Supporting Information

Preparation, Characterization, Molecular and Electronic Structures, TDDFT and TDDFT/PCM Study of the Solvatochromism in Cyanovinylferrocenes

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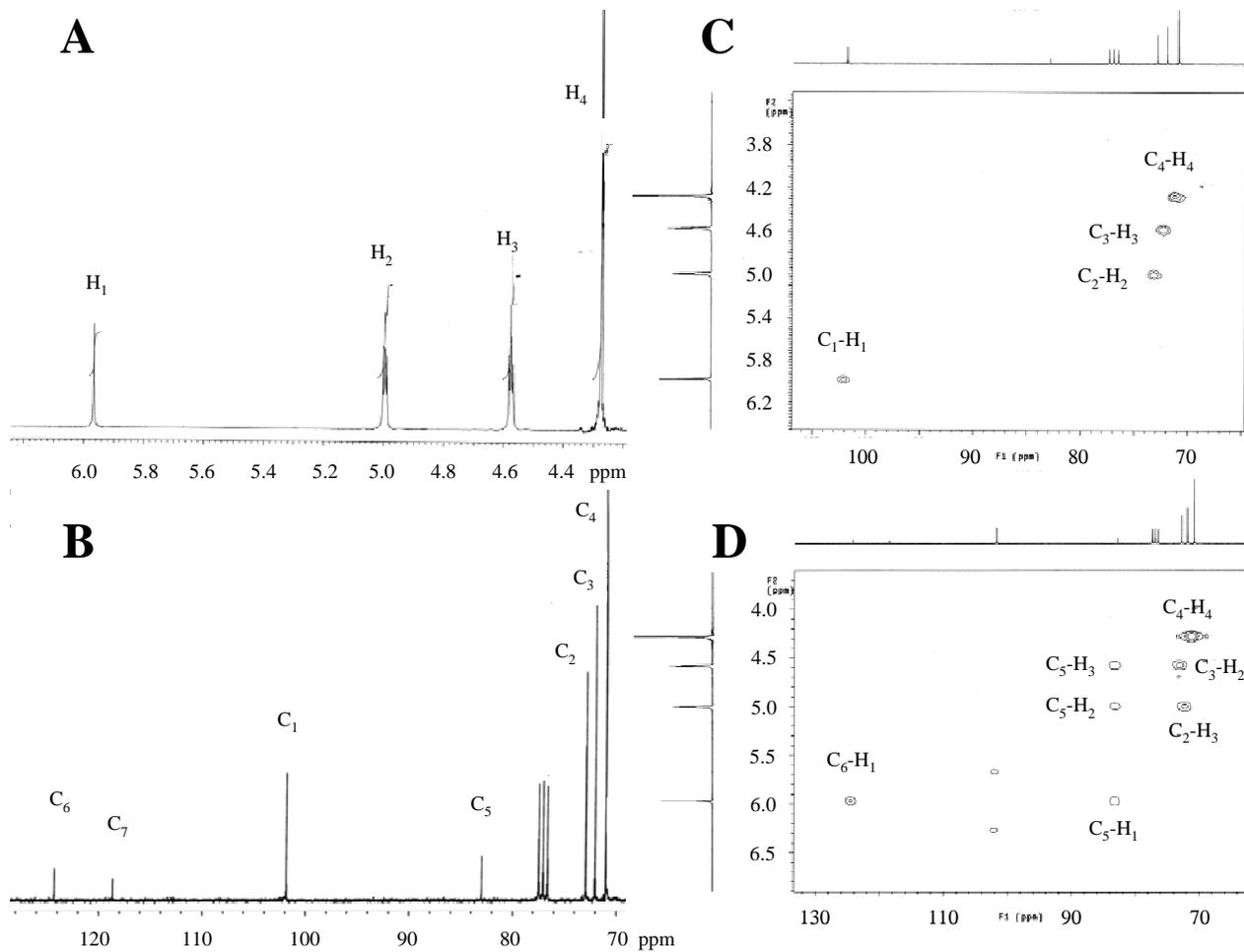
Figure SI 1. ^{1}H (**A**), ^{13}C (**B**), gHMQC (**C**), and gHMBC (**D**) NMR spectra of complex ***trans*-3** in CDCl$_3$. Peak assignments are given in Tables 1 and 2.
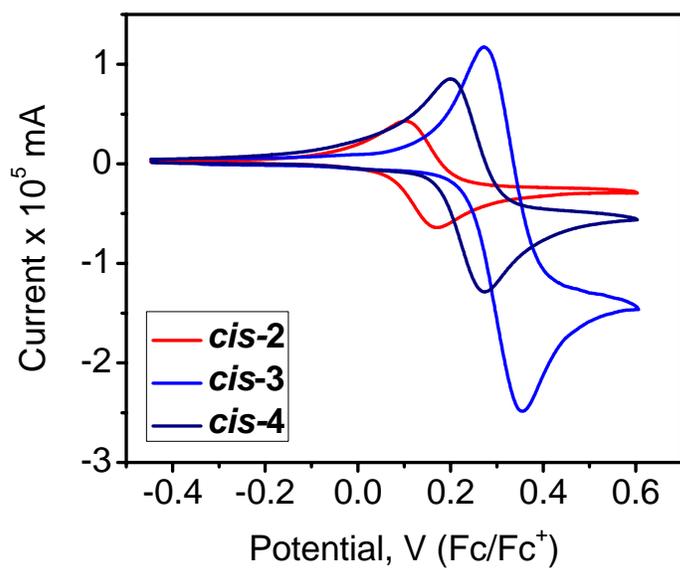
Figure SI 2. Cyclic voltammetry data on complexes *cis*-**2**, *cis*-**3**, and *cis*-**4** in acetonitrile/0.1 M TBAP solution recorded at 100 mV/s scan rate at room temperature.
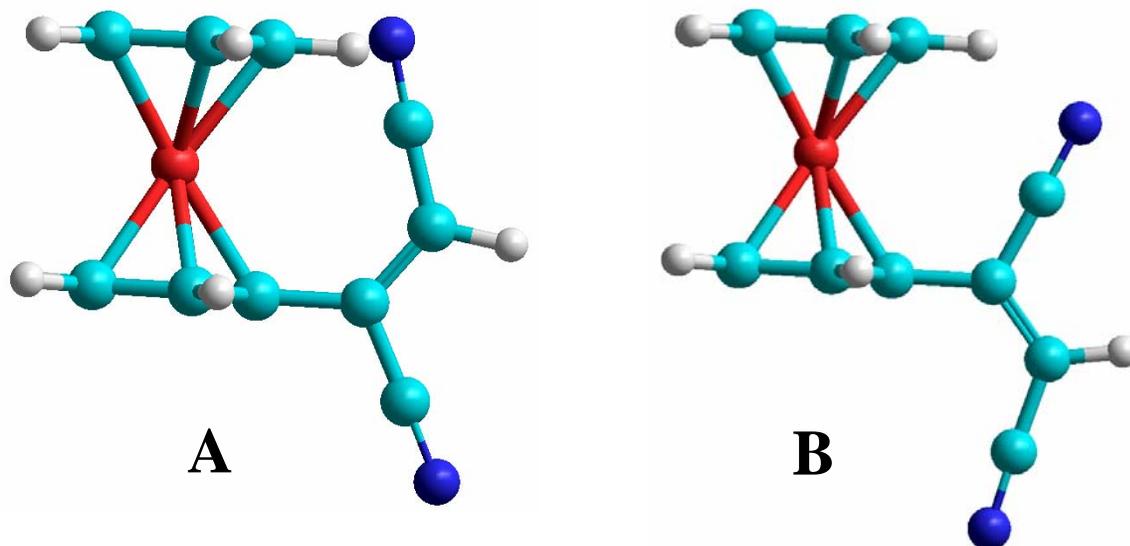
Figure SI 3. High-energy rotational conformers with $\Theta \sim 90^o$ (**A**) $\Theta \sim 270^o$ (**B**) in complex *trans*-**4**. The conformer **A** in *trans*-compounds **2**, **3**, and **4** has very high energy, while conformer **B** represents local maxima on the energy diagram presented in Figure 2.The conformer **A** in *cis*-compounds **2**, **3**, and **4** has low energy, while conformer **B** represents the global maxima because of the different position of substituents.

Supporting Information Table 1. Calculated Using TDDFT Approach Vertical Excitation Energies of Complexes **3** – **5**.[a]

Transition	λ, nm	f	Transitions and expansion coefficients [b]
			cis-**3**
1	548.66	0.0003	63 → **65**, -0.17100; **64** → **65**, 0.66450
2	531.83	0.0001	62 → **65**, 0.28412; 63 → **65**, 0.60403; **64** → **65**, 0.14619
3	479.68	0.0387	61 → **65**, -0.13670; 62 → **65**, 0.59071; 63 → **65**, -0.23089
4	424.49	0.0002	63 → 66, 0.45238; **64** → 66, 0.50793; **64** → 67, 0.15334
5	421.21	0.0011	63 → 66, 0.52490; 63 → 68, -0.11943; **64** → 66, -0.39143; **64** → 67, -0.18786
6	404.41	0.0003	62 → 66, 0.61083; 62 → 67, 0.15468; 63 → 68, -0.10730; **64** → 68, 0.29468
7	397.73	0.0004	63 → 67, 0.46572; 63 → 68, -0.24528; **64** → 67, 0.45192
8	394.24	0.0039	63 → 67, 0.43429; 63 → 68, 0.29849; **64** → 67, -0.32200; **64** → 68, 0.28970
9	388.72	0.0004	62 → 67, 0.50392; 63 → 67, 0.22192; 63 → 68, 0.20289; **64** → 68, -0.37167
10	374.93	0.0075	61 → **65**, -0.10443; 62 → 68, 0.66641
11	325.25	0.0002	62 → 68, -0.12196; 63 → 67, -0.12537; 63 → 68, 0.42220; **64** → 66, -0.20685; **64** → 67, 0.29165; **64** → 68, 0.18004
12	322.32	0.0019	62 → 66, -0.26785; 62 → 67, 0.40363; 63 → 68, -0.16302; **64** → 68, 0.30836
13	311.72	0.0283	60 → **65**, 0.56022; 61 → **65**, 0.35608
14	304.52	0.0044	58 → **65**, 0.16186; 59 → **65**, 0.65373; 60 → **65**, 0.10904; 61 → **65**, -0.14018
15	298.98	0.0617	58 → **65**, 0.37076; 60 → **65**, -0.32953; 61 → **65**, 0.34218; 61 → 66, 0.17480; 61 → 68, -0.19315
16	291.13	0.1211	58 → **65**, 0.53146; 59 → **65**, -0.21458; 60 → **65**, 0.14338; 61 → **65**, -0.14970; 61 → 66, -0.26633; 61 → 67, 0.11348
17	287.38	0.0569	58 → **65**, 0.14582; 60 → **65**, 0.13023; 61 → **65**, -0.16218; 61 → 66, 0.59040; **64** → 69, 0.11731
			trans-**3**
1	564.68	0.0003	62 → **65**, 0.10985; 63 → **65**, 0.56102; **64** → **65**, -0.38308
2	561.00	0.0006	62 → **65**, -0.22771; 63 → **65**, 0.39839; **64** → **65**, 0.50932
3	498.17	0.0288	61 → **65**, 0.11884; 62 → **65**, 0.60490; **64** → **65**, 0.20993
4	470.41	0.0006	**64** → 66, 0.70431
5	459.71	0.0045	63 → 66, 0.69526
6	441.67	0.0012	62 → 66, 0.69859
7	398.44	0.0001	63 → 67, 0.10558; 63 → 68, 0.22589; **64** → 67, 0.61262; **64** → 68, 0.23130
8	392.79	0.0013	62 → 67, -0.15153; 63 → 67, 0.49865; **64** → 68, -0.46158
9	384.75	0.0007	62 → 67, 0.34757; 62 → 68, 0.19177; 63 → 67, -0.18149; 63 → 68, 0.46154; **64** → 68, -0.29654

10	373.52	0.0051	62 → 67, -0.41518; 62 → 68, 0.51763; 63 → 67, -0.15132
11	324.59	0.0032	60 → **65**, 0.61224; 61 → **65**, -0.24456; 63 → 68, 0.11286
12	320.42	0.0000	60 → **65**, -0.23738; 62 → 68, 0.13654; 63 → 67, 0.29475; 63 → 68, 0.28177; **64** → 67, -0.25820; **64** → 68, 0.29775
13	314.22	0.0005	62 → 67, 0.36067; 62 → 68, 0.34720; 63 → 67, 0.18852; 63 → 68, -0.29629
14	306.31	0.0781	59 → **65**, 0.11571; 60 → **65**, -0.19204; 61 → **65**, -0.43070; 61 → 66, 0.41715
15	296.52	0.0275	58 → **65**, 0.43820; 59 → **65**, 0.52396; 61 → 66, -0.11500
16	293.40	0.0292	58 → **65**, 0.42097; 59 → **65**, -0.23826; 61 → **65**, 0.18425; 61 → 66, 0.40002; 61 → 67, -0.14193
17	291.05	0.1242	58 → **65**, -0.34929; 59 → **65**, 0.34108; 60 → **65**, 0.10688; 61 → **65**, 0.24855; 61 → 66, 0.32307
			cis-**4**
1	674.51	0.0002	66 → **68**, -0.14541; **67** → **68**, 0.67946
2	653.71	0.0003	65 → **68**, -0.16979; 66 → **68**, 0.65667; **67** → **68**, 0.12801
3	555.25	0.0393	64 → **68**, -0.14764; 65 → **68**, 0.62338; 66 → **68**, 0.13252
4	403.84	0.0001	66 → 69, 0.48289; **67** → 69, 0.44091; **67** → 70, 0.23766
5	399.90	0.0001	65 → 69, 0.15182; 65 → 70, 0.13166; 66 → 69, 0.31700; 66 → 70, 0.43127; **67** → 69, -0.35137; **67** → 70, 0.20997
6	394.43	0.0002	65 → 69, -0.33280; 65 → 70, -0.15236; 66 → 69, 0.10282; 66 → 70, 0.40484; **67** → 69, 0.15202; **67** → 70, -0.40187
7	383.08	0.0018	65 → 69, -0.39898; 65 → 70, 0.52447; 66 → 69, 0.11285; 66 → 70, -0.16683; **67** → 69, -0.10013
8	343.40	0.0048	63 → **68**, 0.66541; 64 → **68**, 0.21174
9	323.38	0.0336	62 → **68**, 0.17289; 64 → **68**, -0.24512; 65 → 69, -0.10391; 65 → 70, 0.11481; 66 → 69, -0.29151; 66 → 70, 0.24655; **67** → 69, 0.21252; **67** → 70, 0.30121
10	318.33	0.1558	62 → **68**, -0.22813; 63 → **68**, -0.15351; 64 → **68**, 0.42892; 65 → 69, 0.10549; 65 → 70, 0.24390; 66 → 69, -0.13689; 66 → 70, 0.15747; **67** → 69, 0.19539
11	317.37	0.0415	62 → **68**, -0.13067; 63 → **68**, -0.11071; 64 → **68**, 0.21635; 65 → 69, -0.37242; 65 → 70, -0.26938; **67** → 69, -0.14816; **67** → 70, 0.29653
12	281.61	0.0012	**67** → 71, 0.70509
13	280.12	0.0003	66 → 71, 0.70026
14	273.57	0.0028	**67** → 72, 0.69001
15	272.05	0.0009	62 → **68**, 0.10749; 64 → 69, 0.15936; 65 → 71, 0.66407; **67** → 73, -0.10864
			trans-**4**
1	719.62	0.0001	66 → **68**, 0.55858; **67** → **68**, -0.41662
2	671.33	0.0061	65 → **68**, 0.36166; 66 → **68**, 0.36339; **67** → **68**, 0.44846
3	593.02	0.0309	64 → **68**, -0.13034; 65 → **68**, 0.57438;

