1.239605	4.625145
H	-1.972653	0.384544	4.907241
N	-4.321273	3.043826	5.747726
H	-5.233386	2.907854	6.172428
H	-3.973449	3.979330	5.558316
C	2.988289	1.366212	1.900785
C	4.115053	0.552321	2.092976
H	5.010958	0.717933	1.495598
C	4.072228	-0.452551	3.059456
H	4.940321	-1.091486	3.219643
C	2.923040	-0.631728	3.842397
H	2.901341	-1.394551	4.618673
C	1.817198	0.196894	3.627022
C	2.822317	2.458671	0.974882
C	3.845427	2.930689	0.000813
H	4.078746	2.142538	-0.731543
H	3.471923	3.809130	-0.534680
H	4.781648	3.192287	0.515952
C	-0.101912	4.190542	0.503827
C	-0.798494	5.305115	-0.282007
C	0.562407	0.203991	4.368122
C	0.200430	-0.829744	5.383735
H	-0.554164	-1.526735	4.982042
H	-0.224608	-0.363304	6.284465
H	1.067648	-1.426411	5.680131
C	-2.182022	2.373595	4.853671
C	-3.546538	1.983463	5.469991

Fe^{2+} Hdapsox LS OPBE

Fe	0.396575	2.177035	2.480675
O	-1.044005	3.674707	1.509091
O	-0.130797	5.729500	-1.211353
O	-1.415600	3.391528	4.892202
O	-4.191010	1.222404	4.938234
O	-0.551159	0.867152	1.175442
H	-0.149312	-0.011675	1.250325
H	-1.441919	0.743191	1.544281
O	0.756004	3.503115	3.832470
H	0.817311	4.380157	3.429883
H	-0.262070	3.462323	4.377109
N	1.864343	1.200896	2.729968
N	1.443378	2.939094	1.133868
N	0.896349	3.888775	0.341963
H	1.362385	4.363150	-0.428318
N	-2.159123	5.679277	-0.136585
H	-2.707695	5.258023	0.597106
H	-2.567731	6.390550	-0.724601
N	-0.266816	1.102708	3.936957
N	-1.523002	1.100072	4.409934
N	-3.902331	3.265140	5.916268
H	-4.858158	3.304190	6.232775
H	-3.277039	4.034150	6.092539
C	2.951306	1.451263	1.942439
C	4.111674	0.694735	2.122207
H	4.989425	0.871024	1.507982
C	4.128041	-0.290841	3.106728
H	5.028258	-0.882729	3.258283
C	3.008327	-0.523582	3.901656
H	3.027530	-1.284967	4.675953
C	1.859172	0.246312	3.694942
C	2.683037	2.503528	0.981028
C	3.628809	3.012026	-0.049157
H	4.589767	2.500667	0.003522
H	3.235523	2.861398	-1.063581
H	3.822707	4.084882	0.082171
C	-0.388819	4.207638	0.600801
C	-0.893684	5.300065	-0.352574
C	0.583829	0.191971	4.382254
C	0.258606	-0.758319	5.475710
H	0.757282	-1.720660	5.333093
H	-0.822919	-0.909433	5.524587
H	0.577076	-0.354067	6.446208
C	-2.012309	2.260825	4.801520
C	-3.488733	2.179220	5.225570

Fe^{2+} Hdapsox Isomer V OPBE

Fe	-1.992865	4.109737	11.030996
N	-2.829908	5.988481	10.881946
N	-2.758265	4.311717	9.065912
N	-2.634183	3.235712	8.273270
N	-1.586951	-0.176241	8.400963
N	-1.765878	4.961129	12.990911
N	-1.417991	4.203487	14.027788
N	0.965948	1.817083	15.118878
O	-1.739332	2.106395	10.025632
O	-2.450819	1.124761	6.716668
O	0.515554	3.390584	12.966991
O	-1.239455	2.049282	15.677856
O	0.062430	4.416912	10.728503

O	-3.756868	3.004516	12.051031
H	-4.533027	3.569406	12.166392
C	-3.318636	6.434830	9.703443
C	-3.821047	7.735030	9.582027
C	-3.804240	8.559590	10.699869
C	-3.305756	8.086174	11.910497
C	-2.818119	6.776843	11.979596
C	-3.277278	5.438480	8.641084
C	-3.763452	5.652524	7.249397
C	-2.111808	2.131528	8.843753
C	-2.060460	0.955508	7.866909
C	-2.284980	6.152506	13.186433
C	-2.350248	6.794216	14.527378
H	-3.306784	7.301531	14.685406
H	-1.551744	7.537672	14.649810
H	-2.213818	6.031626	15.297457
C	-0.364702	3.396184	13.874546
C	-0.266173	2.355097	15.003057
H	-4.185997	9.576292	10.630139
H	-4.219103	8.101342	8.641262
H	1.682457	2.057349	14.452871
H	-3.291885	8.727193	12.786758
H	1.117003	1.076070	15.784889
H	-4.585765	4.965416	7.009913
H	0.321882	5.346025	10.680726
H	-1.511443	-1.001250	7.824806
H	-1.276368	-0.201574	9.359934
H	-4.130728	6.665424	7.091659
H	0.356425	4.085568	11.669523
H	-2.958958	5.480653	6.522468
H	-3.497278	2.783495	12.960025
H	-2.917764	3.177656	7.298178

Fe^{2+} H_2dapsox Isomer I HS OPBE

Fe	0.030766	2.392155	2.620676
O	-0.919696	4.045648	1.379306
O	0.358533	5.884780	-1.342693
O	-1.993286	2.725191	3.658080
O	-3.515431	1.032521	6.346517
O	-1.114579	0.929633	1.302730
H	-0.711793	0.300413	0.690490
H	-1.955466	1.178106	0.896890
O	0.793969	4.028903	3.982803
H	1.633001	4.041570	4.460339
H	0.218531	4.649152	4.448665
N	1.816075	1.163736	2.756918
N	1.453401	2.982613	1.041290
N	1.043771	3.977860	0.246958
H	1.569757	4.409670	-0.513269
N	-1.706329	6.161939	-0.370588
H	-2.336545	5.856196	0.353944
H	-1.982536	6.911137	-0.990279
N	-0.175524	0.934346	4.310291
N	-1.332034	0.996497	4.975629
H	-1.623072	0.402157	5.752271
N	-4.415216	2.778762	5.150756
H	-5.272823	2.805493	5.684824
H	-4.276111	3.433553	4.397275
C	2.831207	1.349071	1.889165
C	4.007364	0.592759	1.957528
H	4.821070	0.759557	1.257883
C	4.123927	-0.378999	2.939628
H	5.026994	-0.981770	3.014476
C	3.070665	-0.576888	3.827114
H	3.146081	-1.338863	4.597195
C	1.928737	0.216575	3.709549
C	2.607176	2.398015	0.885409
C	3.623798	2.710972	-0.157336
H	3.975085	1.792193	-0.638603
H	3.253563	3.362066	-0.950863
H	4.498091	3.198937	0.293366
C	-0.185097	4.477206	0.478292
C	-0.501680	5.604281	-0.515633
C	0.762817	0.087275	4.605294
C	0.735128	-0.924417	5.697489
H	0.774207	-1.937736	5.278376
H	-0.148928	-0.864903	6.333466
H	1.609764	-0.806439	6.347511
C	-2.216512	1.937896	4.587850
C	-3.478422	1.878083	5.459961

Fe^{2+} H_2dapsox IS OPBE

Fe	0.087457	2.364357	2.624289
O	-0.850100	4.191992	1.522727
O	0.294154	5.750551	-1.423879
O	-2.174276	2.631175	3.512480
O	-3.397796	1.071253	6.428037
O	-0.864567	1.188860	1.274359
H	-0.684675	0.241935	1.376172
H	-1.822091	1.278833	1.406870
O	0.684655	3.750598	3.985364
H	1.643571	3.842821	4.088375
H	0.366638	4.632413	3.736065
N	1.850335	1.174116	2.766861
N	1.447724	2.981443	1.088372
N	1.021233	3.949391	0.266981
H	1.482094	4.262242	-0.589018
N	-1.680661	6.199439	-0.335749
H	-2.277114	5.967160	0.443253
H	-1.975480	6.905903	-0.996124
N	-0.181243	0.999570	4.222812
N	-1.314997	1.080857	4.931880
H	-1.519274	0.561142	5.787245
N	-4.507360	2.640606	5.168096
H	-5.331342	2.643476	5.753708
H	-4.465957	3.246888	4.363729
C	2.854164	1.343400	1.886252
C	3.996237	0.538139	1.922323
H	4.800754	0.665031	1.204463
C	4.086343	-0.447020	2.898720
H	4.964526	-1.087711	2.948377
C	3.051762	-0.611816	3.810622
H	3.122229	-1.381965	4.571962
C	1.932643	0.221493	3.714966
C	2.613089	2.417963	0.914694
C	3.581862	2.786262	-0.154284
H	3.362720	2.240002	-1.082769
H	3.561033	3.857316	-0.379263
H	4.606314	2.545695	0.133730
C	-0.170982	4.515147	0.538369
C	-0.515847	5.574646	-0.521015
C	0.754513	0.159359	4.586194
C	0.626662	-0.744229	5.763419
H	-0.269237	-1.374127	5.685709
H	0.548784	-0.163238	6.692797
H	1.480680	-1.410199	5.872614
C	-2.283039	1.926188	4.520428
C	-3.482810	1.844757	5.480455

Fe^{2+} H_2dapsox LS OPBE

Fe	0.384991	2.201685	2.378273
O	-0.985072	3.578215	1.472716
O	-0.075548	5.749137	-1.156163
O	-1.590720	3.517333	4.808418
O	-3.913460	0.934343	5.394705
O	-0.389851	0.904074	0.985462
H	-0.283489	-0.039120	1.178016
H	-1.345512	1.036865	0.890213
O	0.783388	3.581834	3.739873
H	0.959335	4.461333	3.375229
H	-0.110186	3.652404	4.213434
N	1.834807	1.197471	2.714431
N	1.498543	2.944176	1.094994
N	0.948393	3.915550	0.332006
H	1.396601	4.430419	-0.426360
N	-2.134887	5.659906	-0.137224
H	-2.703948	5.225223	0.572227
H	-2.531327	6.392391	-0.710937
N	-0.318629	1.141604	3.887863
N	-1.558076	1.234182	4.453474
H	-2.160654	0.425036	4.640989
N	-4.145857	3.160366	5.921515
H	-5.058333	3.049370	6.341522
H	-3.699247	4.064986	5.931858
C	2.943310	1.424859	1.958000
C	4.085230	0.651044	2.159938
H	4.979717	0.818723	1.565776
C	4.061005	-0.346643	3.134725
H	4.942787	-0.962624	3.298353
C	2.920036	-0.556792	3.903187
H	2.905636	-1.334398	4.661577
C	1.799761	0.249305	3.679186
C	2.731836	2.496631	0.985093
C	3.776967	2.972500	0.045344
H	4.103125	2.154500	-0.609402
H	3.452515	3.796242	-0.592713
H	4.658249	3.313675	0.603254
C	-0.346543	4.180008	0.582287
C	-0.866065	5.295552	-0.337840
C	0.516735	0.240530	4.376445
C	0.209667	-0.676111	5.501840
H	-0.201286	-1.626926	5.132234
H	-0.520233	-0.240309	6.189135
H	1.111920	-0.912458	6.069741
C	-2.107666	2.398298	4.863070
C	-3.510084	2.093891	5.434836

