

Electronic Supplementary Information (ESI) for:

The interplay between spin states, geometries and biological activity of Fe(III) and Mn(II) complexes with thiosemicarbazone

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Table S1. Crystal data and structure refinement for **1** and **2**.

<i>Identification code</i>	1	2
<i>Empirical formula</i>	C ₁₂ H ₁₆ BF ₄ FeN ₈ OS ₄	C ₁₂ H ₁₄ MnN ₈ S ₄
<i>Formula weight</i>	559.23	453.49
<i>Temperature/K</i>	199.98	199.96
<i>Crystal system</i>	orthorhombic	triclinic
<i>Space group</i>	Pbca	P-1
<i>a/Å</i>	17.8604(10)	7.5680(6)
<i>b/Å</i>	12.1006(7)	14.5498(13)
<i>c/Å</i>	18.9002(11)	17.2336(14)
<i>α/°</i>	90	103.552(3)
<i>β/°</i>	90	102.276(3)
<i>γ/°</i>	90	94.338(3)
<i>Volume/Å³</i>	4084.7(4)	1786.8(3)
<i>Z</i>	8	4
<i>ρ_{calc}/cm³</i>	1.819	1.686
<i>μ/mm⁻¹</i>	1.208	1.220
<i>F(000)</i>	2264.0	924.0
<i>Crystal size/mm³</i>	0.08 × 0.07 × 0.05	0.10 × 0.08 × 0.08
<i>Radiation</i>	MoKα (λ = 0.71073)	MoKα (λ = 0.71073)
<i>2θ range for data collection/°</i>	4.31 to 59.206	4.294 to 59.222
	-24 ≤ h ≤ 24	-10 ≤ h ≤ 10
<i>Index ranges</i>	-16 ≤ k ≤ 1	-20 ≤ k ≤ 19
	-26 ≤ l ≤ 26	0 ≤ l ≤ 23
<i>Reflections collected</i>	133712	10019
	5744	10019
<i>Independent reflections</i>	R _{int} = 0.2018	R _{int} = n/a,
	R _{sigma} = 0.0654	R _{sigma} = 0.0330
<i>Data/restraints/parameters</i>	5744/0/286	10019/0/460
<i>Goodness-of-fit on F²</i>	1.222	1.114
<i>Final R indexes</i>	R ₁ = 0.0997	R ₁ = 0.0792
<i>[I >= 2σ(I)]</i>	wR ₂ = 0.1773	wR ₂ = 0.2588
<i>Final R indexes [all data]</i>	R ₁ = 0.1309	R ₁ = 0.0926
	wR ₂ = 0.1904	wR ₂ = 0.2797
<i>Largest diff. peak/hole / e Å⁻³</i>	1.21/-0.89	1.75/-1.00

Table S2. Selected bond lengths (Å) and angles (°) of complexes **1** and **2**.

1		2			
Fe01–S1	2.2257(16)	Mn1–S1	2.533(2)	Mn2–S5	2.510(2)
Fe01–S3	2.2188(15)	Mn1–S3	2.518(3)	Mn2–S7	2.521(2)
Fe01–N3	1.940(4)	Mn1–N3	2.257(7)	Mn2–N11	2.270(6)
Fe01–N4	1.970(5)	Mn1–N4	2.274(7)	Mn2–N12	2.273(6)
Fe01–N7	1.938(4)	Mn1–N7	2.247(7)	Mn2–N15	2.269(6)

Fe01–N8	1.993(5)	Mn1–N8	2.277(8)	Mn2–N16	2.260(7)
N3–C2	1.300(7)	N3–C2	1.302(10)	N11–C14	1.310(10)
N7–C8	1.301(7)	N7–C8	1.299(14)	N15–C20	1.298(9)
N2–N3	1.379(6)	N2–N3	1.362(9)	N10–N11	1.370(8)
N6–N7	1.375(6)	N6–N7	1.361(14)	N14–N15	1.368(9)
N2–C1	1.322(7)	N2–C1	1.336(10)	N10–C13	1.331(10)
N6–C7	1.329(7)	N6–C7	1.31(2)	N14–C19	1.324(10)
S1–C1	1.755(6)	S1–C1	1.731(8)	S5–C13	1.728(8)
S3–C7	1.739(6)	S3–C7	1.695(13)	S7–C19	1.741(7)
N1–C1	1.318(7)	N1–C1	1.336(10)	N9–C13	1.342(9)
N5–C7	1.343(7)	N5–C7	1.354(15)	N13–C19	1.349(10)
F1–B1	1.383(9)				
F2–B1	1.383(9)				
F3–B1	1.366(10)				
F4–B1	1.374(9)				
S3–Fe01–S1	96.35(6)	S3–Mn1–S1	99.51(9)	S5–Mn2–S7	99.44(9)
N3–Fe01–S1	84.83(15)	N3–Mn1–S1	74.65(16)	N11–Mn2–S7	98.71(18)
N3–Fe01–S3	95.85(14)	N3–Mn1–S3	126.73(19)	N11–Mn2–N12	72.1(2)
N3–Fe01–N4	80.72(19)	N3–Mn1–N4	72.6(3)	N11–Mn2–S5	75.18(16)
N3–Fe01–N8	98.70(18)	N3–Mn1–N8	85.7(3)	N12–Mn2–S5	143.07(18)
N4–Fe01–S1	164.87(14)	N4–Mn1–S1	144.3(2)	N12–Mn2–S7	102.00(18)
N4–Fe01–S3	89.61(14)	N4–Mn1–S3	89.1(2)	N15–Mn2–S5	133.13(18)
N4–Fe01–N8	85.64(19)	N4–Mn1–N8	92.9(3)	N15–Mn2–S7	73.99(16)
N7–Fe01–S1	91.46(14)	N7–Mn1–S1	101.7(2)	N15–Mn2–N11	151.1(2)
N7–Fe01–S3	84.85(14)	N7–Mn1–S3	75.7(3)	N15–Mn2–N12	82.0(2)
N7–Fe01–N3	176.3(2)	N7–Mn1–N3	157.4(3)	N16–Mn2–S5	90.59(18)
N7–Fe01–N4	102.95(19)	N7–Mn1–N4	113.9(3)	N16–Mn2–S7	141.38(19)
N7–Fe01–N8	81.10(19)	N7–Mn1–N8	72.6(4)	N16–Mn2–N11	119.9(2)
N8–Fe01–S1	92.15(14)	N8–Mn1–S1	98.3(2)	N16–Mn2–N12	91.1(3)
N8–Fe01–S3	163.75(13)	N8–Mn1–S3	146.2(3)	N16–Mn2–N15	72.1(2)

Table S3. Comparison of Fe-N_{thiazole}, Fe-N_{imine} and Fe-S_{thiolate} bond lengths (Å) in octahedral Fe(III)-N₄S₂ complexes with thiosemicarbazone based ligands.

Complexes	Fe-N _{thiazole}	mean values	Fe-N _{imine}	mean values	Fe-S _{thiolate}	mean values	References
[Fe(L¹)₂][BF₄·H₂O (1)	1.970	1.982	1.940	1.939	2.2257	2.2222	this work
	1.993		1.938		2.2188		
[Fe(L ²) ₂][NO ₃]	1.987	1.981	1.930	1.9305	2.226	2.223	1
CCDC 1498847	1.975		1.931		2.220		
[Fe(L ³) ₂][NO ₃]	2.034	2.026	1.924	1.926	2.226	2.223	1
CCDC 1498851	2.019		1.928		2.220		
[Fe(L ⁴) ₂][NO ₃]	1.966	1.975	1.916	1.9205	2.207	2.2145	1
CCDC 1498850	1.984		1.925		2.222		
[Fe(L ⁴) ₂](X ¹)	1.976	1.982	1.937	1.935	2.2022	2.2009	2
CCDC 1527317	1.987		1.933		2.1996		
[Fe(L ⁴) ₂](X ²)	1.999	1.993	1.934	1.933	2.2385	2.2351	2
CCDC 1527318	1.987		1.932		2.2318		
[Fe(L ⁴) ₂](X ³)	1.990	1.984	1.931	1.9215	2.206	2.2135	2
CCDC 1527319	1.977		1.912		2.221		
[Fe(L ⁴) ₂](X ⁴)	1.985	1.9795	1.920	1.923	2.2247	2.2232	2
CCDC 1567225	1.974		1.926		2.2217		
[Fe(L ⁴) ₂](X ⁵)	1.989	1.9805	1.925	1.9275	2.248	2.2325	2
CCDC 1527320	1.972		1.930		2.217		

HL¹ = (*E*)-2-(1-(thiazol-2-yl)ethylidene)hydrazine-1-carbothioamide;

HL² = condensation product of 4-phenylthiosemicarbazide and 2-thiazolecarboxaldehyde;

HL³ = condensation product of 4-phenylthiosemicarbazide and 4-methyl-2-thiazolecarboxaldehyde;

HL⁴ = condensation product of 4-phenylthiosemicarbazide and 2-acetylthiazole;

X¹ = *N*-(*p*-aminobenzenesulfonate)-1,8-naphthalimide;

X² = *N*-(*m*-aminobenzenesulfonate)-1,8-naphthalimide;

X³ = *N*-(5-amino-1-naphthalenesulfonate)-1,8-naphthalimide;

X⁴ = *N*-(5-amino-2-naphthalenesulfonate)-1,8-naphthalimide;

X⁵ = hexadecylsulfonate.

Table S4. The M-N_{thiazole}, M-N_{imine} and M-S_{thiolate} bond lengths (Å) in [M(L¹)₂] (M = Mn(II) and Zn(II)) and [M(L¹)₂]⁺ (M = Fe(III) and Co(III)) complexes.

Complexes	M-N _{thiazole}	mean values	M-N _{imine}	mean values	M-S _{thiolate}	mean values	References
[Mn(L ¹) ₂] (2)	2.274		2.257		2.533	2.5205	this work
	2.277		2.247		2.518		
	2.273	2.271	2.270	2.2585	2.510		
	2.260		2.260		2.521		
[Zn(L ¹) ₂]	2.187		2.147		2.4516	2.4312	³
	2.318	2.2525	2.150	2.148	2.4108		
[Fe(L ¹) ₂]BF ₄ ·H ₂ O (1)	1.970		1.940		2.2257	2.2222	this work
	1.993	1.982	1.938	1.939	2.2188		
[Co(L ¹) ₂]BF ₄ ·H ₂ O	1.964		1.909		2.2230	2.2243	⁴
	1.953	1.9585	1.907	1.908	2.2257		
[Co(L ¹) ₂] ₂ [Co(NCS) ₄]·2H ₂ O	1.958		1.903		2.225	2.222	⁵
	1.962	1.960	1.911	1.907	2.220		

Table S5. Hydrogen-bond parameters for complex 1.

D-H...A	D-H (Å)	H...A (Å)	D...A (Å)	D-H...A (°)	Symm. operation on A
N1-H1A...N6	0.88	2.23	3.070(6)	158	1/2+x, y, 1/2-z
N1-H1B...F4	0.88	2.54	3.010(8)	114	1/2+x, 1/2-y, 1-z
N5-H5B...N2	0.88	2.48	3.321(7)	159	-1/2+x, y, 1/2-z
O1-H1C...F2	0.87	1.85	2.707(14)	169	x, 1/2-y, -1/2+z
O1-H1D...N6	0.87	2.19	2.914(14)	141	x, 1/2-y, -1/2+z
Intra C9-H9B...S4	0.98	2.79	3.293(6)	113	

Table S6. Intermolecular π ... π interaction parameters for complex 1.

Cg(I) ^a	Cg(J) ^a	Cg(I)...Cg(J) ^b (Å)	α^c (°)	β^d (°)	γ^e (°)	Slippage ^f (Å)	Sym. code on (J)
Cg(1)	Cg(1)	3.807(3)	0.0(3)	23.0	23.0	1.487	1-x, -y, -z
Cg(2)	Cg(2)	3.904(3)	0.0(3)	25.0	25.0	1.651	1-x, 1-y, -z

^aLabels of aromatic rings: (1) = S(2),C(4),N(4),C(5)C(6); (2) = S(4),C(10),N(8),C(11),C(12).

^bCg(I)...Cg(J) = Distance between ring centroids (Ang.).

^c α = Dihedral angle between planes (I) and (J) (Deg).

^d β = Angle between Cg(I)-Cg(J) vector and normal to plane (I) (Deg).

^e γ = Angle between Cg(I)-Cg(J) vector and normal to plane (J) (Deg).

Slippage = Distance between Cg(I) and perpendicular projection of Cg(J) on ring (I) (Ang.).

Table S7. Intermolecular X–H... π (thiazole ring) interaction parameters for complex **1**.

X–H	Cg(J)	H...Cg (Å)	H...(thiazole ring J) ^a (Å)	X–H...Cg (°)	γ^b (°)	Sym. code on (J)
N5–H5A	Cg(2)	2.73	2.65	160	13.46	1–x, –1/2+ y, 1/2–z

^aPerpendicular distance of H to ring plane (J) (Ang.).^b γ = Angle between H...Cg line and perpendicular H...(ring plane) line (Deg.).**Table S8.** Hydrogen-bond parameters for complex **2**.

D–H...A	D–H (Å)	H...A (Å)	D...A (Å)	D–H...A (°)	Symm. operation on A
N1–H1A...N14	0.89	2.62	3.077(11)	113	
N5–H5B...S6	0.94	2.73	3.287(18)	119	2–x, 1–y, 1–z
N9–H9D...N10	0.89	2.30	3.072(11)	145	–1–x, 1–y, –z
N13–H13A...N2	0.89	2.25	3.082(10)	156	
N13–H13B...S1	0.89	2.74	3.499(8)	143	–1+x, y, z
Intra C3–H3B...S2	0.98	2.71	3.212(10)	112	
Intra C9–H9B...S4	0.98	2.70	3.17(2)	110	
Intra C15–H15B...S6	0.98	2.66	3.184(11)	114	
Intra C21–H21B...S8	0.98	2.76	3.219(9)	109	

Table S9. Intermolecular π ... π interaction parameters for complex **2**.

Cg(I) ^a	Cg(J) ^a	Cg(I)...Cg(J) ^b (Å)	α^c (°)	β^d (°)	γ^e (°)	Slippage ^f (Å)	Sym. code on (J)
Cg(1)	Cg(1)	3.701(9)	0.0(7)	22.7	22.7	1.431	1–x, 1–y, 1–z

^aLabels of aromatic rings: (1) = S(4), C(10), N(8), C(11), C(12).^bCg(I)...Cg(J) = Distance between ring centroids (Ang.).^c α = Dihedral angle between planes (I) and (J) (Deg.).^d β = Angle between Cg(I)–Cg(J) vector and normal to plane (I) (Deg.).^e γ = Angle between Cg(I)–Cg(J) vector and normal to plane (J) (Deg.).

Slippage = Distance between Cg(I) and perpendicular projection of Cg(J) on ring (I) (Ang.).

Table S10. Intermolecular X–H... π (thiazole ring) interaction parameters for complex **2**.

X–H	Cg(J) ^a	H...Cg (Å)	H...(thiazole ring J) ^b (Å)	X–H...Cg (°)	γ^c (°)	Sym. code on (J)
N5–H5B	Cg(1)	2.88	2.80	142	12.82	1+x, y, z
N5–H5A	Cg(2)	2.84	–2.66	162	20.07	1+x, y, z

^aLabels of aromatic rings: (1)(6) = S(4), C(10), N(8), C(11), C(12); (2)(5) = S(2), C(4), N(4), C(5), C(6).^bPerpendicular distance of H to ring plane (J) (Ang.).^c γ = Angle between H...Cg line and perpendicular H...(ring plane) line (Deg.).

Table S11. The Fe-N_{thiazole}, Fe-N_{imine} and Fe-S_{thiolate} bond lengths (Å) in [Fe^{III}(L¹)₂]⁺ from geometry optimizations at different levels of theory

DFA	[Fe ^{III} (L ¹) ₂] ⁺									
	OPBE	OPBE	B97-D	B97-D	SSB-D	SSB-D	B97-D-COSMO	B97-D-COSMO	SSB-D-COSMO	SSB-D-COSMO
Spin-state	LS	HS	LS	HS	LS	HS	LS	HS	LS	HS
Fe-N _{thiazole}	1.963	2.202	1.984	2.185	1.972	2.177	1.976	2.167	1.963	2.161
	1.965	2.203	1.982	2.183	1.969	2.176	1.978	2.163	1.965	2.158
Fe-N _{imine}	1.909	2.198	1.943	2.218	1.928	2.209	1.943	2.217	1.928	2.208
	1.908	2.197	1.942	2.217	1.929	2.208	1.943	2.213	1.929	2.205
Fe-S _{thiolate}	2.204	2.354	2.258	2.387	2.225	2.354	2.262	2.398	2.226	2.364
	2.200	2.354	2.259	2.383	2.226	2.349	2.265	2.397	2.229	2.361

Table S12. The Mn-N_{thiazole}, Mn-N_{imine} and Mn-S_{thiolate} bond lengths (Å) in [Mn^{II}(L¹)₂] from geometry optimizations at different levels of theory

DFA	[Mn ^{II} (L ¹) ₂]									
	OPBE	OPBE	B97-D	B97-D	SSB-D	SSB-D	B97-D-COSMO	B97-D-COSMO	SSB-D-COSMO	SSB-D-COSMO
Spin-state	LS	HS	LS	HS	LS	HS	LS	HS	LS	HS
Mn-N _{thiazole}	1.979	2.347	1.996	2.290	1.989	2.319	1.990	2.264	1.981	2.278
	1.979	2.364	1.997	2.294	1.986	2.295	1.990	2.268	1.980	2.279
Mn-N _{imine}	1.919	2.289	1.949	2.291	1.935	2.293	1.953	2.291	1.938	2.293
	1.917	2.284	1.950	2.294	1.936	2.295	1.953	2.287	1.940	2.293
Mn-S _{thiolate}	2.268	2.497	2.335	2.523	2.290	2.484	2.339	2.548	2.299	2.501
	2.268	2.491	2.333	2.522	2.295	2.485	2.341	2.545	2.295	2.504

Table S13. Intermediate spin (IS) state energies (in kcal/mol relative to the low spin (LS) states) for [Fe^{III}(L¹)₂]⁺ and [Mn(L¹)₂], at B97-D/TZP and SSB-D/TZP levels of theory.

Level of theory	[Fe ^{III} (L ¹) ₂] ⁺		[Mn ^{II} (L ¹) ₂]		
	E _{IS-LS} (X-ray) ^a	E _{IS-LS} (opt.) ^b	E _{IS-LS} (X-ray1) ^a	E _{IS-LS} (X-ray2) ^a	E _{IS-LS} (opt.) ^b
B97-D/TZP	31.26	15.77	-15.68	-19.99	7.03
SSB-D/TZP	27.89	15.44	-17.78	-20.16	7.51
B97-D/TZP-COSMO ^c	30.86	15.30	-17.10	-18.53	5.88
SSB-D/TZP-COSMO ^c	28.05	15.08	-17.14	-18.69	6.74

^a) single-point on X-ray geometries; for Mn(II) complex, two crystallographically independent complexes are considered; ^b) geometry optimization; ^c) DMSO as solvent.