			$66 \rightarrow$ **68**, -0.16729; **67** $\rightarrow$ **68**, -0.25959;
4	413.75	0.0002	$66 \rightarrow 69$, -0.13746; $66 \rightarrow 70$, -0.42446;
			67 $\rightarrow 69$, 0.51929; **67** $\rightarrow 70$, -0.13051
5	412.82	0.0005	$66 \rightarrow 69$, 0.49336; $66 \rightarrow 70$, -0.14442;
			67 $\rightarrow 69$, 0.12975; **67** $\rightarrow 70$, 0.46140
6	392.45	0.0003	$65 \rightarrow 69$, 0.44819; $65 \rightarrow 70$, -0.31894;
			$66 \rightarrow 69$, 0.17183; $66 \rightarrow 70$, -0.28418;
			67 $\rightarrow 69$, -0.14299; **67** $\rightarrow 70$, -0.24171
7	388.10	0.0005	$65 \rightarrow 69$, 0.48937; $65 \rightarrow 70$, 0.39261;
			$66 \rightarrow 69$, -0.19518; **67** $\rightarrow 70$, 0.24178
8	356.90	0.0001	$63 \rightarrow$ **68**, 0.69822
9	338.58	0.1126	$62 \rightarrow$ **68**, -0.35873; $64 \rightarrow$ **68**, 0.53335; $66 \rightarrow 70$, -0.10035
10	330.43	0.0186	$64 \rightarrow$ **68**, 0.16449; $65 \rightarrow 69$, 0.15486; $66 \rightarrow 69$, 0.23111;
			$66 \rightarrow 70$, 0.36536; $66 \rightarrow 71$, -0.10367; **67** $\rightarrow 69$, 0.30776;
			67 $\rightarrow 70$, -0.21584
11	324.69	0.0004	$61 \rightarrow$ **68**, -0.18659; $65 \rightarrow 70$, 0.43118; $66 \rightarrow 69$, 0.23901;
			$66 \rightarrow 70$, -0.15096; **67** $\rightarrow 69$, -0.17654;
			67 $\rightarrow 70$, -0.23392; **67** $\rightarrow 71$, 0.12190
12	302.71	0.0002	$61 \rightarrow$ **68**, 0.27289; $62 \rightarrow$ **68**, -0.11186;
			$66 \rightarrow 71$, -0.12368; **67** $\rightarrow 71$, 0.62222
13	300.67	0.0125	$60 \rightarrow$ **68**, -0.12196; $62 \rightarrow$ **68**, 0.22869;
			$66 \rightarrow 71$, 0.60169; **67** $\rightarrow 71$, 0.20223
14	298.30	0.0045	$61 \rightarrow$ **68**, 0.60741; $62 \rightarrow$ **68**, 0.12276;
			$65 \rightarrow 70$, 0.11594; **67** $\rightarrow 71$, -0.20624
15	296.17	0.0824	$60 \rightarrow$ **68**, -0.25410; $62 \rightarrow$ **68**, 0.46178;
			$64 \rightarrow$ **68**, 0.21219; $66 \rightarrow 71$, -0.31698
		5	
1	811.30	0.0001	**73** $\rightarrow$ **74**, 0.69192
2	749.24	0.0015	$71 \rightarrow$ **74**, 0.35239; $72 \rightarrow$ **74**, 0.58308
3	616.97	0.0465	$70 \rightarrow$ **74**, 0.16512; $71 \rightarrow$ **74**, 0.54737; $72 \rightarrow$ **74**, -0.29074
4	400.37	0.0003	$72 \rightarrow 75$, -0.43223 ; **73** $\rightarrow 76$, 0.54888
5	400.18	0.0000	$72 \rightarrow 75$, 0.55556; **73** $\rightarrow 76$, 0.43298
6	387.58	0.0000	$71 \rightarrow 75$, 0.50225; $72 \rightarrow 75$, -0.30031; **73** $\rightarrow 76$, 0.36653
7	378.52	0.0005	$70 \rightarrow$ **74**, 0.10284; $71 \rightarrow 76$, -0.14392;
			$72 \rightarrow 76$, -0.15579 ; **73** $\rightarrow$ **74**, 0.65865
8	375.55	0.0011	$70 \rightarrow$ **74**, -0.12133; $71 \rightarrow 75$, 0.10425;
			$71 \rightarrow 76$, 0.64474; **73** $\rightarrow$ **74**, 0.19434
9	366.59	0.0036	$70 \rightarrow$ **74**, -0.11547; **73** $\rightarrow$ **74**, 0.67760
10	361.53	0.0003	$72 \rightarrow$ **74**, 0.70158
11	358.19	0.1504	$68 \rightarrow$ **74**, 0.34362; $70 \rightarrow$ **74**, -0.12514;
			$69 \rightarrow$ **74**, 0.51523; **73** $\rightarrow$ **74**, 0.15367
12	345.69	0.0052	$71 \rightarrow 76$ -0.11470; $71 \rightarrow$ **74**, 0.67559
13	325.13	0.0146	$68 \rightarrow$ **74**, -0.27262; $67 \rightarrow$ **74**, 0.13622; $71 \rightarrow 75$, 0.13045;

			$71 \rightarrow 76$ -0.19899; $71 \rightarrow$ **74**, -0.12597;
			$72 \rightarrow 75$, -0.32369; **73** $\rightarrow 76$, 0.35199;
14	323.32	0.0119	$67 \rightarrow$ **74**, -0.31042; $71 \rightarrow 75$, 0.21983;
			$71 \rightarrow 76$, -0.19930; $71 \rightarrow$ **74**, -0.10293;
			$72 \rightarrow 75$, 0.21420; $72 \rightarrow 76$, 0.27546;
			73 $\rightarrow 75$, 0.27109; **73** $\rightarrow 76$, -0.12307
15	308.12	0.1007	$69 \rightarrow$ **74**, 0.19519; $67 \rightarrow$ **74**, 0.23279; $68 \rightarrow$ **74**, -0.47144;
			$70 \rightarrow$ **74**, 0.20252; $71 \rightarrow 76$, -0.14279;
			$72 \rightarrow 75$, -0.11606; **73** $\rightarrow 76$, 0.15674
16	306.25	0.0446	$67 \rightarrow$ **74**, 0.51165; $68 \rightarrow$ **74**, 0.24126;
			$69 \rightarrow$ **74**, -0.11634; $71 \rightarrow 75$, 0.16128;
			$71 \rightarrow 76$, -0.13689; $72 \rightarrow 76$, 0.13101; **73** $\rightarrow 75$ 0.15521

[a] Only transitions important for interpretation of UV-Vis and MCD spectra are shown; complete transition energies lists shown in Supporting Information; in all cases X–ray geometries were used; [b] HOMO and LUMO are labeled in bold. f is an oscillator strength.

Table SI 2. Correlations Between Observed MLCT Band Energy in Complex 1 and Kamlet-Taft Model Parameters.

Parameter	*cis*-2	*trans*-2	*cis*-3	*trans*-3	*cis*-4	*trans*-4	5 [a]
				Eq. (2)			
a	-119.12	-324.03	-241.06	-266.09	-335.58	-339.49	-207.92
b	40.73	360.78	182.53	76.13	338.81	462.07	212.92
s	-291.07	-150.78	-873.52	-367.37	-1243.63	-674.48	-1118.72
d	154.20	-28.11	59.14	-12.91	105.11	-126.99	40.60
r^2	0.217	0.216	0.813	0.773	0.946	0.747	0.948
sd	197.89	213.85	139.10	80.46	94.63	144.76	86.29
				Eq. (3)			
a					-310.76		-198.33
b					300.42		178.78
s					-1190.10		-1098.04
r^2					0.943		0.948
sd					94.18		83.97
				Eq. (4)			
a					-163.65		-110.78
s					-1095.64		-1041.83
r^2					0.908		0.933
sd					116.61		92.17
				Eq. (5)			
s					-1100.28		-1044.96
r					0.942		0.961
sd					124.96		96.41

[a] ref 6.

Full population analysis for complex *trans*-4 (X-ray geometry):

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*************************************************************************
*                          VMOdes                                      *
* Virtual Molecular Orbital description Program, Revision 7.1      *
* Cite this work as: VMOdes Program, Revision A 7.1               *
* V. N. Nemykin, P. Basu, 2001, 2003                             *
* Department of Chemistry, Duquesne University, Pittsburgh, PA    *
*************************************************************************


Input Gaussian file:
C:\Documents and Settings\hp\My Documents\Research Dr.
Nemykin\VMOdes\VModes\trans-CN-CN-pop.gjf.out
Output VMOdes file: trans-CN-CN-xray-pop.out

Full point group is:  C1


Number of Basis Functions = 374

    67 Alpha electrons         67 Beta electrons

Group  1  is: Fe
This group consist of  1  subunits. The Basis Functions range is:
 1            56
Group  2  is: Fc
This group consist of  3  subunits. The Basis Functions range is:
 1            200
 309          344
 348          374
Group  3  is: Lig
This group consist of  2  subunits. The Basis Functions range is:
 201          308
 345          347
Group  4  is: Total
This group consist of  1  subunits. The Basis Functions range is:
 1            374


All MO's will be printed.


Molecular Orbitals Indexes, Energies, and Group Contributions
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	Orbital		Group Number			
Number	Index	Energy,eV	1	2	3	4
1	(A)--O	-6933.009	100.0	100.0	0.0	100.0
2	(A)--O	-803.097	100.0	100.0	0.0	100.0
3	(A)--O	-693.565	100.0	100.0	0.0	100.0
4	(A)--O	-693.209	100.0	100.0	0.0	100.0
5	(A)--O	-693.165	100.0	100.0	0.0	100.0
6	(A)--O	-381.080	0.0	0.0	100.0	100.0
7	(A)--O	-380.824	0.0	0.0	100.0	100.0
8	(A)--O	-271.505	0.0	0.0	100.0	100.0