Mn^{2+} dapsox Isomer I HS OPBE

Mn	-1.918175	3.899812	11.206758
N	-2.849256	5.985787	11.004131
N	-2.676259	4.255556	9.089381
N	-2.546381	3.283586	8.175391
N	-1.292163	-0.058553	8.460498
N	-1.838474	5.048464	13.191361
N	-1.262506	4.454229	14.244461
N	-0.124077	3.080161	16.216296
O	-1.793888	2.021483	9.995290
O	-2.108552	1.015877	6.618174
O	-0.724716	2.772680	12.715360
O	0.579302	1.457840	14.776250
O	0.429906	4.396957	10.674930
O	-3.971947	2.646718	11.749061
H	-3.610990	1.916610	11.219759
C	-3.335326	6.370006	9.814101
C	-3.912731	7.640254	9.650478
C	-3.971122	8.485900	10.749068
C	-3.466672	8.075952	11.976481
C	-2.899849	6.795340	12.071795
C	-3.235140	5.381968	8.733247
C	-3.746704	5.662013	7.359887
C	-2.062748	2.186360	8.760007
C	-1.828673	1.002355	7.808476
C	-2.315594	6.257491	13.308108
C	-2.276233	7.065162	14.562877
H	-3.287998	7.309025	14.910443
H	-1.744464	8.012528	14.410493
H	-1.766497	6.501833	15.344390
C	-0.727951	3.277557	13.869103
C	-0.021458	2.498571	14.994898
H	-4.414308	9.476282	10.648795
H	-4.304033	7.956106	8.687916
H	-0.668019	3.923804	16.309566
H	-3.512164	8.734263	12.839069
H	0.264509	2.609044	17.017049
H	-3.565532	4.792832	6.726085
H	0.683020	5.226367	11.100953
H	-1.020669	-0.870317	7.931032
H	-1.028811	0.047010	9.428147
H	-4.823074	5.875636	7.370586
H	0.710044	3.722340	11.314968
H	-3.243819	6.532744	6.921019
H	-4.679334	2.994473	11.190012

Mn^{2+} dapsox IS OPBE

Mn	0.184111	2.063897	2.848826
O	-1.257492	3.343533	0.159103
O	-0.020426	6.654872	-0.034778
O	-1.550290	2.745395	3.623346
O	-3.729686	1.677463	6.234397
O	-1.000054	1.049285	1.269953
H	-0.434007	0.463010	0.736016
H	-1.110910	1.910874	0.713019
O	0.694821	4.334260	3.653201
H	-0.228921	4.506379	3.924308
H	0.808252	4.843105	2.820461
N	1.806895	1.065291	2.832074
N	1.252141	2.962724	1.246103
N	0.917297	4.131553	0.633577
N	-1.944974	5.688137	-0.829394
H	-2.483890	4.827597	-0.850705
H	-2.342737	6.576427	-1.109376
N	-0.064317	0.895609	4.378826
N	-1.219552	0.990895	5.112589
N	-3.936950	3.294765	4.618917
H	-4.891218	3.500225	4.891123
H	-3.557783	3.650244	3.746859
C	2.777180	1.327109	1.892933
C	3.929062	0.546618	1.845634
H	4.692110	0.750140	1.095978
C	4.097345	-0.503372	2.772963
H	4.996770	-1.118146	2.738276
C	3.120593	-0.748835	3.731679
H	3.237858	-1.549478	4.461699
C	1.962509	0.048859	3.761382
C	2.451445	2.450646	1.029650
C	3.385207	3.010569	0.006568
H	3.145818	2.622787	-0.995965
H	3.255309	4.100143	-0.036168
H	4.428837	2.765648	0.233012
C	-0.350025	4.237216	0.228342
C	-0.726147	5.665982	-0.224551
C	0.860644	-0.036289	4.660626

C	0.726020	-1.017610	5.777514
H	0.762918	-2.050574	5.400369
H	-0.228923	-0.860352	6.289292
H	1.543016	-0.897897	6.505089
C	-1.931701	1.982584	4.626073
C	-3.289400	2.276629	5.258001

Mn^{2+} dapsox LS OPBE

Mn	0.259729	2.178785	2.911191
O	-1.209575	3.194117	0.155225
O	-0.156734	6.550150	-0.235223
O	-1.466345	2.880855	3.644012
O	-3.703523	1.766271	6.155595
O	-0.851218	1.182938	1.560668
H	-0.254073	0.590244	1.083945
H	-0.992966	2.002668	0.896989
O	0.994135	3.750689	4.126003
H	0.130391	4.052536	4.457065
H	1.253481	4.434397	3.487100
N	1.792169	1.120084	2.813512
N	1.214412	3.035745	1.415492
N	0.806421	4.193960	0.835432
N	-1.982137	5.414606	-1.002850
H	-2.452734	4.523312	-1.017314
H	-2.367594	6.224619	-1.458432
N	-0.078557	0.940083	4.306410
N	-1.246881	1.017696	4.997947
N	-3.943093	3.320277	4.501790
H	-4.894370	3.514724	4.768545
H	-3.567951	3.690105	3.642787
C	2.751950	1.395554	1.882251
C	3.888000	0.581904	1.781409
H	4.643710	0.793731	1.030284
C	4.025769	-0.497122	2.649414
H	4.903162	-1.138151	2.580696
C	3.044788	-0.763928	3.605364
H	3.144149	-1.603006	4.288398
C	1.919510	0.060745	3.677643
C	2.406364	2.545903	1.094391
C	3.265442	3.128373	0.028777
H	3.153688	2.578352	-0.915879
H	2.972688	4.164832	-0.155619
H	4.322274	3.092674	0.311122
C	-0.393530	4.167422	0.282253
C	-0.807086	5.519165	-0.335677
C	0.791415	-0.034898	4.557391
C	0.606125	-1.077510	5.600414
H	0.634591	-2.082744	5.160545
H	-0.353342	-0.939728	6.100499
H	1.404478	-1.025341	6.352479
C	-1.903313	2.064163	4.561199
C	-3.272859	2.346148	5.170228

Mn^{2+} dapsox Isomer V OPBE

Mn	-2.014708	3.889692	10.939755
N	-2.867451	5.932733	10.915527
N	-2.838227	4.287117	8.932920
N	-2.817973	3.309153	8.018085
N	-1.528434	-0.029793	8.196236
N	-1.811441	4.863310	13.062853
N	-1.497964	4.133976	14.147567
N	1.144764	2.220323	15.514167
O	-1.943955	2.049965	9.784510
O	-2.640474	0.991100	6.485285
O	0.657434	3.660315	13.344973
O	-1.095463	2.086856	15.961740
O	0.176795	4.138720	10.889165
O	-3.264596	2.456839	12.363374
H	-3.077373	1.536325	12.139222
C	-3.294229	6.418933	9.736079
C	-3.673545	7.763047	9.615082
C	-3.591925	8.580071	10.735960
C	-3.154008	8.063402	11.948615
C	-2.792824	6.709000	12.006818
C	-3.340239	5.454254	8.629805
C	-3.916336	5.797829	7.298313
C	-2.318299	2.202689	8.575273
C	-2.189766	1.006663	7.621061
C	-2.322226	6.052275	13.232725
C	-2.425799	6.719294	14.563857
H	-3.389828	7.222611	14.689457
H	-1.634795	7.470140	14.692445
H	-2.301825	5.969142	15.348329
C	-0.323751	3.517240	14.137511
C	-0.159732	2.533071	15.308948
H	-3.873934	9.630089	10.663827
H	-4.023732	8.159664	8.666731
H	1.800233	2.497940	14.797916
H	-3.088183	8.696720	12.828480
H	1.366867	1.464163	16.141468
H	-3.890823	4.915511	6.657327
H	0.448484	5.037686	10.667127
H	-1.308546	-0.836441	7.635967
H	-1.123669	0.091902	9.110762
H	-4.952900	6.144010	7.391969
H	0.412984	4.034409	11.882431
H	-3.343311	6.598773	6.813794
H	-2.908924	2.579886	13.260998

Mn^{2+} Hdapsox Isomer I HS OPBE

Mn	-0.055436	2.382594	2.738270
O	-1.028772	4.104755	1.176538
O	0.445190	5.854956	-1.507063
O	-1.843815	2.747773	3.878107
O	-3.748916	1.003388	6.297637
O	-1.268564	0.921966	1.267687
H	-1.511918	0.106908	1.728400
H	-2.120212	1.309895	1.024508
O	0.731898	4.163042	4.137723
H	-0.040027	4.304633	4.705087
H	1.435520	3.926713	4.757111
N	1.880394	1.193172	2.793920
N	1.434096	3.020935	1.044936
N	1.048193	4.000821	0.223621
N	-1.674339	6.121337	-0.663461
H	-2.330634	5.822489	0.041048
H	-1.927484	6.847546	-1.316497
N	-0.170679	0.864343	4.339732
N	-1.280158	0.828386	5.088611
N	-4.210192	2.905633	5.123500
H	-5.118878	3.005820	5.546721
H	-3.886257	3.564292	4.435039
C	2.858122	1.393443	1.900426
C	3.993629	0.580550	1.863033
H	4.781647	0.729067	1.131829
C	4.088983	-0.457975	2.786685
H	4.960781	-1.110353	2.781422
C	3.075711	-0.659569	3.708637
H	3.143969	-1.466484	4.432142
C	1.955642	0.189713	3.685413
C	2.621693	2.503197	0.950216
C	3.647778	2.944952	-0.040290

H	3.440991	2.521816	-1.032735
H	3.664181	4.036334	-0.136591
H	4.653389	2.640692	0.249348
C	-0.209635	4.491582	0.342409
C	-0.452381	5.578558	-0.716791
C	0.816955	0.047241	4.602389
C	0.812045	-0.949278	5.709619
H	0.893975	-1.971649	5.319729
H	-0.118678	-0.866124	6.271588
H	1.655701	-0.790552	6.392297
C	-2.086874	1.833912	4.741305
C	-3.433127	1.854970	5.483673
H	1.605263	4.397094	-0.532283