Table S14. Continuous shape measures (CShMs) for Fe(III) and Mn(II) X-ray structures, presenting deviation from ideal OC-6 and TRP-6 polyhedra.

Fe(III)					Mn(II)				
	CCDC	OC-6	TPR-6	Ref.		CCDC	OC-6	TPR-6	Ref.
1	1498847	1.655	12.557	¹	1	1534899	6.528	8.715	¹⁷
2	1498850	1.851	11.394	¹	2	222664	6.983	7.815	¹⁸
3	1498851	1.752	10.894	¹	3	245378	7.278	7.432	¹⁹
4	1527317	1.667	11.119	²	4	261110	5.897	10.775	²⁰
5	1527318	1.661	11.752	²	5	286571_A	7.953	7.084	⁶
6	1527319	1.864	11.326	²	6	286571_B	9.590	4.810	⁶
7	1527320	1.844	11.882	²	7	622077	6.871	9.064	²¹
8	1567225_A	1.823	10.486	²	8	654260	3.108	12.107	²²
9	1567225_B	1.966	11.668	²	9	657940	6.969	7.624	²³
10	286569	1.625	11.324	⁶	10	657941	6.507	8.155	²³
11	115805	2.088	11.037	⁷	11	672181	6.333	10.154	²⁴
12	1164990	1.621	11.734	⁸	12	763553_A	6.945	9.368	²⁵
13	150103	1.804	12.177	⁹	13	763553_B	6.977	10.393	²⁵
14	150104	1.843	10.798	⁹	14	771935	6.306	7.811	²⁶
15	178366	1.716	12.525	¹⁰	15	805046	6.680	10.307	²⁷
16	1990298_A	2.021	9.882	¹¹	16	876299_A	6.771	8.822	²⁸
17	1990298_B	1.763	11.663	¹¹	17	876299_B	6.357	10.167	²⁸
18	217177	1.645	10.661	¹²	18	981824_A	5.824	10.681	²⁹
19	228089	1.634	11.485	¹³	19	981824_B	6.034	9.837	²⁹
20	235994	1.636	12.121	¹⁴	20	632856	3.127	12.538	³⁰
21	782402	2.420	9.524	¹⁵					
22	778260	2.285	9.699	¹⁶					

Table S15. Continuous shape measures (CShMs) for IS state of $[\text{Fe}^{\text{III}}(\text{L}^1)_2]^+$ and $[\text{Mn}^{\text{II}}\text{L}_2]$ presenting deviation from ideal OC-6 and TPR-6 polyhedra for optimized structures at B97-D/TZP and SSB-D/TZP levels of theory. For low spin (LS) and high spin (HS) states see **Table 3** in the main text.

	$[\text{Fe}^{\text{III}}(\text{L}^1)_2]^+$		$[\text{Mn}^{\text{II}}(\text{L}^1)_2]$	
	IS		IS	
	OC-6	TPR-6	OC-6	TPR-6
B97-D/TZP	2.678	12.823	3.740	11.091
SSB-D/TZP	2.699	12.504	3.864	10.228
B97-D/TZP-COSMO ^{a)}	2.691	12.940	3.833	11.557
SSB-D/TZP-COSMO ^{a)}	2.689	13.167	3.957	10.488

^{a)}DMSO as solvent.

Table S16. Gibbs free energy changes ($\Delta_r G$ in kcal mol⁻¹ at T = 298.15 K) calculated at the ZORA-B97-D/TZP-COSMO(DMSO) level of theory.^{a)}

Reaction	$\Delta_r G$
$[\text{Fe}^{\text{III}}(\text{L}^1)_2]^+ + 6\text{H}_2\text{O} \rightarrow [\text{Fe}^{\text{III}}(\text{H}_2\text{O})_6]^{3+} + 2(\text{L}^1)^-$	158.35
$[\text{Fe}^{\text{III}}(\text{L}^1)_2]^+ + 6\text{DMSO} \rightarrow [\text{Fe}^{\text{III}}(\text{DMSO})_6]^{3+} + 2(\text{L}^1)^-$	80.97
$[\text{Mn}^{\text{II}}(\text{L}^1)_2] + 6\text{H}_2\text{O} \rightarrow [\text{Mn}^{\text{II}}(\text{H}_2\text{O})_6]^{2+} + 2(\text{L}^1)^-$	87.96
$[\text{Mn}^{\text{II}}(\text{L}^1)_2] + 6\text{DMSO} \rightarrow [\text{Mn}^{\text{II}}(\text{DMSO})_6]^{2+} + 2(\text{L}^1)^-$	58.97

^{a)} Vibrational analysis with Grimme's scheme³¹ for low-frequency contributions (frequency cut-off 100 cm⁻¹) to the zero-point effects and the entropic and thermal corrections. Because vibrational analysis is done at a standard state of 1 atm, a conversion to 1 mol dm⁻³ solution standard state is done (correction of 1.89 kcal mol⁻¹ to the free energies at 298 K). In reactions where DMSO is involved, the free energy correction due to the conversion to the solvent standard state (13.98 mol dm⁻³) equals 3.46 kcal mol⁻¹ (at 298 K). Entropy correction due to spin-multiplicity ($R \ln(g_s)$, where g_s is the spin-degeneracy of a complex and R is the universal gas constant) was employed when spin-state is changing during a reaction (0.65 kcal mol⁻¹).

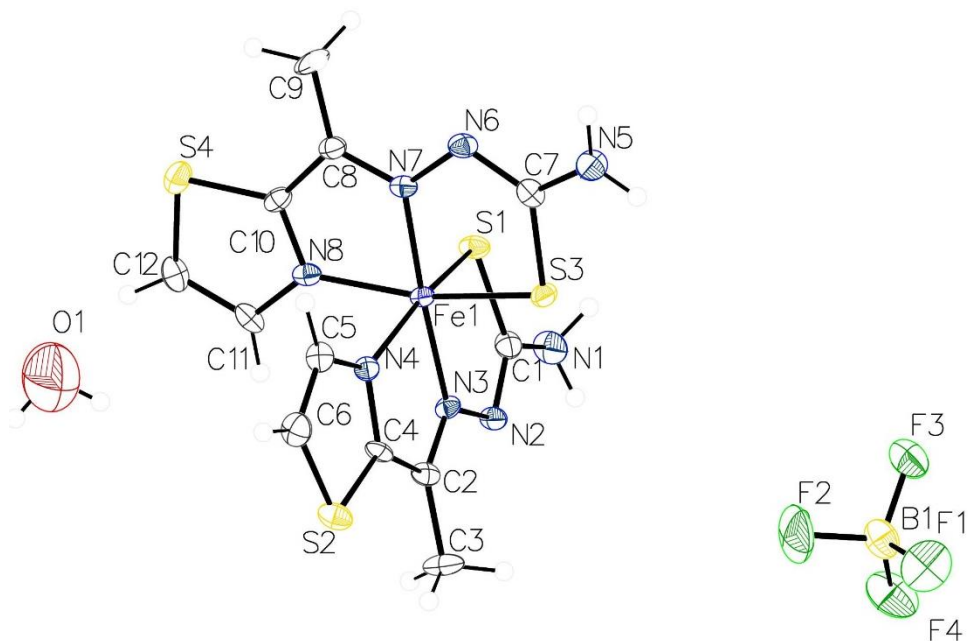


Fig S1. ORTEP drawing of **1**. All non-hydrogen atoms shown as ellipsoids at the 50% probability level. H atoms (isotropically refined) are reported in ball-and-stick style for sake of clarity. Colour code: Fe=purple, N=blue, S=yellow, C=black, O=red, B=light yellow, F=green, H=white.

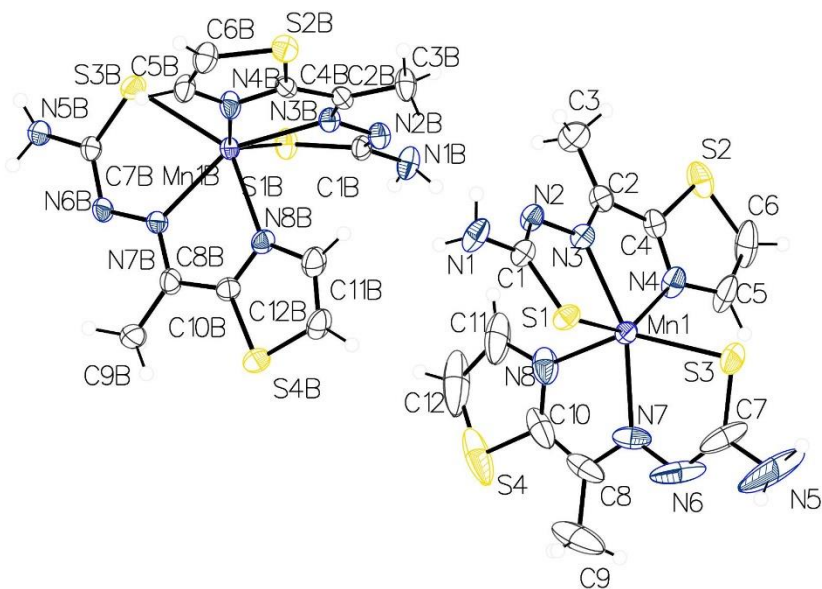
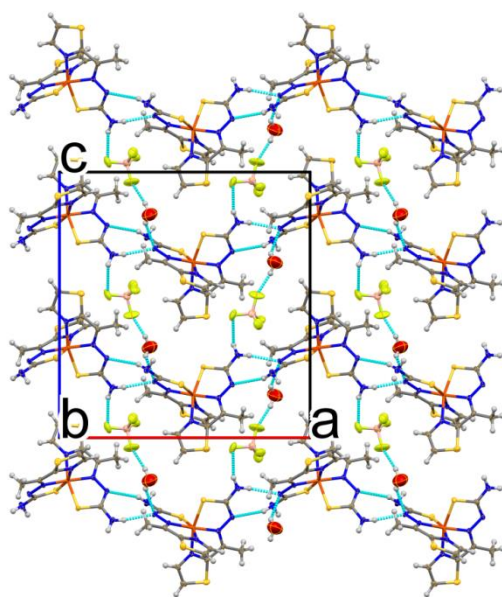
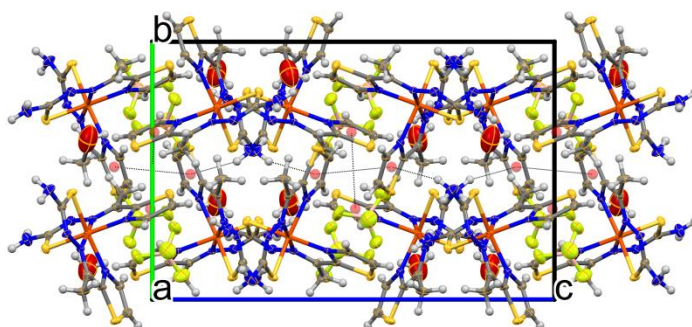


Fig S2. ORTEP drawing of **2**. All non-hydrogen atoms shown as ellipsoids at the 50% probability level. H atoms (isotropically refined) are reported in ball-and-stick style for sake of clarity. Colour code: Mn=purple, N=blue, S=yellow, C=black, H=white.



(a)



(b)

Fig. S1. (a) Crystal packing of **1** showing 2D assembly parallel with the (010) lattice plane generated by hydrogen bonding and (b) Intermolecular $\pi\cdots\pi$ and N-H $\cdots\pi$ interactions between thiazole rings.

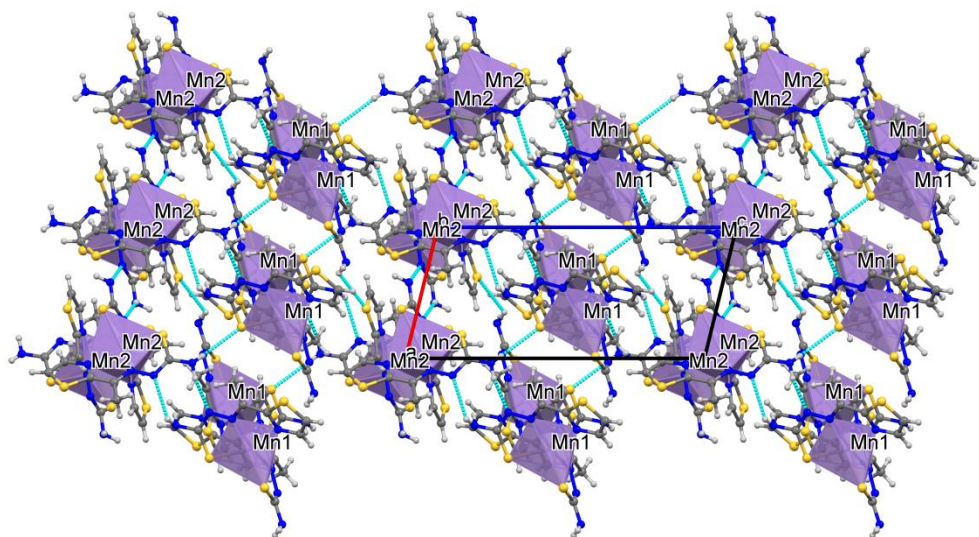


Fig. S2. Crystal packing of **2** showing 2D assembly parallel with the (010) lattice plane generated by intermolecular N–H···N and N–H···S hydrogen bonds.

Cartesian coordinates of all optimized structures

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Complex-1: Xray optimized hydrogens

Fe	9.53691800000000	2.94867400000000	3.03934100000000
S	10.25687100000000	3.67894500000000	5.01479000000000
S	10.46958800000000	1.11373900000000	-0.81535500000000
S	8.68479800000000	1.03859400000000	3.77985100000000
S	8.81625100000000	7.05174600000000	1.70536500000000
N	12.68802800000000	3.22965000000000	5.88741200000000
N	12.30403000000000	2.35598700000000	3.81028000000000
N	11.34671200000000	2.28580300000000	2.82180000000000
N	9.40885900000000	2.27491300000000	1.19260300000000
N	6.25471200000000	0.90391500000000	4.85168100000000
N	6.78159400000000	2.96101700000000	4.02007300000000
N	7.76570200000000	3.66406200000000	3.36612600000000
N	9.77142500000000	4.74343500000000	2.20565300000000
C	11.87359400000000	3.01183900000000	4.87436200000000
C	11.65212500000000	1.69650400000000	1.70290800000000
C	12.97379500000000	1.08663400000000	1.43074500000000
C	10.54299400000000	1.72070500000000	0.78246800000000
C	8.42653700000000	2.24345100000000	0.23436200000000
C	8.84804200000000	1.65052200000000	-0.93178000000000
C	7.14773200000000	1.70376400000000	4.24876500000000
C	7.52815900000000	4.89711300000000	3.02592200000000
C	6.26542800000000	5.66429100000000	3.25839400000000
C	8.67122400000000	5.49730300000000	2.36063500000000
C	10.74124500000000	5.42106900000000	1.53091600000000
C	10.39832500000000	6.67348100000000	1.16803200000000
H	13.62197462784804	2.82182786492997	5.88544137192471
H	12.34460320398741	3.67236010927596	6.73345540581787
H	6.51986885190216	-0.04441544744277	5.09485254501588
H	5.36205055082825	1.28744953648218	5.19882213285152
H	13.77008253303247	1.81753683244910	1.62664354092895
H	13.06137454308391	0.71813873618181	0.40303531027699
H	13.14297780271498	0.25093674872741	2.12565465766406
H	7.44579453507047	2.65851124986261	0.44274957329717
H	8.28183089828665	1.49426805890370	-1.84664104873276
H	5.45370695814917	5.26376078421276	2.63618737528870
H	6.39341600790628	6.72498489737482	3.01635845009395
H	5.97020760359026	5.56907242833582	4.31765678283928
H	11.69444086983174	4.93688671538482	1.33590506883547
H	10.99166258591815	7.41125315422253	0.63465187978244

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Complex-2: Xray optimized hydrogens

Mn	2.89976200000000	1.26653900000000	9.15700000000000
S	3.92497700000000	1.83662700000000	6.91185200000000
S	0.16073500000000	-2.33348900000000	10.21529200000000
S	4.92663500000000	0.31625800000000	10.31082000000000
S	0.53279500000000	5.24193400000000	9.80828200000000
N	2.61467400000000	1.66064600000000	4.64457200000000
N	1.54132000000000	0.58797200000000	6.31590200000000
N	1.60558700000000	0.22753900000000	7.62757900000000
N	1.60746600000000	-0.23839300000000	10.26883300000000
N	6.58123000000000	1.69008800000000	11.75138600000000

N	4.84838800000000	2.93764500000000	11.08090100000000
N	3.64646900000000	2.95249300000000	10.44133600000000
N	1.27696500000000	2.86327300000000	9.19475500000000
C	2.58946700000000	1.32571700000000	5.93672000000000
C	0.75787700000000	-0.67687300000000	8.02791700000000
C	-0.24578900000000	-1.36003200000000	7.18167400000000
C	0.87754300000000	-0.97459700000000	9.45839300000000
C	1.58516500000000	-0.74438900000000	11.54958900000000
C	0.88847600000000	-1.86971700000000	11.68954500000000
C	5.42566300000000	1.75808500000000	11.04835300000000
C	2.96664700000000	4.05834100000000	10.46737500000000
C	3.42409100000000	5.32181000000000	11.11182100000000
C	1.68103300000000	3.96682300000000	9.81316400000000
C	0.01905100000000	3.01729100000000	8.67561800000000
C	-0.49921700000000	4.28696700000000	8.91484400000000
H	1.82107998251425	1.43570221615392	4.01821165362432
H	3.26953376014914	2.38071507355088	4.36439955959976
H	7.19258168236040	0.89818394768996	11.58795305313429
H	6.99779382834163	2.56973919403251	12.05023852332114
H	-1.16612379238908	-0.76207865007645	7.08935072254007
H	-0.52976073660251	-2.33655485886641	7.59521956980808
H	0.15166273366410	-1.50429370560896	6.16924443465356
H	2.16048768410289	-0.23860826268597	12.32032959570974
H	0.72543954121986	-2.44920346510162	12.59371436556337
H	4.02756934252354	5.08338889290804	11.99552753494774
H	2.58176248214359	5.95958393833742	11.40897108186737
H	4.06329722559665	5.89164579356651	10.41991232805773
H	-0.44911283283703	2.21288389863359	8.11871588288451
H	-1.47341997747577	4.65424488551238	8.60255684968401

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C12H14FeN8S4 optimized with ADF in AMS. HS OPBE/TZP