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9   (A)--O   -270.648   0.0     0.0     100.0   100.0
10  (A)--O   -270.607   0.0     0.2     99.8    100.0
11  (A)--O   -270.605   0.1     99.8    0.2     100.0
12  (A)--O   -270.304   0.0     0.0     100.0   100.0
13  (A)--O   -270.079   0.1     100.0   0.0     100.0
14  (A)--O   -270.001   0.1     100.0   0.0     100.0
15  (A)--O   -269.933   0.1     100.0   0.0     100.0
16  (A)--O   -269.873   0.1     100.0   0.0     100.0
17  (A)--O   -269.866   0.0     100.0   0.0     100.0
18  (A)--O   -269.851   0.1     100.0   0.0     100.0
19  (A)--O   -269.786   0.1     100.0   0.0     100.0
20  (A)--O   -269.774   0.1     100.0   0.0     100.0
21  (A)--O   -269.746   0.1     100.0   0.0     100.0
22  (A)--O   -88.375    100.0   100.0   0.0     100.0
23  (A)--O   -56.947    99.8    100.0   0.0     100.0
24  (A)--O   -55.939    99.9    100.0   0.0     100.0
25  (A)--O   -55.848    99.9    100.0   0.0     100.0
26  (A)--O   -23.458    1.5     16.4    83.6    100.0
27  (A)--O   -23.089    4.7     48.7    51.3    100.0
28  (A)--O   -22.954    1.5     15.2    84.8    100.0
29  (A)--O   -22.630    8.7     92.8    7.2     100.0
30  (A)--O   -21.389    1.4     14.8    85.2    100.0
31  (A)--O   -18.754    1.5     66.2    33.8    100.0
32  (A)--O   -18.282    2.2     97.0    3.0     100.0
33  (A)--O   -18.220    1.9     99.4    0.6     100.0
34  (A)--O   -18.057    1.8     100.0   0.0     100.0
35  (A)--O   -17.340    0.6     33.4    66.6    100.0
36  (A)--O   -14.754    0.9     58.1    41.9    100.0
37  (A)--O   -14.324    0.5     77.7    22.3    100.0
38  (A)--O   -13.918    1.4     97.8    2.2     100.0
39  (A)--O   -13.867    0.9     98.2    1.8     100.0
40  (A)--O   -13.757    0.7     99.2    0.8     100.0
41  (A)--O   -13.542    1.1     98.7    1.3     100.0
42  (A)--O   -13.140    0.2     38.5    61.5    100.0
43  (A)--O   -12.405    1.2     41.5    58.5    100.0
44  (A)--O   -11.076    31.1    79.5    20.5    100.0
45  (A)--O   -10.733    5.3     66.5    33.5    100.0
46  (A)--O   -10.588    9.0     97.3    2.7     100.0
47  (A)--O   -10.426    3.9     88.3    11.7    100.0
48  (A)--O   -10.237    15.7    53.4    46.6    100.0
49  (A)--O   -10.177    2.2     98.7    1.3     100.0
50  (A)--O   -9.995     1.1     95.0    5.0     100.0
51  (A)--O   -9.769     0.4     98.9    1.1     100.0
52  (A)--O   -9.551     0.8     92.6    7.4     100.0
53  (A)--O   -9.498     0.3     83.9    16.1    100.0
54  (A)--O   -9.469     10.4    88.2    11.8    100.0
55  (A)--O   -9.218     0.4     6.4     93.6    100.0
56  (A)--O   -8.978     0.2     5.7     94.3    100.0
57  (A)--O   -8.879     0.5     8.2     91.8    100.0
58  (A)--O   -8.658     0.1     3.2     96.8    100.0
59  (A)--O   -8.374     0.4     8.6     91.4    100.0
60  (A)--O   -7.727     10.5    47.5    52.5    100.0
61  (A)--O   -7.299     31.9    99.5    0.5     100.0
62  (A)--O   -7.104     23.9    82.5    17.5    100.0
63  (A)--O   -6.666     7.2     99.4    0.6     100.0
64  (A)--O   -6.451     6.1     66.4    33.6    100.0
65  (A)--O   -5.114     83.4    96.6    3.4     100.0
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 66 (A)--O    -4.912   64.9   99.0    1.0   100.0
 67 (A)--O    -4.876   60.1   97.9    2.1   100.0
 68 (A)--V    -3.213    8.7   20.5   79.5   100.0
 69 (A)--V    -1.960   40.6   93.2    6.8   100.0
 70 (A)--V    -1.863   42.6   99.2    0.8   100.0
 71 (A)--V    -0.795    4.2   26.1   73.9   100.0
 72 (A)--V    -0.469    0.3   23.6   76.4   100.0
 73 (A)--V     0.114    2.6   79.5   20.5   100.0
 74 (A)--V     0.380    5.8   97.3    2.7   100.0
 75 (A)--V     0.472   30.3   94.7    5.3   100.0
 76 (A)--V     0.563   37.5   84.0   16.0   100.0
 77 (A)--V     0.675   11.8   88.6   11.4   100.0
 78 (A)--V     1.179    3.1   41.5   58.5   100.0
 79 (A)--V     1.420   14.1   90.8    9.2   100.0
 80 (A)--V     1.525    4.9   34.0   66.0   100.0
 81 (A)--V     1.637    2.7   95.5    4.5   100.0
 82 (A)--V     2.001   10.5   78.3   21.7   100.0
 83 (A)--V     2.124    2.2   65.2   34.8   100.0
 84 (A)--V     2.358    2.0   78.8   21.2   100.0
 85 (A)--V     2.623   16.8   79.7   20.3   100.0
 86 (A)--V     2.754   45.7   81.2   18.8   100.0
 87 (A)--V     2.792   10.8   98.1    1.9   100.0
 88 (A)--V     3.080    7.0   82.3   17.7   100.0
 89 (A)--V     3.196   24.9   89.4   10.6   100.0
 90 (A)--V     3.647   16.4   71.1   28.9   100.0
 91 (A)--V     3.816   35.1   70.4   29.6   100.0
 92 (A)--V     4.215   55.8   94.5    5.5   100.0
 93 (A)--V     4.345   65.6   96.6    3.4   100.0
 94 (A)--V     4.572   62.0   91.5    8.5   100.0
 95 (A)--V     5.065   28.5   89.9   10.1   100.0
 96 (A)--V     5.149   45.3   90.0   10.0   100.0
 97 (A)--V     5.312   35.5   97.3    2.7   100.0
 98 (A)--V     5.452   68.9   95.5    4.5   100.0
 99 (A)--V     5.629    6.3   84.9   15.1   100.0
100 (A)--V     5.807    6.3   66.2   33.8   100.0
101 (A)--V     6.221    3.0   75.9   24.1   100.0
102 (A)--V     6.716    2.1   85.1   14.9   100.0
103 (A)--V     6.880    1.6   81.9   18.1   100.0
104 (A)--V     7.480   18.5   47.8   52.2   100.0
105 (A)--V     7.685    5.2   87.3   12.7   100.0
106 (A)--V     8.082   49.6   83.8   16.2   100.0
107 (A)--V     8.179   25.8   85.9   14.1   100.0
108 (A)--V     8.225   14.9   72.6   27.4   100.0
109 (A)--V     8.307   23.2   58.3   41.7   100.0
110 (A)--V     8.464   39.2   97.2    2.8   100.0
111 (A)--V     8.745   47.2   91.1    8.9   100.0
112 (A)--V     8.793    9.1   63.3   36.7   100.0
113 (A)--V     8.920   12.7   70.0   30.0   100.0
114 (A)--V     9.259   39.0   66.1   33.9   100.0
115 (A)--V     9.639    3.9   30.7   69.3   100.0
116 (A)--V     9.898   31.7   57.3   42.7   100.0
117 (A)--V    10.180    4.1   82.4   17.6   100.0
118 (A)--V    10.294   20.9   80.5   19.5   100.0
119 (A)--V    10.395    7.9   46.4   53.6   100.0
120 (A)--V    10.671   41.0   86.4   13.6   100.0
121 (A)--V    10.910   15.3   79.9   20.1   100.0
122 (A)--V    11.217   19.7   91.5    8.5   100.0
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123 (A)--V    11.511    18.3    51.9    48.1    100.0
124 (A)--V    11.650     4.2    38.2    61.8    100.0
125 (A)--V    12.064     7.1    58.7    41.3    100.0
126 (A)--V    12.268    12.0    94.5     5.5    100.0
127 (A)--V    12.643    10.3    79.9    20.1    100.0
128 (A)--V    12.801    15.3    96.6     3.4    100.0
129 (A)--V    12.902    17.9    92.9     7.1    100.0
130 (A)--V    13.179     8.0    79.6    20.4    100.0
131 (A)--V    13.324    31.1    93.7     6.3    100.0
132 (A)--V    13.557    26.5    89.5    10.5    100.0
133 (A)--V    13.740    35.6    75.3    24.7    100.0
134 (A)--V    13.872    20.8    90.8     9.2    100.0
135 (A)--V    14.317    14.7    63.7    36.3    100.0
136 (A)--V    14.505    13.8    61.2    38.8    100.0
137 (A)--V    14.544    26.1    67.2    32.8    100.0
138 (A)--V    14.635     4.2    62.3    37.7    100.0
139 (A)--V    14.703    32.4    63.8    36.2    100.0
140 (A)--V    14.971     9.2    69.8    30.2    100.0
141 (A)--V    15.404     2.8    56.0    44.0    100.0
142 (A)--V    15.606     3.3    90.0    10.0    100.0
143 (A)--V    15.736     1.7    59.8    40.2    100.0
144 (A)--V    15.798     8.8    82.1    17.9    100.0
145 (A)--V    15.985     7.6    81.9    18.1    100.0
146 (A)--V    16.103    20.7    72.9    27.1    100.0
147 (A)--V    16.369     6.5    92.9     7.1    100.0
148 (A)--V    16.611     6.2    97.4     2.6    100.0
149 (A)--V    16.767     6.5    93.6     6.4    100.0
150 (A)--V    16.873     8.8    83.3    16.7    100.0
151 (A)--V    16.949    12.2    87.6    12.4    100.0
152 (A)--V    17.241     1.2    77.7    22.3    100.0
153 (A)--V    17.403     5.2    61.4    38.6    100.0
154 (A)--V    17.941     5.5    78.1    21.9    100.0
155 (A)--V    18.191     6.3    50.7    49.3    100.0
156 (A)--V    18.263     8.9    83.8    16.2    100.0
157 (A)--V    18.917    10.7    67.6    32.4    100.0
158 (A)--V    19.133     7.4    77.1    22.9    100.0
159 (A)--V    19.288     2.6    96.1     3.9    100.0
160 (A)--V    19.368    26.0    72.0    28.0    100.0
161 (A)--V    19.799     5.8    70.1    29.9    100.0
162 (A)--V    19.931     5.9    82.0    18.0    100.0
163 (A)--V    20.132     2.7    42.1    57.9    100.0
164 (A)--V    20.401    10.1    75.7    24.3    100.0
165 (A)--V    20.513    31.3    75.9    24.1    100.0
166 (A)--V    20.783    21.9    50.2    49.8    100.0
167 (A)--V    20.944    31.3    83.3    16.7    100.0
168 (A)--V    21.590    23.2    91.6     8.4    100.0
169 (A)--V    22.088    15.2    76.8    23.2    100.0
170 (A)--V    22.374    25.7    80.9    19.1    100.0
171 (A)--V    22.871     9.6    75.3    24.7    100.0
172 (A)--V    23.022    29.0    83.2    16.8    100.0
173 (A)--V    23.711     8.2    65.0    35.0    100.0
174 (A)--V    24.020     3.7    52.1    47.9    100.0
175 (A)--V    24.355     1.1    38.6    61.4    100.0
176 (A)--V    24.744     3.3    63.3    36.7    100.0
177 (A)--V    25.410     2.4    72.9    27.1    100.0
178 (A)--V    25.564     2.0    64.9    35.1    100.0
179 (A)--V    26.154     0.8    95.3     4.7    100.0
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180 (A)--V    26.644    1.2    47.5    52.5    100.0
181 (A)--V    26.695    1.0    92.4     7.6    100.0
182 (A)--V    27.347   10.1    95.3     4.7    100.0
183 (A)--V    27.790    4.1    85.4    14.6    100.0
184 (A)--V    28.017    3.4    74.1    25.9    100.0
185 (A)--V    28.164    1.4    94.2     5.8    100.0
186 (A)--V    28.404    3.2    87.9    12.1    100.0
187 (A)--V    28.619    0.7    95.0     5.0    100.0
188 (A)--V    28.849    2.1    30.2    69.8    100.0
189 (A)--V    28.966   26.5    92.4     7.6    100.0
190 (A)--V    29.132    1.9    71.3    28.7    100.0
191 (A)--V    29.542   15.5    95.9     4.1    100.0
192 (A)--V    30.478   11.0    95.0     5.0    100.0
193 (A)--V    30.641    5.5    75.4    24.6    100.0
194 (A)--V    30.961    8.8    79.0    21.0    100.0
195 (A)--V    31.156    0.9    72.4    27.6    100.0
196 (A)--V    31.507    5.6    84.7    15.3    100.0
197 (A)--V    32.225   19.0    83.5    16.5    100.0
198 (A)--V    32.446   24.0    92.1     7.9    100.0
199 (A)--V    33.000    5.3    36.9    63.1    100.0
200 (A)--V    33.746   14.3    74.1    25.9    100.0
201 (A)--V    34.162    5.7    48.0    52.0    100.0
202 (A)--V    34.742    5.3    33.2    66.8    100.0
203 (A)--V    35.353    2.8    32.0    68.0    100.0
204 (A)--V    35.732   10.4    41.9    58.1    100.0
205 (A)--V    36.200    3.6    74.7    25.3    100.0
206 (A)--V    36.424    6.5    56.6    43.4    100.0
207 (A)--V    37.079   11.5    95.2     4.8    100.0
208 (A)--V    37.428    0.9    43.9    56.1    100.0
209 (A)--V    37.941    6.0    51.5    48.5    100.0
210 (A)--V    37.952    5.0    64.7    35.3    100.0
211 (A)--V    39.706    6.6    93.0     7.0    100.0
212 (A)--V    40.149    2.0    54.9    45.1    100.0
213 (A)--V    40.377    2.2    77.2    22.8    100.0
214 (A)--V    40.569    2.0    97.2     2.8    100.0
215 (A)--V    41.209   12.3    52.4    47.6    100.0
216 (A)--V    41.725    9.1    62.8    37.2    100.0
217 (A)--V    42.197   15.5    88.7    11.3    100.0
218 (A)--V    42.371   13.2    94.5     5.5    100.0
219 (A)--V    42.517   13.8    97.9     2.1    100.0
220 (A)--V    42.620    6.2    95.9     4.1    100.0
221 (A)--V    42.871    9.7    80.2    19.8    100.0
222 (A)--V    43.039    3.7    78.8    21.2    100.0
223 (A)--V    43.758    1.2    49.6    50.4    100.0
224 (A)--V    44.382   11.4    95.8     4.2    100.0
225 (A)--V    44.631    9.8    85.6    14.4    100.0
226 (A)--V    44.833   11.4    94.8     5.2    100.0
227 (A)--V    45.584    2.4    57.9    42.1    100.0
228 (A)--V    45.664    7.9    54.8    45.2    100.0
229 (A)--V    46.083    9.8    76.2    23.8    100.0
230 (A)--V    46.821    9.3    71.5    28.5    100.0
231 (A)--V    47.560    4.7    71.0    29.0    100.0
232 (A)--V    47.622   12.5    73.1    26.9    100.0
233 (A)--V    48.131   21.9    85.1    14.9    100.0
234 (A)--V    48.286   18.6    84.7    15.3    100.0
235 (A)--V    48.675    4.9    59.1    40.9    100.0
236 (A)--V    49.051    2.0    85.1    14.9    100.0
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237 (A)--V    49.711    1.7    66.9    33.1    100.0
238 (A)--V    50.399   12.0    49.0    51.0    100.0
239 (A)--V    50.972   12.7    69.6    30.4    100.0
240 (A)--V    51.360   17.0    84.3    15.7    100.0
241 (A)--V    51.792   12.7    33.0    67.0    100.0
242 (A)--V    52.194   34.6    75.2    24.8    100.0
243 (A)--V    52.823    7.9    93.8     6.2    100.0
244 (A)--V    52.988    1.2    71.0    29.0    100.0
245 (A)--V    53.107    4.7    81.3    18.7    100.0
246 (A)--V    53.721    0.4    95.5     4.5    100.0
247 (A)--V    54.445    5.1    74.4    25.6    100.0
248 (A)--V    54.471   15.4    74.3    25.7    100.0
249 (A)--V    54.706    6.6    74.8    25.2    100.0
250 (A)--V    55.006    1.9    50.0    50.0    100.0
251 (A)--V    55.401   17.9    83.1    16.9    100.0
252 (A)--V    56.175   35.5    69.1    30.9    100.0
253 (A)--V    56.433   48.5    96.2     3.8    100.0
254 (A)--V    56.501   15.4    71.2    28.8    100.0
255 (A)--V    56.554    5.9    75.2    24.8    100.0
256 (A)--V    56.931   17.4    85.0    15.0    100.0
257 (A)--V    57.613   10.0    91.3     8.7    100.0
258 (A)--V    57.792   16.3    78.5    21.5    100.0
259 (A)--V    58.097    4.8    97.5     2.5    100.0
260 (A)--V    58.136    7.4    98.6     1.4    100.0
261 (A)--V    58.218    7.9    98.4     1.6    100.0
262 (A)--V    58.335   28.3    86.1    13.9    100.0
263 (A)--V    58.389    7.2    93.6     6.4    100.0
264 (A)--V    59.030   16.0    98.1     1.9    100.0
265 (A)--V    59.467    7.4    90.3     9.7    100.0
266 (A)--V    60.970    1.1    59.3    40.7    100.0
267 (A)--V    61.149    6.7    75.2    24.8    100.0
268 (A)--V    61.850    0.4    94.8     5.2    100.0
269 (A)--V    61.903    0.2    95.7     4.3    100.0
270 (A)--V    62.442    1.6    94.4     5.6    100.0
271 (A)--V    64.766    6.7    35.2    64.8    100.0
272 (A)--V    65.695    4.1    35.3    64.7    100.0
273 (A)--V    66.450    3.3    32.4    67.6    100.0
274 (A)--V    67.262   29.4    92.1     7.9    100.0
275 (A)--V    67.469   15.1    68.0    32.0    100.0
276 (A)--V    67.907   10.9    74.0    26.0    100.0
277 (A)--V    68.215   14.5    67.6    32.4    100.0
278 (A)--V    68.382    0.9    12.9    87.1    100.0
279 (A)--V    69.012   16.7    52.4    47.6    100.0
280 (A)--V    70.456    3.1    65.2    34.8    100.0
281 (A)--V    70.845   21.9    71.4    28.6    100.0
282 (A)--V    71.981   29.8    76.5    23.5    100.0
283 (A)--V    72.028   29.3    92.3     7.7    100.0
284 (A)--V    72.766   41.0    78.5    21.5    100.0
285 (A)--V    73.525    9.4    29.3    70.7    100.0
286 (A)--V    73.839   11.3    41.3    58.7    100.0
287 (A)--V    74.128    1.3    61.3    38.7    100.0
288 (A)--V    74.481    3.9    61.1    38.9    100.0
289 (A)--V    74.932    1.6    81.9    18.1    100.0
290 (A)--V    75.184    5.2    66.4    33.6    100.0
291 (A)--V    76.270    1.3    43.2    56.8    100.0
292 (A)--V    77.711    1.2    27.3    72.7    100.0
293 (A)--V    78.740    3.0    27.8    72.2    100.0
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294 (A)--V    79.089     5.4    34.2    65.8    100.0
295 (A)--V    79.436     1.7    38.2    61.8    100.0
296 (A)--V    79.935     4.4    72.9    27.1    100.0
297 (A)--V    80.279    14.6    74.9    25.1    100.0
298 (A)--V    80.861     6.3    82.3    17.7    100.0
299 (A)--V    82.101     8.7    96.7     3.3    100.0
300 (A)--V    82.325    14.6    99.0     1.0    100.0
301 (A)--V    82.501     9.4    95.6     4.4    100.0
302 (A)--V    82.701    11.1    98.8     1.2    100.0
303 (A)--V    83.478    18.7    93.5     6.5    100.0
304 (A)--V    83.891     1.2    14.8    85.2    100.0
305 (A)--V    84.233     0.6    84.8    15.2    100.0
306 (A)--V    84.318     5.7    61.7    38.3    100.0
307 (A)--V    84.801     4.6    97.5     2.5    100.0
308 (A)--V    85.040     0.5    87.7    12.3    100.0
309 (A)--V    85.263     5.9    76.9    23.1    100.0
310 (A)--V    85.416     6.0    45.9    54.1    100.0
311 (A)--V    85.560     0.5    96.8     3.2    100.0
312 (A)--V    85.996     1.9    78.1    21.9    100.0
313 (A)--V    86.860     3.4    84.9    15.1    100.0
314 (A)--V    88.498     0.6    80.5    19.5    100.0
315 (A)--V    88.935     3.9    46.6    53.4    100.0
316 (A)--V    89.794    12.6    72.4    27.6    100.0
317 (A)--V    90.316     2.5    56.1    43.9    100.0
318 (A)--V    90.714     4.9    91.6     8.4    100.0
319 (A)--V    91.154    15.2    91.5     8.5    100.0
320 (A)--V    91.775    18.3    99.3     0.7    100.0
321 (A)--V    94.685     3.5    79.4    20.6    100.0
322 (A)--V    96.283     2.3    95.6     4.4    100.0
323 (A)--V    96.594     5.8    66.3    33.7    100.0
324 (A)--V    97.717     1.1    88.4    11.6    100.0
325 (A)--V    99.184     1.2    96.9     3.1    100.0
326 (A)--V   100.695    13.4    91.1     8.9    100.0
327 (A)--V   101.466     7.8    92.6     7.4    100.0
328 (A)--V   101.733     8.6    71.8    28.2    100.0
329 (A)--V   102.294    52.8    88.1    11.9    100.0
330 (A)--V   102.580    22.8    75.0    25.0    100.0
331 (A)--V   103.171     1.5    28.2    71.8    100.0
332 (A)--V   103.335     3.1    39.9    60.1    100.0
333 (A)--V   104.117     2.7    93.1     6.9    100.0
334 (A)--V   104.659     1.3    69.0    31.0    100.0
335 (A)--V   104.978     5.3    97.7     2.3    100.0
336 (A)--V   105.289     0.9    98.4     1.6    100.0
337 (A)--V   105.407     6.2    88.4    11.6    100.0
338 (A)--V   105.714     3.8    71.9    28.1    100.0
339 (A)--V   106.050     8.4    84.4    15.6    100.0
340 (A)--V   109.257    52.3    87.8    12.2    100.0
341 (A)--V   116.381     7.4    59.1    40.9    100.0
342 (A)--V   120.753     0.5    39.9    60.1    100.0
343 (A)--V   121.083     0.0    98.4     1.6    100.0
344 (A)--V   121.288     1.5    55.0    45.0    100.0
345 (A)--V   121.876     0.8    15.5    84.5    100.0
346 (A)--V   158.211    12.7    98.9     1.1    100.0
347 (A)--V   158.580    19.3    97.8     2.2    100.0
348 (A)--V   166.070    82.6    98.7     1.3    100.0
349 (A)--V   169.189    64.1    93.7     6.3    100.0
350 (A)--V   169.304    78.0    99.5     0.5    100.0
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351 (A)--V    234.516    93.9    99.6    0.4    100.0
352 (A)--V    235.122    88.5    96.2    3.8    100.0
353 (A)--V    250.338    80.2    94.9    5.1    100.0
354 (A)--V    629.850     2.7    24.7   75.3    100.0
355 (A)--V    632.506     9.5    93.1    6.9    100.0
356 (A)--V    635.062     5.9    80.0   20.0    100.0
357 (A)--V    644.027     5.6    99.5    0.5    100.0
358 (A)--V    644.168     5.2    99.5    0.5    100.0
359 (A)--V    644.970     8.5    99.9    0.1    100.0
360 (A)--V    645.630     8.8    95.5    4.5    100.0
361 (A)--V    646.295     2.0    98.8    1.2    100.0
362 (A)--V    646.456     6.6    99.4    0.6    100.0
363 (A)--V    646.928     0.6    98.6    1.4    100.0
364 (A)--V    648.867     1.8    99.9    0.1    100.0
365 (A)--V    651.184     1.2     7.0   93.0    100.0
366 (A)--V    657.172     0.3     5.5   94.5    100.0
367 (A)--V    660.934     0.2     0.8   99.2    100.0
368 (A)--V    760.037    91.3    97.5    2.5    100.0
369 (A)--V    966.144     0.0     0.4   99.6    100.0
370 (A)--V    966.547     0.0     0.8   99.2    100.0
371 (A)--V   4856.133    98.5    99.9    0.1    100.0
372 (A)--V   4856.590    96.8    99.0    1.0    100.0
373 (A)--V   4869.947    91.9    97.9    2.1    100.0
374 (A)--V  12038.935    98.0    99.4    0.6    100.0
```

Full population analysis for complex *cis*-4 (X-ray geometry):