Mn^{2+} Hdapsox IS OPBE

Mn	0.380331	2.349273	2.398360
O	-0.745006	3.667334	1.408574
O	-0.173825	5.903471	-1.303277
O	-1.902008	3.416976	4.502693
O	-3.821456	0.693962	5.698477
O	-1.268862	0.946263	1.322521
H	-0.949374	0.226025	0.747233
H	-1.675932	1.594737	0.714144
O	0.648132	4.020614	3.866005
H	1.262790	3.861827	4.606075
H	-0.270408	3.962309	4.256356
N	1.873633	1.199891	2.692826
N	1.579963	2.911711	0.961081
N	1.172829	3.908507	0.119931
N	-1.936623	5.723908	0.160087
H	-2.274275	5.303178	1.018706
H	-2.421949	6.513828	-0.251863
N	-0.237255	1.138907	4.064473
N	-1.463502	1.142560	4.670012
H	-1.927906	0.281624	4.991855
N	-4.375493	2.936121	5.645131
H	-5.291583	2.806101	6.062664
H	-4.050016	3.863662	5.389510
C	2.982891	1.354710	1.877669
C	4.115927	0.568498	2.070126
H	4.982899	0.707349	1.425020
C	4.125042	-0.393701	3.090897
H	5.005866	-1.014057	3.251376
C	2.999067	-0.554891	3.897695
H	2.996043	-1.304921	4.686910
C	1.869021	0.251547	3.694472
C	2.793323	2.374407	0.876370
C	3.807847	2.793522	-0.129357
H	4.200395	1.921721	-0.671981
H	3.361424	3.496208	-0.839546
H	4.658235	3.286879	0.366285
C	-0.054654	4.248775	0.450623
C	-0.713872	5.387698	-0.334242
C	0.643691	0.215641	4.450616
C	0.364551	-0.755792	5.552472
H	-0.357416	-1.525065	5.232227
H	-0.066479	-0.240575	6.423617
H	1.271168	-1.273921	5.876757
C	-2.221582	2.255510	4.808500
C	-3.577595	1.875478	5.435458

Mn^{2+} Hdapsox LS OPBE

Mn	0.346882	2.290669	2.379894
O	-0.829125	3.548842	1.436517
O	-0.343859	5.726262	-1.313144
O	-1.625566	3.498882	4.895093
O	-3.932764	0.873864	5.398118
O	-0.530020	0.909018	1.061070
H	0.145302	0.497772	0.501047
H	-1.036040	1.475909	0.455506
O	0.730106	3.827475	3.666591
H	1.463205	3.595614	4.253932
H	-0.086492	3.791194	4.241363
N	1.841774	1.217019	2.717825
N	1.542900	2.968466	1.088205
N	1.115972	3.953602	0.258137
N	-2.093270	5.560793	0.146494
H	-2.440210	5.172658	1.007996
H	-2.613828	6.283714	-0.325455
N	-0.285404	1.168804	3.922033
N	-1.532634	1.228071	4.472293
H	-2.121800	0.400078	4.574888
N	-4.167319	3.093832	5.933189
H	-5.087119	2.979935	6.331750
H	-3.723275	3.999096	5.929441
C	2.965027	1.417133	1.955409
C	4.087086	0.612362	2.140517
H	4.978755	0.777472	1.542824
C	4.042683	-0.407912	3.094276
H	4.910050	-1.047751	3.243126
C	2.899606	-0.610745	3.854230
H	2.865545	-1.405764	4.592849
C	1.790961	0.226402	3.659210
C	2.774063	2.482917	1.001508
C	3.800111	2.970343	0.047052
H	4.139420	2.159405	-0.609399
H	3.392678	3.773287	-0.567789
H	4.679429	3.346076	0.585100
C	-0.146152	4.190240	0.527547
C	-0.858710	5.251528	-0.316447
C	0.533176	0.205195	4.352109
C	0.177880	-0.774649	5.413549
H	-0.362812	-1.636934	4.997310
H	-0.459709	-0.320962	6.178802
H	1.070657	-1.160030	5.908800
C	-2.115416	2.363788	4.899424
C	-3.521282	2.030192	5.440067

Mn^{2+} Hdapsox Isomer V OPBE

Mn	0.147925	2.578596	2.346189
O	-0.720815	3.911342	0.954443
O	0.358564	5.731400	-1.867318
O	-2.084238	3.252707	4.888267
O	-3.581909	0.399770	6.317882
O	-1.355193	1.068367	1.232641
H	-0.947316	0.316228	0.782579
H	-1.707740	1.608669	0.510379
O	0.276782	4.212109	3.877973
H	1.021264	4.206001	4.493331
H	-0.514667	4.012551	4.424066
N	1.794940	1.157344	2.678575
N	1.666968	3.024518	0.889311
N	1.397761	3.949942	-0.035030
N	-1.519610	5.960767	-0.588471
H	-1.999090	5.689449	0.253767
H	-1.875749	6.711267	-1.158653
N	-0.305492	1.099494	4.291476
N	-1.467003	1.021406	4.965235
H	-1.817950	0.162294	5.393930
N	-4.387529	2.547895	6.284744

H	-5.219899	2.323384	6.808687
H	-4.217260	3.495936	5.986728
C	2.914510	1.391226	1.958723
C	4.089627	0.669284	2.221068
H	4.988403	0.849661	1.639016
C	4.087341	-0.274187	3.234756
H	4.992771	-0.834412	3.462578
C	2.924851	-0.509389	3.963601
H	2.928095	-1.240470	4.765611
C	1.784133	0.236646	3.654877
C	2.816451	2.401708	0.900106
C	3.924561	2.665897	-0.058678
H	4.216471	1.754435	-0.593944
H	3.605244	3.415132	-0.784052
H	4.813622	3.042812	0.462446
C	0.131243	4.352622	0.104477
C	-0.313390	5.427211	-0.896342
C	0.515178	0.091904	4.399725
C	0.224261	-1.116321	5.230049
H	-0.725066	-1.575793	4.923887
H	0.137783	-0.857013	6.293271
H	0.986153	-1.886857	5.126329
C	-2.274619	2.081593	5.209809
C	-3.503027	1.585548	6.004303

Mn^{2+} H_2dapsox Isomer I HS OPBE

Mn	-0.075130	2.443815	2.620550
O	-0.894033	4.161516	1.305554
O	0.489658	5.878532	-1.444086
O	-2.079142	2.664580	3.715950
O	-3.465642	0.914990	6.442253
O	-1.227988	0.919701	1.230153
H	-2.096268	1.094798	0.844367
H	-0.856505	0.206135	0.695569
O	0.705128	4.081402	4.137206
H	1.624883	4.288996	4.347690
H	0.220304	4.897505	4.317870
N	1.832596	1.145845	2.745354
N	1.483282	3.005049	0.999549
N	1.089044	3.989875	0.190948
H	1.615925	4.398339	-0.583447
N	-1.573371	6.253152	-0.500130
H	-2.224759	5.978140	0.218325
H	-1.818689	6.995087	-1.140987
N	-0.178065	0.908744	4.339639
N	-1.320621	0.957189	5.025855
H	-1.585413	0.369855	5.818603
N	-4.438679	2.660117	5.305652
H	-5.282712	2.651575	5.861468
H	-4.343921	3.321913	4.551521
C	2.841592	1.345949	1.883005
C	4.029239	0.610723	1.962398
H	4.848358	0.780618	1.270209
C	4.150648	-0.349234	2.958761
H	5.064335	-0.934773	3.046146
C	3.099627	-0.559088	3.842268
H	3.188454	-1.311177	4.620497
C	1.942941	0.215648	3.706280
C	2.618439	2.393816	0.855809
C	3.641172	2.665248	-0.193002
H	3.967682	1.731367	-0.662601
H	3.285442	3.316625	-0.992816
H	4.528944	3.136174	0.249412
C	-0.128644	4.533987	0.405661
C	-0.389417	5.647329	-0.620838
C	0.771769	0.067780	4.608132
C	0.772180	-0.962627	5.684488
H	0.957729	-1.956777	5.261050
H	-0.163518	-1.018967	6.242055
H	1.573035	-0.760970	6.406848
C	-2.241166	1.874861	4.657683
C	-3.474071	1.775142	5.568258

Mn^{2+} H_2dapsox IS OPBE

Mn	0.168515	2.088886	2.853885
O	-0.502507	5.220874	1.849902
O	-0.095985	5.204459	-1.649613
O	-1.814640	2.458972	3.381882
O	-3.566891	1.164486	6.161844
O	-1.111201	0.714180	1.033929
H	-2.053227	0.790247	0.833894
H	-0.872311	-0.159710	0.698495
O	0.560285	3.962736	4.049392
H	1.459842	4.224986	4.287676
H	0.244339	4.645807	3.417432
N	1.791571	1.128972	2.844911
N	1.149269	2.937070	1.212795
N	0.630673	3.846997	0.363284
H	0.776196	3.816567	-0.654871
N	-1.255022	6.745213	-0.398474
H	-1.517769	7.034435	0.531506
H	-1.518540	7.311434	-1.193020
N	-0.062415	0.877736	4.347986
N	-1.252722	0.983225	4.984708
H	-1.526184	0.471499	5.822286
N	-4.354222	2.734752	4.675767
H	-5.247900	2.830501	5.139178
H	-4.149184	3.312237	3.875458
C	2.726198	1.382631	1.876747
C	3.928136	0.685944	1.875248
H	4.669806	0.869036	1.103756
C	4.182025	-0.263769	2.869829
H	5.124600	-0.806502	2.874619
C	3.229954	-0.513157	3.844402
H	3.420554	-1.250486	4.618826
C	2.017802	0.188339	3.824769
C	2.324647	2.403406	0.929045
C	3.132182	2.806673	-0.249834
H	2.747326	2.331736	-1.164080
H	3.092687	3.891136	-0.398726
H	4.177876	2.518501	-0.148859
C	-0.151351	4.901361	0.718038
C	-0.511985	5.654876	-0.583503
C	0.914238	0.052487	4.724562
C	0.819808	-0.842977	5.905095
H	1.727393	-1.430613	6.039816
H	-0.015690	-1.548373	5.801983
H	0.665124	-0.264702	6.826168
C	-2.122037	1.825721	4.424778
C	-3.451422	1.888859	5.182120

Mn^{2+} H_2dapsox LS OPBE

Mn	0.321994	2.226277	2.384849
O	-0.938042	3.506625	1.348769
O	0.035242	5.892472	-1.062869
O	-1.726784	3.548919	4.650685
O	-3.795916	0.839374	5.544297
O	-0.606132	0.758724	1.231091
H	-0.059607	0.011029	0.948376
H	-1.035374	1.082847	0.425560
O	0.649120	3.829576	3.576333
H	1.350909	3.686448	4.228457
H	-0.210102	3.828704	4.104800

N	1.835777	1.192270	2.704742
N	1.524064	2.915284	1.079385
N	1.023660	3.929516	0.331968
H	1.549010	4.513163	-0.317475
N	-2.058383	5.690953	-0.130742
H	-2.642631	5.202283	0.529598
H	-2.448055	6.458831	-0.661030
N	-0.253780	1.180849	3.998279
N	-1.493052	1.248628	4.546103
H	-2.045264	0.420554	4.801846
N	-4.235902	3.075024	5.846664
H	-5.129665	2.919239	6.292151
H	-3.883731	4.015495	5.752281
C	2.946694	1.380903	1.920339
C	4.079287	0.591208	2.116247
H	4.966478	0.743737	1.508736
C	4.064522	-0.392270	3.102180
H	4.940691	-1.018008	3.257003
C	2.939003	-0.564593	3.900413
H	2.932176	-1.320639	4.679764
C	1.822377	0.250145	3.692963
C	2.749908	2.432783	0.946024
C	3.756209	2.925718	-0.028920
H	4.537963	2.183760	-0.198378
H	3.306548	3.143653	-1.004237
H	4.244462	3.841190	0.334463
C	-0.269061	4.196172	0.538688
C	-0.773828	5.368456	-0.309254
C	0.578384	0.246968	4.434793
C	0.266798	-0.688266	5.544830
H	-0.277508	-1.570426	5.177424
H	-0.354206	-0.207565	6.307084
H	1.175638	-1.046646	6.030303
C	-2.141646	2.401174	4.831608
C	-3.506348	2.029747	5.454910