Fe	9.56286154055822	2.89749569514950	3.33030249156539
S	10.76494222797682	3.39787739194552	5.29291904146192
S	10.43967451641650	0.76163684384230	-0.65772843724603
S	8.32184430302316	1.16468345593798	4.33036430445121
S	8.74646991819160	7.23517285645845	2.00237556946008
N	13.38751900117230	3.24861894654319	5.57361923633274
N	12.65964384240883	2.43325893359289	3.57903861292288
N	11.59616075133200	2.24965859642382	2.80511560371906
N	9.43002695448830	2.05797187774015	1.29893143315421
N	5.68587097604408	1.05722326990282	4.48693838005890
N	6.44950407359032	3.05302935542933	3.70825923146397
N	7.53077306975668	3.73324906959438	3.34460707412529
N	9.73586895677067	4.93557691275855	2.51118504410898
C	12.35499308621744	2.99567929961662	4.75084737478081
C	11.78529813966824	1.64616812540681	1.64826235460494
C	13.10569373490595	1.13417924417742	1.19279522270879
C	10.57864565086434	1.54271750134738	0.86844842607169
C	8.41699762732133	1.83283971629848	0.42056843263101
C	8.77782599588449	1.14779997677609	-0.70771884889316
C	6.73544357392311	1.82472513173997	4.14651739919897
C	7.36059725441793	4.98142931454453	2.95607166421280
C	6.04248278420883	5.67127343016962	2.95287027054011
C	8.58615919712524	5.60474466275834	2.52595480448251
C	10.76761031292063	5.71574620857300	2.09334915756566

C	10.42013057793872	6.99817760387168	1.76543340220662
H	14.30317074483597	2.90114226943355	5.32799204187646
H	13.21571515869645	3.56117169915342	6.51499517880785
H	5.83585492809434	0.16497931938548	4.92819855723496
H	4.76457609254236	1.46990568900599	4.50636849343819
H	13.83373664704633	1.95308187632342	1.14602841974903
H	13.04809659503425	0.65902531944951	0.21115414246157
H	13.49815810894289	0.40909022495576	1.91560545253321
H	7.41492907603818	2.18905644937177	0.63757735697317
H	8.16073239224416	0.85712506068179	-1.55126295675748
H	5.34689261266782	5.15980226930035	2.27616040961154
H	6.12446570084200	6.71626760122914	2.64645544288949
H	5.59357686557979	5.62787681365945	3.95201074490449
H	11.77276710241192	5.30955493975218	2.03766434831418
H	11.05296948004771	7.80071471660009	1.40184716815821

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C12H14FeN8S4 optimized with ADF in AMS. LS OPBE/TZP

Fe	9.56385654665290	3.01317203383363	3.03510869195857
S	10.30479381708315	3.77150555462549	4.96687603940434
S	10.41395750319337	1.08580916930248	-0.78849276791995
S	8.77843597665446	1.12553011089883	3.84749692305379
S	8.80672096471744	7.09418320378992	1.67322343000292
N	12.72104292525136	3.13844122495324	5.87985378439621
N	12.26924265455230	2.34812567670269	3.78335074530010
N	11.32835069872848	2.31404493319976	2.83415198089167
N	9.39500192037831	2.30951823278021	1.21044614301422
N	6.32021217660822	0.94998713886784	4.84799991834945
N	6.82506582931832	2.98535213678213	3.93893355996311
N	7.79649392245959	3.67096209046554	3.32705225731109
N	9.77767624024154	4.79952077462851	2.24426764706348
C	11.86171012974217	3.01951094891432	4.85573859321544
C	11.63511513391794	1.69296826098232	1.69598415157865
C	12.94635526236372	1.04700864159778	1.42882767709248
C	10.52842849226170	1.72301138785635	0.80082009001222
C	8.41955336607483	2.25761483132779	0.26097100859086
C	8.79349829910095	1.62888916359639	-0.89208576328665
C	7.20992460506029	1.74950511013525	4.23968868193390
C	7.51465003885925	4.91726512674648	2.94983926524092
C	6.19840908541095	5.57183473496936	3.16756415653442
C	8.64986216783498	5.51798040392892	2.33499210444772
C	10.78105494105128	5.49545826092838	1.64054616134960
C	10.43538134946606	6.76158182790874	1.26275492129936
H	13.61414892877190	2.67228150401953	5.83396286449484
H	12.43352665492131	3.56674816308809	6.74359486952839
H	6.58625204667480	0.03274227695139	5.16430287082096
H	5.41798553688510	1.31870221274988	5.10671292925844
H	13.76797654078710	1.75238947972226	1.59598641260474
H	13.00471591114754	0.67293592915008	0.40395795078479
H	13.10618107486948	0.20667670074391	2.11591452312943
H	7.44028961594063	2.68076650269905	0.45611012424862
H	8.20360509177126	1.44877561298312	-1.78415966772513
H	5.38703846884701	4.94765321929826	2.77738010274592
H	6.15473037691052	6.55105183305040	2.68506702555063
H	6.00869723522404	5.70340809462153	4.24020396894988
H	11.75824871103156	5.04451297359083	1.50629989042782

H 11.05048933138412 7.51230218651003 0.77887878026700

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C12H14FeN8S4 optimized with ADF in AMS. HS OLYP/TZP

Fe	9.53626237618471	2.83394815673056	3.34616479289151
S	10.75439568403585	3.25615966183671	5.35539943496460
S	10.47954031935563	0.76270041350990	-0.70542709031088
S	8.21526822461568	1.10622279039424	4.34643236908586
S	8.78500086379810	7.23123833572556	2.00564556775364
N	13.40465992967701	3.28851780991065	5.56926223308047
N	12.68529544795375	2.47812802374202	3.56177960439857
N	11.61664204660335	2.24856683131019	2.78986683945411
N	9.43142131232879	1.98346921353000	1.29644625688920
N	5.56279436439198	1.10158398438358	4.51713785666646
N	6.39540390237326	3.07183824389054	3.72766239276406
N	7.49975372915516	3.73162745179907	3.35851689627584
N	9.74620082367731	4.90983859161932	2.54274323273146
C	12.36872537626823	2.98633381607510	4.75868283284247
C	11.81645970317974	1.67194902732445	1.61885236475443
C	13.15914634257080	1.22133019330846	1.13470478598129
C	10.60179740881570	1.52777887337311	0.84662032643031
C	8.41348126499406	1.72675377696653	0.42199606671340
C	8.78869476702336	1.07766798961828	-0.72427994173117
C	6.64236280574041	1.83351559201301	4.16881377707442
C	7.35762313934505	4.98464789964367	2.96474638666635
C	6.04587007610992	5.70476995938680	2.95135899506811
C	8.59999570083410	5.59152819699083	2.54272914104995
C	10.79593261344308	5.67866959492370	2.12640705325963
C	10.46950104044297	6.96494201964070	1.78611276111778
H	14.33889081230667	3.01882983061107	5.29266916825417
H	13.23709617758426	3.56962472707115	6.52233122987576
H	5.68040611324664	0.20515279230086	4.96205644783652
H	4.65552179293176	1.54693172258389	4.53948817337563
H	13.84341275324970	2.07474751142468	1.06445056925204
H	13.10399017186315	0.73693068916576	0.15852459076418
H	13.60318268104898	0.52274208873959	1.85202996860144
H	7.40141877981895	2.03465069316446	0.65996415593902
H	8.17329339896253	0.77485575904502	-1.56285048422937
H	5.33402698728656	5.18633200285725	2.29910662889740
H	6.14606738775058	6.73639373468238	2.61038429111125
H	5.60680168414211	5.70566821751713	3.95514997385897
H	11.79474555846413	5.25898397111484	2.08392496657441
H	11.11759601057595	7.75415748097566	1.42451742990094

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C12H14FeN8S4 optimized with ADF in AMS. LS OLYP/TZP

Fe	9.56483651708731	3.00361605008527	3.06523745248126
S	10.34850706346844	3.76980118985425	5.01919835939112
S	10.43640364648376	1.06412364567735	-0.80570039358369
S	8.73808239544804	1.09340734664526	3.89721779245716
S	8.77837573164673	7.11665649074123	1.66070133139946
N	12.79403062510645	3.12656387770472	5.88726038227249
N	12.30992127438117	2.33811047953439	3.79146678836974
N	11.35479364960463	2.29438375857220	2.84259944157837
N	9.39669799644653	2.28398575978005	1.20191380496511
N	6.25085952140611	0.95834796485864	4.86797485675796

N	6.78665413932604	2.98879318671216	3.95364694874961
N	7.77173478939788	3.68173277236841	3.35028943582034
N	9.77459609428535	4.82300878749790	2.25193059693415
C	11.91522472268620	3.01095027651594	4.87156035638648
C	11.65351079413209	1.68085340028778	1.69619429924221
C	12.97555785125219	1.04504076960363	1.40944754339528
C	10.53941160533198	1.70516928554130	0.79900087929151
C	8.42199072097750	2.22833326383936	0.24324443332004
C	8.80077415732478	1.60101091222680	-0.91114294353397
C	7.16085041038888	1.74893645756404	4.26514951379603
C	7.49738715318025	4.92766746448363	2.96050096791496
C	6.17098831559595	5.58918921929374	3.15465915441194
C	8.63677936518239	5.53063238823569	2.34027267973060
C	10.77662642487093	5.52791804979946	1.64229546747625
C	10.42182730503140	6.78967438829826	1.25156418334526
H	13.68883797931089	2.66293634012263	5.82599624926485
H	12.52338176757235	3.55692614538608	6.75659713952132
H	6.49929951476162	0.03608021699968	5.18710560407625
H	5.34642073295313	1.33575629087985	5.11008386379147
H	13.79067128970589	1.76081475025687	1.55862560423418
H	13.02257396211479	0.66642173380247	0.38667896159309
H	13.15697326468694	0.21140761785796	2.09795338822997
H	7.44142744306733	2.64662891233665	0.43657309363916
H	8.21408458666818	1.41958763251370	-1.80323235917545
H	5.38836797284683	5.06398143184120	2.59459003265947
H	6.19294445749400	6.63041579707104	2.82759513520068
H	5.87962551652053	5.55788921526027	4.20952270425142
H	11.75645205095872	5.08371235931839	1.51357796287177
H	11.03119676344577	7.53926203953249	0.76197133335639

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C12H14FeN8S4 optimized with ADF in AMS. HS B97-D/TZP

Fe	9.55138277525136	2.78615917207027	3.54414886140227
S	10.86231350094919	3.16740874919509	5.50222698059657
S	10.22600396226817	1.01737461569181	-0.67153599647945
S	8.18789088112408	1.12904356518563	4.58054956129507
S	8.98823642636924	7.08017108007755	1.92850446257757
N	13.52466993671368	3.29364457343702	5.52899573233766
N	12.70144501898041	2.57097547878476	3.52935375610413
N	11.59382101160804	2.30290691251910	2.82700079994547
N	9.31806117781736	1.99893128428475	1.52105150907441
N	5.52898730504612	1.04440799691736	4.40276741580024
N	6.40206985820078	2.98189717225792	3.57597642948657
N	7.52711809140881	3.66466838460967	3.32909357872934
N	9.83887064321167	4.79329849468889	2.72983303196936
C	12.44695775271419	2.99141359343604	4.77439015263384
C	11.72854668720925	1.83121756834375	1.60411112256660
C	13.05375301849449	1.51992495413908	0.97745439725247
C	10.46217500076701	1.65875909561804	0.92722025071647
C	8.22745653559362	1.75181696953829	0.73725085454767
C	8.51812243477987	1.22319757172791	-0.49328670310684
C	6.62369447730779	1.78958513517848	4.14179193578028
C	7.42425597383012	4.87619394981139	2.82219532663332
C	6.11471011453184	5.55690752677412	2.56253021587732
C	8.70952531555319	5.47337972542568	2.53246679051751
C	10.95086560099681	5.52268868500780	2.41970732835831

C	10.69257899578668	6.78825075645144	1.96172488535343
H	14.44949990248776	3.08840033075471	5.17267710158132
H	13.41235811161964	3.53624005498349	6.50185573979095
H	5.61474394460188	0.17217174685984	4.90252299566384
H	4.61179720051224	1.45034048747800	4.26725806669285
H	13.64543481862373	2.43928964772895	0.87963833335458
H	12.94112726388565	1.05994366457867	-0.00823472866883
H	13.62086960367486	0.84742608952467	1.63162175076355
H	7.23539067338501	1.97552742804128	1.11454459811050
H	7.83581004436501	0.94728481818777	-1.28828266508312
H	5.53104174226287	4.97549203435926	1.83751162905369
H	6.25084163836469	6.57286947681267	2.18167440943497
H	5.52635697950705	5.58974894904176	3.48725862214188
H	11.93343158591441	5.08101856725271	2.54646994325451
H	11.39646356643134	7.54975136212508	1.64808356982396

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C12H14FeN8S4 optimized with ADF in AMS. LS B97-D/TZP

Fe	9.56248190672322	2.97685191109574	3.12201546288339
S	10.36889508439002	3.74744791856479	5.08639741645309
S	10.39312970261282	1.19378239715134	-0.81550151261242
S	8.70831583293777	1.05356747976024	3.94172793395969
S	8.82403524266307	7.03272464785747	1.57137449599684
N	12.84129315899875	3.10625764616326	5.90054913744025
N	12.33733197363480	2.35247056222272	3.79782940365086
N	11.36585161436213	2.30202000209735	2.86518903166453
N	9.37852610854862	2.29928420677794	1.26868359509044
N	6.19871783172494	0.95732165610166	4.88157643940377
N	6.75740512840104	2.97078695608003	3.94553187616736
N	7.75781049390223	3.65609004030878	3.35725306980961
N	9.79391581505196	4.76725090509692	2.29718464184237
C	11.94883442537495	3.00021591006949	4.89679079025530
C	11.65359050973284	1.73434171872579	1.69439695879047
C	12.98725914313871	1.14367266705061	1.36171744064678
C	10.52333017157938	1.76186751263198	0.81876749993610
C	8.37863195907126	2.27812039043049	0.33653255751874
C	8.73897457887417	1.71486670653899	-0.85698533006152
C	7.12161544874731	1.73252439367432	4.27973818828065
C	7.49670286945348	4.88696080212927	2.91865326086443
C	6.16263717093812	5.55115520822865	3.05040487685668
C	8.65414616937928	5.47571017930670	2.31970913159814
C	10.82113999206594	5.43219070992384	1.68745907873776
C	10.48761560896360	6.67790330277559	1.23056912537670
H	13.74782135355129	2.66802397614796	5.81035862098584
H	12.58701954570603	3.54217787406083	6.77346586925040
H	6.42906387955605	0.02616912294839	5.19221103578285
H	5.28516738379857	1.33784006042939	5.08785961384015
H	13.77857338956360	1.89114019841848	1.49459295929278
H	13.00837459845389	0.77178031762710	0.33319004815870
H	13.21177391835095	0.31692738399852	2.04735290798295
H	7.40190036902537	2.67513627686827	0.58695162342892
H	8.13235669385803	1.56746326584841	-1.74204006889718
H	5.38420379408174	4.93888874154903	2.57934165765247
H	6.16941389262202	6.54408671465543	2.59133201213010
H	5.89501778211347	5.64699148582975	4.11010032412916
H	11.79675078630956	4.96561886133494	1.61713567793781

H 11.11905424388899 7.40209755842024 0.73070519365928

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C12H14FeN8S4 optimized with ADF in AMS. IS B97-D/TZP

Fe	9.47392114726212	2.97743303074024	3.27622098945059
S	10.56468862494006	3.60680002005757	5.36806232966170
S	10.41026632428815	0.84471309113198	-0.73574900547936
S	8.51147694488798	1.07346079892137	4.01571092134401
S	8.89353975779574	7.11671214346538	1.81860507843784
N	13.19041615223134	3.26412236843822	5.66415598583177
N	12.41642824927030	2.47429999115973	3.67693717373062
N	11.37284660190025	2.29352183675764	2.85785423264146
N	9.32627413998798	2.22205236359796	1.14998721977452
N	5.93110199127844	0.98977318911586	4.73618754631918
N	6.57084663958779	3.01336372071324	3.87715012411314
N	7.62488468423458	3.69077242377432	3.38606588526921
N	9.79314518066948	4.80368261409886	2.47534868155130
C	12.13277169250074	3.07067739488287	4.84285122455131
C	11.62252806456932	1.72803771478426	1.68209585651534
C	12.98776335141145	1.24108809486521	1.29974090990466
C	10.48213853169931	1.65948765398213	0.80750266083190
C	8.35148075447978	2.01338397683825	0.22103305059056
C	8.74841663155454	1.29519932332425	-0.87928365038237
C	6.90119264489851	1.76728986372894	4.22056800874161
C	7.44421932382528	4.93278645729885	2.94704381208675
C	6.11904492224448	5.62339101671731	2.98138999012669
C	8.65962104058747	5.51984643811296	2.45047910938516
C	10.86899949227660	5.50035051508093	2.00586907172308
C	10.57600481562657	6.77529094371667	1.59835635195984
H	14.08375317952352	2.85467408184022	5.42317848795834
H	13.04463794498658	3.61618288286268	6.59804119661312
H	6.13301106037440	0.05244699172011	5.04915212538139
H	5.00832062166490	1.37443011972154	4.88699048649868
H	13.69786838434670	2.07777475797741	1.29420954565986
H	12.98414998138957	0.76901552289647	0.31321321932399
H	13.35037723660193	0.52486049284737	2.04651120004941
H	7.35457245344163	2.41020060326216	0.38339667379587
H	8.16643711505763	1.01853592206254	-1.75040400840094
H	5.37136080097231	5.02241716397270	2.44949068377299
H	6.17361065273207	6.61960451375425	2.53408495834477
H	5.77427324656441	5.70880825989724	4.01984502153892
H	11.84628018937488	5.03202588330534	1.98989110474318
H	11.24600900111116	7.52121348747570	1.18833779192414

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C12H14FeN8S4 optimized with ADF in AMS. HS B97-D-COSMO(DMSO)/TZP

Fe	9.54887360094052	2.77722474041520	3.56315032781185
S	10.87048692149513	3.13760215284296	5.53171439424984
S	10.21020257847073	1.12178779153486	-0.67710620549367
S	8.17097917061114	1.12727062014926	4.62272245737041
S	9.01040735027643	7.00509535097927	1.82400290270444
N	13.53776060205495	3.25296763456841	5.56186692095179
N	12.70641108981869	2.53832946940828	3.55894184841799
N	11.59082153238136	2.28375713428076	2.85508964711741
N	9.30891913619187	2.00393564707297	1.55689521271493
N	5.50765132979078	1.05556927579079	4.45297570956869

N	6.39445649863946	2.98709514915032	3.61794347855964
N	7.52921093103751	3.65776085683147	3.35616807823061
N	9.84813125122426	4.76320970895596	2.74850032736193
C	12.46518184678055	2.95771720780012	4.80412305586222
C	11.71911726530855	1.85112715633090	1.61831418813675
C	13.03896701396468	1.57627625345799	0.96743018948713
C	10.45090419569392	1.69256287174819	0.94081562212612
C	8.21525796319492	1.79131789069399	0.76685977504134
C	8.50594943904410	1.31547240620611	-0.48589247394555
C	6.59961178576441	1.79542195861372	4.18490299584319
C	7.43549166706393	4.85360376377325	2.81370513773522
C	6.13334901823805	5.53107674678350	2.51990704443146
C	8.72308052414992	5.43883754415149	2.50931729037676
C	10.96508319492276	5.46936864537769	2.40438228852981
C	10.70998657068068	6.71096981399373	1.88061689332569
H	14.46844098193941	3.09537806234505	5.19701756875219
H	13.42861172158594	3.53606337046263	6.52380813225470
H	5.58942755334523	0.16716463992354	4.92362158194617
H	4.58696175685958	1.44013126369360	4.28395622685713
H	13.61964716776226	2.50553350166651	0.90661116083578
H	12.91606593287638	1.16345163264887	-0.03677904443857
H	13.61466385121344	0.87542020978603	1.58294696160691
H	7.22413447535704	2.00279308173765	1.15170853999384
H	7.82402952789527	1.07628824306555	-1.29194556286802
H	5.55611672161981	4.92620200558973	1.80935146999979
H	6.28205661586311	6.53065395597473	2.10441819214587
H	5.53994402627253	5.60262106081451	3.43896161055377
H	11.94588691751059	5.03124013556621	2.55110086154425
H	11.41639984431007	7.45142871471496	1.52799724018438