```
**********************************************************************
*                        VMOdes                                      *
* Virtual Molecular Orbital description Program, Revision 7.1        *
* Cite this work as: VMOdes Program, Revision A 7.1                  *
* V. N. Nemykin, P. Basu, 2001, 2003                                *
* Department of Chemistry, Duquesne University, Pittsburgh, PA       *
**********************************************************************

Input Gaussian file:
C:\Documents and Settings\hp\My Documents\Research Dr.
Nemykin\VMOdes\VModes\cis-CN-CN-pop.gjf.out
Output VMOdes file: cis-CN-CN-xray-pop.out


Full point group is:  C1


Number of Basis Functions = 374

    67 Alpha electrons          67 Beta electrons


Group  1  is: Fe
This group consist of  1  subunits. The Basis Functions range is:
 1          56
Group  2  is: Fc
This group consist of  2  subunits. The Basis Functions range is:
 1         236
 348        374
Group  3  is: Lig
This group consist of  1  subunits. The Basis Functions range is:
```

```
 237           347
Group  4  is: Total
This group consist of  1  subunits. The Basis Functions range is:
 1             374

All MO's will be printed.

Molecular Orbitals Indexes, Energies, and Group Contributions


        Orbital                              Group Number
_____    _____

Number Index    Energy,eV     1         2         3         4


 1    (A)--O    -6933.217    100.0     100.0       0.0     100.0
 2    (A)--O     -803.293    100.0     100.0       0.0     100.0
 3    (A)--O     -693.747    100.0     100.0       0.0     100.0
 4    (A)--O     -693.416    100.0     100.0       0.0     100.0
 5    (A)--O     -693.368    100.0     100.0       0.0     100.0
 6    (A)--O     -381.068      0.0       0.0     100.0     100.0
 7    (A)--O     -380.819      0.0       0.0     100.0     100.0
 8    (A)--O     -271.649      0.0       0.1      99.9     100.0
 9    (A)--O     -271.028      0.0       0.0     100.0     100.0
10    (A)--O     -270.937      0.1     100.0       0.0     100.0
11    (A)--O     -270.605      0.0       0.0     100.0     100.0
12    (A)--O     -270.404      0.0       0.0     100.0     100.0
13    (A)--O     -270.382      0.1     100.0       0.0     100.0
14    (A)--O     -270.360      0.1     100.0       0.0     100.0
15    (A)--O     -270.318      0.1     100.0       0.0     100.0
16    (A)--O     -270.297      0.0     100.0       0.0     100.0
17    (A)--O     -270.169      0.1     100.0       0.0     100.0
18    (A)--O     -270.136      0.1     100.0       0.0     100.0
19    (A)--O     -270.122      0.1     100.0       0.0     100.0
20    (A)--O     -270.097      0.1     100.0       0.0     100.0
21    (A)--O     -270.076      0.0     100.0       0.0     100.0
22    (A)--O      -88.637    100.0     100.0       0.0     100.0
23    (A)--O      -57.174     99.9     100.0       0.0     100.0
24    (A)--O      -56.238     99.8     100.0       0.0     100.0
25    (A)--O      -56.147     99.9     100.0       0.0     100.0
26    (A)--O      -23.691      7.4      78.4      21.6     100.0
27    (A)--O      -23.402      2.6      29.0      71.0     100.0
28    (A)--O      -23.120      6.2      72.8      27.2     100.0
29    (A)--O      -23.009      0.1       1.2      98.8     100.0
30    (A)--O      -21.523      1.3      17.1      82.9     100.0
31    (A)--O      -19.035      1.4      71.4      28.6     100.0
32    (A)--O      -18.818      1.9      95.5       4.5     100.0
33    (A)--O      -18.790      1.8      99.8       0.2     100.0
34    (A)--O      -18.642      1.9     100.0       0.0     100.0
35    (A)--O      -17.230      0.6      33.3      66.7     100.0
36    (A)--O      -15.245      0.6      45.3      54.7     100.0
37    (A)--O      -14.538      1.4      94.6       5.4     100.0
38    (A)--O      -14.418      2.2      89.2      10.8     100.0
39    (A)--O      -14.179      0.5      97.4       2.6     100.0
40    (A)--O      -14.149      0.6      88.9      11.1     100.0
41    (A)--O      -13.873      1.7      94.6       5.4     100.0
42    (A)--O      -13.618      1.0      59.1      40.9     100.0
43    (A)--O      -12.198      1.4      26.7      73.3     100.0
44    (A)--O      -11.419     26.3      77.2      22.8     100.0
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45  (A)--O   -10.870    2.7    71.1    28.9    100.0
46  (A)--O   -10.739    1.3    82.0    18.0    100.0
47  (A)--O   -10.672   14.7    81.1    18.9    100.0
48  (A)--O   -10.401    3.6    94.3     5.7    100.0
49  (A)--O   -10.362    2.7    85.4    14.6    100.0
50  (A)--O   -10.232    2.3    98.3     1.7    100.0
51  (A)--O   -10.033    0.8    89.2    10.8    100.0
52  (A)--O    -9.956    0.6    97.7     2.3    100.0
53  (A)--O    -9.829    6.4    84.6    15.4    100.0
54  (A)--O    -9.738    1.6    84.6    15.4    100.0
55  (A)--O    -9.130    0.5     6.0    94.0    100.0
56  (A)--O    -8.909    1.0     7.9    92.1    100.0
57  (A)--O    -8.847    0.3     4.4    95.6    100.0
58  (A)--O    -8.647    0.1     1.1    98.9    100.0
59  (A)--O    -8.528    0.1     1.6    98.4    100.0
60  (A)--O    -8.273   26.5    74.3    25.7    100.0
61  (A)--O    -8.098   42.1    99.4     0.6    100.0
62  (A)--O    -7.609   19.8    65.5    34.5    100.0
63  (A)--O    -6.941   10.0    98.3     1.7    100.0
64  (A)--O    -6.682    8.0    65.1    34.9    100.0
65  (A)--O    -5.299   72.8    95.3     4.7    100.0
66  (A)--O    -5.167   80.6    99.3     0.7    100.0
67  (A)--O    -5.147   73.5    99.5     0.5    100.0
68  (A)--V    -3.353   10.4    22.9    77.1    100.0
69  (A)--V    -2.123   44.7    96.4     3.6    100.0
70  (A)--V    -2.072   42.2    94.3     5.7    100.0
71  (A)--V    -0.748    6.1    36.4    63.6    100.0
72  (A)--V    -0.629   16.3    84.4    15.6    100.0
73  (A)--V    -0.568    4.3    86.1    13.9    100.0
74  (A)--V    -0.403   18.0    95.4     4.6    100.0
75  (A)--V    -0.237   28.7    96.5     3.5    100.0
76  (A)--V    -0.130   46.4    83.0    17.0    100.0
77  (A)--V     0.136   34.7    62.4    37.6    100.0
78  (A)--V     0.719   14.7    60.4    39.6    100.0
79  (A)--V     0.919    4.2    72.6    27.4    100.0
80  (A)--V     1.170   18.8    76.4    23.6    100.0
81  (A)--V     1.523    3.5    53.4    46.6    100.0
82  (A)--V     1.976   16.0    68.4    31.6    100.0
83  (A)--V     2.080    7.1    87.9    12.1    100.0
84  (A)--V     2.326   71.2    94.2     5.8    100.0
85  (A)--V     2.446   67.7    93.5     6.5    100.0
86  (A)--V     2.826   23.1    81.6    18.4    100.0
87  (A)--V     3.019   13.2    74.9    25.1    100.0
88  (A)--V     3.469   16.4    97.3     2.7    100.0
89  (A)--V     3.559   17.4    93.7     6.3    100.0
90  (A)--V     3.617   75.1    99.6     0.4    100.0
91  (A)--V     3.794   40.0    98.3     1.7    100.0
92  (A)--V     3.908   18.3    76.4    23.6    100.0
93  (A)--V     4.305   21.1    95.8     4.2    100.0
94  (A)--V     4.499   25.8    79.6    20.4    100.0
95  (A)--V     4.667   48.3    96.2     3.8    100.0
96  (A)--V     4.752   50.3    96.1     3.9    100.0
97  (A)--V     5.009   25.0    84.9    15.1    100.0
98  (A)--V     5.193   26.7    69.5    30.5    100.0
99  (A)--V     5.369   42.0    96.8     3.2    100.0
100 (A)--V     5.485    4.4    89.8    10.2    100.0
101 (A)--V     5.905   27.4    75.5    24.5    100.0
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102 (A)--V    6.552    18.0    73.8    26.2    100.0
103 (A)--V    6.661     3.4    70.9    29.1    100.0
104 (A)--V    7.042    57.4    94.9     5.1    100.0
105 (A)--V    7.454    63.5    90.7     9.3    100.0
106 (A)--V    7.515    38.5    88.2    11.8    100.0
107 (A)--V    7.759    22.0    85.1    14.9    100.0
108 (A)--V    7.972    26.7    74.8    25.2    100.0
109 (A)--V    8.029    16.8    76.0    24.0    100.0
110 (A)--V    8.103    35.3    82.8    17.2    100.0
111 (A)--V    8.409    34.1    60.9    39.1    100.0
112 (A)--V    8.685    21.7    48.7    51.3    100.0
113 (A)--V    8.924    28.2    62.1    37.9    100.0
114 (A)--V    9.060     8.7    62.3    37.7    100.0
115 (A)--V    9.356     9.9    88.3    11.7    100.0
116 (A)--V    9.600    12.7    78.3    21.7    100.0
117 (A)--V    9.891    18.1    58.8    41.2    100.0
118 (A)--V   10.324     1.2    95.8     4.2    100.0
119 (A)--V   10.786     7.0    53.7    46.3    100.0
120 (A)--V   10.985    16.6    55.8    44.2    100.0
121 (A)--V   11.255    12.6    63.8    36.2    100.0
122 (A)--V   11.406    11.2    61.3    38.7    100.0
123 (A)--V   11.613     4.9    44.0    56.0    100.0
124 (A)--V   11.690     4.6    49.1    50.9    100.0
125 (A)--V   11.990    26.7    74.1    25.9    100.0
126 (A)--V   12.123    14.9    60.0    40.0    100.0
127 (A)--V   12.436    29.6    93.4     6.6    100.0
128 (A)--V   12.523    23.4    94.0     6.0    100.0
129 (A)--V   12.754    21.7    91.5     8.5    100.0
130 (A)--V   12.804     8.5    93.8     6.2    100.0
131 (A)--V   13.041    30.2    83.1    16.9    100.0
132 (A)--V   13.196    18.8    91.2     8.8    100.0
133 (A)--V   13.290    13.1    67.3    32.7    100.0
134 (A)--V   13.582    10.5    95.6     4.4    100.0
135 (A)--V   14.040    15.7    73.3    26.7    100.0
136 (A)--V   14.142    20.3    83.1    16.9    100.0
137 (A)--V   14.263    10.5    62.2    37.8    100.0
138 (A)--V   14.670    26.1    62.5    37.5    100.0
139 (A)--V   14.869     2.9    81.4    18.6    100.0
140 (A)--V   14.983    19.7    82.2    17.8    100.0
141 (A)--V   15.253    14.7    87.7    12.3    100.0
142 (A)--V   15.298    28.4    86.6    13.4    100.0
143 (A)--V   15.375     9.3    75.8    24.2    100.0
144 (A)--V   15.502    57.2    83.1    16.9    100.0
145 (A)--V   15.597    39.9    73.2    26.8    100.0
146 (A)--V   15.798    29.0    95.9     4.1    100.0
147 (A)--V   16.023    17.7    84.3    15.7    100.0
148 (A)--V   16.351    13.4    93.1     6.9    100.0
149 (A)--V   16.492    21.3    88.2    11.8    100.0
150 (A)--V   16.568    34.3    92.1     7.9    100.0
151 (A)--V   16.758    15.9    76.6    23.4    100.0
152 (A)--V   16.903    35.7    86.8    13.2    100.0
153 (A)--V   17.140    14.9    88.2    11.8    100.0
154 (A)--V   17.280    17.1    95.2     4.8    100.0
155 (A)--V   17.443     8.5    92.0     8.0    100.0
156 (A)--V   17.885     9.9    72.1    27.9    100.0
157 (A)--V   18.325     1.3    86.5    13.5    100.0
158 (A)--V   18.413    11.2    90.7     9.3    100.0
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159 (A)--V    18.918    7.4     97.1    2.9     100.0
160 (A)--V    19.032    12.1    90.7    9.3     100.0
161 (A)--V    19.248    2.5     79.2    20.8    100.0
162 (A)--V    19.545    3.0     87.7    12.3    100.0
163 (A)--V    19.638    1.7     85.4    14.6    100.0
164 (A)--V    19.903    2.1     90.3    9.7     100.0
165 (A)--V    20.063    1.7     75.8    24.2    100.0
166 (A)--V    20.160    3.9     73.5    26.5    100.0
167 (A)--V    20.458    4.0     98.3    1.7     100.0
168 (A)--V    20.842    3.3     79.2    20.8    100.0
169 (A)--V    20.866    4.4     67.6    32.4    100.0
170 (A)--V    21.368    10.4    83.3    16.7    100.0
171 (A)--V    21.783    9.3     60.1    39.9    100.0
172 (A)--V    22.127    11.0    50.0    50.0    100.0
173 (A)--V    22.521    27.8    68.3    31.7    100.0
174 (A)--V    22.652    9.3     70.3    29.7    100.0
175 (A)--V    22.910    37.9    90.3    9.7     100.0
176 (A)--V    23.414    12.1    48.4    51.6    100.0
177 (A)--V    24.307    2.2     93.8    6.2     100.0
178 (A)--V    24.469    3.8     48.7    51.3    100.0
179 (A)--V    25.018    1.5     66.6    33.4    100.0
180 (A)--V    25.666    2.4     11.3    88.7    100.0
181 (A)--V    25.688    4.5     77.2    22.8    100.0
182 (A)--V    26.191    2.0     97.2    2.8     100.0
183 (A)--V    26.592    17.4    63.4    36.6    100.0
184 (A)--V    27.304    3.0     65.5    34.5    100.0
185 (A)--V    27.776    4.2     76.3    23.7    100.0
186 (A)--V    27.939    8.8     83.7    16.3    100.0
187 (A)--V    28.824    17.5    92.6    7.4     100.0
188 (A)--V    28.865    7.0     26.1    73.9    100.0
189 (A)--V    29.655    1.0     14.2    85.8    100.0
190 (A)--V    30.121    26.7    96.4    3.6     100.0
191 (A)--V    30.503    23.0    96.1    3.9     100.0
192 (A)--V    30.731    24.1    82.1    17.9    100.0
193 (A)--V    31.070    11.6    78.4    21.6    100.0
194 (A)--V    31.442    6.0     75.3    24.7    100.0
195 (A)--V    31.579    8.2     71.0    29.0    100.0
196 (A)--V    32.218    12.2    72.7    27.3    100.0
197 (A)--V    32.895    1.8     43.6    56.4    100.0
198 (A)--V    33.279    12.8    59.3    40.7    100.0
199 (A)--V    33.508    1.3     17.8    82.2    100.0
200 (A)--V    33.916    2.7     36.1    63.9    100.0
201 (A)--V    34.372    4.2     63.3    36.7    100.0
202 (A)--V    34.622    2.2     63.5    36.5    100.0
203 (A)--V    35.086    12.9    74.1    25.9    100.0
204 (A)--V    35.158    6.4     70.4    29.6    100.0
205 (A)--V    35.616    5.1     46.8    53.2    100.0
206 (A)--V    35.994    4.3     45.9    54.1    100.0
207 (A)--V    36.108    3.6     73.1    26.9    100.0
208 (A)--V    36.659    8.0     32.5    67.5    100.0
209 (A)--V    37.071    1.6     39.8    60.2    100.0
210 (A)--V    37.812    11.4    53.0    47.0    100.0
211 (A)--V    38.212    2.6     43.9    56.1    100.0
212 (A)--V    39.565    7.6     75.4    24.6    100.0
213 (A)--V    40.201    4.8     63.3    36.7    100.0
214 (A)--V    40.524    4.0     35.4    64.6    100.0
215 (A)--V    40.904    10.6    46.0    54.0    100.0
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216 (A)--V    41.048    6.9    56.6    43.4    100.0
217 (A)--V    41.968    9.2    48.8    51.2    100.0
218 (A)--V    42.261    6.1    59.5    40.5    100.0
219 (A)--V    42.487    6.4    72.3    27.7    100.0
220 (A)--V    43.110    5.5    74.2    25.8    100.0
221 (A)--V    43.361    3.0    60.8    39.2    100.0
222 (A)--V    43.465    5.2    67.9    32.1    100.0
223 (A)--V    43.954    5.4    73.9    26.1    100.0
224 (A)--V    44.458    6.4    85.0    15.0    100.0
225 (A)--V    44.719    2.6    69.4    30.6    100.0
226 (A)--V    44.783    3.9    85.0    15.0    100.0
227 (A)--V    45.178    3.6    90.5     9.5    100.0
228 (A)--V    45.714    2.9    71.6    28.4    100.0
229 (A)--V    46.053   10.2    91.5     8.5    100.0
230 (A)--V    46.262   11.2    62.9    37.1    100.0
231 (A)--V    46.598    4.9    81.5    18.5    100.0
232 (A)--V    46.825    3.4    83.5    16.5    100.0
233 (A)--V    47.241   24.7    60.6    39.4    100.0
234 (A)--V    47.403   10.7    83.7    16.3    100.0
235 (A)--V    47.879    0.7    94.8     5.2    100.0
236 (A)--V    48.447    2.0    77.7    22.3    100.0
237 (A)--V    48.743    2.2    71.7    28.3    100.0
238 (A)--V    49.302    2.0    60.4    39.6    100.0
239 (A)--V    50.756    9.6    64.2    35.8    100.0
240 (A)--V    51.648   12.8    56.2    43.8    100.0
241 (A)--V    51.956   61.9    94.1     5.9    100.0
242 (A)--V    52.230   21.4    90.0    10.0    100.0
243 (A)--V    52.441    2.9    95.9     4.1    100.0
244 (A)--V    52.707    5.4    86.1    13.9    100.0
245 (A)--V    53.241    7.5    98.3     1.7    100.0
246 (A)--V    53.478   12.6    94.1     5.9    100.0
247 (A)--V    53.790    0.8    98.5     1.5    100.0
248 (A)--V    54.021   16.8    88.0    12.0    100.0
249 (A)--V    54.491    4.4    89.5    10.5    100.0
250 (A)--V    54.723    8.4    40.1    59.9    100.0
251 (A)--V    54.926   26.2    89.2    10.8    100.0
252 (A)--V    55.253    7.4    86.2    13.8    100.0
253 (A)--V    55.429   48.5    95.4     4.6    100.0
254 (A)--V    56.093   38.3    67.6    32.4    100.0
255 (A)--V    56.533   25.2    99.2     0.8    100.0
256 (A)--V    56.691   18.0    71.4    28.6    100.0
257 (A)--V    56.894    4.0    62.1    37.9    100.0
258 (A)--V    57.210    0.9    90.5     9.5    100.0
259 (A)--V    57.420   25.6    93.0     7.0    100.0
260 (A)--V    57.737    4.7    81.0    19.0    100.0
261 (A)--V    58.040    7.8    86.2    13.8    100.0
262 (A)--V    58.533   11.1    92.4     7.6    100.0
263 (A)--V    59.347    2.3    61.0    39.0    100.0
264 (A)--V    60.204    4.2    78.5    21.5    100.0
265 (A)--V    60.649    8.3    92.7     7.3    100.0
266 (A)--V    60.806   11.4    94.3     5.7    100.0
267 (A)--V    61.583    4.2    64.9    35.1    100.0
268 (A)--V    62.225    3.8    81.6    18.4    100.0
269 (A)--V    62.493   30.1    78.0    22.0    100.0
270 (A)--V    64.207   20.0    97.3     2.7    100.0
271 (A)--V    64.247   26.7    90.3     9.7    100.0
272 (A)--V    64.485   13.7    84.0    16.0    100.0
```