Mn^{2+} H_2dapsox Isomer V OPBE

Mn	0.077298	2.476403	2.481150
O	-0.849359	4.030651	0.932304
O	0.700963	5.766767	-1.712982
O	-2.008561	3.214180	4.991150
O	-3.665357	0.276896	5.997077
O	-1.580478	1.215079	1.414080
H	-1.571436	0.253009	1.323247
H	-1.965521	1.542047	0.590119
O	0.123633	4.152362	3.854008
H	0.877070	4.292816	4.442669
H	-0.646839	3.894811	4.442151
N	1.842651	1.196515	2.704876
N	1.590075	2.979755	0.873391
N	1.228662	3.923745	0.001771
H	1.813424	4.336060	-0.727105
N	-1.429024	6.116457	-0.927763
H	-2.117575	5.868550	-0.234623
H	-1.627646	6.857801	-1.585301
N	-0.292225	1.035081	4.281259
N	-1.450249	0.898016	4.967264
H	-2.807024	-0.095510	5.624867
N	-4.340662	2.429640	6.206014
H	-5.214691	2.174494	6.650152
H	-4.112348	3.403452	6.041888
C	2.899551	1.364052	1.890954
C	4.084707	0.653641	2.088528
H	4.946529	0.799305	1.444958
C	4.149937	-0.248711	3.143991
H	5.062710	-0.814023	3.322921
C	3.048136	-0.425785	3.967820
H	3.095362	-1.132422	4.790007
C	1.890722	0.325515	3.723997
C	2.720728	2.346949	0.794940
C	3.751615	2.559850	-0.258253
H	4.299151	1.640127	-0.473388
H	3.310831	2.895445	-1.201091
H	4.482689	3.315745	0.060491
C	-0.023958	4.429250	0.102066
C	-0.229975	5.529197	-0.951042
C	0.679592	0.208835	4.566493
C	0.645714	-0.788539	5.670770
H	-0.309506	-0.765284	6.191417
H	1.432154	-0.574896	6.404677
H	0.819284	-1.801990	5.291443
C	-2.174707	1.988218	5.178356
C	-3.466017	1.543705	5.832155

Co^{2+} dapsox Isomer I HS OPBE

Co	0.090752	2.292338	2.626667
O	-1.001673	3.609040	1.193930
O	-0.065299	6.114208	-1.125519
O	-1.727958	2.848661	3.691015
O	-3.754548	1.441671	6.229488
O	-0.961304	0.795726	1.121360
H	-0.238235	0.474623	0.567048
H	-1.258798	1.598602	0.661680
O	0.734963	4.126733	3.978382
H	-0.200961	4.212387	4.221892
H	0.875442	4.842433	3.344089
N	1.843486	1.131782	2.766704
N	1.455906	3.021506	1.153492
N	1.119150	4.053244	0.357520
N	-2.045589	5.668408	-0.074123
H	-2.525543	5.014410	0.524876
H	-2.550306	6.356736	-0.607571
N	-0.193007	0.921095	4.226436
N	-1.317423	0.946620	4.955664
N	-4.013579	3.306486	4.935724
H	-4.938357	3.485648	5.290417
H	-3.660585	3.800971	4.131589
C	2.877959	1.387116	1.949837
C	4.044681	0.610128	1.998117
H	4.882946	0.823963	1.341586
C	4.100759	-0.443267	2.902130
H	4.990646	-1.069850	2.952567
C	3.025416	-0.698205	3.743699
H	3.060517	-1.516352	4.457253
C	1.896469	0.129870	3.660035
C	2.650926	2.500778	1.036584
C	3.682778	2.970411	0.069840
H	3.931814	2.182701	-0.653026
H	3.308702	3.838529	-0.473808
H	4.610373	3.241931	0.588717
C	-0.184681	4.275132	0.474864
C	-0.734048	5.451772	-0.345853
C	0.711613	0.015515	4.498720
C	0.580384	-1.014922	5.566822
H	0.655563	-2.026337	5.147679
H	-0.384953	-0.908285	6.062605
H	1.377177	-0.908749	6.314138
C	-2.037435	1.998761	4.591462
C	-3.357549	2.192027	5.350589

Co^{2+} dapsox LS OPBE

Co	-2.178414	4.301225	10.928658
N	-2.849203	5.998799	10.896489
N	-2.743569	4.301416	9.158782
N	-2.559467	3.193196	8.389718

N	-1.224050	0.000444	9.376059
N	-1.837109	4.791792	12.820265
N	-1.454752	3.969241	13.822246
N	0.973814	1.441523	14.508462
O	-1.792482	2.356437	10.435147
O	-1.917961	0.689344	7.296687
O	0.474998	3.257995	12.667629
O	-0.968688	1.937577	15.627021
O	-0.046353	4.605761	10.507522
O	-3.978595	3.035028	11.961057
H	-3.628808	3.022114	12.876086
C	-3.363530	6.440129	9.711193
C	-3.883652	7.737969	9.635133
C	-3.863114	8.538602	10.786263
C	-3.344134	8.054878	11.990682
C	-2.832884	6.744869	12.028786
C	-3.285711	5.414577	8.681452
C	-3.763714	5.577994	7.279438
C	-2.043224	2.244884	9.163440
C	-1.724472	0.905394	8.488738
C	-2.263390	6.010516	13.146861
C	-2.194781	6.538189	14.541545
H	-2.928752	7.336735	14.703916
H	-1.193253	6.938682	14.765393
H	-2.370820	5.715846	15.248213
C	-0.384186	3.200575	13.602711
C	-0.178569	2.136864	14.706263
H	-4.263342	9.552119	10.742321
H	-4.296150	8.109639	8.697894
H	1.556151	1.694908	13.715775
H	-3.333965	8.676740	12.884561
H	1.242592	0.721137	15.167081
H	-3.559902	4.663160	6.713166
H	0.175112	5.540516	10.671710
H	-0.889449	-0.888615	9.023527
H	-0.990176	0.312873	10.313769
H	-4.846812	5.777107	7.258458
H	0.241633	4.116581	11.362814
H	-3.261803	6.426230	6.789240
H	-3.538796	2.261747	11.547456

Co^{2+} dapsox Isomer V OPBE

Co	-2.118886	4.042960	11.013319
N	-2.896575	5.932093	10.927676
N	-2.752006	4.301550	9.055888
N	-2.621640	3.277739	8.199900
N	-1.298274	-0.000123	8.789339
N	-1.820294	4.832704	12.951083
N	-1.460023	4.048882	13.975123
N	1.127921	1.831938	14.957700
O	-1.949264	2.186847	10.137273
O	-2.223488	0.842343	6.880175
O	0.547429	3.416769	12.928264
O	-1.000253	2.012201	15.772734
O	0.005356	4.474903	10.589777
O	-3.872804	2.848967	12.136065
H	-3.700306	1.979472	11.749116
C	-3.306761	6.419669	9.741630
C	-3.703362	7.756054	9.622581
C	-3.653816	8.567617	10.753225
C	-3.218384	8.052982	11.968001
C	-2.833701	6.704630	12.024061
C	-3.267503	5.437259	8.662958
C	-3.752516	5.719102	7.283800
C	-2.173342	2.228437	8.875847
C	-1.908395	0.963439	8.054232
C	-2.320951	6.020491	13.202453
C	-2.358127	6.628471	14.562311
H	-3.311979	7.134132	14.745699
H	-1.557746	7.370864	14.685388
H	-2.208275	5.849006	15.312688
C	-0.341395	3.339581	13.821718
C	-0.133455	2.326630	14.967511
H	-3.952256	9.613059	10.683023
H	-4.036589	8.152935	8.667731
H	1.712846	2.062382	14.168213
H	-3.164987	8.683119	12.851291
H	1.362995	1.073115	15.575895
H	-3.642776	4.826952	6.665987
H	0.113313	5.433514	10.626368
H	-0.997444	-0.842263	8.327122
H	-0.997390	0.208507	9.728059
H	-4.806964	6.022166	7.291970
H	0.312463	4.158941	11.494438
H	-3.179453	6.535731	6.825930
H	-3.544915	2.771268	13.044681

Co^{2+} Hdapsox Isomer I HS OPBE

Co	0.152026	2.402835	2.537200
O	-0.728237	3.957893	1.486952
O	0.041670	5.983694	-1.307618
O	-2.202652	2.785414	3.623158
O	-3.482173	1.024916	6.400856
O	-1.025108	1.007197	1.147567
H	-0.435514	0.629379	0.480837
H	-1.577363	1.620902	0.642132
O	0.895439	4.083205	3.905610
H	0.528010	4.118530	4.797947
H	0.537847	4.871726	3.473645
N	1.842507	1.156666	2.746727
N	1.512278	2.952052	1.017459
N	1.175880	3.932693	0.170680
N	-1.822502	5.899440	0.008437
H	-2.263817	5.479232	0.809591
H	-2.272920	6.648477	-0.492707
N	-0.206210	1.050480	4.208925
N	-1.353452	1.097281	4.899739
H	-1.575692	0.492202	5.687871
N	-4.503046	2.723417	5.242208
H	-5.335785	2.713860	5.811533
H	-4.425546	3.364355	4.467993
C	2.868370	1.313662	1.890623
C	4.014414	0.511559	1.984046
H	4.838105	0.643442	1.288820
C	4.076970	-0.450808	2.980487
H	4.956080	-1.086118	3.073686
C	3.013806	-0.603449	3.862675
H	3.062422	-1.356381	4.642220
C	1.897794	0.228038	3.714815
C	2.669732	2.358079	0.891102
C	3.685250	2.689253	-0.144210
H	3.923773	1.809406	-0.754879
H	3.310637	3.480191	-0.794080
H	4.619231	3.027738	0.321710
C	-0.022415	4.384757	0.504560
C	-0.582322	5.512298	-0.372969
C	0.700480	0.178624	4.557651

C	0.524423	-0.768394	5.696630
H	-0.338984	-1.426521	5.531402
H	0.357670	-0.223822	6.635909
H	1.393539	-1.406280	5.846173
C	-2.311421	1.989647	4.551186
C	-3.513531	1.861257	5.502610