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C12H14FeN8S4 optimized with ADF in AMS. LS B97-D-COSMO(DMSO)/TZP

Fe	9.56490646856669	2.97189274938790	3.14790534206802
S	10.39028852191412	3.75229252261942	5.10425993136097
S	10.38751714649313	1.26323547003961	-0.81601014532192
S	8.70527294578228	1.04895323456769	3.98042890666502
S	8.82337891004661	6.98520503859511	1.51825418223015
N	12.85892690121877	3.09049590905704	5.91878216519888
N	12.34266679245060	2.32813885915535	3.81826985101651
N	11.36555161480981	2.29199948116010	2.88175000914989
N	9.37039423208154	2.30532991201528	1.29580304211869
N	6.19230637617963	0.95593427666914	4.91476123575096
N	6.75351913630784	2.96960806224695	3.97278865406327
N	7.75929763312580	3.65314883925236	3.37754234394024
N	9.79753884379959	4.74713280764718	2.31013755617910
C	11.97046614613218	2.98468458885332	4.91619627443886
C	11.64805796809078	1.74297974699205	1.70420194899891
C	12.98110345737457	1.16819296430007	1.34762260241129
C	10.51443628214589	1.77984132681175	0.83015080981717
C	8.37256791241473	2.31935264620800	0.36135943410461
C	8.73908308765908	1.78960100656042	-0.84690084285518
C	7.10934173344850	1.73146188786923	4.31215949867498
C	7.49814134405567	4.87168839991176	2.91394401458734
C	6.16027668286982	5.53221608334725	3.00528052026240
C	8.65723111839701	5.45539889661763	2.30918780103681
C	10.82560611561275	5.39493225851831	1.68355141293226

C	10.48506341575902	6.62702679330925	1.19235951954321
H	13.76972758334738	2.65928715242278	5.83474918830939
H	12.61112217484000	3.54415549340450	6.78481243047407
H	6.41976965797878	0.01975995720281	5.21310022801814
H	5.26914897007135	1.32123448753304	5.10637661297431
H	13.76605631664835	1.92140716700135	1.48472792182672
H	12.99048626540786	0.81922718567232	0.31178596922107
H	13.21630084905605	0.32729313728377	2.01203944774598
H	7.39856147525681	2.71875684075919	0.61646229051262
H	8.13799373549891	1.67356117550118	-1.73946357150619
H	5.41180007699548	4.94859587410439	2.45477253747678
H	6.19730135298322	6.54524972300003	2.59621899242520
H	5.83530515894875	5.57546698321547	4.05146769865867
H	11.80059680875124	4.92724818092742	1.62025638250584
H	11.11156835962935	7.33774054916030	0.66902984886918

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C12H14FeN8S4 optimized with ADF in AMS. IS B97-D-COSMO(DMSO)/TZP

Fe	9.65405572829764	2.87956553851088	3.22615557289934
S	10.55776012936131	3.66832060583987	5.13496294732878
S	10.35598368147022	1.06097331846053	-0.73679292663183
S	8.49582124990273	0.91196842340099	4.19411738065661
S	8.75563494424037	7.16470167716777	1.76038631937226
N	13.07822585898543	3.08941747913910	5.85025496687254
N	12.51081297742477	2.30074090785631	3.77148330202591
N	11.48885153024519	2.21962036344347	2.89015765736739
N	9.38749226012536	2.18640802588884	1.35322158068824
N	5.87925349286355	1.02971387270310	4.70422910572429
N	6.69943631954883	2.97435240336186	3.85745159601306
N	7.75607872511556	3.65812183973414	3.38449295189975
N	9.84151305279410	4.89151719692247	2.27454153647317
C	12.16325272477169	2.95317487900179	4.87900230270141
C	11.70487966788222	1.67391296882935	1.69896197004862
C	13.03218999334811	1.13822632718573	1.27668761051543
C	10.52728821191703	1.67002515379814	0.87006081327980
C	8.35495816006406	2.10865157467433	0.46514038697522
C	8.69457312757859	1.52555170251371	-0.72936328407930
C	6.94705516154406	1.71823472589269	4.24471530135575
C	7.52194838610090	4.87723493398786	2.91782825684409
C	6.15972907427001	5.50040902489534	2.93946156092757
C	8.67787681626946	5.53072039999980	2.36010387593680
C	10.82745901250383	5.67126386822722	1.74735669321646
C	10.42842102228133	6.93871933659866	1.40101831317742
H	14.01880822874685	2.74467691416963	5.71097870057179
H	12.87045306670439	3.61322390707628	6.68710028615593
H	5.99468998791643	0.10356602577190	5.08649675283523
H	4.98964370035688	1.49940485647376	4.81362776237264
H	13.78573970353247	1.93355502308531	1.33349196424214
H	12.99529345339904	0.74229199541706	0.25932829282673
H	13.34574896719336	0.34658966985154	1.96802071630233
H	7.37768717632434	2.48853898233397	0.73677893628097
H	8.06695059060797	1.34923456673546	-1.59333028417336
H	5.46172942131416	4.88964661762491	2.35337836877942
H	6.17907352152421	6.51385968248783	2.53068953445579
H	5.77852160600759	5.52831140067087	3.96707700159867
H	11.82887323386847	5.27249787511981	1.62502069992856

H 11.01491560574738 7.73278360404843 0.95582752211862

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C12H14FeN8S4 optimized with ADF in AMS. HS SSB-D/TZP

Fe	9.55177436370100	2.77909818869555	3.56288818312573
S	10.86790166772798	3.12632373457173	5.48370464781381
S	10.21565061023664	1.04505307676214	-0.63663101961255
S	8.18449269689994	1.16833084857512	4.58883449394374
S	8.99525449170367	7.03480664474940	1.92929626167438
N	13.50062246687511	3.27828095310547	5.50575025784580
N	12.68680310764855	2.57314303177026	3.51018448488135
N	11.58052364172089	2.31256084912332	2.82531433240167
N	9.31240295613753	2.00805496175082	1.54215613365990
N	5.55706017530798	1.06175453998920	4.38088812650885
N	6.41828327610557	2.99023540180426	3.55501033810090
N	7.54064117590032	3.65772403678323	3.31864017837915
N	9.84357414162135	4.77802933934953	2.75069210392198
C	12.42869284220257	2.97278933814752	4.75757095567055
C	11.71216215699206	1.85728214831366	1.60022144671500
C	13.02030590063691	1.56720766344164	0.96718298729200
C	10.44908874958233	1.67940044478171	0.93839101709763
C	8.23342649215811	1.74941609401047	0.76506245485740
C	8.52909779068937	1.22603988363333	-0.46215890839613
C	6.64446808280770	1.80875907598759	4.13355486638574
C	7.44044550995250	4.86211360882185	2.80470943865331
C	6.14815398387584	5.53337659042912	2.52937692713409
C	8.72132758940950	5.45417060351070	2.53202015487708
C	10.94287000785668	5.51056731227996	2.45217096370631
C	10.67847089461017	6.76711887361156	1.98429204519223
H	14.41315911880358	3.04459093356803	5.15607064893536
H	13.38619314787446	3.46154412099986	6.48380418332755
H	5.64361189102858	0.22552983052813	4.92540897442574
H	4.65068984261411	1.48121474949447	4.27050993404085
H	13.60686039537784	2.48418517464915	0.89209780942050
H	12.90612125233742	1.13476419267719	-0.02337609604056
H	13.58888329797419	0.88459054247791	1.59883471774741
H	7.24253938995771	1.96161694018374	1.13903787127071
H	7.85455124926420	0.94479933662743	-1.25502931974801
H	5.57677076084219	4.95261708659437	1.80380164682905
H	6.28615297274133	6.54252074141272	2.15011305537259
H	5.55132140523916	5.56635167075687	3.44107841182256
H	11.92455192199989	5.08240790403928	2.59298328179281
H	11.37377815373511	7.53135720089243	1.67566405485777

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C12H14FeN8S4 optimized with ADF in AMS. LS SSB-D/TZP

Fe	9.56216117805275	2.98319593056892	3.10397395817172
S	10.35134871512707	3.74322824218109	5.04170019371445
S	10.40527822542529	1.19734782090403	-0.78858989208622
S	8.72598149553585	1.08804414655167	3.91669239204988
S	8.81398955929243	7.01083792315575	1.59088135603372
N	12.79008627959108	3.11844451887489	5.87313929621782
N	12.30909267699034	2.34498122855348	3.78611409692085
N	11.35092169629647	2.30629908782415	2.85771536484182
N	9.38387856942294	2.30696754039045	1.26255511067813
N	6.25334377296790	0.97229015282093	4.86652630676838

N	6.78482393300925	2.98448209264727	3.94434695422818
N	7.77165178292391	3.65741350440786	3.34882151024463
N	9.78749126292305	4.76258494904218	2.28481512809045
C	11.90649169737486	2.99875433729293	4.87245850607199
C	11.64296878024905	1.73416068837681	1.69671966853035
C	12.95961052743788	1.13760081535092	1.37946969717727
C	10.52249763790146	1.76480726512112	0.82124829644931
C	8.40317071243297	2.28332706123123	0.32695084747640
C	8.77650981867513	1.71314744323549	-0.85482690329231
C	7.16416754920973	1.75133590365821	4.26818787898890
C	7.50659718696785	4.88458119926089	2.91983382273127
C	6.18938043816043	5.54266931209373	3.06794371017394
C	8.65464952874361	5.46992794517966	2.31806984732859
C	10.79724497688168	5.43185514807221	1.67629763087272
C	10.45245269691060	6.67589692702748	1.23489946681040
H	13.66241151492848	2.62605885493255	5.81226549110696
H	12.50238608617610	3.49183484430765	6.75623991598736
H	6.51199925595617	0.07330197168949	5.22233887317484
H	5.36773059862761	1.36665622158930	5.12518152128609
H	13.75436820713304	1.86435295252110	1.54726749209787
H	12.99660017843684	0.79155949906819	0.34949020489088
H	13.15665852524523	0.29589307110165	2.04519951298045
H	7.42863781729741	2.68325324588788	0.56047074562123
H	8.18459509109924	1.56171336812471	-1.74293749236720
H	5.40628990385240	4.92502815520530	2.62801640233280
H	6.18429570884814	6.52246427347993	2.59676683548722
H	5.94604580214434	5.65416318320018	4.12549046447938
H	11.77046556718830	4.97375584790803	1.59129065829280
H	11.07040461671301	7.40551099606137	0.73709717532091

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C12H14FeN8S4 optimized with ADF in AMS. IS SSB-D-COSMO(DMSO)/TZP

Fe	9.63137699469386	2.83274909357731	3.23510675733489
S	10.53228830786612	3.62666888795592	5.11209769352237
S	10.32515533457152	0.95873927344817	-0.67487174687679
S	8.46966166668830	0.97109433097406	4.19979940206056
S	8.82513673407360	7.17004885492353	1.88821593304535
N	13.06559741957933	3.19265963237466	5.75394874454147
N	12.50677558103357	2.38609950088786	3.70023635402514
N	11.48339494036206	2.26427817848259	2.85542926971913
N	9.36787700087555	2.13366918536139	1.37043686537102
N	5.85756527528276	1.04026768144633	4.56152523118816
N	6.68355291304430	2.98986488293557	3.76621562693649
N	7.75086915131653	3.65919677214714	3.35021380091289
N	9.85728985426027	4.86860029705979	2.28548158677345
C	12.13081129838915	3.00982859013009	4.81477427289174
C	11.69795556553436	1.70743747025216	1.67351199493463
C	13.02381496027484	1.21133123870348	1.24586040701032
C	10.50911733136024	1.64424334695083	0.88113205822897
C	8.32871129015242	1.96474900184447	0.51930220398084
C	8.66289774618686	1.34530650292085	-0.65137295168985
C	6.93723059096098	1.74170148703500	4.16789994625864
C	7.54530558593971	4.89238643094994	2.92059652845912
C	6.20973071884240	5.53514637757217	2.95713231446878
C	8.71417279894997	5.53021546648746	2.39619729625330
C	10.84811145074069	5.65732625616601	1.81242964110043

C	10.47509673697099	6.94291016139154	1.52840144089928
H	13.98149875168696	2.80488952000958	5.62146183454812
H	12.82600145290713	3.59971997116118	6.63656213363711
H	5.99086273606034	0.16186858149569	5.02399963961322
H	4.99539425556320	1.53557465586341	4.70578558304268
H	13.76442076241392	2.00571089827172	1.34301858363126
H	13.00553516243447	0.85282053835145	0.22005100664289
H	13.34492185859320	0.40373808488562	1.90580393153092
H	7.34434615542804	2.30545156667639	0.80158094484087
H	8.02669964785977	1.10093149436553	-1.48683912704198
H	5.51002534324124	4.98292691840769	2.32791230229877
H	6.25282158625357	6.56724891735130	2.61888930923572
H	5.81086034592794	5.50049921431857	3.97097286812272
H	11.84225990142839	5.25498329454315	1.68110921258488
H	11.07353436440136	7.74684511122112	1.13011315184669

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C12H14FeN8S4 optimized with ADF in AMS. HS SSB-D-COSMO(DMSO)/TZP

Fe	9.54678180272425	2.76076525305806	3.58424004625901
S	10.87261663777478	3.08511122457061	5.51456457375501
S	10.20595023874530	1.17535556489822	-0.65466903341428
S	8.16161940405566	1.16265892147238	4.63321097199966
S	9.02198739932342	6.95067280789291	1.82314392993662
N	13.50897940377467	3.23243380307263	5.54159546301609
N	12.68956024497562	2.54322928296248	3.53937638525369
N	11.57739832807025	2.29559162865408	2.85227335957546
N	9.30408229194580	2.00890675764986	1.57552746727561
N	5.52930312333646	1.07432587677468	4.43784599884846
N	6.40836444284714	2.99444572762628	3.60159251966468
N	7.54080336902554	3.64643265321737	3.34882353124286
N	9.85255137427485	4.73618306617167	2.76421838663607
C	12.44347160525787	2.93465237396731	4.78924949953470
C	11.70409487541995	1.88416083106996	1.61249654054617
C	13.00767335041029	1.63813773831458	0.95473960636313
C	10.43988996414364	1.72030034704088	0.94849778940632
C	8.22328052315126	1.79073844889653	0.78795645963045
C	8.52137195290485	1.33756081497943	-0.46708870814498
C	6.61570086195505	1.81401455550596	4.18342173989394
C	7.45193322941918	4.83403481141589	2.79743208583667
C	6.16829328113499	5.50446613479630	2.48820121641131
C	8.73655402111611	5.41028419248043	2.50655673660056
C	10.95859568760648	5.44340602248842	2.43034809896437
C	10.70076257918463	6.67625579202014	1.89824524365910
H	14.42904394670920	3.04314716695868	5.18518959351206
H	13.39839307101343	3.44279847128789	6.51432406433256
H	5.60931838247195	0.23291840589930	4.97517009711704
H	4.62032128927885	1.48395795576390	4.31236336320667
H	13.57426025935113	2.56927663278305	0.90609193846410
H	12.88357375677467	1.24266897351993	-0.04926667908393
H	13.59332699063492	0.93980794595480	1.55211396559574
H	7.23217454062287	1.98124426416084	1.17146071533936
H	7.84830687583788	1.09958721973504	-1.27439447578911
H	5.60345717693065	4.90291269761246	1.77472047694859
H	6.32177830048615	6.49805106706024	2.07704179066705
H	5.56533853579506	5.57414575738113	3.39347587723972
H	11.93743660796866	5.01672215556311	2.58968638433847

H 11.40032984569654 7.41836432422330 1.55034502524524

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C12H14FeN8S4 optimized with ADF in AMS. LS SSB-D-COSMO(DMSO)/TZP

Fe	9.56323117247958	2.97581422123122	3.13201186995490
S	10.36810941727984	3.74121738441269	5.06152557333665
S	10.39667345449819	1.26319824910854	-0.78801100362965
S	8.71841476655559	1.08229916997598	3.94892319067887
S	8.81964709670988	6.96225440355931	1.53761976608071
N	12.80215270346865	3.09815763133403	5.89516448343403
N	12.31512295666909	2.32835436699190	3.80413235632607
N	11.35031858671594	2.29875005831239	2.87522995261786
N	9.37367054222637	2.31204317593350	1.29198307265153
N	6.24384759892648	0.97089658464573	4.89674478487077
N	6.77917386558140	2.98260111266858	3.96702479886077
N	7.77278377292633	3.65289989174252	3.36907726271583
N	9.79405768992140	4.73797056327243	2.29879089469633
C	11.92635569014569	2.98560333144847	4.89266770873214
C	11.63717372609681	1.74708186609724	1.70584876975110
C	12.95557647613658	1.17148941496317	1.36242881711845
C	10.51230181520886	1.78461584295557	0.83374655659117
C	8.39212430459687	2.31675615450148	0.35682533065027
C	8.76945601436203	1.77699741905941	-0.83906454326751
C	7.14915308085915	1.74905793824860	4.29768154275433
C	7.51124292940431	4.87012600284390	2.91761916215222
C	6.19220076055710	5.52976426338674	3.02820480322383
C	8.66185975393702	5.44704026545160	2.30914342625257
C	10.80560953596437	5.38776929548819	1.67189762352999
C	10.45647359634267	6.61844555609410	1.19482721432014
H	13.68892705868872	2.63218439329724	5.83397425997670
H	12.52727968824146	3.50557900578488	6.76731031868804
H	6.49353928923734	0.06009336875546	5.22862772217408
H	5.34479182712769	1.34748982737872	5.13543040102863
H	13.74027768824560	1.91176710460614	1.51831921876567
H	12.97545130828206	0.83550760929418	0.32928511668752
H	13.17474288274358	0.32651531479711	2.01667642933019
H	7.41924911442280	2.71589529427015	0.59682873787944
H	8.18089651865859	1.65130873316215	-1.73270968466367
H	5.44147198123067	4.96584555246384	2.47275490981360
H	6.23271693204224	6.54502828615990	2.64311686708114
H	5.87370131177011	5.55116949936454	4.07031573504532
H	11.77777462002250	4.92685028038633	1.59489627338743
H	11.07112804386639	7.33328923545282	0.67325232628676

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C12H14FeN8S4 optimized with ADF in AMS. IS SSB-D-COSMO(DMSO)/TZP