```
273 (A)--V    64.869    5.5    50.1    49.9    100.0
274 (A)--V    65.298   14.6    80.8    19.2    100.0
275 (A)--V    65.381    9.6    69.4    30.6    100.0
276 (A)--V    65.918    2.9    23.2    76.8    100.0
277 (A)--V    66.532    1.5    18.9    81.1    100.0
278 (A)--V    66.770    0.3     5.2    94.8    100.0
279 (A)--V    70.127   15.3    53.6    46.4    100.0
280 (A)--V    70.768    0.8    15.9    84.1    100.0
281 (A)--V    71.039    7.5    58.3    41.7    100.0
282 (A)--V    71.589   39.6    89.4    10.6    100.0
283 (A)--V    71.857   21.4    65.8    34.2    100.0
284 (A)--V    72.973    6.3    31.3    68.7    100.0
285 (A)--V    73.676    1.8    33.6    66.4    100.0
286 (A)--V    73.813   70.7    92.8     7.2    100.0
287 (A)--V    74.122   56.1    80.3    19.7    100.0
288 (A)--V    74.452   10.6    69.7    30.3    100.0
289 (A)--V    74.676    1.8    77.5    22.5    100.0
290 (A)--V    75.511    1.2    38.6    61.4    100.0
291 (A)--V    76.016    4.1    43.1    56.9    100.0
292 (A)--V    76.609   16.1    73.1    26.9    100.0
293 (A)--V    76.968    1.6    80.5    19.5    100.0
294 (A)--V    78.253    2.3    36.6    63.4    100.0
295 (A)--V    78.799    0.8    73.1    26.9    100.0
296 (A)--V    79.262    2.2    78.1    21.9    100.0
297 (A)--V    79.437    2.2    73.2    26.8    100.0
298 (A)--V    79.796    4.1    76.3    23.7    100.0
299 (A)--V    79.984    0.8    80.1    19.9    100.0
300 (A)--V    80.013    1.2    84.6    15.4    100.0
301 (A)--V    80.749    1.3    63.5    36.5    100.0
302 (A)--V    81.432    8.8    58.5    41.5    100.0
303 (A)--V    82.264    2.0    60.3    39.7    100.0
304 (A)--V    83.309   25.6    85.8    14.2    100.0
305 (A)--V    83.421   20.5    55.0    45.0    100.0
306 (A)--V    83.613   26.9    77.1    22.9    100.0
307 (A)--V    83.894   15.8    57.9    42.1    100.0
308 (A)--V    84.231   13.7    59.5    40.5    100.0
309 (A)--V    84.440   12.1    72.7    27.3    100.0
310 (A)--V    84.847   12.4    78.0    22.0    100.0
311 (A)--V    84.878   14.6    55.4    44.6    100.0
312 (A)--V    85.266   13.7    72.1    27.9    100.0
313 (A)--V    85.690   10.8    40.5    59.5    100.0
314 (A)--V    86.749    5.1    58.9    41.1    100.0
315 (A)--V    88.040    7.3    66.0    34.0    100.0
316 (A)--V    88.273   35.9    74.7    25.3    100.0
317 (A)--V    89.384   12.9    96.5     3.5    100.0
318 (A)--V    90.087    4.1    59.6    40.4    100.0
319 (A)--V    90.922   10.0    71.8    28.2    100.0
320 (A)--V    91.543    5.1    74.0    26.0    100.0
321 (A)--V    95.175    2.7    66.1    33.9    100.0
322 (A)--V    96.036    3.0    89.6    10.4    100.0
323 (A)--V    96.567    6.6    73.8    26.2    100.0
324 (A)--V    98.747    2.7    72.2    27.8    100.0
325 (A)--V    99.570   66.1    97.2     2.8    100.0
326 (A)--V   101.818    4.5    98.4     1.6    100.0
327 (A)--V   102.073    7.9    98.0     2.0    100.0
328 (A)--V   102.141    3.2    97.7     2.3    100.0
329 (A)--V   102.657    2.6    33.3    66.7    100.0
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330 (A)--V    103.211     3.3   74.6   25.4   100.0
331 (A)--V    103.325     2.5   73.6   26.4   100.0
332 (A)--V    103.712     2.2   81.0   19.0   100.0
333 (A)--V    104.135     3.4   67.0   33.0   100.0
334 (A)--V    104.613     1.4   85.1   14.9   100.0
335 (A)--V    105.024     7.3   91.8    8.2   100.0
336 (A)--V    105.278    10.8   97.8    2.2   100.0
337 (A)--V    105.933     2.7   41.1   58.9   100.0
338 (A)--V    107.392    50.1   91.5    8.5   100.0
339 (A)--V    108.477     8.9   97.6    2.4   100.0
340 (A)--V    108.789     0.9   98.4    1.6   100.0
341 (A)--V    117.250     3.7   59.1   40.9   100.0
342 (A)--V    120.208     2.7   24.8   75.2   100.0
343 (A)--V    120.530     0.2   81.3   18.7   100.0
344 (A)--V    121.110     0.0   99.8    0.2   100.0
345 (A)--V    121.741     0.2   13.5   86.5   100.0
346 (A)--V    157.511    40.6   81.7   18.3   100.0
347 (A)--V    157.966    23.9   90.7    9.3   100.0
348 (A)--V    166.672    85.2   99.2    0.8   100.0
349 (A)--V    169.209    54.3   95.5    4.5   100.0
350 (A)--V    169.372    48.9   97.2    2.8   100.0
351 (A)--V    235.653    92.5   99.4    0.6   100.0
352 (A)--V    236.521    86.7   95.0    5.0   100.0
353 (A)--V    250.561    91.9   98.0    2.0   100.0
354 (A)--V    629.479     4.0   37.3   62.7   100.0
355 (A)--V    632.605    13.0   93.5    6.5   100.0
356 (A)--V    635.742     6.9   69.6   30.4   100.0
357 (A)--V    644.269     5.0   99.6    0.4   100.0
358 (A)--V    644.444     2.8   97.8    2.2   100.0
359 (A)--V    644.846     8.4   99.0    1.0   100.0
360 (A)--V    645.250     5.8   98.3    1.7   100.0
361 (A)--V    645.481     7.9   99.3    0.7   100.0
362 (A)--V    646.709     0.8   99.7    0.3   100.0
363 (A)--V    648.150     3.2  100.0    0.0   100.0
364 (A)--V    649.376     0.3   99.4    0.6   100.0
365 (A)--V    650.967     0.7    3.9   96.1   100.0
366 (A)--V    656.100     0.3    6.1   93.9   100.0
367 (A)--V    657.453     0.2    2.9   97.1   100.0
368 (A)--V    759.202    96.9   99.4    0.6   100.0
369 (A)--V    966.233     0.0    0.9   99.1   100.0
370 (A)--V    966.852     0.0    0.4   99.6   100.0
371 (A)--V   4857.096    97.8   99.9    0.1   100.0
372 (A)--V   4857.685    96.1   98.7    1.3   100.0
373 (A)--V   4870.185    97.0   99.3    0.7   100.0
374 (A)--V  12038.120    99.3   99.9    0.1   100.0
```

Full population analysis for complex *trans*-3 (X-ray geometry):

```
***********************************************************************
*                       VMOdes                                       *
* Virtual Molecular Orbital description Program, Revision 7.1         *
* Cite this work as: VMOdes Program, Revision A 7.1                   *
* V. N. Nemykin, P. Basu, 2001, 2003                                 *
* Department of Chemistry, Duquesne University, Pittsburgh, PA        *
***********************************************************************
```

```
Input Gaussian file:
C:\Documents and Settings\hp\My Documents\Research Dr.
Nemykin\VMOdes\VModes\trans-I-CN-pop.gjf.out
Output VMOdes file: trans-I-CN-xray-pop.out

Full point group is:  C1


Number of Basis Functions = 349

     64 Alpha electrons          64 Beta electrons

Group  1  is: Fe
This group consist of  1  subunits. The Basis Functions range is:
 1            56
Group  2  is: Fc
This group consist of  2  subunits. The Basis Functions range is:
 1            236
 323          349
Group  3  is: Lig
This group consist of  1  subunits. The Basis Functions range is:
 237          322
Group  4  is: Total
This group consist of  1  subunits. The Basis Functions range is:
 1            349


All MO's will be printed.