Co^{2+} Hdapsox LS OPBE

Co	0.472722	2.286566	2.430830
O	-0.832101	3.535946	1.573776
O	-0.431740	5.744418	-1.181659
O	-1.692816	3.575001	4.749861
O	-3.965981	0.923220	5.301341
O	-0.741225	0.799784	1.059999
H	-0.249382	0.481783	0.278845
H	-1.331897	1.496409	0.706865
O	0.824703	4.015376	3.769634
H	1.495303	3.884159	4.465078
H	-0.055274	3.977914	4.236893
N	1.907367	1.192708	2.745868
N	1.543581	2.918918	1.065002
N	1.055762	3.877105	0.239333
N	-2.196574	5.434765	0.259639
H	-2.503905	4.997302	1.121410
H	-2.748809	6.166340	-0.174845
N	-0.242384	1.212222	3.974960
N	-1.499781	1.265890	4.527318
H	-2.076904	0.424266	4.669582
N	-4.291977	3.189901	5.602472
H	-5.244114	3.094766	5.941667
H	-3.848402	4.102777	5.554409
C	2.994236	1.368569	1.937742
C	4.116078	0.551069	2.116130
H	4.995446	0.683692	1.486939
C	4.081581	-0.440460	3.105553
H	4.947730	-1.085783	3.251406
C	2.945361	-0.619990	3.899153
H	2.914720	-1.402693	4.655172
C	1.846999	0.230574	3.696684
C	2.766693	2.418390	0.949365
C	3.755604	2.851067	-0.074672
H	4.059415	2.001531	-0.705822
H	3.319220	3.629451	-0.708874
H	4.664131	3.246522	0.404838
C	-0.196715	4.134424	0.604032
C	-0.940340	5.203641	-0.208863
C	0.560920	0.245565	4.393811
C	0.197430	-0.741433	5.452045
H	-0.421011	-1.554178	5.036038
H	-0.378976	-0.261923	6.255378
H	1.090210	-1.199917	5.889560
C	-2.147542	2.426793	4.807100
C	-3.586069	2.097225	5.270492

Co^{2+} Hdapsox Isomer V OPBE

Co	-2.042737	4.032816	10.978898
N	-2.909583	5.899763	10.974175
N	-2.717867	4.311857	9.046912
N	-2.578006	3.307601	8.177657
N	-1.402858	-0.051858	8.696272
N	-1.725792	4.874821	12.985548
N	-1.215431	4.168511	14.006197
N	0.813152	1.459369	15.097197
O	-1.891976	2.204650	10.095023
O	-2.146734	0.959830	6.790385
O	0.044779	2.732774	12.723892
O	-0.475926	3.003929	16.203626
O	0.064207	4.504828	10.362270
O	-3.901549	2.965488	11.905365
H	-3.872912	2.149613	11.384116
C	-3.353473	6.383918	9.795047
C	-3.809071	7.704740	9.695038
C	-3.778323	8.510626	10.825217
C	-3.309473	8.002750	12.032141
C	-2.875266	6.673448	12.072966
C	-3.302057	5.427715	8.693594
C	-3.849309	5.707157	7.338848
C	-2.118735	2.249615	8.830842
C	-1.889066	0.990407	7.980797
C	-2.315910	6.010143	13.255582
C	-2.405275	6.574069	14.633201
H	-2.897451	7.544852	14.653112
H	-1.408722	6.689689	15.078388
H	-2.988257	5.910879	15.287216
C	-0.373048	3.120539	13.810127
C	-0.012143	2.508792	15.179422
H	-4.115670	9.543948	10.766622
H	-4.170816	8.092865	8.747203
H	1.139385	1.142067	14.197587
H	-3.268829	8.640486	12.909141
H	1.114742	0.993158	15.939479
H	-3.738609	4.826019	6.706021
H	0.333475	5.421992	10.502452
H	-1.170483	-0.901347	8.206261
H	-1.141545	0.063715	9.661328
H	-4.910440	5.979675	7.390401
H	0.550229	4.000328	11.033942
H	-3.316996	6.542810	6.867050
H	-4.720293	3.392555	11.619308
H	-1.423837	4.358669	14.986528

Co^{2+} H_2dapsox Isomer I HS OPBE

Co	0.051382	2.349694	2.622286
O	-0.965725	3.957291	1.392204
O	0.306964	5.914466	-1.246430
O	-1.927437	2.780445	3.629248
O	-3.527556	1.083518	6.270972
O	-1.081741	0.868011	1.306266
H	-0.632435	0.214479	0.754736
H	-1.780453	1.225274	0.742464
O	0.871295	4.043017	3.918281
H	1.576521	3.906100	4.564126
H	0.227300	4.601056	4.373865
N	1.826464	1.151628	2.758113
N	1.431952	2.962070	1.059792
N	1.007075	3.961808	0.282568
H	1.542825	4.432015	-0.446993
N	-1.771642	6.126441	-0.288952
H	-2.407934	5.782301	0.412745
H	-2.052625	6.892581	-0.885353
N	-0.170267	0.949280	4.271333
N	-1.332211	1.023262	4.925498
H	-1.640697	0.417719	5.685949
N	-4.378727	2.870815	5.103062
H	-5.243127	2.899144	5.626140
H	-4.226108	3.531496	4.357408
C	2.838575	1.351050	1.897526
C	4.017852	0.604414	1.971276
H	4.836371	0.778638	1.279130
C	4.128949	-0.373023	2.951685
H	5.035390	-0.970884	3.029122
C	3.076077	-0.581203	3.833707
H	3.149856	-1.345819	4.601437

C	1.929770	0.209385	3.709808
C	2.594369	2.405584	0.897239
C	3.607107	2.747297	-0.138778
H	3.985313	1.837773	-0.617516
H	3.222688	3.387702	-0.934523
H	4.465252	3.258037	0.318214
C	-0.232708	4.433761	0.515847
C	-0.558335	5.591086	-0.441456
C	0.753005	0.092911	4.589739
C	0.702807	-0.910085	5.688475
H	0.710905	-1.927079	5.275340
H	-0.174273	-0.821480	6.331150
H	1.584565	-0.812786	6.332285
C	-2.188773	1.989863	4.545615
C	-3.464643	1.944622	5.401576

Co^{2+} H_2dapsox LS OPBE

Co	0.425055	2.238195	2.433342
O	-0.941638	3.573005	1.542687
O	-0.091725	5.748579	-1.114049
O	-1.687493	3.575612	4.734537
O	-3.896317	0.883255	5.321633
O	-0.743524	0.670103	1.144419
H	-0.304681	0.095886	0.488202
H	-1.545721	0.995725	0.693245
O	0.752296	3.973677	3.699582
H	1.456574	3.929543	4.373987
H	-0.113726	3.951137	4.207116
N	1.890898	1.175644	2.720611
N	1.521948	2.900918	1.069976
N	0.966292	3.899099	0.331733
H	1.422522	4.440681	-0.414406
N	-2.127606	5.679945	-0.017855
H	-2.661589	5.262887	0.738208
H	-2.541970	6.425301	-0.573605
N	-0.245261	1.191670	3.975278
N	-1.496795	1.262160	4.522532
H	-2.087889	0.429128	4.697928
N	-4.280057	3.127240	5.717084
H	-5.214621	2.987505	6.093496
H	-3.873703	4.058374	5.703625
C	2.978451	1.368698	1.920487
C	4.119911	0.586080	2.111462
H	5.005327	0.736398	1.494548
C	4.104283	-0.395417	3.111082
H	4.985254	-1.017370	3.269506
C	2.969370	-0.586126	3.904551
H	2.955548	-1.358119	4.672634
C	1.851849	0.233844	3.692147
C	2.744213	2.429734	0.929597
C	3.743921	2.902260	-0.066622
H	4.428488	2.092588	-0.347260
H	3.270258	3.268288	-0.987396
H	4.352214	3.721215	0.352641
C	-0.321878	4.186749	0.639941
C	-0.862332	5.309507	-0.260420
C	0.571036	0.244053	4.409077
C	0.237497	-0.713951	5.497902
H	-0.317475	-1.580212	5.098585
H	-0.391260	-0.239967	6.263804
H	1.143007	-1.099635	5.978726
C	-2.138472	2.429527	4.818907
C	-3.558635	2.071064	5.324007

Co^{2+} H_2dapsox Isomer V OPBE

Co	0.155182	2.313284	2.363494
O	-0.928525	3.655592	1.003485
O	0.459254	5.993567	-1.241722
O	-2.003817	3.380557	4.591016
O	-3.540382	0.634678	6.175020
O	-0.946847	0.743056	1.226986
H	-0.494371	-0.048992	0.906620
H	-1.486149	1.039183	0.480772
O	0.423490	4.063666	3.583531
H	1.139275	4.033831	4.233232
H	-0.406281	4.003547	4.112966
N	1.800356	1.138670	2.652125
N	1.591180	3.011130	1.014719
N	1.174782	4.015855	0.237750
H	1.748259	4.598606	-0.374007
N	-1.745212	5.893614	-0.595178
H	-2.430967	5.426368	-0.022595
H	-2.027799	6.676154	-1.169743
N	-0.271525	1.137913	4.189341
N	-1.436839	1.149931	4.853569
H	-1.831787	0.335462	5.339864
N	-4.338831	2.785862	6.078854
H	-5.168633	2.582470	6.618537
H	-4.172434	3.726926	5.756967
C	2.911293	1.383170	1.930141
C	4.092050	0.678013	2.166411
H	4.991587	0.877936	1.591502
C	4.103363	-0.282701	3.171949
H	5.012850	-0.843105	3.381116
C	2.957536	-0.512276	3.922587
H	2.979363	-1.241066	4.726391
C	1.804141	0.230355	3.643758
C	2.759292	2.448948	0.920873
C	3.835657	2.814169	-0.037913
H	4.360588	1.923289	-0.393744
H	3.453187	3.336430	-0.918296
H	4.578428	3.464085	0.445544
C	-0.139427	4.310775	0.300355
C	-0.467416	5.509460	-0.602666
C	0.555084	0.149059	4.419149
C	0.275162	-0.937087	5.399246
H	-0.618768	-1.503906	5.103980
H	0.089184	-0.523945	6.399175
H	1.088361	-1.656135	5.477081
C	-2.227173	2.247616	5.008083
C	-3.464725	1.811792	5.828239

Zn^{2+} dapsox Isomer I OPBE

Zn	0.184139	2.266096	2.631428
O	-0.870419	4.453811	0.949868
O	0.760214	5.907537	-1.844624
O	-2.384615	2.575851	4.057670
O	-3.466273	0.669936	6.846240
O	-1.567983	1.888638	1.550229
H	-2.139454	2.038879	2.341264
H	-1.546306	2.776816	1.119927
O	-0.184040	4.102879	3.563274
H	-0.449282	4.529358	2.713201
H	-1.044547	3.792593	3.934423
N	1.856219	1.127243	2.757835
N	1.449292	3.004944	0.950109
N	1.243988	3.957358	0.026715
N	-1.255938	6.328819	-0.859866
H	-1.887135	6.055475	-0.123750
H	-1.496883	7.045712	-1.523415
N	-0.219013	0.936232	4.376890
N	-1.272673	0.837325	5.202511
N	-4.426704	2.403249	5.712705
H	-5.266648	2.375498	6.265925
H	-4.330633	3.029453	4.929279
C	2.839225	1.337165	1.873537
C	4.013055	0.573312	1.946213
H	4.822874	0.726986	1.240088
C	4.117170	-0.386672	2.945624
H	5.020715	-0.991011	3.021122