Fe	9.64494572491755	2.85518276064597	3.22841943517884
S	10.54505755935398	3.63301231757868	5.11532014554627
S	10.35284395423798	1.05329469046031	-0.70176028691016
S	8.48187056949060	0.94972129511083	4.18900575432985
S	8.78140393727483	7.13090249867806	1.80279638625153
N	13.03992512294465	3.07811544241746	5.82411396705291
N	12.49528893641176	2.31669981334772	3.74413084820471
N	11.47749791113302	2.23114408801008	2.88148476914328
N	9.37982137784111	2.17425616859959	1.36337757761878
N	5.87594194638405	1.03272019381601	4.62468857129635

N	6.69793787887307	2.98551798378890	3.82660540089916
N	7.75663564885592	3.65164020700124	3.37039008651790
N	9.84833000028487	4.86625171765168	2.29311360446358
C	12.13327586500264	2.95247760959757	4.85367785255653
C	11.69406594241055	1.69220850484765	1.69296153731827
C	13.01202258772448	1.17803509147988	1.26928639995638
C	10.51810193405380	1.67260174106030	0.87760801010387
C	8.35681862053064	2.07156576838458	0.48361541869559
C	8.70536347263360	1.48300041646581	-0.70064174815165
C	6.94893154777726	1.73450363168677	4.21179064596826
C	7.53624849644995	4.87267458264877	2.91929657784657
C	6.19546404869633	5.50293786903846	2.94136497568314
C	8.69560976346084	5.51559876552452	2.37778219787810
C	10.82661305998955	5.64389666581941	1.77731473827407
C	10.43099176666004	6.91126781991761	1.44259567674855
H	13.98719911883494	2.79182377293500	5.65495994018145
H	12.84175932881131	3.63406809484668	6.63329495450425
H	6.02298230283263	0.16994112602210	5.11310648368623
H	5.02747799105340	1.53775561648932	4.81458027312877
H	13.75700799003915	1.97026797815690	1.35020098096561
H	12.98311495595028	0.80683423015679	0.24906649653868
H	13.32482914334948	0.37663238899133	1.93985022317611
H	7.37662785623268	2.43531341585789	0.74920754092172
H	8.08515946336149	1.28642151191188	-1.55953883867894
H	5.50033144490293	4.91728190451512	2.33805029603271
H	6.22890180490396	6.51979839695390	2.56016186208911
H	5.80521061040766	5.50838267648780	3.95918608791234
H	11.82407846539840	5.24847623265839	1.65235815842009
H	11.01299142267850	7.70750267933978	1.00729904453541

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C12H14FeN8S4 optimized with ADF in AMS. HS B3LYP*/TZP

Fe	9.54257196078190	2.82755485348492	3.39674943437750
S	10.78281348441512	3.21979284000019	5.39782146866305
S	10.37158738039610	0.81275625049451	-0.67657432482741
S	8.22375760702049	1.13333905596011	4.43922386313103
S	8.87677216208644	7.19713133548407	2.03895986007838
N	13.43687835043127	3.30375989185255	5.53571941329867
N	12.68223879445649	2.54255994435669	3.52982683673504
N	11.59229409821772	2.28916718174686	2.78429751286549
N	9.37547544321482	1.98190704199477	1.37451709350186
N	5.56562592861135	1.08167494636016	4.44671336859362
N	6.40567267675987	3.03094680680790	3.63150410893283
N	7.52526967192398	3.70660152397682	3.31793188982490
N	9.79292297750304	4.87289361758911	2.60911888672744
C	12.39349532343499	3.00455630637444	4.74168767091506
C	11.76721485185892	1.73876288809556	1.61073164135790
C	13.10122146205684	1.32961029404570	1.07759474086289
C	10.53192086804182	1.56556358107511	0.87540652154395
C	8.32431810532778	1.70525756431060	0.54388824649530
C	8.66676580799987	1.08023503588291	-0.61746345643565
C	6.64241407486403	1.82325432523447	4.13119206088070
C	7.39680652973172	4.94130974326371	2.90507508565764
C	6.08580028605689	5.65005011893980	2.80911132625175
C	8.65783436523632	5.55630285965140	2.54909063354409
C	10.87397052048540	5.63524265621251	2.26069711371579

C	10.57621328043546	6.91924256352512	1.91405801048664
H	14.37211088388112	3.07964925536606	5.22373335248876
H	13.28682082440483	3.57509161178467	6.49466974797101
H	5.67583448230498	0.19535672898073	4.91361805740548
H	4.64716055792802	1.50014308264255	4.38680449351507
H	13.75108771583701	2.20315516826264	0.97031652962907
H	13.01745006697919	0.83208957841620	0.11088948374715
H	13.59523221146720	0.65775516901590	1.78437826225103
H	7.31994629422758	1.98138477403770	0.83632657454125
H	8.02381624705877	0.76641928872875	-1.42651710460814
H	5.42014828009126	5.12248128880068	2.11995732962519
H	6.20361934817955	6.67913279920766	2.46832260534844
H	5.58895032008277	5.65098595150447	3.78317289772895
H	11.86575371458292	5.20308066108574	2.27798946353968
H	11.24889261377614	7.70352908434698	1.59958134552281

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C12H14FeN8S4 optimized with ADF in AMS. LS B3LYP*/TZP

Fe	9.56363311924267	3.00262281776972	3.06078034759261
S	10.35411913132790	3.77910168330893	5.03409347599299
S	10.44206347754879	1.04157694780972	-0.79468233266487
S	8.72575910415840	1.07085280620464	3.89647365048670
S	8.77361024575175	7.12081123685609	1.68492072747379
N	12.79819459402679	3.12275191937051	5.87879019563431
N	12.32096191029552	2.34519324310453	3.78987670273800
N	11.37200902051759	2.29205421372540	2.83471466446805
N	9.40096167178845	2.28280932439788	1.19042954999849
N	6.24401344151519	0.96792440428412	4.87030938228518
N	6.77384012343725	2.98392977599348	3.94923491139977
N	7.75259016153220	3.68630999866989	3.34576573175286
N	9.77074082271354	4.82757171103116	2.24489848495960
C	11.92317760923327	3.01410916917612	4.86598787515052
C	11.65752141433909	1.68479846153171	1.70153977359163
C	12.97321187644664	1.04401724205907	1.40973481655255
C	10.53800604515224	1.70451962547939	0.80020964905749
C	8.42500334543980	2.21788063864308	0.23301768620502
C	8.80195380478312	1.58030906309762	-0.90885722417666
C	7.14975381872996	1.74879027975717	4.25972361120451
C	7.49274206959757	4.91866452166195	2.96135179094152
C	6.17516262133953	5.59164024649184	3.15813141818541
C	8.63837072514188	5.52642316820352	2.34133540644639
C	10.77518840074478	5.53918024746606	1.64644320015412
C	10.42273985691128	6.79964395535776	1.27251144158661
H	13.70146368170994	2.67676870122799	5.80467148882449
H	12.53873366434766	3.57541108050664	6.74055021337096
H	6.48183172988738	0.03575472943466	5.16916360750114
H	5.33405152707979	1.34465173890047	5.09438924703541
H	13.78792457326257	1.75701444331561	1.55952984708018
H	13.01486939099640	0.66527720743129	0.38782502520353
H	13.15082292988816	0.21358684693533	2.09980536198759
H	7.44861728088261	2.63962521499449	0.42735317333763
H	8.21656207382348	1.39225552608310	-1.79655569737290
H	5.38920363736025	5.06966240503594	2.60435818288061
H	6.20562427960201	6.63097466923671	2.82874064591329
H	5.89075479594067	5.56134330131194	4.21299475553922
H	11.75115763273441	5.09224960257151	1.51730323545915

H 11.03173396291946 7.55166550046369 0.79325802210734

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C12H14MnN8S4 optimized with ADF in AMS. HS OPBE/TZP

Mn	2.89235101017946	1.48390440785022	8.85318308488235
S	3.44795815940463	2.30887429213218	6.56321782668621
S	0.09069562262092	-2.03448714072976	10.37772008754618
S	5.04889224350442	0.50093904641405	9.62021981369089
S	0.47869169796334	5.34358205245712	10.25268395077601
N	2.57054739157190	1.24043666115107	4.32044207964383
N	1.70668274080568	0.21158180265111	6.13839434007162
N	1.68484485908121	0.12320496291316	7.46326111364982
N	1.60904811222829	0.01728311746813	10.16174440318256
N	6.65311556713228	1.58394029517079	11.41006121405334
N	4.78099368954876	2.81561647881737	11.09552788824327
N	3.61322130032901	2.93174557540107	10.47295939166229
N	1.22823315483691	3.12323984800887	9.21513671127773
C	2.50801360036008	1.19179262445437	5.67858340805497
C	0.93408993882043	-0.82747652370568	7.98168715840827
C	0.14932123722659	-1.79339064517936	7.15817557384801
C	0.938127111018230	-0.85696228427968	9.42460547045834
C	1.47227756893530	-0.23354622730915	11.48870000567654
C	0.68063515324611	-1.30312049175329	11.80803875853438
C	5.47373099798513	1.71785011110716	10.73865767867931
C	2.87720161834989	3.97834055539534	10.78739543558137
C	3.29797664289418	5.00747845141776	11.78288303206939
C	1.62182197103153	4.04799041943491	10.07950429380226
C	0.02108784995455	3.42450996882751	8.67301799731702
C	-0.55062344152209	4.58747010767572	9.11330892623398
H	1.877111114443558	0.71513249597316	3.80779963905400
H	2.96506509199270	2.06428474281554	3.89775616032926
H	7.32781174160749	0.94567231314266	11.01947639089624
H	7.00235303541018	2.41337430278762	11.86997921504344
H	-0.61062410060820	-1.26559087151154	6.56799449895346
H	-0.34891565133339	-2.54925082244260	7.77063680649422
H	0.80702140202422	-2.29589225409913	6.43929290519677
H	1.98114285987321	0.39969706064958	12.21074550152247
H	0.42310034331718	-1.69343836438360	12.78641537852697
H	3.55055474364348	4.52943247537988	12.73668187422678
H	2.52023841853687	5.75535204702578	11.95801225400536
H	4.20670438871964	5.51902666779294	11.44151009705667
H	-0.42073114977421	2.75500812980384	7.93952320406988
H	-1.49996714120390	5.03030150932067	8.83293458599025

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C12H14MnN8S4 optimized with ADF in AMS. LS OPBE/TZP

Mn	2.57045509826881	1.53070498839858	9.01415458597553
S	3.34650197027646	2.59324577289001	7.16685648770421
S	0.06315502167856	-1.74584729285460	10.57824156637362
S	4.46259364503407	0.31775729320827	9.31634502674736
S	0.24704002825425	5.07148516987397	10.25239907711221
N	3.05381648945067	1.58272713371770	4.71419187058340
N	1.99333037106838	0.40726306204646	6.37463998359901
N	1.80717743497656	0.34212567135521	7.71515861877022
N	1.55959388049687	0.31095251935259	10.20073092020679
N	6.46934429046676	1.15754953331595	10.86228523256975

N	4.66480275177458	2.57272509248735	10.76885745063531
N	3.41597484090157	2.71468992094001	10.26292928299923
N	1.14594539386517	2.88713510127115	9.23564505286647
C	2.73373841852497	1.44636253509736	6.03724451884860
C	1.04814686794087	-0.69157238944930	8.13072312137012
C	0.45700389616478	-1.71058916704655	7.22183265278904
C	0.92367196105626	-0.67101765652520	9.53176902757677
C	1.36737788124081	0.21299859071226	11.54727219125919
C	0.58759016765067	-0.83264902641317	11.94193382179715
C	5.22761955368595	1.44966848259049	10.36440561682401
C	2.77092738283818	3.83168966133945	10.65651035206897
C	3.35456088676904	4.85364693902154	11.56691658501351
C	1.49423728946459	3.88731658617181	10.06930521526822
C	-0.11289206188602	3.05707636571422	8.73988731614139
C	-0.75530742409429	4.17854085910877	9.17274773533987
H	2.45532842590770	1.08165971248524	4.07206285718526
H	3.33260370233970	2.50596534073493	4.41931483466565
H	7.01946870467069	0.51669107911967	10.31045005276179
H	6.97624888365841	1.95212738954132	11.22800456947529
H	-0.19488842556628	-1.24412188339697	6.47317773294786
H	-0.12840737951793	-2.44311891199746	7.78464363128235
H	1.24084758889971	-2.24335347976552	6.66895538349864
H	1.83111347460295	0.93460292054886	12.21172676859146
H	0.30093852855417	-1.11988729950004	12.94682407073104
H	3.67693953051795	4.40253129967738	12.51289046409961
H	2.62941200929873	5.64279548584582	11.78521337460796
H	4.24384007228411	5.31538826765199	11.11912793778548
H	-0.52246976196857	2.32883948013925	8.04761193389483
H	-1.74758046623823	4.52980175063699	8.91488123342848

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C12H14MnN8S4 optimized with ADF in AMS. HS OLYP/TZP

Mn	2.95264193917584	1.53388225017697	8.75386457318110
S	3.44624830694094	2.28297832313369	6.39053718708136
S	0.14078885650892	-1.97677470604092	10.44827402745373
S	5.21701286219124	0.64674045754014	9.44695329931051
S	0.44272485010427	5.33226932624744	10.27014829016428
N	2.46138721898293	1.15139426237242	4.20655183014350
N	1.65511587846605	0.18374150263353	6.09187601475032
N	1.68131911083144	0.11927954558597	7.42841593316256
N	1.71142501172597	0.04277782594024	10.14611102137468
N	6.63853573051887	1.55063519157292	11.49531156824386
N	4.75076622670093	2.76819853048731	11.17259268299635
N	3.61303512968490	2.92812034048728	10.48674552478738
N	1.28404227356854	3.19011795371760	9.11366362500476
C	2.45089600869423	1.14281461431912	5.57314811444686
C	0.93050999030329	-0.80838216627329	7.99398974589589
C	0.08604192259061	-1.77345490112294	7.21377519518993
C	0.99059929832113	-0.82185566302427	9.44097565993167
C	1.61578481925243	-0.18744668605940	11.48736573248517
C	0.80953471099402	-1.23281519191347	11.85279562552564
C	5.50622955678991	1.73357023834733	10.74668197827800
C	2.84064265049857	3.93966776835849	10.83971234511606
C	3.18683271526497	4.89597966278793	11.94387106388912
C	1.62094935579842	4.05165078160576	10.06714237109735
C	0.09945832286828	3.51941256486020	8.52297481163819

C	-0.51398596547722	4.64229345148157	9.01193752136147
H	1.74841184590453	0.61416039365314	3.73230562967100
H	2.85089328794494	1.95522635119535	3.74068131527966
H	7.36293414431157	0.97103144316950	11.10024373995718
H	6.92302312083394	2.32445332123752	12.08187574852829
H	-0.64306808044745	-1.23231619537480	6.59951261544479
H	-0.45199187981641	-2.46851754803166	7.86160910169253
H	0.70999355354351	-2.34886149134502	6.52059508500478
H	2.16627311903247	0.44271117102649	12.17896847509071
H	0.58100215059456	-1.60042386841925	12.84554120517452
H	3.35267325953162	4.35092430747050	12.88000248043062
H	2.40428325683928	5.64003713084873	12.10633835816747
H	4.12449024023179	5.41685845005021	11.71759507515686
H	-0.28728871319688	2.90037124607591	7.71943386276610
H	-1.45036516329530	5.09345690926756	8.70774972052135

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C12H14MnN8S4 optimized with ADF in AMS. LS OLYP/TZP

Mn	2.59882980499044	1.53122962506303	8.99414740957405
S	3.37867734069240	2.59341589254976	7.09046656048818
S	0.05082720998966	-1.76703831594157	10.57682628193086
S	4.54032501134370	0.31134839710021	9.32397191662219
S	0.24203989937631	5.09484641587477	10.26602036558235
N	3.01807814903294	1.55240939711607	4.64509866927852
N	1.97830469171483	0.39538509133655	6.33700748784680
N	1.80716100261480	0.32467057493909	7.68913640917958
N	1.57298944792895	0.28968762548969	10.20587871470050
N	6.51056093179610	1.18583174846945	10.91980633682969
N	4.69005902766917	2.58463010036401	10.79621800358040
N	3.43869776720445	2.73265018362796	10.27228067670276
N	1.14746801035939	2.91031739352736	9.22059827483873
C	2.72309475962591	1.42948959064028	5.98138466746364
C	1.04016750168325	-0.70065834024342	8.11973470841661
C	0.41851973643420	-1.71897677654350	7.21649238752050
C	0.92691581837649	-0.68296405175868	9.52697349550355
C	1.38033731625793	0.18607353689346	11.55763393126370
C	0.59143299378599	-0.85523393174302	11.95228212439124
C	5.26961144576172	1.46444051949451	10.39621067355404
C	2.77635069146415	3.84164030058391	10.66854281055232
C	3.34004408096893	4.86374379681015	11.60509234637110
C	1.49924622812673	3.90076508374758	10.06946915168168
C	-0.11592826104687	3.08687710578810	8.72278642525295
C	-0.76296384618496	4.20376692755489	9.16581246399185
H	2.41109929592939	1.04316157020577	4.01596029892771
H	3.30470855507973	2.46784550708969	4.33137718133129
H	7.08148037509150	0.54702784566077	10.38542060240208
H	7.00108958586763	1.98256993156297	11.30563634281889
H	-0.23913813773366	-1.24536717480051	6.47839037542731
H	-0.16717616488173	-2.44320962753507	7.78812884557522
H	1.18562852080340	-2.26189660191431	6.65194475042440
H	1.85203743989233	0.89990671318722	12.22323530906070
H	0.30672655686770	-1.14267895176319	12.95616785931028
H	3.64608861117862	4.40566647917910	12.55232050139297
H	2.60763621200746	5.64660089503693	11.81740451070671
H	4.23472250701671	5.33419575306789	11.17970881572710
H	-0.52207566642311	2.36582134726303	8.02260821094977

H -1.75387352735090 4.55591532106489 8.90969225822337

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C12H14MnN8S4 optimized with ADF in AMS. HS B97-D/TZP