Molecular Orbitals Indexes, Energies, and Group Contributions


        Orbital                          Group Number

_____   _____
Number Index   Energy,eV    1        2        3        4

  1   (A)--O   -6932.980   100.0    100.0    0.0      100.0
  2   (A)--O   -803.058    100.0    100.0    0.0      100.0
  3   (A)--O   -693.511    100.0    100.0    0.0      100.0
  4   (A)--O   -693.188    100.0    100.0    0.0      100.0
  5   (A)--O   -693.127    100.0    100.0    0.0      100.0
  6   (A)--O   -380.586    0.0      0.0      100.0    100.0
  7   (A)--O   -271.752    0.0      0.1      99.9     100.0
  8   (A)--O   -270.689    0.1      100.0    0.0      100.0
  9   (A)--O   -270.657    0.0      0.0      100.0    100.0
 10   (A)--O   -270.240    0.0      0.0      100.0    100.0
 11   (A)--O   -270.129    0.1      100.0    0.0      100.0
 12   (A)--O   -270.096    0.1      100.0    0.0      100.0
 13   (A)--O   -270.085    0.0      100.0    0.0      100.0
 14   (A)--O   -270.065    0.1      100.0    0.0      100.0
 15   (A)--O   -270.004    0.1      100.0    0.0      100.0
 16   (A)--O   -269.961    0.1      100.0    0.0      100.0
 17   (A)--O   -269.933    0.1      100.0    0.0      100.0
 18   (A)--O   -269.927    0.1      100.0    0.0      100.0
 19   (A)--O   -269.885    0.1      100.0    0.0      100.0
 20   (A)--O   -88.400     100.0    100.0    0.0      100.0
 21   (A)--O   -56.935     99.9     100.0    0.0      100.0
 22   (A)--O   -56.014     99.9     100.0    0.0      100.0
 23   (A)--O   -55.898     99.9     100.0    0.0      100.0
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24  (A)--O  -23.371   9.1   96.0    4.0   100.0
25  (A)--O  -22.933   6.5   71.7   28.3   100.0
26  (A)--O  -22.772   1.7   20.4   79.6   100.0
27  (A)--O  -21.134   2.4   21.8   78.2   100.0
28  (A)--O  -18.734   1.3   64.1   35.9   100.0
29  (A)--O  -18.621   1.9   99.3    0.7   100.0
30  (A)--O  -18.577   1.8   90.0   10.0   100.0
31  (A)--O  -18.352   1.9  100.0    0.0   100.0
32  (A)--O  -18.034   0.9   28.0   72.0   100.0
33  (A)--O  -15.849   0.6   35.1   64.9   100.0
34  (A)--O  -14.368   0.9   95.6    4.4   100.0
35  (A)--O  -14.229   1.7   35.2   64.8   100.0
36  (A)--O  -14.177   1.6   85.7   14.3   100.0
37  (A)--O  -13.933   0.3   96.0    4.0   100.0
38  (A)--O  -13.911   0.6   95.0    5.0   100.0
39  (A)--O  -13.581   2.5   97.4    2.6   100.0
40  (A)--O  -12.420   1.8   40.2   59.8   100.0
41  (A)--O  -11.269   6.8   53.6   46.4   100.0
42  (A)--O  -10.962  27.1   82.4   17.6   100.0
43  (A)--O  -10.465   1.8   97.2    2.8   100.0
44  (A)--O  -10.436   4.2   92.8    7.2   100.0
45  (A)--O  -10.172   2.0   75.0   25.0   100.0
46  (A)--O  -10.129   3.6   96.6    3.4   100.0
47  (A)--O   -9.995   7.2   78.6   21.4   100.0
48  (A)--O   -9.928   1.9   89.8   10.2   100.0
49  (A)--O   -9.762   0.8   95.1    4.9   100.0
50  (A)--O   -9.591   1.1   97.5    2.5   100.0
51  (A)--O   -9.389   4.3   42.6   57.4   100.0
52  (A)--O   -9.271   2.3   46.2   53.8   100.0
53  (A)--O   -8.478   1.5    5.4   94.6   100.0
54  (A)--O   -8.365  10.0   37.9   62.1   100.0
55  (A)--O   -8.346   1.6    8.8   91.2   100.0
56  (A)--O   -7.785  41.6   97.9    2.1   100.0
57  (A)--O   -7.708  29.2   77.2   22.8   100.0
58  (A)--O   -6.999   0.5   14.0   86.0   100.0
59  (A)--O   -6.874   4.7   50.0   50.0   100.0
60  (A)--O   -6.608  10.0   97.3    2.7   100.0
61  (A)--O   -6.311   5.0   28.8   71.2   100.0
62  (A)--O   -5.061  76.0   95.8    4.2   100.0
63  (A)--O   -4.947  72.4   99.4    0.6   100.0
64  (A)--O   -4.898  79.3   99.1    0.9   100.0
65  (A)--V   -2.815  14.6   31.0   69.0   100.0
66  (A)--V   -2.268   1.4    7.3   92.7   100.0
67  (A)--V   -1.841  39.5   88.8   11.2   100.0
68  (A)--V   -1.765  37.5   86.4   13.6   100.0
69  (A)--V   -0.370   8.9   86.2   13.8   100.0
70  (A)--V   -0.212   2.6   97.7    2.3   100.0
71  (A)--V   -0.159  53.2   92.8    7.2   100.0
72  (A)--V   -0.064  17.2   90.9    9.1   100.0
73  (A)--V   -0.022  29.5   55.6   44.4   100.0
74  (A)--V    0.438  38.3   88.5   11.5   100.0
75  (A)--V    0.850   7.8   48.6   51.4   100.0
76  (A)--V    0.904  22.0   58.3   41.7   100.0
77  (A)--V    1.204  17.6   30.4   69.6   100.0
78  (A)--V    1.406  18.5   83.9   16.1   100.0
79  (A)--V    1.559   1.8   76.7   23.3   100.0
80  (A)--V    1.986  66.0   90.7    9.3   100.0
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81  (A)--V    2.241    4.0    47.8    52.2    100.0
82  (A)--V    2.494   15.9    90.7     9.3    100.0
83  (A)--V    2.665   74.0    97.1     2.9    100.0
84  (A)--V    2.811   15.2    61.0    39.0    100.0
85  (A)--V    2.969   39.4    95.0     5.0    100.0
86  (A)--V    3.610   45.6    79.6    20.4    100.0
87  (A)--V    3.684   10.6    94.6     5.4    100.0
88  (A)--V    3.802    8.3    97.8     2.2    100.0
89  (A)--V    4.013   72.7    98.8     1.2    100.0
90  (A)--V    4.170    9.1    92.8     7.2    100.0
91  (A)--V    4.271   47.5    91.6     8.4    100.0
92  (A)--V    4.462   30.9    89.2    10.8    100.0
93  (A)--V    4.808   12.3    96.6     3.4    100.0
94  (A)--V    5.034   68.1    91.8     8.2    100.0
95  (A)--V    5.147   20.2    87.5    12.5    100.0
96  (A)--V    5.313   42.1    96.3     3.7    100.0
97  (A)--V    5.556   12.0    87.6    12.4    100.0
98  (A)--V    5.756   32.3    97.5     2.5    100.0
99  (A)--V    6.088    2.7    89.5    10.5    100.0
100 (A)--V    6.380    4.5    69.0    31.0    100.0
101 (A)--V    7.118   68.5    96.5     3.5    100.0
102 (A)--V    7.353    5.6    71.3    28.7    100.0
103 (A)--V    7.408   33.3    54.3    45.7    100.0
104 (A)--V    7.710   31.9    86.2    13.8    100.0
105 (A)--V    7.875   47.7    93.5     6.5    100.0
106 (A)--V    8.034   58.1    79.6    20.4    100.0
107 (A)--V    8.146   20.8    90.2     9.8    100.0
108 (A)--V    8.450   38.3    97.2     2.8    100.0
109 (A)--V    8.860   42.3    93.9     6.1    100.0
110 (A)--V    9.182   18.0    75.2    24.8    100.0
111 (A)--V    9.273   10.7    79.0    21.0    100.0
112 (A)--V    9.446   21.7    82.0    18.0    100.0
113 (A)--V    9.633   23.1    72.8    27.2    100.0
114 (A)--V   10.033   14.8    51.7    48.3    100.0
115 (A)--V   10.402    1.4    91.4     8.6    100.0
116 (A)--V   10.650   16.5    76.9    23.1    100.0
117 (A)--V   10.867    2.6    57.8    42.2    100.0
118 (A)--V   11.276    7.3    49.1    50.9    100.0
119 (A)--V   11.457   25.5    84.0    16.0    100.0
120 (A)--V   11.689   15.2    74.4    25.6    100.0
121 (A)--V   11.824   24.8    81.9    18.1    100.0
122 (A)--V   12.150   16.0    78.3    21.7    100.0
123 (A)--V   12.480   13.2    82.5    17.5    100.0
124 (A)--V   12.525   14.4    72.3    27.7    100.0
125 (A)--V   12.592   26.8    91.4     8.6    100.0
126 (A)--V   12.721   17.6    95.2     4.8    100.0
127 (A)--V   13.076   27.3    95.9     4.1    100.0
128 (A)--V   13.188   23.6    87.9    12.1    100.0
129 (A)--V   13.499   12.7    80.6    19.4    100.0
130 (A)--V   13.811   12.7    95.5     4.5    100.0
131 (A)--V   13.986   31.3    81.8    18.2    100.0
132 (A)--V   14.351   18.4    89.9    10.1    100.0
133 (A)--V   14.655    8.4    77.6    22.4    100.0
134 (A)--V   14.793   13.3    85.5    14.5    100.0
135 (A)--V   14.883    2.5    90.6     9.4    100.0
136 (A)--V   14.907   36.2    93.9     6.1    100.0
137 (A)--V   15.225    8.4    69.9    30.1    100.0
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138 (A)--V    15.548    29.9    92.1     7.9    100.0
139 (A)--V    15.605    26.2    90.8     9.2    100.0
140 (A)--V    15.750    10.4    75.3    24.7    100.0
141 (A)--V    15.826    61.4    97.1     2.9    100.0
142 (A)--V    16.058    12.5    85.9    14.1    100.0
143 (A)--V    16.233    13.1    89.4    10.6    100.0
144 (A)--V    16.366    14.9    75.6    24.4    100.0
145 (A)--V    16.551    33.0    78.5    21.5    100.0
146 (A)--V    16.716    17.6    92.4     7.6    100.0
147 (A)--V    16.910    40.1    96.9     3.1    100.0
148 (A)--V    16.965    16.2    83.5    16.5    100.0
149 (A)--V    17.340    24.2    81.0    19.0    100.0
150 (A)--V    17.545     6.5    84.5    15.5    100.0
151 (A)--V    17.711    13.5    49.1    50.9    100.0
152 (A)--V    17.942    10.0    82.9    17.1    100.0
153 (A)--V    18.486     5.5    94.9     5.1    100.0
154 (A)--V    18.579     3.1    86.6    13.4    100.0
155 (A)--V    19.065     5.7    92.9     7.1    100.0
156 (A)--V    19.256     2.8    91.8     8.2    100.0
157 (A)--V    19.416    13.6    95.0     5.0    100.0
158 (A)--V    19.510     6.0    88.9    11.1    100.0
159 (A)--V    19.887     0.9    93.1     6.9    100.0
160 (A)--V    20.432     0.7    51.4    48.6    100.0
161 (A)--V    20.484     6.1    90.7     9.3    100.0
162 (A)--V    20.901     3.3    89.4    10.6    100.0
163 (A)--V    21.153     6.7    80.0    20.0    100.0
164 (A)--V    21.694     3.9    85.6    14.4    100.0
165 (A)--V    21.946    10.2    79.2    20.8    100.0
166 (A)--V    22.117    17.5    84.9    15.1    100.0
167 (A)--V    22.309    18.6    94.5     5.5    100.0
168 (A)--V    22.913     2.2    92.2     7.8    100.0
169 (A)--V    23.032    34.9    89.8    10.2    100.0
170 (A)--V    23.359    42.9    77.8    22.2    100.0
171 (A)--V    23.979    13.5    83.5    16.5    100.0
172 (A)--V    24.971     5.2    40.1    59.9    100.0
173 (A)--V    25.616     5.8    64.5    35.5    100.0
174 (A)--V    26.211     1.7    91.1     8.9    100.0
175 (A)--V    26.373     0.9    99.2     0.8    100.0
176 (A)--V    26.890     2.9    89.4    10.6    100.0
177 (A)--V    27.059    20.1    94.7     5.3    100.0
178 (A)--V    28.154    25.8    93.1     6.9    100.0
179 (A)--V    28.722     6.3    82.4    17.6    100.0
180 (A)--V    29.115    19.9    82.2    17.8    100.0
181 (A)--V    29.888    24.8    80.6    19.4    100.0
182 (A)--V    30.238    25.5    99.4     0.6    100.0
183 (A)--V    30.547    22.9    99.2     0.8    100.0
184 (A)--V    30.819     6.5    73.9    26.1    100.0
185 (A)--V    31.144    23.7    96.1     3.9    100.0
186 (A)--V    31.559     5.7    94.8     5.2    100.0
187 (A)--V    32.377    30.2    95.0     5.0    100.0
188 (A)--V    32.890     2.9    70.3    29.7    100.0
189 (A)--V    33.065    18.4    78.1    21.9    100.0
190 (A)--V    33.517     2.5    45.5    54.5    100.0
191 (A)--V    33.960     7.1    74.8    25.2    100.0
192 (A)--V    34.151     2.1    54.0    46.0    100.0
193 (A)--V    34.566     5.9    48.5    51.5    100.0
194 (A)--V    35.211     2.8    43.5    56.5    100.0
```