C	3.080034	-0.583409	3.849530
H	3.161175	-1.332841	4.630368
C	1.930057	0.209942	3.729623
C	2.601472	2.380747	0.869456
C	3.633563	2.685014	-0.162846
H	3.855491	1.798235	-0.769272
H	3.265236	3.479789	-0.812181
H	4.571335	3.010224	0.304631
C	0.084888	4.600036	0.117776
C	-0.073968	5.676458	-0.980830
C	0.768648	0.106902	4.620802
C	0.752605	-0.891868	5.727882
H	0.862862	-1.911359	5.338271
H	-0.193101	-0.813562	6.265016
H	1.577791	-0.713689	6.428682
C	-2.268876	1.681988	4.959773
C	-3.439690	1.505872	5.954148

Zn^{2+} dapsox Isomer V OPBE

Zn	-1.943060	3.979490	11.192669
N	-2.857231	5.997826	10.992434
N	-2.641026	4.251744	9.117578
N	-2.501190	3.255062	8.237610
N	-1.327073	-0.106732	8.639178
N	-1.862031	5.011005	13.146785
N	-1.300380	4.397948	14.192585
N	0.464849	1.291715	14.443810
O	-1.786276	2.037570	10.103808
O	-2.095177	0.934178	6.758878
O	-0.644935	2.814602	12.599873
O	-0.010672	2.812338	16.078825
O	0.303409	4.655051	10.660832
O	-3.915125	2.747947	11.829758
H	-3.549555	2.021805	11.297707
C	-3.305478	6.382158	9.794550
C	-3.867268	7.656855	9.624446
C	-3.947735	8.491432	10.733600
C	-3.480663	8.070117	11.973500
C	-2.923173	6.785023	12.069397
C	-3.175615	5.376921	8.728037
C	-3.642362	5.639967	7.336572
C	-2.043795	2.167706	8.864253
C	-1.829865	0.949937	7.951886
C	-2.357050	6.209082	13.298816
C	-2.340128	6.960796	14.586532
H	-3.355765	7.238719	14.894258
H	-1.759287	7.887932	14.497880
H	-1.891737	6.337788	15.361711
C	-0.720302	3.265042	13.787493
C	-0.061354	2.450773	14.912317
H	-4.381054	9.485900	10.630088
H	-4.231294	7.987878	8.656120
H	0.342433	1.060470	13.470658
H	-3.545281	8.722220	12.839714
H	0.891121	0.648173	15.089296
H	-3.449139	4.761577	6.719296
H	0.420665	5.519593	11.076015
H	-1.079952	-0.944008	8.138520
H	-1.081738	0.015525	9.608966
H	-4.716961	5.861460	7.312882
H	0.580379	4.033237	11.354357
H	-3.120337	6.502206	6.903180
H	-4.632468	3.087071	11.278261

Zn^{2+} Hdapsox Isomer I OPBE

Zn	-0.122115	2.146677	2.995344
O	-1.043162	4.611079	0.770966
O	1.037446	5.861678	-1.798860
O	-2.072500	2.426422	4.019819
O	-3.532555	0.747504	6.772135
O	-1.406629	1.652694	1.335462
H	-2.248899	1.492057	1.789789
H	-1.537530	2.519035	0.913068
O	0.128865	4.217600	3.584010
H	-0.261426	4.702669	2.837295
H	-0.544331	4.295065	4.278784
N	1.788529	1.193450	2.781618
N	1.328308	3.077777	0.942193
N	1.084125	4.061783	0.062105
H	1.745740	4.362078	-0.657010
N	-1.101454	6.513403	-1.273171
H	-1.888030	6.358843	-0.661659
H	-1.151670	7.211960	-1.999590
N	-0.152003	0.785476	4.520956
N	-1.202520	0.698809	5.336613
N	-4.318709	2.473046	5.498522
H	-5.198132	2.504748	5.989206
H	-4.152306	3.073051	4.708152
C	2.735820	1.427349	1.857538
C	3.891365	0.643027	1.795702
H	4.648456	0.809577	1.037982
C	4.060846	-0.384706	2.715721
H	4.954399	-1.005786	2.681603
C	3.090505	-0.607629	3.674276
H	3.207878	-1.398735	4.407944
C	1.944353	0.202753	3.684145
C	2.506569	2.531860	0.899188
C	3.572269	2.970497	-0.057118
H	4.554369	2.573246	0.190130
H	3.334311	2.660332	-1.083766
H	3.671834	4.062876	-0.049707
C	-0.074390	4.755349	0.019683
C	0.010205	5.784060	-1.129060
C	0.878466	-0.000128	4.674415
C	0.981778	-1.026654	5.746856
H	1.073704	-2.033971	5.322509
H	0.086334	-0.991494	6.368131
H	1.859918	-0.849524	6.379552
C	-2.136981	1.590073	4.982988
C	-3.400505	1.544660	5.859445

Zn^{2+} Hdapsox Isomer V OPBE

Zn	0.042500	2.274033	2.834102
O	-1.131074	3.813185	-0.298903
O	1.237853	6.043760	-1.643592
O	-1.823789	3.017911	5.335200
O	-3.928512	0.293674	5.991979
O	-1.595263	2.063949	1.617730
H	-1.821439	1.176715	1.311331
H	-1.454227	2.629991	0.810523
O	-0.217152	4.011569	3.777597
H	0.556328	4.336598	4.255857
H	-0.878572	3.604180	4.525125
N	1.782800	1.250519	2.758409
N	1.389585	3.068279	0.878129
N	1.155543	4.075725	0.021298
H	1.891371	4.662723	-0.381124
N	-1.022416	5.974555	-2.034566
H	-1.891154	5.511712	-1.816209
H	-1.009516	6.749748	-2.680236
N	-0.309909	0.882614	4.365080
N	-1.400292	0.707649	5.100536
N	-3.973778	2.418463	6.833065
H	-4.888404	2.291811	7.236932
H	-3.573787	3.340983	6.775398
C	2.817717	1.551060	1.957979

C	3.984833	0.788771	1.990276
H	4.823300	1.003422	1.336880
C	4.048381	-0.292293	2.869215
H	4.948712	-0.903266	2.909890
C	2.973839	-0.589225	3.686933
H	3.025415	-1.418943	4.384507
C	1.817787	0.209538	3.616378
C	2.625049	2.684586	1.026389
C	3.772266	3.301990	0.294705
H	4.735847	2.917543	0.623632
H	3.686152	3.133691	-0.786746
H	3.798627	4.387033	0.460362
C	-0.056019	4.374925	-0.503669
C	0.117337	5.569380	-1.467790
C	0.652463	-0.012276	4.468290
C	0.585222	-1.161318	5.412658
H	-0.442785	-1.272499	5.763222
H	1.221502	-0.993043	6.291528
H	0.907099	-2.092552	4.935897
C	-2.107073	1.784920	5.438976
C	-3.437372	1.404950	6.116777

Zn^{2+} H_2dapsox Isomer I OPBE

Zn	0.131460	2.321125	2.630319
O	-0.929157	4.619261	0.781675
O	1.140017	5.668638	-1.879552
O	-2.538534	2.645331	4.289017
O	-3.104868	0.356079	6.915600
O	-1.606690	1.923987	1.575871
H	-2.322743	1.993840	2.231792
H	-1.730782	2.713544	1.018492
O	-0.134000	4.142256	3.578032
H	-0.399420	4.752254	2.866596
H	-0.951713	4.024610	4.094772
N	1.788411	1.159751	2.739346
N	1.448604	3.046142	0.920587
N	1.167236	4.004414	0.029470
N	-0.952608	6.471232	-1.370752
H	-1.743325	6.406560	-0.748305
H	-0.970246	7.135497	-2.132625
N	-0.256177	0.943066	4.383788
N	-1.336418	0.882582	5.172716
N	-4.522198	2.028555	6.223483
H	-5.233183	1.820018	6.911287
H	-4.662793	2.790158	5.577667
C	2.796029	1.379316	1.881961
C	3.970450	0.624185	1.955824
H	4.790381	0.789920	1.264682
C	4.076118	-0.350376	2.938075
H	4.982442	-0.947996	3.020466
C	3.022156	-0.562730	3.817509
H	3.114865	-1.320429	4.587614
C	1.868786	0.216145	3.692733
C	2.600981	2.440976	0.864395
C	3.698833	2.716971	-0.105286
H	3.899542	1.827846	-0.715660
H	3.504908	3.541726	-0.790700
H	4.621350	2.962928	0.433907
C	0.018371	4.720794	-0.001167
C	0.115609	5.693386	-1.200740
C	0.694296	0.071138	4.582674
C	0.612348	-0.986127	5.629977
H	1.428457	-1.703158	5.581308
H	-0.317654	-1.560319	5.526703
H	0.622499	-0.540584	6.634528
C	-2.399573	1.721469	5.092211
C	-3.406547	1.300516	6.189311
H	-1.457970	0.202246	5.933231
H	1.791771	4.287150	-0.736130

Zn^{2+} H_2dapsox Isomer V OPBE

Zn	0.085254	2.292227	2.591449
O	-1.153119	3.990182	-0.117444
O	1.355261	6.032983	-1.501893
O	-2.179772	3.057787	5.044013
O	-3.283690	0.137317	6.665436
O	-1.602947	2.000360	1.509197
H	-1.735699	1.158214	1.051879
H	-1.516782	2.700903	0.792957
O	-0.321957	4.051217	3.525840
H	0.379042	4.489129	4.028357
H	-1.017906	3.772153	4.196246
N	1.743591	1.161969	2.726310
N	1.405978	3.050851	0.910665
N	1.168565	4.050441	0.045276
H	1.903975	4.628278	-0.389849
N	-0.904723	6.202649	-1.858757
H	-1.819193	5.829041	-1.655971
H	-0.817579	6.990585	-2.485844
N	-0.300582	0.952907	4.389405
N	-1.408822	0.864797	5.137805
H	-1.692564	0.022073	5.658702
N	-4.281920	2.203065	6.729802
H	-5.022233	1.904243	7.349743
H	-4.247135	3.163535	6.424576
C	2.803278	1.475415	1.961769
C	4.021053	0.816700	2.150170
H	4.896975	1.065229	1.560584
C	4.104297	-0.174643	3.120177
H	5.046409	-0.694799	3.285938
C	2.989114	-0.501539	3.879633
H	3.064097	-1.266292	4.645566
C	1.801176	0.203075	3.664421
C	2.601058	2.526956	0.936149
C	3.705735	2.924986	0.018964
H	4.403611	2.105812	-0.156918
H	3.322706	3.229254	-0.959545
H	4.279649	3.765309	0.435150
C	-0.050622	4.463602	-0.386353
C	0.192717	5.669767	-1.326941
C	0.582121	-0.003962	4.481251
C	0.420303	-1.189301	5.369693
H	-0.548491	-1.675439	5.196948
H	0.458017	-0.894155	6.427454
H	1.179944	-1.950501	5.200816
C	-2.255811	1.890035	5.419907
C	-3.356902	1.324113	6.350615