Mn	3.20440680073366	1.49894219390866	8.62734579393729
S	3.73714461120610	2.01876286837991	6.21664768028060
S	0.25680716253176	-1.56238336080336	10.70777614131402
S	5.49718680914982	0.77954023265494	9.39343830719619
S	0.27842333367353	4.95895133484100	9.97851506285719
N	2.15083549784492	1.34306586609405	4.19115299703607
N	1.47908001718989	0.39150288842146	6.13882798806195
N	1.67939283786489	0.25515253720032	7.45482955129413
N	2.07842540802857	0.15644033606616	10.10877939495026
N	6.52368678804131	1.44812833269369	11.75484678792017
N	4.61986163619078	2.60040273948694	11.30943232370337
N	3.60067073192149	2.80918782044187	10.46828477343528
N	1.52258078477050	3.04583704676134	8.78553415580040
C	2.38576423886043	1.18790439001073	5.53156707654352
C	0.85946625403499	-0.53020396800096	8.12116370899287
C	-0.26114551778410	-1.29461894052534	7.47353051553029
C	1.12517793014747	-0.57433280143232	9.54410199151024
C	2.16016627831628	-0.03561500004516	11.45638336168101
C	1.25698106751577	-0.92672308242229	11.97451202573380
C	5.50551526659793	1.67952970242431	10.86920809806257
C	2.70350591896863	3.71231364778983	10.80291444656084
C	2.78640206932548	4.53371674538257	12.05911999572596
C	1.61258147802158	3.82398629049761	9.85727374641297
C	0.41876489216426	3.31518353423019	8.03133415777239
C	-0.38510512359592	4.31660775032539	8.51005612821547
H	1.51979177269439	0.68278561259013	3.75327061862948
H	2.88869595961364	1.74251506736968	3.63008464124114
H	7.32776089169007	0.93695552416389	11.42190606713588
H	6.65922140112997	2.12842930584956	12.49283945354849
H	-0.99057304706099	-0.59637152199181	7.04175837253435
H	-0.77377539507360	-1.95181779915061	8.18296046108316
H	0.13142123699806	-1.89218853848220	6.64187761202270
H	2.90925436709601	0.50938765891210	12.02285886111165
H	1.12757995490529	-1.24035509682113	13.00320089192251
H	2.71648176727051	3.88085575023335	12.93954730920617
H	1.99396017482904	5.28696428052787	12.11067575183063
H	3.76341551829708	5.02905428097213	12.11267391924794
H	-1.30507282878996	4.70575156087136	8.09114236365275
H	0.24506197799215	2.74066170861996	7.12649562170001

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C12H14MnN8S4 optimized with ADF in AMS. LS B97-D/TZP

Mn	2.67241188477864	1.50859590233201	8.97559565590296
S	3.47131470416412	2.56342842385025	7.05124704279908
S	0.03387837321338	-1.67347634629773	10.61219694702561
S	4.63045707293605	0.29767234268910	9.35575524462313
S	0.19252295980163	4.98536233606664	10.21391283511135
N	2.95154794949946	1.58102758764077	4.60412015513184
N	1.93751698180981	0.43250995815502	6.31466333569686
N	1.81933248768007	0.33562556074612	7.67219638408376
N	1.64921044500566	0.30047573478368	10.19154298105905
N	6.54075554933633	1.21058547286843	11.01355552504977

N	4.70024328221361	2.57657643842894	10.85067865896599
N	3.46452769789570	2.71499353719109	10.28540802163005
N	1.20473054143145	2.84890367020889	9.16727499629410
C	2.71355227767396	1.44116747837344	5.94913299039726
C	1.00723095923113	-0.64548236077595	8.11973238734673
C	0.29350845298948	-1.61132729632756	7.22419208859748
C	0.93426545835690	-0.63539227761903	9.52955617552867
C	1.49647832206359	0.21722573437335	11.54863705148989
C	0.66732602547267	-0.78067650444858	11.97356679348339
C	5.30889077787507	1.46780610922255	10.45965642286545
C	2.75844794630372	3.79691860158338	10.67908454182569
C	3.26355273586464	4.81387351324270	11.65609908880851
C	1.50023375083931	3.83574978851182	10.04159109703409
C	-0.04672661863371	2.97884044899744	8.62996822306422
C	-0.74955323649030	4.06553931835456	9.06560326869198
H	2.31726350635112	1.09162697444581	3.98521098592074
H	3.28412237567410	2.48080174897638	4.28844881752176
H	7.13528892606250	0.56849842275002	10.50838186446283
H	7.00602110880074	2.00635639336860	11.43317536434416
H	-0.36621800865840	-1.07969866795740	6.52626075149841
H	-0.30255684651226	-2.31661475916102	7.81315056887142
H	1.01337027896159	-2.17228956538044	6.61459786446931
H	2.03070477950846	0.91510276468264	12.18375681770872
H	0.40054372160035	-1.04884522990378	12.98781139904018
H	3.54229075669818	4.33583434906620	12.60364378490904
H	2.50124179933625	5.57646441130327	11.84878450725010
H	4.16712479216582	5.30314130628122	11.26951052902585
H	-0.39071779747397	2.24423990291795	7.91032430202734
H	-1.74433525051519	4.38276567450505	8.77984268583889

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C12H14MnN8S4 optimized with ADF in AMS. IS B97-D/TZP

Mn	2.73865248610285	1.42429496829817	8.89693669714829
S	3.48636073446285	2.49705295072799	6.93364630147425
S	-0.26395250647422	-1.56052559616448	10.44341856285897
S	4.85560510210496	0.21757781183283	9.58095384340453
S	0.13529380154179	4.93124019820829	10.67657801185403
N	3.41627176344491	1.18439188151500	4.58805418428011
N	2.18524370436815	0.18609071310403	6.24942167736322
N	1.89132072673456	0.21168151233386	7.57935779216902
N	1.56107432003923	0.25202666189352	10.14191447391648
N	6.76556555670548	1.65024525343971	10.78231091976657
N	4.77115676174389	2.74138752455371	10.68074250105256
N	3.49243577285757	2.76124107910589	10.24859079819518
N	0.99962216828898	2.95894670081131	9.24246891007917
C	2.96514003096896	1.18967946648868	5.88367538433687
C	0.94065437467093	-0.63535194141083	8.01882286252693
C	0.17912906772853	-1.54364964170594	7.10259567236714
C	0.78520204678935	-0.58958778851230	9.42571149154587
C	1.37204750532669	0.11992809744913	11.48738818887415
C	0.42606129624966	-0.79663182730680	11.85293012561626
C	5.45665569047635	1.63446923877654	10.36528985937181
C	2.72278074943055	3.73898904197108	10.73778454032660
C	3.23274819720571	4.70497636999047	11.76656611187092
C	1.39898006571640	3.79803709451094	10.19383725407048
C	-0.28940568480844	3.17762502408345	8.86528447165212

C	-0.93105016206566	4.19943175399092	9.51838262481293
H	2.93105616342517	0.57108252219539	3.94531119223949
H	3.75248738462478	2.05983483278850	4.21356956773217
H	7.38176591120396	0.96784153227289	10.36532700860415
H	7.16111135205704	2.55554636809579	11.00534973134063
H	-0.31029410866095	-0.96447311486237	6.30963258191722
H	-0.57730546794932	-2.11078736636174	7.65430828796174
H	0.86377798936448	-2.24379687570618	6.60649029778062
H	1.95477241316025	0.73164293104663	12.16769636975408
H	0.09220981786317	-1.05975714345410	12.84856562987209
H	3.64541086262597	4.16004099460869	12.62420450247697
H	2.44222785392102	5.37966657567368	12.10934040739965
H	4.05618660214467	5.29867996984975	11.34854422289840
H	-0.73208614590021	2.55833177443839	8.09073819137687
H	-1.94511327417838	4.55648734947530	9.38612690310704

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C12H14MnN8S4 optimized with ADF in AMS. HS B97-D-COSMO(DMSO)/TZP

Mn	3.17013412644247	1.48519268623347	8.65966301123627
S	3.77912589684943	1.97056373184873	6.23353976002586
S	0.21046148604193	-1.55347593451943	10.68359760354023
S	5.51718818197675	0.81135472065989	9.37804713799646
S	0.28318155285091	4.94130409383348	9.99927106394525
N	2.25528979768134	1.25191782422981	4.16351720239183
N	1.52025199986076	0.34633108803803	6.11508785865072
N	1.70589813055620	0.21545751679861	7.44487262793669
N	2.07071796967410	0.12623576028621	10.10405367423359
N	6.55515126008696	1.45637290098799	11.75277165285746
N	4.65743018081068	2.62722162607698	11.30549654959403
N	3.61855146212632	2.82010566145141	10.46695172768463
N	1.52346841091060	3.03224374498411	8.80187967247761
C	2.41882805227617	1.13677268253143	5.51014376154624
C	0.87664755834445	-0.56503763581050	8.09936477286190
C	-0.23625437127371	-1.33278761539835	7.44532910857380
C	1.11582672140283	-0.60178963022907	9.53266597251428
C	2.11275609643089	-0.04358968309772	11.45842372355105
C	1.18229887358638	-0.91608864467425	11.96289097136748
C	5.53880752020404	1.70952968367275	10.88276206243360
C	2.73102748727465	3.72980263710457	10.79683171925679
C	2.82480801461809	4.57668271626826	12.03369747984628
C	1.62044572010313	3.82706012258955	9.86360328287833
C	0.39526574648118	3.27650246685674	8.07202555363407
C	-0.40652426626836	4.27640519078806	8.56038963081783
H	1.39803656257612	0.90228414588902	3.75179627319067
H	2.76038708278370	1.97127935456931	3.66695814585298
H	7.35649364989179	0.93319552369244	11.43082635999383
H	6.68630716454543	2.08943770881064	12.53315121408997
H	-0.93540379658446	-0.63539432079629	6.96624181931331
H	-0.78452372960575	-1.95074876606198	8.16165968103699
H	0.16987008046751	-1.97333884418077	6.65329210821216
H	2.84853492382385	0.50100559126646	12.04143192605660
H	1.01810780749875	-1.21279622738228	12.99145805397691
H	2.78511539585306	3.93725114638985	12.92509141018463
H	2.01855045891376	5.31329646984031	12.08882140226060
H	3.79018024027170	5.09616669763808	12.05485023895647
H	0.19990249020944	2.68791660908976	7.18134884213050

H -1.34254101638144 4.65006409777045 8.16406309828783

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C12H14MnN8S4 optimized with ADF in AMS. LS B97-D-COSMO(DMSO)/TZP

Mn	2.66910895784008	1.51821490929580	8.96636202469776
S	3.44223297213181	2.59180146419921	7.03564828795500
S	-0.00742953487881	-1.62556018055850	10.59624278567226
S	4.63352109394227	0.30242665684606	9.33402051116264
S	0.17518481626781	4.94618414303583	10.28404275400769
N	3.01118219108702	1.55108760247846	4.58717585370065
N	1.98382029896401	0.40571595281216	6.29820355399954
N	1.83050976339672	0.33172288292215	7.66178610235759
N	1.63946470213903	0.32016149839953	10.17685004100354
N	6.57366052914944	1.22352183294541	10.96122317005210
N	4.72721785682630	2.59012358377443	10.82071972833423
N	3.47179705776579	2.72218132453519	10.27747068649233
N	1.20162757627292	2.84515603925951	9.18548632990404
C	2.73654407255010	1.42463032778503	5.92248723473716
C	1.01772090241423	-0.64495640658859	8.10613080237543
C	0.31010006894019	-1.62369458091867	7.22024403794806
C	0.92643641076594	-0.61945897274894	9.51947994216147
C	1.45013345868288	0.26778244371195	11.53361093246921
C	0.60071568786547	-0.71696766713385	11.95253506052719
C	5.33957987999818	1.48633267470194	10.43016179661083
C	2.76472337156038	3.79017555757851	10.69169519973993
C	3.26045874031911	4.80108271151977	11.67935489096119
C	1.49362776276554	3.82420091379136	10.06841241380953
C	-0.06649416056928	2.95889532188929	8.67727589484176
C	-0.77362528158304	4.03035954731680	9.14513945922962
H	2.40294282383671	1.04798202194844	3.95086696589570
H	3.32235520735743	2.45692467455094	4.26234471288912
H	7.16379987782157	0.57316831486634	10.45980264291870
H	7.05603628702363	2.00355985815427	11.39317929164215
H	-0.32116090443870	-1.09908671171852	6.49220727857046
H	-0.31532331939694	-2.29795138160660	7.81345485424854
H	1.03287711725500	-2.22142306856250	6.64998107864145
H	1.96728242698552	0.97538829356427	12.17171879996642
H	0.30208705431471	-0.96511264674734	12.96312194266379
H	3.52061045042301	4.31735835864443	12.62927259364179
H	2.49772910065372	5.56344668801101	11.86597558948672
H	4.16851358105273	5.29228331232831	11.30690528238772
H	-0.42025734895225	2.22848741335465	7.95847306039765
H	-1.77951062523857	4.33776219040823	8.88880456729469

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C12H14MnN8S4 optimized with ADF in AMS. IS B97-D-COSMO(DMSO)/TZP

Mn	2.74388339200408	1.43150025532809	8.87701822181656
S	3.52404520018151	2.46542097863261	6.90462026770322
S	-0.32288480304692	-1.43966994246595	10.44021885451439
S	4.92302431219428	0.22445745607788	9.57276342580510
S	0.09788841769033	4.80731104574058	10.74782309204796
N	3.44492122234463	1.13973496036461	4.55870990446159
N	2.20539523772153	0.15750892680118	6.23034127038099
N	1.90247706780963	0.20328005935185	7.56485596072771
N	1.59206833854393	0.26954450171763	10.12687107206128
N	6.81238944577888	1.69766038577557	10.77897359002912

N	4.80087416006225	2.76031070244714	10.65180238581845
N	3.50558734843481	2.75574599116533	10.23307589228294
N	1.02756796232360	2.94459488380105	9.21566794626759
C	2.99010707624214	1.14824592333442	5.84719523929489
C	0.93272011191587	-0.61224197345086	8.00969561354528
C	0.13320082271388	-1.50307572396128	7.11028958143249
C	0.77958440092182	-0.54705071187049	9.42152809111730
C	1.37441562730580	0.18277864278054	11.47442139899310
C	0.38077725688958	-0.68375178539702	11.83973718494174
C	5.50759906009177	1.67108507139257	10.35591447190444
C	2.72518884958120	3.70823134903090	10.74735117886427
C	3.20945409703671	4.65905811058820	11.80133790998469
C	1.39562204798267	3.75529805001666	10.20684246217571
C	-0.27613161972971	3.12499245861432	8.86024084300463
C	-0.94821772142795	4.08887580268844	9.57052784907021
H	2.95751945563729	0.53606146462261	3.90622031356245
H	3.78289504591863	2.01350068688664	4.17807521038904
H	7.44746412197974	1.03155569535664	10.36131323466604
H	7.20362171306579	2.60416631490003	11.01060778785409
H	-0.33593213197050	-0.91569398570527	6.31151278746541
H	-0.64373147771805	-2.02932156223762	7.67231060434322
H	0.78633239099692	-2.24155522044757	6.62727618719247
H	1.96726929938799	0.78647503811117	12.15266164849825
H	0.01827154418653	-0.91308844264184	12.83385194276791
H	3.63019439365537	4.10263510722601	12.64725230443758
H	2.40147738537780	5.30360174831129	12.15867821953603
H	4.01520045889727	5.28755740629608	11.40014906211020
H	-0.70569312884429	2.52536783059185	8.06348712256976
H	-1.97664545882514	4.41279939827181	9.46664802175749

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C12H14MnN8S4 optimized with ADF in AMS. HS SSB-D/TZP

Mn	3.28733234410524	1.42075674352721	8.63128850623160
S	3.81045939606075	1.90234697918607	6.25066630481487
S	0.16260359719869	-1.44211731433675	10.68646303749250
S	5.50094989140212	0.70605169622366	9.50452564070556
S	0.32032111664338	4.87045563858610	9.92592249963693
N	2.30233396962290	1.19817931565086	4.21342582253412
N	1.50837115886544	0.37534015658153	6.15875389894125
N	1.70911993081986	0.23184578460074	7.46356050996525
N	2.08802821027385	0.13018806704437	10.10240178286620
N	6.52637597638935	1.49261733244883	11.79967268417494
N	4.62986385261555	2.61203952026254	11.30554520269130
N	3.62300387155296	2.77046234496398	10.45431528395350
N	1.56040192815031	2.96241817312117	8.76547420675992
C	2.45869142601776	1.11814150040652	5.56158884601018
C	0.84050721510481	-0.49495463824422	8.12681883618188
C	-0.31498110881077	-1.18289739759161	7.49304096149414
C	1.09477841519799	-0.54198498328568	9.54317577634093
C	2.13689562102868	-0.05994250705362	11.44058040202450
C	1.16974788138399	-0.88142484015580	11.94884257917784
C	5.51223314878435	1.67789420510110	10.90823040145743
C	2.71979834100981	3.67080275085319	10.76652803115687
C	2.79061113922698	4.51015062141454	11.99148545770638
C	1.63932754135207	3.75745141440037	9.81987982762392
C	0.45988556613514	3.21782078483875	8.02230713349057

C	-0.34324685975143	4.21988051941368	8.49115778176954
H	1.41486017990133	0.90591979695808	3.84306802602009
H	2.80016076735042	1.92406512095956	3.73518269778491
H	7.33950630230057	1.01791580473897	11.45510622162724
H	6.67491036609691	2.24112536163607	12.45530691952170
H	-1.05676138952393	-0.45077862187083	7.16614640095691
H	-0.79310243003634	-1.88540616679970	8.17241150705461
H	0.01978428716627	-1.70888054573614	6.59953456334790
H	2.91048943180783	0.43195272003932	12.01403867197866
H	1.00370173557322	-1.18132590925332	12.97088196419763
H	2.79757548421552	3.87211215324756	12.87672118046895
H	1.95847778595358	5.20706657403633	12.06050293834427
H	3.72902926268494	5.06581612611766	12.00470201872802
H	0.28136768421482	2.63280201886876	7.13049325339732
H	-1.26361211477331	4.60000059714594	8.07812037676537

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C12H14MnN8S4 optimized with ADF in AMS. LS SSB-D/TZP

Mn	2.67119392820097	1.51978534848669	8.96282709169838
S	3.43990792867912	2.54732086089480	7.06000680760345
S	0.07553912718531	-1.64703837043399	10.60313361196685
S	4.60294103425229	0.34280718613183	9.31867347385618
S	0.22044401945236	4.97259885389747	10.20529124618592
N	2.96857473149057	1.55158784372275	4.63684355205968
N	1.94278380041160	0.41638342096781	6.33567444764125
N	1.82719812180200	0.33968554021933	7.68080735966329
N	1.66264813785739	0.31857390959514	10.18114184948122
N	6.48375420286971	1.18987935736913	11.00274844662473
N	4.66701881729914	2.57080507262401	10.84690665699952
N	3.44981631644068	2.70994269272679	10.27482737802188
N	1.21058396521864	2.85507304690575	9.15734809923546
C	2.71170268192086	1.42644376343444	5.97366259779971
C	1.02563251303104	-0.64085072962917	8.12985344786430
C	0.32817594890327	-1.60773546552250	7.25008328010476
C	0.95440164761494	-0.62130493597371	9.53248123581901
C	1.51014440202505	0.23544684357690	11.52673755917304
C	0.68748428416580	-0.76490581368336	11.94737908383222
C	5.26989777699655	1.47005179007231	10.43658993413462
C	2.74661050894493	3.78095682127490	10.68059144692975
C	3.23963268207863	4.77140422599782	11.66636641561298
C	1.49909522492142	3.82920195831078	10.03713731151224
C	-0.02537157169621	3.00420384273650	8.61802160021492
C	-0.71401713195983	4.09308740772630	9.05952884284982
H	2.30867576714233	1.08504190857069	4.03790794199180
H	3.24442645236240	2.46801300542943	4.33482252397333
H	7.07641283081081	0.58963178537700	10.45805540992303
H	6.94763677514679	1.99077762078391	11.39775348757180
H	-0.34431387019309	-1.09222683572567	6.56262078039463
H	-0.24484819037715	-2.32050844962508	7.83988332148216
H	1.04785916431821	-2.15029886102103	6.63564012659328
H	2.03604836522005	0.93327420973712	12.16054063513875
H	0.42050911683003	-1.03522567726659	12.95532243785645
H	3.53947923994782	4.27717582749064	12.59096878049296
H	2.47070832199530	5.50919919237485	11.88735657276621
H	4.12360297787689	5.28560662503395	11.28490931058085
H	-0.37398728665060	2.28442136565444	7.89282158662261