```
195 (A)--V    35.548    22.6    80.5    19.5    100.0
196 (A)--V    35.790    20.8    92.3     7.7    100.0
197 (A)--V    35.942     7.9    63.2    36.8    100.0
198 (A)--V    36.787    15.2    76.4    23.6    100.0
199 (A)--V    38.127     7.3    57.0    43.0    100.0
200 (A)--V    38.647    10.2    82.1    17.9    100.0
201 (A)--V    38.990    12.1    80.7    19.3    100.0
202 (A)--V    39.131     5.2    56.1    43.9    100.0
203 (A)--V    40.284     4.5    78.5    21.5    100.0
204 (A)--V    41.067     9.7    53.0    47.0    100.0
205 (A)--V    41.168    18.5    61.1    38.9    100.0
206 (A)--V    41.330     3.1    50.3    49.7    100.0
207 (A)--V    42.008     7.4    69.7    30.3    100.0
208 (A)--V    42.110    14.1    97.7     2.3    100.0
209 (A)--V    42.918     3.3    46.4    53.6    100.0
210 (A)--V    43.635     8.9    84.8    15.2    100.0
211 (A)--V    43.684     7.5    94.5     5.5    100.0
212 (A)--V    43.963     8.1    88.7    11.3    100.0
213 (A)--V    44.385     7.2    65.0    35.0    100.0
214 (A)--V    44.651     2.9    87.2    12.8    100.0
215 (A)--V    45.710     2.3    95.6     4.4    100.0
216 (A)--V    45.890     8.1    91.3     8.7    100.0
217 (A)--V    46.083     5.0    87.0    13.0    100.0
218 (A)--V    46.339     2.0    58.9    41.1    100.0
219 (A)--V    46.862    10.3    60.6    39.4    100.0
220 (A)--V    47.088     2.7    70.5    29.5    100.0
221 (A)--V    47.187     3.7    46.3    53.7    100.0
222 (A)--V    47.615    53.4    95.2     4.8    100.0
223 (A)--V    47.960     8.4    83.8    16.2    100.0
224 (A)--V    48.061     4.0    69.2    30.8    100.0
225 (A)--V    48.312     3.3    52.7    47.3    100.0
226 (A)--V    48.745     7.1    83.7    16.3    100.0
227 (A)--V    48.985     6.9    89.4    10.6    100.0
228 (A)--V    49.540     5.3    66.2    33.8    100.0
229 (A)--V    52.152    30.3    78.6    21.4    100.0
230 (A)--V    52.459    62.3    91.3     8.7    100.0
231 (A)--V    52.504    37.4    88.6    11.4    100.0
232 (A)--V    52.755     0.4    99.2     0.8    100.0
233 (A)--V    53.206     0.8    98.6     1.4    100.0
234 (A)--V    53.995    18.9    90.1     9.9    100.0
235 (A)--V    54.162     0.9    98.8     1.2    100.0
236 (A)--V    54.760    13.0    62.3    37.7    100.0
237 (A)--V    54.966     9.9    94.1     5.9    100.0
238 (A)--V    55.271    44.7    92.8     7.2    100.0
239 (A)--V    55.419    38.5    97.8     2.2    100.0
240 (A)--V    56.290     4.7    91.4     8.6    100.0
241 (A)--V    56.322    41.7    81.8    18.2    100.0
242 (A)--V    56.532    15.6    89.4    10.6    100.0
243 (A)--V    56.719    11.6    87.4    12.6    100.0
244 (A)--V    57.247     6.1    97.5     2.5    100.0
245 (A)--V    57.519    24.3    87.7    12.3    100.0
246 (A)--V    57.730     8.0    97.8     2.2    100.0
247 (A)--V    57.991    15.2    68.1    31.9    100.0
248 (A)--V    58.108     9.2    80.6    19.4    100.0
249 (A)--V    58.971     3.1    65.7    34.3    100.0
250 (A)--V    60.202     3.3    68.2    31.8    100.0
251 (A)--V    60.527     8.5    98.6     1.4    100.0
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252 (A)--V    60.911    22.6    98.6    1.4    100.0
253 (A)--V    62.035     9.9    77.6   22.4    100.0
254 (A)--V    62.472     5.8    55.8   44.2    100.0
255 (A)--V    62.593    16.8    86.7   13.3    100.0
256 (A)--V    64.037     8.4    35.8   64.2    100.0
257 (A)--V    64.393    28.9    81.4   18.6    100.0
258 (A)--V    64.589    16.1    84.0   16.0    100.0
259 (A)--V    65.100     4.3    39.0   61.0    100.0
260 (A)--V    65.574    15.2    68.9   31.1    100.0
261 (A)--V    65.713    10.4    82.7   17.3    100.0
262 (A)--V    67.165     2.7    29.0   71.0    100.0
263 (A)--V    67.864     0.9    16.9   83.1    100.0
264 (A)--V    68.214     5.6    57.8   42.2    100.0
265 (A)--V    71.160    21.8    83.5   16.5    100.0
266 (A)--V    71.532    13.1    94.1    5.9    100.0
267 (A)--V    71.864    45.0    92.3    7.7    100.0
268 (A)--V    72.571    15.9    57.4   42.6    100.0
269 (A)--V    73.714    65.6    84.2   15.8    100.0
270 (A)--V    73.932    29.1    44.4   55.6    100.0
271 (A)--V    74.498    17.7    82.8   17.2    100.0
272 (A)--V    74.701    43.8    86.5   13.5    100.0
273 (A)--V    75.029     1.3    61.4   38.6    100.0
274 (A)--V    76.235     3.3    33.6   66.4    100.0
275 (A)--V    77.728     6.9    34.0   66.0    100.0
276 (A)--V    78.099     5.8    92.8    7.2    100.0
277 (A)--V    78.474     2.4    46.4   53.6    100.0
278 (A)--V    79.266     4.2    49.8   50.2    100.0
279 (A)--V    79.295     1.1    97.1    2.9    100.0
280 (A)--V    79.698     1.6    86.5   13.5    100.0
281 (A)--V    79.940     2.0    96.1    3.9    100.0
282 (A)--V    80.761     1.5    85.4   14.6    100.0
283 (A)--V    81.547     1.7    26.7   73.3    100.0
284 (A)--V    82.076    15.2    95.5    4.5    100.0
285 (A)--V    83.072    14.3    71.9   28.1    100.0
286 (A)--V    83.527    38.2    96.1    3.9    100.0
287 (A)--V    83.546    33.9    97.0    3.0    100.0
288 (A)--V    84.028    29.0    96.8    3.2    100.0
289 (A)--V    84.103    14.6    84.2   15.8    100.0
290 (A)--V    84.343    27.8    97.6    2.4    100.0
291 (A)--V    84.704    11.0    60.9   39.1    100.0
292 (A)--V    84.969    14.9    86.4   13.6    100.0
293 (A)--V    85.467     4.8    78.9   21.1    100.0
294 (A)--V    87.611     6.5    63.2   36.8    100.0
295 (A)--V    88.281    37.7    81.5   18.5    100.0
296 (A)--V    88.787    23.8    77.2   22.8    100.0
297 (A)--V    89.358    11.0    94.8    5.2    100.0
298 (A)--V    90.474    10.7    67.3   32.7    100.0
299 (A)--V    90.967     8.3    67.8   32.2    100.0
300 (A)--V    91.857     5.7    76.4   23.6    100.0
301 (A)--V    94.761     4.7    71.0   29.0    100.0
302 (A)--V    96.157     2.0    98.4    1.6    100.0
303 (A)--V    96.761    11.4    85.8   14.2    100.0
304 (A)--V    99.645    59.9    97.8    2.2    100.0
305 (A)--V   100.495     7.8    75.3   24.7    100.0
306 (A)--V   102.053     8.5    97.5    2.5    100.0
307 (A)--V   102.238     2.6    99.4    0.6    100.0
308 (A)--V   102.353     4.9    99.4    0.6    100.0
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309 (A)--V    103.228    4.2    50.6    49.4    100.0
310 (A)--V    103.540    4.1    90.3     9.7    100.0
311 (A)--V    104.209    1.7    38.7    61.3    100.0
312 (A)--V    104.653    0.9    99.6     0.4    100.0
313 (A)--V    105.268    9.8    97.0     3.0    100.0
314 (A)--V    105.432    9.8    97.1     2.9    100.0
315 (A)--V    107.090   64.7    95.2     4.8    100.0
316 (A)--V    108.365    5.6    99.3     0.7    100.0
317 (A)--V    109.111    0.4    99.9     0.1    100.0
318 (A)--V    116.782    6.1    54.4    45.6    100.0
319 (A)--V    120.645    0.5    67.9    32.1    100.0
320 (A)--V    121.031    0.0   100.0     0.0    100.0
321 (A)--V    121.191    0.8    42.3    57.7    100.0
322 (A)--V    157.651   46.2    91.3     8.7    100.0
323 (A)--V    157.919   26.2    95.3     4.7    100.0
324 (A)--V    166.774   85.3    99.1     0.9    100.0
325 (A)--V    169.417   53.3    98.9     1.1    100.0
326 (A)--V    169.672   54.8    98.4     1.6    100.0
327 (A)--V    235.784   93.4    99.9     0.1    100.0
328 (A)--V    236.430   86.7    96.7     3.3    100.0
329 (A)--V    250.644   91.6    97.7     2.3    100.0
330 (A)--V    374.836    9.5    44.9    55.1    100.0
331 (A)--V    628.825    4.2    33.6    66.4    100.0
332 (A)--V    632.696   12.4    93.1     6.9    100.0
333 (A)--V    635.589    8.2    77.3    22.7    100.0
334 (A)--V    643.245    6.4    99.8     0.2    100.0
335 (A)--V    644.681    7.6    98.0     2.0    100.0
336 (A)--V    644.901    6.0    99.7     0.3    100.0
337 (A)--V    645.686    1.7    98.8     1.2    100.0
338 (A)--V    646.265    5.8    99.6     0.4    100.0
339 (A)--V    646.478    5.1    99.9     0.1    100.0
340 (A)--V    647.760    1.7   100.0     0.0    100.0
341 (A)--V    648.989    1.5    99.9     0.1    100.0
342 (A)--V    649.598    1.5     7.3    92.7    100.0
343 (A)--V    656.288    0.3     2.5    97.5    100.0
344 (A)--V    759.325   96.9    99.6     0.4    100.0
345 (A)--V    966.516    0.0     0.4    99.6    100.0
346 (A)--V   4857.272   98.0    99.9     0.1    100.0
347 (A)--V   4857.799   96.4    99.2     0.8    100.0
348 (A)--V   4870.350   96.9    99.2     0.8    100.0
349 (A)--V  12038.239   99.3    99.9     0.1    100.0
```

Full population analysis for complex *cis*-3 (X-ray geometry):

```
**********************************************************************
*                          VMOdes                                    *
* Virtual Molecular Orbital description Program, Revision 7.1         *
* Cite this work as: VMOdes Program, Revision A 7.1                   *
* V. N. Nemykin, P. Basu, 2001, 2003                                 *
* Department of Chemistry, Duquesne University, Pittsburgh, PA        *
**********************************************************************


Input Gaussian file:
C:\Documents and Settings\hp\My Documents\Research Dr.
Nemykin\VMOdes\VModes\cis-I-CN-pop.gjf.out
```

```
Output VMOdes file: cis-I-CN-xray-pop.out

Full point group is:  C1


Number of Basis Functions = 349

    64 Alpha electrons          64 Beta electrons

Group  1  is: Fe
This group consist of  1  subunits. The Basis Functions range is:
 1           56
Group  2  is: Fc
This group consist of  2  subunits. The Basis Functions range is:
 1           236
 320          346
Group  3  is: Lig
This group consist of  2  subunits. The Basis Functions range is:
 237          319
 347          349
Group  4  is: Total
This group consist of  1  subunits. The Basis Functions range is:
 1           349


All MO's will be printed.

Molecular Orbitals Indexes, Energies, and Group Contributions


        Orbital                        Group Number
_____    _____
Number Index   Energy,eV   1        2        3        4