[Fe(dapsox)Cl] HS OPBE

Fe	1.278436	1.110268	2.423840
O	0.027993	2.542890	3.010167
O	-0.302133	3.747353	-0.262995
O	1.059247	1.406700	5.809473
O	-1.134094	1.893317	7.416484
N	-1.269871	4.262078	2.303952
N	0.903986	1.970106	0.664215
N	1.452295	1.706032	-0.499530
N	1.639067	-0.584277	1.301179
N	0.630246	-0.397085	3.711060
N	-0.161190	-0.245178	4.745991
N	-2.287010	0.288971	6.286729
C	-0.424056	3.292101	2.097461
C	0.042361	3.053898	0.676742
C	2.059178	0.602382	-0.806366
C	2.662037	0.567108	-2.174432
C	2.093059	-0.603878	0.037066

C	2.536998	-1.811581	-0.533859
C	2.489393	-2.982100	0.201327
C	1.982107	-2.950675	1.491430
C	1.547582	-1.733155	2.019760
C	0.937375	-1.630653	3.331922
C	0.613031	-2.786177	4.193549
C	0.018714	0.773784	5.630568
C	-1.207790	1.035896	6.532809
H	-1.612029	4.470522	3.232184
H	-1.576139	4.824668	1.521773
H	2.143443	-0.154578	-2.814755
H	3.718432	0.284833	-2.132271
H	2.576850	1.553991	-2.630435
H	2.902441	-1.827499	-1.552677
H	2.830742	-3.917817	-0.233359
H	1.920406	-3.859865	2.075758
H	1.071959	-3.711984	3.859008
H	-0.477694	-2.919967	4.203075
H	0.915871	-2.581462	5.224409
H	-2.274713	-0.416965	5.566335
H	-3.124471	0.418083	6.836481
Cl	3.327108	1.797028	2.972949

[Fe(dapsox)Cl] IS OPBE

Fe	1.176490	1.031027	2.306620
O	-0.051305	2.406855	2.999131
O	-0.170572	3.844927	-0.202572
O	1.088619	1.400501	5.860044
O	-1.105290	1.881591	7.465913
N	-1.143843	4.291429	2.360807
N	0.903837	1.945829	0.658275
N	1.463894	1.715124	-0.526384
N	1.647598	-0.564516	1.309641
N	0.613434	-0.324719	3.682123
N	-0.235324	-0.132228	4.694611
N	-2.252923	0.253424	6.376401
C	-0.384041	3.252890	2.120660
C	0.119904	3.074787	0.706863
C	2.064079	0.601643	-0.810465
C	2.665501	0.539047	-2.179573
C	2.108724	-0.598102	0.043465
C	2.567463	-1.808915	-0.496396
C	2.533489	-2.965526	0.266755
C	2.027563	-2.918047	1.557129
C	1.577330	-1.695886	2.056108
C	0.960382	-1.552177	3.363367
C	0.683550	-2.731219	4.220929
C	0.034068	0.783631	5.636515
C	-1.173146	1.018375	6.581257
H	-1.508895	4.474548	3.284952
H	-1.369019	4.916918	1.599798
H	2.149423	-0.197513	-2.805470
H	3.723310	0.260179	-2.139206
H	2.575944	1.516331	-2.655628
H	2.934557	-1.845739	-1.514481
H	2.889286	-3.904647	-0.149734
H	1.974063	-3.813450	2.165996
H	1.593278	-3.323652	4.359775
H	-0.064396	-3.382178	3.751964
H	0.312948	-2.416298	5.195530
H	-2.252363	-0.427658	5.632369
H	-3.073206	0.369493	6.953245
Cl	3.229657	1.814599	2.933757

[Fe(dapsox)Cl] LS OPBE

Fe	1.045566	0.989892	2.223574
O	0.056102	2.493621	3.024280
O	-0.247449	3.820373	-0.210142
O	1.237183	1.083103	6.001612
O	-0.904047	1.702038	7.611827
N	-1.133369	4.317703	2.380714
N	0.857354	1.930514	0.640718
N	1.426134	1.725356	-0.550543
N	1.676794	-0.524750	1.349908
N	0.628300	-0.283429	3.624642
N	-0.258067	-0.037609	4.599734
N	-2.305286	0.674304	6.149948
C	-0.356008	3.290151	2.138187
C	0.075813	3.070584	0.701049
C	2.082107	0.625448	-0.790518
C	2.709878	0.569624	-2.148857
C	2.174715	-0.548882	0.085077
C	2.719355	-1.736883	-0.424562
C	2.736618	-2.891896	0.342099
C	2.184099	-2.865154	1.613207
C	1.653283	-1.670588	2.096383
C	0.991395	-1.522302	3.369485
C	0.644757	-2.644600	4.276152
C	0.104307	0.705834	5.654907
C	-1.095554	1.067484	6.566402
H	-1.441435	4.530373	3.319048
H	-1.420377	4.909244	1.614017
H	2.242238	-0.198334	-2.774762
H	3.778994	0.343141	-2.085561
H	2.583848	1.535568	-2.639664
H	3.125534	-1.755287	-1.428341
H	3.166327	-3.808059	-0.054812
H	2.162091	-3.760364	2.224267
H	1.170368	-3.562711	4.019930
H	-0.434567	-2.838612	4.222919
H	0.874562	-2.381867	5.312693
H	-2.396628	0.148654	5.293917
H	-3.123923	0.877275	6.704755
Cl	3.007274	1.625788	2.928419

$[Fe(Hdapsox)Cl]^+$ HS OPBE

Fe	1.347138	1.205927	2.476895
O	-0.187621	2.483212	2.874976
O	-0.262790	3.604458	-0.459938
O	0.959525	1.714552	5.527958
O	-1.827050	0.002628	6.871587
N	-1.584728	4.008522	1.946547
N	1.015191	1.986173	0.641460
N	1.782207	1.808410	-0.439745
N	1.600178	-0.551259	1.317819
N	0.531211	-0.360912	3.695521
N	-0.170769	-0.152406	4.825817
N	-0.768915	1.864679	7.686719
C	-0.602994	3.145126	1.882514
C	0.065356	2.956149	0.532315
C	2.390513	0.680632	-0.653063
C	3.292609	0.659338	-1.845862
C	2.164888	-0.570693	0.095673
C	2.463752	-1.796111	-0.525717
C	2.132667	-2.981939	0.101461
C	1.501422	-2.942647	1.338354
C	1.256656	-1.706338	1.928891

C	0.591380	-1.578365	3.231129
C	0.004262	-2.737364	3.945277
C	0.066965	0.885811	5.661602
C	-0.950981	0.875032	6.819109
H	-2.070217	4.187919	2.814348
H	-1.852928	4.507374	1.109710
H	2.863094	0.065248	-2.660248
H	4.267811	0.229540	-1.596812
H	3.433027	1.678834	-2.207901
H	2.930698	-1.813159	-1.503146
H	2.348482	-3.935115	-0.374272
H	1.215593	-3.865214	1.828112
H	0.405941	-3.686485	3.601238
H	-1.082162	-2.761261	3.785939
H	0.188815	-2.657319	5.020596
H	-0.017211	2.523673	7.549885
H	-1.371334	1.958245	8.490966
Cl	3.390049	1.878166	2.962882
H	-0.928998	-0.775579	5.086450

$[Fe(Hdapsox)Cl]^+$ IS OPBE

Fe	1.171643	1.082647	2.280354
O	-0.147260	2.396279	2.882455
O	-0.100949	3.784340	-0.342773
O	1.013336	1.731332	5.719097
O	-1.884495	0.002196	6.763165
N	-1.344926	4.173679	2.135650
N	0.997688	1.964664	0.635075
N	1.691047	1.753941	-0.473503
N	1.602446	-0.548322	1.306157
N	0.593600	-0.278770	3.670614
N	-0.130990	-0.050612	4.791791
N	-0.863188	1.818625	7.713868
C	-0.483506	3.205616	1.968792
C	0.144773	3.050633	0.603461
C	2.318400	0.646250	-0.711218
C	3.126088	0.613543	-1.968018
C	2.184900	-0.580442	0.094680
C	2.587836	-1.809074	-0.453592
C	2.348135	-2.983886	0.234968
C	1.704052	-2.934143	1.465088
C	1.348174	-1.694550	1.984722
C	0.692526	-1.525806	3.279813
C	0.155761	-2.660698	4.063201
C	0.095143	0.926224	5.707532
C	-1.001381	0.869245	6.795271
H	-1.797045	4.327869	3.026330
H	-1.564497	4.774537	1.353179
H	2.684182	-0.060343	-2.709907
H	4.146079	0.269508	-1.768204
H	3.167867	1.616180	-2.395223
H	3.067410	-1.838266	-1.424208
H	2.652045	-3.938245	-0.186621
H	1.497661	-3.847415	2.009146
H	0.560281	-3.616100	3.740634
H	-0.934958	-2.710012	3.943511
H	0.372450	-2.526297	5.127170
H	-0.099123	2.473789	7.643588
H	-1.512820	1.888008	8.482964
Cl	3.205543	1.837972	2.924768
H	-0.935943	-0.639466	4.991356

$[Fe(Hdapsox)Cl]^+$ LS OPBE

Fe	1.026618	1.014364	2.193181
O	0.002665	2.489933	2.956389
O	-0.109861	3.843056	-0.278559
O	1.165008	1.459148	5.892099
O	-2.123451	0.306735	6.483944
N	-1.134832	4.336525	2.278266
N	0.936043	1.950159	0.627855
N	1.586708	1.751424	-0.513868
N	1.646964	-0.524335	1.354620
N	0.609792	-0.255180	3.622131
N	-0.175338	-0.006691	4.714098
N	-0.843957	1.746978	7.722477
C	-0.355014	3.308983	2.063312
C	0.158497	3.102519	0.652165
C	2.225132	0.636410	-0.735898
C	2.950167	0.585243	-2.042939
C	2.199650	-0.556448	0.114756
C	2.683927	-1.771545	-0.397471
C	2.563489	-2.943866	0.327084
C	1.956206	-2.903412	1.574969
C	1.517757	-1.680684	2.069261
C	0.858778	-1.516824	3.348694
C	0.454787	-2.648890	4.211142
C	0.117179	0.851538	5.719514
C	-1.082099	0.942684	6.692125
H	-1.501653	4.533227	3.199259
H	-1.378239	4.939731	1.505049
H	2.491725	-0.139269	-2.724682
H	3.997838	0.299589	-1.904467
H	2.912713	1.569571	-2.511204
H	3.143547	-1.792822	-1.378013
H	2.931672	-3.882207	-0.078572
H	1.824035	-3.809585	2.154514
H	1.134695	-3.493509	4.106042
H	-0.547949	-2.992315	3.923357
H	0.421277	-2.345181	5.259303
H	0.047747	2.213925	7.794480
H	-1.543879	1.891909	8.434732
Cl	2.981117	1.686031	2.831639
H	-1.098077	-0.432394	4.751136