H -1.69819976253600 4.42561781175761 8.77460330772699

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C12H14MnN8S4 optimized with ADF in AMS. IS SSB-D/TZP

Mn	2.73648684157392	1.43039377233421	8.89224711219410
S	3.41415996068696	2.50532473191501	6.94793111269696
S	-0.27380476549322	-1.53591067760685	10.39185868147425
S	4.78450258999576	0.24696521740499	9.56545056057736
S	0.17699726930966	4.91431105831901	10.73401977099268
N	3.50197786611330	1.14866984972273	4.65777675264235
N	2.24814234168459	0.14689950842778	6.28603378466114
N	1.92276717162041	0.19998324002895	7.59321162087623
N	1.52176831366199	0.27952494176582	10.13025110447454
N	6.73393998093528	1.64284932393492	10.69412838572756
N	4.76350224996821	2.76028198390543	10.62896398491534
N	3.48563352955192	2.76685202917569	10.22767986187951
N	0.98826654774467	2.96847614372254	9.27185191113443
C	2.99862990651418	1.17153578219127	5.92783991014156
C	0.97508371964446	-0.64759933304435	8.01775766982158
C	0.26083904915981	-1.57339661466040	7.10722357896242
C	0.78141371865303	-0.58030941112738	9.41212814258781
C	1.28354264134177	0.16296382930857	11.45800072437077
C	0.33857321428305	-0.75930063580853	11.79717037249201
C	5.42287615965728	1.64773359637591	10.30711542901304
C	2.72694807600671	3.73287442999101	10.73936977902524
C	3.24606705443754	4.68035484372132	11.75739637215130
C	1.40115697693757	3.79694039403610	10.22113688906293
C	-0.29845988906495	3.20129530692011	8.93566209460893
C	-0.91343519778915	4.21614125251503	9.61726871779417
H	3.02044138110072	0.53117089696111	4.02592468633881
H	3.75103082786406	2.04318231995629	4.27634198366526
H	7.31689359419228	0.97809901541081	10.22041861398527
H	7.13821628041783	2.55149166306883	10.84744762603105
H	-0.18394642444671	-1.02299101375448	6.27744498706589
H	-0.51887452016454	-2.11597423525146	7.63780616139400
H	0.95946966790972	-2.28916706479185	6.66967472034781
H	1.82608862994134	0.78955171685167	12.15058237037633
H	-0.03090326359327	-1.01328877472692	12.77699145993686
H	3.72493479986670	4.13274614960938	12.56896530393455
H	2.45272753645903	5.30735642907559	12.15857462720466
H	4.01573083116091	5.31879005580767	11.31885652735707
H	-0.76654412195302	2.59772288773060	8.17042371243303
H	-1.92303962257811	4.58136228862969	9.51894105104682

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C12H14MnN8S4 optimized with ADF in AMS. HS SSB-D-COSMO(DMSO)/TZP

Mn	3.23209129930024	1.46190775214910	8.64061878510837
S	3.79729134733810	1.89004428868728	6.23938553577265
S	0.18460314456155	-1.46409762542877	10.67476066603448
S	5.53510648517036	0.85243041797813	9.40259901057486
S	0.30165228471703	4.87293723554810	9.97471594981109
N	2.28214246760451	1.19553752887740	4.18933134729069
N	1.51789289423122	0.33687009833152	6.13780684512932
N	1.71531320605284	0.21664472882180	7.45390339254177
N	2.09693485822836	0.12454511392381	10.09479400316991
N	6.53346739690102	1.48440377815142	11.76703059760300

N	4.63507948025781	2.62908692609849	11.31177891931469
N	3.61779977664489	2.79969130330735	10.46214908938390
N	1.56024507754118	3.00368040972544	8.77504605504583
C	2.43548527825777	1.09711406986642	5.53209709026474
C	0.86765219443391	-0.53270323745177	8.11389555168796
C	-0.26065348179311	-1.26228179760108	7.47989503393380
C	1.11414851808144	-0.56800752280729	9.53659762214515
C	2.12642940692363	-0.04419237663968	11.43820663921170
C	1.16313815945936	-0.87548032069537	11.94082247190356
C	5.53041470655987	1.73102671114682	10.88980140026354
C	2.71668276159814	3.69227963444387	10.78852441092240
C	2.77991703454026	4.52135701411342	12.01968134095639
C	1.62882494588932	3.78516140163672	9.84338062114283
C	0.44748155544706	3.25374655391508	8.04462070398541
C	-0.36261738056430	4.23976518715222	8.53771318616582
H	1.39636870626541	0.90842463136725	3.80759362381860
H	2.76496212559038	1.93556180841442	3.71518631686072
H	7.35552641065010	1.02628864411074	11.42040091900123
H	6.66244276226629	2.14881488929528	12.51199738356016
H	-0.94093012554910	-0.55115397200808	7.00852546043999
H	-0.81536100616949	-1.86093995335027	8.19762546586855
H	0.11700968558882	-1.90947151821274	6.68804451324513
H	2.87727456664599	0.46994966036122	12.02170563599174
H	0.98272441159448	-1.16480985839559	12.96352356763449
H	2.78644634637030	3.87528472861063	12.89875499309748
H	1.94304641465543	5.21103477315992	12.09209026605848
H	3.71240685203295	5.08621401932203	12.03671752196458
H	0.26296683813055	2.68156298804782	7.14623631928957
H	-1.29160648214289	4.61567878407270	8.14030989920107

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C12H14MnN8S4 optimized with ADF in AMS. LS SSB-D-COSMO/TZP

Mn	2.66519111588208	1.51909234318077	8.97028964524567
S	3.41985672923433	2.57169941865678	7.07119966766521
S	0.01297147051528	-1.61402014317331	10.56908681314390
S	4.59500874024357	0.33194864735385	9.33462073548842
S	0.20093076297047	4.92828747119834	10.27979443980402
N	3.04636439876493	1.53822426731933	4.64020786750837
N	1.99632895165388	0.39748371262400	6.32631834259756
N	1.83931504745302	0.33498419251103	7.67422777238131
N	1.63726038019475	0.32583407609617	10.17067653052615
N	6.52578829790080	1.21641944127696	10.94835246265757
N	4.70285922630536	2.59714856625300	10.80666883884811
N	3.46116983940701	2.71906935703470	10.26813071599025
N	1.20378033054494	2.83827690165436	9.19055909124578
C	2.74728022867153	1.41822126767130	5.96451253907367
C	1.02914433151020	-0.63919624887348	8.11049293112062
C	0.33722136475188	-1.61034098628102	7.23082028225530
C	0.93215568938664	-0.61168721658064	9.51601300356250
C	1.44325327887387	0.26133048962893	11.51445385725790
C	0.59833185471475	-0.72867678841721	11.91844519780562
C	5.30333924873318	1.49195325329253	10.41292390564624
C	2.76244680072702	3.78630680332416	10.67924241753251
C	3.25964666897063	4.79209456358259	11.64709118573777
C	1.49582918063006	3.81719110440912	10.06296893162408
C	-0.05696070506879	2.95759663879043	8.69664568039939

C	-0.75088322688174	4.03187689118602	9.16746833366140
H	2.42003454431350	1.05757768114282	4.01481883777518
H	3.31332283467700	2.45649413992785	4.33167942088560
H	7.10947949280144	0.59749058867761	10.41385525524173
H	7.00996714276826	2.00755824629991	11.34051605544300
H	-0.28686213782149	-1.09186806968812	6.50202345227540
H	-0.28626734750489	-2.28192613162184	7.81686118615715
H	1.06038071395126	-2.20272248785208	6.66816689070576
H	1.95017998429055	0.96248121841453	12.15993786268166
H	0.29516268992230	-0.98719005579526	12.91967966286560
H	3.54198070289365	4.31532384040280	12.58638621666691
H	2.49742414471955	5.54232281429511	11.84567804436898
H	4.15047106436517	5.29003240016534	11.26087313053745
H	-0.42118263312742	2.23181694644923	7.98539921394896
H	-1.75192027902687	4.34539774350924	8.92078173706297

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C12H14MnN8S4 optimized with ADF in AMS. IS SSB-D-COSMO/TZP

Mn	2.73986775058854	1.44019491597279	8.87618191789719
S	3.44132728546136	2.48596397662281	6.91189287230540
S	-0.35842553237954	-1.40690119677293	10.37114111538227
S	4.83807504443816	0.26427989176630	9.54289111913053
S	0.13397165858629	4.76622417169000	10.85461200713651
N	3.55996909673978	1.09084523668394	4.64064904773856
N	2.28956284402951	0.11270359065912	6.27602802845470
N	1.94131181437707	0.19395063222936	7.58210802934855
N	1.53335548110433	0.30627389564712	10.11582786389774
N	6.78437682709166	1.69552482295801	10.64910121507580
N	4.79587407762491	2.78712194393671	10.58187747586761
N	3.50133160922523	2.76788957871129	10.20587218089323
N	1.00916044218355	2.96006416248063	9.25656717762937
C	3.03921391661136	1.12846642919952	5.89741207930007
C	0.97229566052248	-0.62503761549603	8.00546833184575
C	0.23153209304878	-1.53920020023285	7.10537023185402
C	0.76592000610681	-0.53241291120383	9.40129285136298
C	1.24765746741821	0.24464684068385	11.44032518553851
C	0.25103104932636	-0.62635619541672	11.77111909164376
C	5.47367272541556	1.68909358670040	10.27324501127855
C	2.73409644448206	3.70622063184520	10.74942731779480
C	3.23812913659544	4.63947293068356	11.78698591698466
C	1.39682697945703	3.75096825410660	10.24986858950866
C	-0.29889567493257	3.14197707560373	8.96421103339808
C	-0.94395804100797	4.08340367410420	9.72070884034392
H	3.10055316784330	0.46283951933254	4.00119733639749
H	3.81980512170474	1.97634128022222	4.24337669256822
H	7.38281953508468	1.04094583761254	10.17910325359492
H	7.18799397810168	2.60220107655266	10.82012325043195
H	-0.19843931261595	-0.98350563541978	6.27167357412320
H	-0.56367398059903	-2.05128720681190	7.64158706903341
H	0.90688582381301	-2.28321532132826	6.67905767286111
H	1.79189673441191	0.86734495841119	12.13482009189003
H	-0.15811465366616	-0.84170696790037	12.74465238285108
H	3.69868998581313	4.08174709396551	12.60222987107083
H	2.43993941521091	5.26284247111428	12.18157640015933
H	4.01362335124356	5.28258779219886	11.36716663085076
H	-0.75845570456395	2.56401013558521	8.17460622469547

H -1.97100270058454 4.40738374134833 9.66651317325659

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C12H14MnN8S4 optimized with ADF in AMS. HS B3LYP*/TZP

Mn	2.98190059149696	1.49820316073437	8.77394645329440
S	3.52338151434758	2.21420446029071	6.39735116959729
S	0.15901548307693	-1.92496795802000	10.47815036094664
S	5.24850225398974	0.62117688257858	9.51616265522770
S	0.43632163232375	5.26815886532948	10.17099046448837
N	2.26894011202605	1.33021510366232	4.23636433965151
N	1.55482015317789	0.28405102737168	6.10949205728772
N	1.62866019268444	0.17713088616513	7.44376114865991
N	1.78809869802050	0.03302052791087	10.13727812881616
N	6.62163051855707	1.56133412773819	11.57898681598552
N	4.72862108989257	2.74440989104687	11.22087312427973
N	3.60412441482516	2.89314910781515	10.50558878732488
N	1.32832535514032	3.12996940420960	9.05890451561126
C	2.38220014064140	1.20335650423167	5.58841654838867
C	0.87728435262764	-0.72916992430006	8.01389324715329
C	-0.03076086392877	-1.64590570604302	7.25254228261621
C	1.00277783804120	-0.78225298108564	9.45652777201655
C	1.75749103401363	-0.21965013089980	11.47973654199096
C	0.93421272166115	-1.23459672011983	11.86435651986322
C	5.50096628883550	1.72299797939682	10.82054989372015
C	2.82242147557768	3.89273267925613	10.82277226894263
C	3.13296540889614	4.86586396228541	11.91900310494084
C	1.62503340204501	3.99354597683630	10.01312453606979
C	0.16415072601886	3.44644018058655	8.41800537626926
C	-0.46985575548437	4.56234440048595	8.87539185420881
H	1.76602544868680	0.60408124591695	3.74430520578970
H	2.98805020216178	1.83886902684077	3.74669881505584
H	7.34975758942519	0.96120811725783	11.22503973386410
H	6.87440432732934	2.32008484666453	12.19764403524529
H	-0.72904919936852	-1.06629849526137	6.64239000012186
H	-0.59842709666012	-2.30094999871897	7.91557486475119
H	0.54991104604441	-2.26208644192311	6.55934385405158
H	2.37223772115202	0.37370398103392	12.14461007500242
H	0.74800596053214	-1.61252704291248	12.85835154592146
H	3.29942166433007	4.33432416528810	12.85990105154099
H	2.33091427260079	5.59253831367786	12.05897416781583
H	4.06067045596879	5.40221513434914	11.69719223619562
H	-0.18030842302657	2.81977829856084	7.60512426586229
H	-1.39304182436846	5.00320403980832	8.53054833682600

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C12H14MnN8S4 optimized with ADF in AMS. LS B3LYP*/TZP

Mn	2.59138485620487	1.52991237204544	9.00172087039567
S	3.37685367179792	2.60852185145316	7.07236519140836
S	0.04883481874988	-1.78712808214253	10.55215419293797
S	4.55810570285180	0.29417940760808	9.34973072749657
S	0.25733668342270	5.10574599768221	10.27945661031056
N	2.99234978629769	1.54828300057279	4.64848990568913
N	1.96923612766578	0.39599490397522	6.33117056539597
N	1.79014307680899	0.31856802187654	7.67942225282769
N	1.55524960481846	0.27867664344153	10.20751500761168
N	6.52699233443891	1.23568578003228	10.89604353071635

N	4.69603319063648	2.59626142388561	10.79909304533408
N	3.44063748741464	2.74237049015558	10.29050431850234
N	1.13672827608783	2.91385659949660	9.23962624781054
C	2.71574789315883	1.42905754218348	5.97808127367315
C	1.03403178595121	-0.69237321282718	8.10828368313117
C	0.41385372088726	-1.71340495813355	7.20993075823499
C	0.92083660127533	-0.68206913413027	9.52117769041520
C	1.36374432463850	0.16016579790873	11.55887962656249
C	0.58359649427879	-0.88426736223656	11.94139855952102
C	5.27769890079878	1.47832412180067	10.39926223371165
C	2.78120897085786	3.83545604735196	10.67701431681493
C	3.34212435625800	4.86905092998921	11.59962113378822
C	1.49796089072781	3.89494226289332	10.07931488313401
C	-0.12555660286843	3.10077986127774	8.74068985928623
C	-0.76006414795807	4.21915703163340	9.17927554533134
H	2.444014488930629	0.98933546858171	4.01018409129123
H	3.35679281346484	2.42661599026928	4.31543117574408
H	7.09286480882479	0.55582617380536	10.41186669595621
H	7.00656132630769	2.02369524770758	11.30948136968789
H	-0.22107427980559	-1.23712281031446	6.45760208398807
H	-0.18882613560631	-2.42245199621046	7.78128849623958
H	1.18395849501934	-2.26809202717766	6.66542448169970
H	1.83361500627717	0.87057174682210	12.22574140088713
H	0.30098505143214	-1.18051342121890	12.93987673077045
H	3.67008204656976	4.41599335481677	12.53908861201685
H	2.60139776005201	5.64079242834218	11.81911006474114
H	4.22192695226845	5.34630788111177	11.15702618175247
H	-0.53197670678389	2.38092686870456	8.04294363557034
H	-1.74558950921687	4.57627465501252	8.92258110500926

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H2O optimized with ADF in AMS. B97-D-COSMO(DMSO)/TZP

O	0.00000000000000	0.00000000000000	0.06730816142554
H	-0.00000000000000	-0.76263008915630	-0.53365408071277
H	0.00000000000000	0.76263008915630	-0.53365408071277

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C2H6OS optimized with ADF in AMS. DMSO. B97-D-COSMO(DMSO)/TZP

S	-0.54786477734165	-0.39869777102979	-2.38198541482390
O	0.05748271333491	-1.61015814167836	-3.09594528683669
C	-0.23594141558371	1.05081684964832	-3.45415413476395
H	-0.76120872973028	1.90907264213632	-3.02180274648288
H	0.84399640686887	1.22177294689514	-3.45201339198903
H	-0.60110976149291	0.82743638289763	-4.46211571587860
C	-2.35514009739744	-0.47597486227581	-2.66018532370716
H	-2.72315177298242	-1.3522239529278	-2.11951648362068
H	-2.79823834034789	0.43955717527969	-2.25402292836891
H	-2.54206122532749	-0.56526582658035	-3.73555057352818

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C12H36FeO6S6 optimized with ADF in AMS. Fe(DMSO)6+. HS B97-D-COSMO(DMSO)/TZP

Fe	5.69565482675156	9.86515200824992	-0.00000536145739
S	3.63085108903666	8.06352758113308	1.63777611190583
O	5.11345869952791	8.27896705752146	1.16187579393732
C	3.03886069783878	6.67814546255904	0.62604695076685
H	2.99993287981922	7.04257738330038	-0.40310755586765

H	2.03923049598273	6.41792350105390	0.98763458271381
H	3.73289696236306	5.84003630699149	0.73362490573287
C	3.83074216056582	7.20367651407974	3.21873831837098
H	4.50189437921255	6.35316515104304	3.07033112212767
H	2.83331309353472	6.88117654940578	3.53295877892412
H	4.24245554620936	7.92795417154529	3.92592698452324
S	8.30697975683975	8.99802298078708	1.62747679852423
O	7.36387241490945	10.16449552681600	1.15686398074862
C	9.80613439052766	9.21429201879704	0.62819419990662
H	9.52255613080616	8.99948514120543	-0.40478277196528
H	10.54361247439359	8.49125906811313	0.98999501720555
H	10.16353281699183	10.24086598183725	0.74639786411967
C	8.93044087136864	9.59373251149742	3.21976350765166
H	9.32637744303775	10.60399246362473	3.08406721689357
H	9.70897687680752	8.89340688853908	3.53799161554349
H	8.08899732980555	9.57740274196343	3.91682564115431
S	5.15017479692152	12.56450718649589	1.62281640348713
O	4.60358649634576	11.16986557940895	1.14583865838700
C	4.21740818658184	13.76556498822265	0.63310702336736
H	4.54068600223774	13.63091502397474	-0.40179930835905
H	4.48409012932302	14.76176782178502	0.99966130317288
H	3.14857440157567	13.56871999709733	0.75352422654947
C	4.32795533389123	12.80089175653916	3.21883970767853
H	3.25458849869788	12.64006742667959	3.08556589388181
H	4.54694289454364	13.82373667916448	3.54082231117572
H	4.76442188586574	12.07729592813886	3.91181229224251
S	7.76048613255330	11.66677201657073	-1.63775402435017
O	6.27787343475937	11.45135068556859	-1.16185701153967
C	8.35254848940912	13.05203317608745	-0.62590107471129
H	8.39147148836241	12.68750175266913	0.40321824716153
H	9.35218622059606	13.31224476056987	-0.98747548417932
H	7.65854869679603	13.89018365573475	-0.73339188096024
C	7.56061214972159	12.52678451263786	-3.21863047588651
H	6.88950217285972	13.37731311111057	-3.07013103388651
H	8.55805178606728	12.84926884800780	-3.53283333892698
H	7.14885393164621	11.80259614700244	-3.92588514390941
S	3.08431120861464	10.73224058902506	-1.62749067950184
O	4.02744659076746	9.56578797970466	-1.15688411055125
C	1.58522815136332	10.51604077550706	-0.62808513902654
H	1.86888495331875	10.73090758313815	0.40485756982904
H	0.84772693279965	11.23905524244557	-0.98987545376878
H	1.22781628665610	9.48946138204437	-0.74620060923776
C	2.46072779168808	10.13643946324926	-3.21969494717835
H	2.06479511227432	9.12619025226908	-3.08390733712014
H	1.68217178153534	10.83675014712840	-3.53790673678036
H	3.30211901314680	10.15272209083568	-3.91682125101607
S	6.24109167040435	7.16579057999337	-1.62282317892023
O	6.78769653489231	8.56043225960608	-1.14586612232269
C	7.17411147674984	5.96473091892540	-0.63335532332195
H	6.85102002100941	6.09930022373665	0.40161996755229
H	6.90741875669108	4.96853327350707	-0.99991578526878
H	8.24291137782140	6.16164472073804	-0.75396205509281
C	7.06302136719142	6.92953781579385	-3.21901538641596
H	8.13640373363670	7.09042043717331	-3.08593755240869
H	6.84403407378790	5.90669662500232	-3.54101013286044
H	6.62637870056570	7.65314357664701	-3.91186672844359

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C12H36FeO6S6 optimized with ADF in AMS. Fe(dmso)6+:LS B97-D-COSMO(DMSO)/TZP

Fe	0.000000000000000	0.000000000000000	0.000000000000000
S	2.63164007265381	-0.10531831486081	-1.58274440601975
O	1.40660427392122	0.78160355686904	-1.11703309078883
C	4.06454546099978	0.72708850589992	-0.85010654476878
H	4.95980023609138	0.24681574231670	-1.25708248774001
H	3.99654568126592	0.57261448267290	0.22923875425732
H	4.02733624190454	1.78853499811530	-1.11050567498561
C	2.83778260053523	0.40359809465120	-3.30673427024923
H	3.78110917341701	-0.02600368166578	-3.65723818063636
H	2.85297295673486	1.49620744925656	-3.34811590042044
H	1.99512628094251	-0.01249934468342	-3.86446115043840
S	-1.22461170130127	2.33172631322278	-1.58274440601975
O	-1.38019066816893	0.82735325408530	-1.11703309078883
C	-2.66194984741615	3.15645537602427	-0.85010654476878
H	-2.69364882425999	4.17190513491925	-1.25708248774001
H	-2.49417152850450	3.17480284912814	0.22923875425732
H	-3.56258486116562	2.59350799626949	-1.11050567498561
C	-1.76841750673785	2.25579277577535	-3.30673427024923
H	-1.86803474170360	3.28753843636564	-3.65723818063636
H	-2.72224013418785	1.72264333270670	-3.34811590042044
H	-0.98673839141383	1.73407971745659	-3.86446115043840
S	-1.40702837135254	-2.22640799836197	-1.58274440601975
O	-0.02641360575230	-1.60895681095434	-1.11703309078883
C	-1.40259561358363	-3.88354388192419	-0.85010654476878
H	-2.26615141183139	-4.41872087723594	-1.25708248774001
H	-1.50237415276142	-3.74741733180104	0.22923875425732
H	-0.46475138073893	-4.38204299438479	-1.11050567498561
C	-1.06936509379737	-2.65939087042655	-3.30673427024923
H	-1.91307443171342	-3.26153475469986	-3.65723818063636
H	-0.13073282254700	-3.21885078196326	-3.34811590042044
H	-1.00838788952868	-1.72158037277317	-3.86446115043840
S	-2.63164007265381	0.10531831486081	1.58274440601975
O	-1.40660427392122	-0.78160355686904	1.11703309078883
C	-4.06454546099978	-0.72708850589992	0.85010654476878
H	-4.95980023609138	-0.24681574231670	1.25708248774001
H	-3.99654568126592	-0.57261448267290	-0.22923875425732
H	-4.02733624190454	-1.78853499811530	1.11050567498561
C	-2.83778260053523	-0.40359809465120	3.30673427024923
H	-3.78110917341701	0.02600368166578	3.65723818063636
H	-2.85297295673486	-1.49620744925656	3.34811590042044
H	-1.99512628094251	0.01249934468342	3.86446115043840
S	1.22461170130127	-2.33172631322278	1.58274440601975
O	1.38019066816893	-0.82735325408530	1.11703309078883
C	2.66194984741615	-3.15645537602427	0.85010654476878
H	2.69364882425999	-4.17190513491925	1.25708248774001
H	2.49417152850450	-3.17480284912814	-0.22923875425732
H	3.56258486116562	-2.59350799626949	1.11050567498561
C	1.76841750673785	-2.25579277577535	3.30673427024923
H	1.86803474170360	-3.28753843636564	3.65723818063636
H	2.72224013418785	-1.72264333270670	3.34811590042044
H	0.98673839141383	-1.73407971745659	3.86446115043840
S	1.40702837135254	2.22640799836197	1.58274440601975
O	0.02641360575230	1.60895681095434	1.11703309078883

C	1.40259561358363	3.88354388192419	0.85010654476878
H	2.26615141183139	4.41872087723594	1.25708248774001
H	1.50237415276142	3.74741733180104	-0.22923875425732
H	0.46475138073893	4.38204299438479	1.11050567498561
C	1.06936509379737	2.65939087042655	3.30673427024923
H	1.91307443171342	3.26153475469986	3.65723818063636
H	0.13073282254700	3.21885078196326	3.34811590042044
H	1.00838788952868	1.72158037277317	3.86446115043840

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C12H36MnO6S6 optimized with ADF in AMS. Mn(dmso)6. HS- B97-D-COSMO(DMSO)/TZP

Mn	-0.00000000000000	-0.00000000000000	0.00000000000000
S	2.88436604345433	0.03213238044879	-1.58532281918838
O	1.61552193601782	0.84639601392252	-1.22973365032348
C	4.14171778041894	0.52688384049989	-0.36255307368056
H	5.08190780105992	0.03420443376271	-0.63140461136550
H	3.77438351792449	0.17525418533983	0.60457723468275
H	4.24648321334831	1.61586738764404	-0.38151581287455
C	3.58832916486708	0.89196302742780	-3.02510327938049
H	4.56463396650236	0.44261725529485	-3.23398192817639
H	3.68116984103412	1.95593197586648	-2.78604505715156
H	2.90319669377191	0.72935254643012	-3.86119094750435
S	-1.47001048060748	2.48186807647731	-1.58532281918838
O	-1.54076141299915	0.97588502823346	-1.22973365032348
C	-2.52715368093314	3.32339089781025	-0.36255307368056
H	-2.57057581240466	4.38395904245326	-0.63140461136550
H	-2.03896633488800	3.18108492058129	0.60457723468275
H	-3.52262380980863	2.86962864593785	-0.38151581287455
C	-2.56662722700580	2.66160270082157	-3.02510327938049
H	-2.66563477439944	3.73178034319218	-3.23398192817639
H	-3.53447169512445	2.21002061054003	-2.78604505715156
H	-2.08323618137838	2.14956581783510	-3.86119094750435
S	-1.41435556284685	-2.51400045692611	-1.58532281918838
O	-0.07476052301867	-1.82228104215598	-1.22973365032348
C	-1.61456409948580	-3.85027473831014	-0.36255307368056
H	-2.51133198865526	-4.41816347621597	-0.63140461136550
H	-1.73541718303649	-3.35633910592112	0.60457723468275
H	-0.72385940353968	-4.48549603358189	-0.38151581287455
C	-1.02170193786128	-3.55356572824937	-3.02510327938049
H	-1.89899919210292	-4.17439759848702	-3.23398192817639
H	-0.14669814590967	-4.16595258640651	-2.78604505715156
H	-0.81996051239353	-2.87891836426522	-3.86119094750435
S	-2.88436604345433	-0.03213238044879	1.58532281918838
O	-1.61552193601782	-0.84639601392252	1.22973365032348
C	-4.14171778041894	-0.52688384049989	0.36255307368056
H	-5.08190780105992	-0.03420443376271	0.63140461136550
H	-3.77438351792449	-0.17525418533983	-0.60457723468275
H	-4.24648321334831	-1.61586738764404	0.38151581287455
C	-3.58832916486708	-0.89196302742780	3.02510327938049
H	-4.56463396650236	-0.44261725529485	3.23398192817639
H	-3.68116984103412	-1.95593197586648	2.78604505715156
H	-2.90319669377191	-0.72935254643012	3.86119094750435
S	1.47001048060748	-2.48186807647731	1.58532281918838
O	1.54076141299915	-0.97588502823346	1.22973365032348
C	2.52715368093314	-3.32339089781025	0.36255307368056
H	2.57057581240466	-4.38395904245326	0.63140461136550

H	2.03896633488800	-3.18108492058129	-0.60457723468275
H	3.52262380980863	-2.86962864593785	0.38151581287455
C	2.56662722700580	-2.66160270082157	3.02510327938049
H	2.66563477439944	-3.73178034319218	3.23398192817639
H	3.53447169512445	-2.21002061054003	2.78604505715156
H	2.08323618137838	-2.14956581783510	3.86119094750435
S	1.41435556284685	2.51400045692611	1.58532281918838
O	0.07476052301867	1.82228104215598	1.22973365032348
C	1.61456409948580	3.85027473831014	0.36255307368056
H	2.51133198865526	4.41816347621597	0.63140461136550
H	1.73541718303649	3.35633910592112	-0.60457723468275
H	0.72385940353968	4.48549603358189	0.38151581287455
C	1.02170193786128	3.55356572824937	3.02510327938049
H	1.89899919210292	4.17439759848702	3.23398192817639
H	0.14669814590967	4.16595258640651	2.78604505715156
H	0.81996051239353	2.87891836426522	3.86119094750435

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C12H36MnO6S6 optimized with ADF in AMS. Mn(dmsO)6. LS B97-D-COSMO(DMSO)/TZP

Mn	-0.00000000000000	0.00000000000000	0.00000000000000
S	2.71627099927667	-0.02023003959223	-1.57495489837167
O	1.46524190410749	0.82454339154738	-1.16666829054744
C	4.05379680710979	0.52558055480897	-0.46263059512355
H	4.97871686401736	0.03326368060081	-0.78117767399802
H	3.75949643414814	0.20503268854322	0.53912881658154
H	4.14452082882791	1.61422831133526	-0.52425889244164
C	3.29932761940838	0.79890563936970	-3.08834886710796
H	4.27065972696102	0.36604571520948	-3.34800878247061
H	3.38017240396445	1.87297050398770	-2.89468352247996
H	2.56365491797719	0.59035709597551	-3.86958795418903
S	-1.34061577255949	2.36247470798971	-1.57495489837167
O	-1.44669647092781	0.85666501410515	-1.16666829054744
C	-2.48206451576184	3.24790074424453	-0.46263059512355
H	-2.51816562774649	4.29506344611503	-0.78117767399802
H	-2.05731173326065	3.15330307624101	0.53912881658154
H	-3.47022313582629	2.78214616886714	-0.52425889244164
C	-2.34153639220830	2.45784871475042	-3.08834886710796
H	-2.45233475570794	3.51547695373385	-3.34800878247061
H	-3.31212623440724	1.99082991950307	-2.89468352247996
H	-1.79309170237686	1.92501173957810	-3.86958795418903
S	-1.37565522671718	-2.34224466839748	-1.57495489837167
O	-0.01854543317968	-1.68120840565254	-1.16666829054744
C	-1.57173229134795	-3.77348129905350	-0.46263059512355
H	-2.46055123627088	-4.32832712671585	-0.78117767399802
H	-1.70218470088749	-3.35833576478423	0.53912881658154
H	-0.67429769300163	-4.39637448020240	-0.52425889244164
C	-0.95779122720008	-3.25675435412012	-3.08834886710796
H	-1.81832497125308	-3.88152266894333	-3.34800878247061
H	-0.06804616955721	-3.86380042349077	-2.89468352247996
H	-0.77056321560033	-2.51536883555361	-3.86958795418903
S	-2.71627099927667	0.02023003959223	1.57495489837167
O	-1.46524190410749	-0.82454339154738	1.16666829054744
C	-4.05379680710979	-0.52558055480897	0.46263059512355
H	-4.97871686401736	-0.03326368060081	0.78117767399802
H	-3.75949643414814	-0.20503268854322	-0.53912881658154
H	-4.14452082882791	-1.61422831133526	0.52425889244164

C	-3.29932761940838	-0.79890563936970	3.08834886710796
H	-4.27065972696102	-0.36604571520948	3.34800878247061
H	-3.38017240396445	-1.87297050398770	2.89468352247996
H	-2.56365491797719	-0.59035709597551	3.86958795418903
S	1.34061577255949	-2.36247470798971	1.57495489837167
O	1.44669647092781	-0.85666501410515	1.16666829054744
C	2.48206451576184	-3.24790074424453	0.46263059512355
H	2.51816562774649	-4.29506344611503	0.78117767399802
H	2.05731173326065	-3.15330307624101	-0.53912881658154
H	3.47022313582629	-2.78214616886714	0.52425889244164
C	2.34153639220830	-2.45784871475042	3.08834886710796
H	2.45233475570794	-3.51547695373385	3.34800878247061
H	3.31212623440724	-1.99082991950307	2.89468352247996
H	1.79309170237686	-1.92501173957810	3.86958795418903
S	1.37565522671718	2.34224466839748	1.57495489837167
O	0.01854543317968	1.68120840565254	1.16666829054744
C	1.57173229134795	3.77348129905350	0.46263059512355
H	2.46055123627088	4.32832712671585	0.78117767399802
H	1.70218470088749	3.35833576478423	-0.53912881658154
H	0.67429769300163	4.39637448020240	0.52425889244164
C	0.95779122720008	3.25675435412012	3.08834886710796
H	1.81832497125308	3.88152266894333	3.34800878247061
H	0.06804616955721	3.86380042349077	2.89468352247996
H	0.77056321560033	2.51536883555361	3.86958795418903

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H12FeO6 optimized with ADF in AMS. Fe(H₂O)₆³⁺. B97-D-COSMO(DMSO)/TZP

Fe	0.00000000000000	0.00000000000000	0.00000000000000
O	1.19873258700715	-1.46734286221175	0.70082162917649
H	1.88905443586423	-1.35007504317748	1.37675116243261
H	1.17153721342310	-2.40353063504879	0.43636220042426
O	0.92131836690548	1.33570549708566	1.20504011357424
H	1.72462959772063	1.83947450690627	0.98599710625092
H	0.67482838093775	1.52426872745588	2.12763684762418
O	-1.19873258700715	1.46734286221175	-0.70082162917649
H	-1.17153721342310	2.40353063504879	-0.43636220042426
H	-1.88905443586423	1.35007504317748	-1.37675116243261
O	-0.92131836690548	-1.33570549708566	-1.20504011357424
H	-0.67482838093775	-1.52426872745588	-2.12763684762418
H	-1.72462959772063	-1.83947450690627	-0.98599710625092
O	1.34354744559289	0.38968068893062	-1.45828597146466
H	2.18729060270263	-0.08026000336628	-1.57895919755452
H	1.26278940607796	1.07501483420543	-2.14441381776849
O	-1.34354744559289	-0.38968068893062	1.45828597146466
H	-1.26278940607796	-1.07501483420543	2.14441381776849
H	-2.18729060270263	0.08026000336628	1.57895919755452

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H12MnO6 optimized with ADF in AMS. Mn(H₂O)₆. B97-D-COSMO(DMSO)/TZP

Mn	-0.00007115335731	-0.00000878684221	-0.00046489137791
O	0.00882682623699	0.11377617885384	2.18669025970501
H	0.29687206456542	-0.63634307706705	2.73136109894564
H	0.38917680789375	0.90420543330020	2.60379141286633
O	-0.11328062135862	-2.18711471848584	0.00917292353721
H	-0.90347806692070	-2.60444438777979	0.38975053699661
H	0.63709341227104	-2.73151551462142	0.29708059404840

O	-0.00876261858100	-0.11376609265819	-2.18746530600898
H	-0.38910098461003	-0.90433676590185	-2.60429757642176
H	-0.29720110737112	0.63619687020571	-2.73217390057261
O	0.11303504298461	2.18710290612204	-0.01040543632232
H	-0.63717602766331	2.73134386287511	-0.29901891014168
H	0.90347897679649	2.60445156461113	-0.39044661302276
O	-2.18712911323688	0.00929113411114	0.11304056463536
H	-2.60404890121819	0.38955953029957	0.90360205088379
H	-2.73176754825942	0.29753167237386	-0.63702343230649
O	2.18709134687280	-0.00922811057315	-0.11168494931029
H	2.73017205288898	-0.29673696862890	0.63979065368026
H	2.60569261206653	-0.39025773019417	-0.90099007981380

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C6H7N4S2 optimized with ADF in AMS. Ligand. B97-D-COSMO(DMSO)/TZP

S	5.22380877329839	0.21933130895397	10.25901353487173
S	0.56829738877248	5.29942374797889	9.77999618515342
N	6.69814105530236	1.81376166654906	11.81951269016678
N	4.81285357380534	2.85847025663017	11.10532467142268
N	3.61585748051063	2.79211083289113	10.46612938563817
N	1.09573084626167	2.83554815073524	9.17456558117293
C	5.54170401240626	1.73480338339444	11.06895592850146
C	2.93448374617696	3.91252004714500	10.46098617123699
C	3.43854097851570	5.18827452516847	11.10113235686548
C	1.62855654513201	3.87569131614502	9.79936290548922
C	-0.14321736299700	3.12895401586586	8.67009683847037
C	-0.60533805608932	4.40301935221421	8.88978868228372
H	7.42826268515593	1.14909448169280	11.60106566034907
H	7.00543254624965	2.74700126921919	12.07548421701314
H	3.57776336659584	5.03414422114820	12.17874908626633
H	2.76556391376882	6.03675196008923	10.94962984214422
H	4.42355833386918	5.44026874062534	10.69012851477135
H	-0.69508192548070	2.36368544137524	8.12950392563890
H	-1.54469615060121	4.84782383285895	8.58310407644085

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