$[Fe(dapsox)H_2O]^+$ HS OPBE

Fe	1.149007	1.196360	2.357682
O	2.509187	1.735649	3.531826
O	-0.382364	2.504965	2.662094
O	-0.077811	3.723050	-0.629172
O	1.316106	1.363326	5.737449
O	-0.312909	1.640658	7.811035
N	-1.550332	4.175866	1.666347
N	1.033985	2.026523	0.534598
N	1.843737	1.820096	-0.516844
N	1.628926	-0.536200	1.274324
N	0.466421	-0.346979	3.639082
N	-0.227649	-0.161093	4.789044
N	-1.797959	0.146048	6.943543
C	-0.639856	3.236521	1.661995
C	0.139795	3.040754	0.371177
C	2.428861	0.678127	-0.709193
C	3.340263	0.635362	-1.896596
C	2.217577	-0.563982	0.063009
C	2.608115	-1.791689	-0.498605
C	2.367729	-2.970602	0.183502
C	1.741706	-2.923629	1.422232
C	1.381112	-1.683595	1.941690

C	0.715033	-1.564029	3.246923
C	0.387601	-2.768076	4.045174
C	0.209142	0.668183	5.685093
C	-0.669923	0.861097	6.923128
H	-2.103227	4.368979	2.489794
H	-1.688785	4.723520	0.828366
H	2.923491	0.012450	-2.696135
H	4.321084	0.227946	-1.632315
H	3.467129	1.646291	-2.286555
H	3.090370	-1.819628	-1.468157
H	2.663981	-3.923678	-0.247135
H	1.543009	-3.835365	1.973364
H	-0.097490	-3.524766	3.423570
H	-0.260504	-2.511456	4.882038
H	1.309472	-3.207781	4.444837
H	-2.036623	-0.461039	6.174648
H	-2.430903	0.237125	7.723911
H	1.827406	1.434417	4.837725
H	2.729252	2.679263	3.505020

$[Fe(dapsox)H_2O]^+$ IS OPBE

Fe	0.936421	0.993681	2.214690
O	2.470409	1.766476	3.320023
O	-0.540337	2.212085	2.667389
O	0.173620	3.960022	-0.301687
O	1.341501	1.512422	5.516143
O	-0.223346	1.840789	7.700707
N	-1.564124	4.076783	1.877894
N	1.031421	1.991772	0.635990
N	1.854638	1.832298	-0.399614
N	1.602996	-0.558041	1.282757
N	0.487780	-0.340313	3.616036
N	-0.174249	-0.116599	4.765344
N	-1.684865	0.277313	6.930242
C	-0.676163	3.122699	1.795416
C	0.219613	3.106595	0.572039
C	2.465559	0.714167	-0.632904
C	3.388756	0.720558	-1.808423
C	2.266846	-0.546232	0.112105
C	2.730615	-1.753366	-0.429921
C	2.484971	-2.946661	0.230564
C	1.791354	-2.937340	1.433416
C	1.364602	-1.716218	1.947475
C	0.689530	-1.580235	3.234329
C	0.315755	-2.758699	4.049120
C	0.289436	0.813459	5.587080
C	-0.576720	1.021420	6.845364
H	-2.190711	4.143726	2.668352
H	-1.611917	4.769621	1.143440
H	3.008438	0.084715	-2.615454
H	4.381160	0.350849	-1.531097
H	3.481050	1.738982	-2.187575
H	3.269171	-1.756597	-1.369450
H	2.835509	-3.884840	-0.191830
H	1.598706	-3.859447	1.969610
H	-0.071965	-3.562334	3.419491
H	-0.428664	-2.482154	4.795323
H	1.199724	-3.140855	4.575802
H	-1.916569	-0.377420	6.199196
H	-2.294089	0.370700	7.729524
H	2.042809	1.668819	4.277984
H	2.612537	2.715033	3.181968

$[Fe(dapsox)H_2O]^+$ LS OPBE

Fe	0.843326	0.932326	2.148447
O	2.287863	1.514040	3.083907
O	-0.360276	2.325212	2.801582
O	0.185604	4.012993	-0.230151
O	1.284628	1.482672	5.443338
O	-0.238630	1.858707	7.603335
N	-1.330634	4.254690	2.106176
N	0.978095	1.980206	0.637492
N	1.737184	1.812514	-0.444228
N	1.635500	-0.547169	1.339023
N	0.449747	-0.358204	3.555302
N	-0.262891	-0.124889	4.692110
N	-1.775455	0.347447	6.862276
C	-0.523849	3.239211	1.941228
C	0.250747	3.157074	0.640186
C	2.365818	0.691403	-0.661604
C	3.179660	0.675965	-1.919127
C	2.279661	-0.530455	0.143839
C	2.833399	-1.721382	-0.357080
C	2.702090	-2.909807	0.339288
C	2.011597	-2.915006	1.544868
C	1.492007	-1.718971	2.024054
C	0.774895	-1.597820	3.277534
C	0.481699	-2.753763	4.157101
C	0.185635	0.772115	5.512029
C	-0.639515	1.043262	6.767438
H	-1.867612	4.365103	2.955235
H	-1.411497	4.944221	1.371902
H	2.769536	-0.028204	-2.651293
H	4.217285	0.388293	-1.722166
H	3.169878	1.673312	-2.360752
H	3.362866	-1.710150	-1.301844
H	3.130361	-3.827359	-0.055395
H	1.883883	-3.832516	2.108627
H	0.208105	-3.632880	3.570899
H	-0.324731	-2.509759	4.849109
H	1.370542	-3.007006	4.748561
H	-2.046617	-0.296250	6.135014
H	-2.378473	0.483680	7.659596
H	1.720035	1.420418	4.512886
H	2.351957	2.468945	2.910692

$[Fe(Hdapsox)H_2O]^{2+}$ HS OPBE

Fe	1.132278	1.177261	2.383813
O	2.674804	1.829558	3.525205
O	-0.388288	2.438505	2.619828
O	0.172593	3.769919	-0.591887
O	1.178004	1.505564	5.657611
O	-1.592535	-0.202009	7.013777
N	-1.514623	4.121791	1.598197
N	1.258264	2.120405	0.659487
N	2.180031	1.933519	-0.290614
N	1.552247	-0.518727	1.254122
N	0.488968	-0.404865	3.655218
N	-0.119910	-0.226329	4.847749
N	-0.386218	1.528603	7.912904
C	-0.580883	3.213551	1.632255
C	0.324464	3.091861	0.415638
C	2.674562	0.758920	-0.523001
C	3.773181	0.710282	-1.531966
C	2.195814	-0.511696	0.072958
C	2.402046	-1.710971	-0.624949

C	1.905176	-2.894993	-0.111378
C	1.251721	-2.885171	1.114875
C	1.106619	-1.676830	1.788405
C	0.483181	-1.595892	3.121626
C	-0.088676	-2.791621	3.778954
C	0.244370	0.703264	5.749759
C	-0.684344	0.636332	6.976801
H	-2.151644	4.251413	2.372661
H	-1.604085	4.702534	0.775412
H	3.430596	0.250296	-2.465460
H	4.618912	0.122601	-1.161742
H	4.105601	1.725074	-1.754705
H	2.929007	-1.708095	-1.571674
H	2.034461	-3.826785	-0.655413
H	0.868587	-3.807815	1.533040
H	-1.126365	-2.931428	3.449283
H	-0.077397	-2.697994	4.865651
H	0.466065	-3.691329	3.516043
H	0.379058	2.171979	7.778030
H	-0.929076	1.576742	8.762552
H	2.261090	1.762161	4.434422
H	2.919913	2.761471	3.410725
H	-0.905623	-0.809396	5.126668

$[Fe(Hdapsox)H_2O]^{2+}$ IS OPBE

Fe	1.002153	1.027495	2.225737
O	2.595011	1.728886	3.369035
O	-0.409101	2.283313	2.702541
O	0.362291	4.035030	-0.246031
O	1.207924	1.495383	5.614995
O	-1.718787	-0.032353	6.859291
N	-1.421741	4.153311	1.911192
N	1.188521	2.061001	0.705196
N	2.048548	1.900084	-0.292030
N	1.584147	-0.535195	1.252162
N	0.479861	-0.357430	3.574368
N	-0.169176	-0.139323	4.743809
N	-0.438845	1.611491	7.815283
C	-0.535421	3.201505	1.834422
C	0.379657	3.186719	0.627120
C	2.611237	0.765295	-0.556221
C	3.609734	0.771439	-1.664495
C	2.271075	-0.515172	0.099323
C	2.616916	-1.724292	-0.523624
C	2.210875	-2.924759	0.030098
C	1.487901	-2.922855	1.218104
C	1.205275	-1.706328	1.824805
C	0.530727	-1.585470	3.120206
C	-0.038017	-2.738901	3.845918
C	0.218933	0.761710	5.667902
C	-0.758292	0.746496	6.860542
H	-2.060718	4.213315	2.692668
H	-1.463925	4.849235	1.178816
H	3.234690	0.225839	-2.537292
H	4.544498	0.296990	-1.349343
H	3.812556	1.800391	-1.963309
H	3.180884	-1.716932	-1.448190
H	2.455843	-3.863456	-0.459273
H	1.166223	-3.856229	1.662938
H	-1.126447	-2.759493	3.699791
H	0.156729	-2.648929	4.918281
H	0.360495	-3.687263	3.495516
H	0.373204	2.202073	7.717886
H	-1.005434	1.682619	8.647601
H	2.199122	1.699329	4.284443
H	2.822309	2.658412	3.213032
H	-1.006794	-0.669465	4.973642

$[Fe(Hdapsox)H_2O]^{2+}$ LS OPBE

Fe	0.868277	0.986738	2.150357
O	2.348682	1.478545	3.238208
O	-0.293120	2.393340	2.785811
O	0.338304	4.045659	-0.244316
O	1.305605	1.283680	5.515279
O	-1.810770	0.258511	6.808870
N	-1.368005	4.226107	1.983298
N	1.138109	2.046925	0.696321
N	2.034693	1.924008	-0.272835
N	1.577931	-0.515404	1.308685
N	0.336003	-0.343942	3.469738
N	-0.318932	-0.083044	4.641609
N	-0.173929	1.512361	7.811755
C	-0.480271	3.275693	1.892814
C	0.373657	3.214668	0.642492
C	2.629673	0.782334	-0.492768
C	3.652422	0.805728	-1.579016
C	2.313012	-0.484949	0.169583
C	2.734408	-1.692334	-0.413841
C	2.377823	-2.906589	0.141766
C	1.623712	-2.922092	1.309512
C	1.255663	-1.712795	1.882421
C	0.530703	-1.597536	3.134339
C	0.077793	-2.758345	3.926583
C	0.206337	0.709365	5.584472
C	-0.706621	0.811124	6.817551
H	-1.961817	4.312123	2.797416
H	-1.459811	4.892466	1.228307
H	3.308060	0.249509	-2.457691
H	4.592730	0.356288	-1.244084
H	3.836710	1.838137	-1.877974
H	3.331179	-1.670166	-1.317420
H	2.688399	-3.837129	-0.325220
H	1.329656	-3.859392	1.768288
H	-0.924414	-3.057511	3.591103
H	0.022778	-2.514958	4.988807
H	0.741062	-3.611555	3.791004
H	0.739426	1.929541	7.714888
H	-0.685596	1.637969	8.672813
H	1.976127	1.373465	4.208981
H	2.506222	2.432602	3.131748
H	-1.236793	-0.483458	4.819636