  1  (A)--O   -6933.040  100.0    100.0    0.0      100.0
  2  (A)--O    -803.108  100.0    100.0    0.0      100.0
  3  (A)--O    -693.570  100.0    100.0    0.0      100.0
  4  (A)--O    -693.228  100.0    100.0    0.0      100.0
  5  (A)--O    -693.182  100.0    100.0    0.0      100.0
  6  (A)--O    -380.416    0.0      0.0    100.0    100.0
  7  (A)--O    -271.615    0.0      0.1     99.9    100.0
  8  (A)--O    -270.734    0.1    100.0    0.0      100.0
  9  (A)--O    -270.591    0.0      0.0    100.0    100.0
 10  (A)--O    -270.236    0.1    100.0    0.0      100.0
 11  (A)--O    -270.196    0.1    100.0    0.0      100.0
 12  (A)--O    -270.183    0.1    100.0    0.0      100.0
 13  (A)--O    -270.176    0.0    100.0    0.0      100.0
 14  (A)--O    -270.056    0.0      0.0    100.0    100.0
 15  (A)--O    -269.991    0.1    100.0    0.0      100.0
 16  (A)--O    -269.967    0.1    100.0    0.0      100.0
 17  (A)--O    -269.954    0.0    100.0    0.0      100.0
 18  (A)--O    -269.934    0.1    100.0    0.0      100.0
 19  (A)--O    -269.898    0.1    100.0    0.0      100.0
 20  (A)--O     -88.447  100.0    100.0    0.0      100.0
 21  (A)--O     -56.991   99.9    100.0    0.0      100.0
 22  (A)--O     -56.039   99.9    100.0    0.0      100.0
 23  (A)--O     -55.953   99.9    100.0    0.0      100.0
 24  (A)--O     -23.487    8.8     98.6    1.4      100.0
 25  (A)--O     -23.000    7.7     85.3    14.7     100.0
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26   (A)--O   -22.812   0.6    7.7    92.3   100.0
27   (A)--O   -21.124   2.5    23.3   76.7   100.0
28   (A)--O   -18.774   1.6    75.8   24.2   100.0
29   (A)--O   -18.649   1.8    99.9   0.1    100.0
30   (A)--O   -18.552   1.7    89.0   11.0   100.0
31   (A)--O   -18.522   2.0    97.6   2.4    100.0
32   (A)--O   -17.986   1.0    18.0   82.0   100.0
33   (A)--O   -16.010   0.7    39.2   60.8   100.0
34   (A)--O   -14.409   0.9    91.8   8.2    100.0
35   (A)--O   -14.306   2.5    98.2   1.8    100.0
36   (A)--O   -14.122   1.3    97.6   2.4    100.0
37   (A)--O   -13.940   0.2    96.9   3.1    100.0
38   (A)--O   -13.761   1.4    93.3   6.7    100.0
39   (A)--O   -13.419   1.4    42.0   58.0   100.0
40   (A)--O   -12.805   0.7    20.8   79.2   100.0
41   (A)--O   -11.369   14.7   68.3   31.7   100.0
42   (A)--O   -10.935   19.5   74.7   25.3   100.0
43   (A)--O   -10.595   2.0    96.1   3.9    100.0
44   (A)--O   -10.446   4.7    95.8   4.2    100.0
45   (A)--O   -10.253   2.1    91.9   8.1    100.0
46   (A)--O   -10.149   2.8    92.9   7.1    100.0
47   (A)--O   -10.108   4.0    78.8   21.2   100.0
48   (A)--O   -9.997    2.9    82.1   17.9   100.0
49   (A)--O   -9.829    0.9    95.7   4.3    100.0
50   (A)--O   -9.696    0.6    98.2   1.8    100.0
51   (A)--O   -9.425    5.9    41.6   58.4   100.0
52   (A)--O   -9.197    2.1    43.9   56.1   100.0
53   (A)--O   -8.389    6.0    22.2   77.8   100.0
54   (A)--O   -8.377    7.4    24.9   75.1   100.0
55   (A)--O   -8.352    0.3    2.9    97.1   100.0
56   (A)--O   -7.887    41.8   99.2   0.8    100.0
57   (A)--O   -7.663    27.6   75.3   24.7   100.0
58   (A)--O   -6.863    5.0    47.6   52.4   100.0
59   (A)--O   -6.809    1.8    25.6   74.4   100.0
60   (A)--O   -6.744    7.8    75.6   24.4   100.0
61   (A)--O   -6.280    6.9    31.3   68.7   100.0
62   (A)--O   -5.093    74.9   95.3   4.7    100.0
63   (A)--O   -4.982    77.2   98.9   1.1    100.0
64   (A)--O   -4.945    72.9   99.4   0.6    100.0
65   (A)--V   -2.763    16.7   36.4   63.6   100.0
66   (A)--V   -2.068    11.5   27.9   72.1   100.0
67   (A)--V   -1.871    13.8   30.9   69.1   100.0
68   (A)--V   -1.849    32.9   86.0   14.0   100.0
69   (A)--V   -0.449    4.2    86.3   13.7   100.0
70   (A)--V   -0.268    52.3   95.7   4.3    100.0
71   (A)--V   -0.151    30.7   96.6   3.4    100.0
72   (A)--V   -0.072    2.6    96.9   3.1    100.0
73   (A)--V   0.010     17.5   38.3   61.7   100.0
74   (A)--V   0.422     45.6   89.2   10.8   100.0
75   (A)--V   0.818     3.3    74.5   25.5   100.0
76   (A)--V   1.246     47.7   84.0   16.0   100.0
77   (A)--V   1.322     51.8   69.1   30.9   100.0
78   (A)--V   1.395     7.6    66.2   33.8   100.0
79   (A)--V   1.602     2.9    78.3   21.7   100.0
80   (A)--V   2.000     35.9   73.2   26.8   100.0
81   (A)--V   2.196     16.8   46.8   53.2   100.0
82   (A)--V   2.455     55.3   94.8   5.2    100.0
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 83  (A)--V    2.571    61.8    95.2     4.8    100.0
 84  (A)--V    2.687    33.5    77.0    23.0    100.0
 85  (A)--V    2.954    52.0    97.8     2.2    100.0
 86  (A)--V    3.579     3.7    87.7    12.3    100.0
 87  (A)--V    3.656     1.3    92.6     7.4    100.0
 88  (A)--V    3.687    30.0    94.0     6.0    100.0
 89  (A)--V    3.894    67.2    97.8     2.2    100.0
 90  (A)--V    4.027    65.0    94.3     5.7    100.0
 91  (A)--V    4.233    29.8    88.9    11.1    100.0
 92  (A)--V    4.493    20.7    81.8    18.2    100.0
 93  (A)--V    4.838    21.1    96.0     4.0    100.0
 94  (A)--V    4.928    65.1    94.9     5.1    100.0
 95  (A)--V    5.029    32.6    97.2     2.8    100.0
 96  (A)--V    5.176    51.9    97.7     2.3    100.0
 97  (A)--V    5.413    37.0    88.9    11.1    100.0
 98  (A)--V    5.658     9.8    78.3    21.7    100.0
 99  (A)--V    6.077     2.2    79.3    20.7    100.0
100  (A)--V    6.372     6.8    82.6    17.4    100.0
101  (A)--V    6.814    44.8    77.9    22.1    100.0
102  (A)--V    7.160    57.6    85.4    14.6    100.0
103  (A)--V    7.503     7.3    74.1    25.9    100.0
104  (A)--V    7.687    54.5    95.8     4.2    100.0
105  (A)--V    7.877    34.5    85.0    15.0    100.0
106  (A)--V    7.940    28.2    92.3     7.7    100.0
107  (A)--V    8.209    26.6    81.6    18.4    100.0
108  (A)--V    8.414    36.7    88.7    11.3    100.0
109  (A)--V    8.771    11.6    41.4    58.6    100.0
110  (A)--V    9.149    20.1    76.1    23.9    100.0
111  (A)--V    9.182    19.8    76.0    24.0    100.0
112  (A)--V    9.289    39.4    70.4    29.6    100.0
113  (A)--V    9.425    11.8    91.4     8.6    100.0
114  (A)--V   10.021    10.5    49.6    50.4    100.0
115  (A)--V   10.533     0.8    87.8    12.2    100.0
116  (A)--V   10.678     8.3    58.3    41.7    100.0
117  (A)--V   10.931    12.5    64.7    35.3    100.0
118  (A)--V   11.398     7.9    66.3    33.7    100.0
119  (A)--V   11.488     5.9    45.4    54.6    100.0
120  (A)--V   11.700    19.2    92.9     7.1    100.0
121  (A)--V   11.777    22.2    86.8    13.2    100.0
122  (A)--V   12.015    19.9    62.7    37.3    100.0
123  (A)--V   12.235    23.2    86.0    14.0    100.0
124  (A)--V   12.647    36.1    93.7     6.3    100.0
125  (A)--V   12.782    22.2    94.3     5.7    100.0
126  (A)--V   12.809    23.5    81.6    18.4    100.0
127  (A)--V   12.954    28.3    97.8     2.2    100.0
128  (A)--V   13.185     6.2    93.8     6.2    100.0
129  (A)--V   13.335    11.2    76.0    24.0    100.0
130  (A)--V   13.413    15.0    93.4     6.6    100.0
131  (A)--V   13.730    26.8    88.7    11.3    100.0
132  (A)--V   14.027     7.5    90.7     9.3    100.0
133  (A)--V   14.364    23.1    86.6    13.4    100.0
134  (A)--V   14.408    13.1    86.1    13.9    100.0
135  (A)--V   14.829     4.7    90.2     9.8    100.0
136  (A)--V   14.984    23.1    89.7    10.3    100.0
137  (A)--V   15.081    21.7    92.2     7.8    100.0
138  (A)--V   15.297    11.7    80.5    19.5    100.0
139  (A)--V   15.543    33.4    97.4     2.6    100.0
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140 (A)--V    15.677    28.8    93.3     6.7   100.0
141 (A)--V    15.769    11.6    95.1     4.9   100.0
142 (A)--V    16.014    43.2    96.9     3.1   100.0
143 (A)--V    16.128    59.9    89.5    10.5   100.0
144 (A)--V    16.211    40.6    91.5     8.5   100.0
145 (A)--V    16.345     5.8    92.3     7.7   100.0
146 (A)--V    16.585    35.3    77.1    22.9   100.0
147 (A)--V    16.784    21.4    90.5     9.5   100.0
148 (A)--V    17.006     9.0    79.3    20.7   100.0
149 (A)--V    17.179    14.0    94.4     5.6   100.0
150 (A)--V    17.514     3.8    80.2    19.8   100.0
151 (A)--V    17.652    15.3    98.3     1.7   100.0
152 (A)--V    17.859    12.2    65.6    34.4   100.0
153 (A)--V    18.558     2.7    91.1     8.9   100.0
154 (A)--V    18.904    10.6    90.8     9.2   100.0
155 (A)--V    19.139    11.6    97.5     2.5   100.0
156 (A)--V    19.255     7.9    96.3     3.7   100.0
157 (A)--V    19.555     4.7    98.5     1.5   100.0
158 (A)--V    19.721     1.7    97.2     2.8   100.0
159 (A)--V    19.980     4.2    81.0    19.0   100.0
160 (A)--V    20.177     3.8    76.5    23.5   100.0
161 (A)--V    20.333     3.6    68.9    31.1   100.0
162 (A)--V    20.805     1.8    87.4    12.6   100.0
163 (A)--V    21.514    10.5    67.1    32.9   100.0
164 (A)--V    21.791     8.0    73.9    26.1   100.0
165 (A)--V    22.100    11.3    67.6    32.4   100.0
166 (A)--V    22.252    13.4    88.0    12.0   100.0
167 (A)--V    22.832    36.7    81.4    18.6   100.0
168 (A)--V    23.139    34.0    87.8    12.2   100.0
169 (A)--V    23.598     8.1    97.8     2.2   100.0
170 (A)--V    23.948     7.9    98.0     2.0   100.0
171 (A)--V    24.644     4.3    52.8    47.2   100.0
172 (A)--V    25.034     4.4    54.6    45.4   100.0
173 (A)--V    25.725     2.3    77.9    22.1   100.0
174 (A)--V    26.031     6.1    94.3     5.7   100.0
175 (A)--V    26.499     1.0    90.1     9.9   100.0
176 (A)--V    26.894    23.1    92.3     7.7   100.0
177 (A)--V    27.063     5.2    86.3    13.7   100.0
178 (A)--V    28.238     6.7    82.6    17.4   100.0
179 (A)--V    28.510    16.1    84.8    15.2   100.0
180 (A)--V    29.188    19.8    98.5     1.5   100.0
181 (A)--V    29.535    18.5    81.4    18.6   100.0
182 (A)--V    29.938    25.7    96.8     3.2   100.0
183 (A)--V    30.650    19.2    94.6     5.4   100.0
184 (A)--V    30.854    19.6    74.3    25.7   100.0
185 (A)--V    31.349    14.6    85.2    14.8   100.0
186 (A)--V    31.485     9.6    93.5     6.5   100.0
187 (A)--V    31.986     3.7    83.3    16.7   100.0
188 (A)--V    32.404    12.0    82.7    17.3   100.0
189 (A)--V    32.711    19.5    54.2    45.8   100.0
190 (A)--V    33.355     5.5    87.8    12.2   100.0
191 (A)--V    33.663     4.8    84.7    15.3   100.0
192 (A)--V    34.453     1.4    17.8    82.2   100.0
193 (A)--V    34.686     3.3    40.2    59.8   100.0
194 (A)--V    35.406    12.3    62.7    37.3   100.0
195 (A)--V    35.542    26.9    92.0     8.0   100.0
196 (A)--V    35.864    17.2    95.4     4.6   100.0
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197 (A)--V    36.066    1.8    58.9    41.1    100.0
198 (A)--V    37.153    6.2    66.7    33.3    100.0
199 (A)--V    37.558    5.8    62.0    38.0    100.0
200 (A)--V    38.227   20.1    83.6    16.4    100.0
201 (A)--V    38.587    1.9    82.0    18.0    100.0
202 (A)--V    39.040    7.7    45.2    54.8    100.0
203 (A)--V    39.862    7.5    72.4    27.6    100.0
204 (A)--V    40.472    5.1    78.5    21.5    100.0
205 (A)--V    40.921   42.3    83.9    16.1    100.0
206 (A)--V    41.548   14.3    83.3    16.7    100.0
207 (A)--V    41.929    9.9    93.8     6.2    100.0
208 (A)--V    42.123    5.0    65.5    34.5    100.0
209 (A)--V    42.742    7.8    69.6    30.4    100.0
210 (A)--V    43.362    4.3    76.2    23.8    100.0
211 (A)--V    43.557    3.0    54.1    45.9    100.0
212 (A)--V    44.072    3.2    73.2    26.8    100.0
213 (A)--V    44.267    7.9    99.0     1.0    100.0
214 (A)--V    44.544    7.9    96.2     3.8    100.0
215 (A)--V    45.146    4.3    93.4     6.6    100.0
216 (A)--V    45.257    3.6    96.9     3.1    100.0
217 (A)--V    46.096    4.0    96.9     3.1    100.0
218 (A)--V    46.328    2.8    97.9     2.1    100.0
219 (A)--V    46.524    9.2    72.2    27.8    100.0
220 (A)--V    46.788    8.7    76.0    24.0    100.0
221 (A)--V    47.235   25.9    98.4     1.6    100.0
222 (A)--V    47.650    9.5    95.6     4.4    100.0
223 (A)--V    47.919    6.2    86.1    13.9    100.0
224 (A)--V    48.314    2.2    97.8     2.2    100.0
225 (A)--V    48.673    4.0    77.1    22.9    100.0
226 (A)--V    48.705    1.9    92.1     7.9    100.0
227 (A)--V    50.610   10.0    63.5    36.5    100.0
228 (A)--V    50.958    6.3    41.8    58.2    100.0
229 (A)--V    51.988   25.6    96.5     3.5    100.0
230 (A)--V    52.272    5.9    84.7    15.3    100.0
231 (A)--V    52.370   52.7    89.0    11.0    100.0
232 (A)--V    52.601    1.3    94.4     5.6    100.0
233 (A)--V    53.090    3.5    95.4     4.6    100.0
234 (A)--V    53.351   11.2    96.2     3.8    100.0
235 (A)--V    53.812    3.4    99.0     1.0    100.0
236 (A)--V    54.432    9.9    92.9     7.1    100.0
237 (A)--V    54.890   37.4    76.8    23.2    100.0
238 (A)--V    55.344   41.0    85.7    14.3    100.0
239 (A)--V    55.367   31.0    85.8    14.2    100.0
240 (A)--V    55.896   20.7    62.7    37.3    100.0
241 (A)--V    56.372   43.5    90.4     9.6    100.0
242 (A)--V    56.649   39.4    96.3     3.7    100.0
243 (A)--V    56.843   13.6    99.2     0.8    100.0
244 (A)--V    57.264    8.0    90.8     9.2    100.0
245 (A)--V    57.458   14.8    90.1     9.9    100.0
246 (A)--V    57.633    1.7    77.3    22.7    100.0
247 (A)--V    57.919    5.2    88.6    11.4    100.0
248 (A)--V    58.328    4.1    89.4    10.6    100.0
249 (A)--V    58.967    2.7    46.1    53.9    100.0
250 (A)--V    59.846    6.9    84.9    15.1    100.0
251 (A)--V    60.429    1.5    98.5     1.5    100.0
252 (A)--V    61.067   32.7    93.5     6.5    100.0
253 (A)--V    61.422    7.3    69.8    30.2    100.0
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254 (A)--V    62.345    2.0    95.5    4.5    100.0
255 (A)--V    62.676   29.1    76.9   23.1    100.0
256 (A)--V    64.236   30.2    83.2   16.8    100.0
257 (A)--V    64.563   11.0    73.2   26.8    100.0
258 (A)--V    64.632    5.8    91.8    8.2    100.0
259 (A)--V    64.768   15.8    73.7   26.3    100.0
260 (A)--V    65.360   13.5    90.1    9.9    100.0
261 (A)--V    65.543   22.1    94.6    5.4    100.0
262 (A)--V    66.701    5.2    25.9   74.1    100.0
263 (A)--V    67.221    0.9    17.3   82.7    100.0
264 (A)--V    68.810    3.0    30.7   69.3    100.0
265 (A)--V    70.746   21.5    83.3   16.7    100.0
266 (A)--V    71.294   11.2    78.4   21.6    100.0
267 (A)--V    71.826   47.2    94.7    5.3    100.0
268 (A)--V    73.234   73.2    87.3   12.7    100.0
269 (A)--V    73.360   36.5    63.2   36.8    100.0
270 (A)--V    73.559   53.5    69.7   30.3    100.0
271 (A)--V    74.466    8.9    80.5   19.5    100.0
272 (A)--V    74.648   13.6    89.8   10.2    100.0
273 (A)--V    75.357    6.5    75.3   24.7    100.0
274 (A)--V    76.910    2.6    79.8   20.2    100.0
275 (A)--V    77.753    4.5    59.9   40.1    100.0
276 (A)--V    77.975   14.5    27.1   72.9    100.0
277 (A)--V    78.571    3.1    22.5   77.5    100.0
278 (A)--V    79.124    1.4    90.6    9.4    100.0
279 (A)--V    79.684    1.2    96.2    3.8    100.0
280 (A)--V    80.002    2.7    98.8    1.2    100.0
281 (A)--V    80.062    0.9    94.8    5.2    100.0
282 (A)--V    80.617    1.1    97.7    2.3    100.0
283 (A)--V    81.387    7.5    90.9    9.1    100.0
284 (A)--V    82.277   26.6    87.3   12.7    100.0
285 (A)--V    82.871   35.9    94.7    5.3    100.0
286 (A)--V    83.044   24.2    90.5    9.5    100.0
287 (A)--V    83.335   33.1    90.5    9.5    100.0
288 (A)--V    83.999    9.2    42.2   57.8    100.0
289 (A)--V    84.307   21.4    96.9    3.1    100.0
290 (A)--V    84.493    4.3    63.8   36.2    100.0
291 (A)--V    84.696   10.1    51.1   48.9    100.0
292 (A)--V    84.892   16.0    90.6    9.4    100.0
293 (A)--V    85.449   10.5    72.5   27.5    100.0
294 (A)--V    87.490   13.4    80.9   19.1    100.0
295 (A)--V    87.865   10.5    63.1   36.9    100.0
296 (A)--V    88.451   25.8    86.4   13.6    100.0
297 (A)--V    89.433   11.8    94.5    5.5    100.0
298 (A)--V    90.057   12.7    72.9   27.1    100.0
299 (A)--V    90.567   16.1    77.7   22.3    100.0
300 (A)--V    91.650    4.9    77.4   22.6    100.0
301 (A)--V    95.005    4.2    81.9   18.1    100.0
302 (A)--V    96.218    3.2    96.7    3.3    100.0
303 (A)--V    97.230   11.5    86.4   13.6    100.0
304 (A)--V    99.651   61.0    98.4    1.6    100.0
305 (A)--V   101.148    7.0    62.1   37.9    100.0
306 (A)--V   101.977   18.2    95.4    4.6    100.0
307 (A)--V   102.406    5.2    97.3    2.7    100.0
308 (A)--V   102.501    2.1    97.6    2.4    100.0
309 (A)--V   103.362    1.7    39.4   60.6    100.0
310 (A)--V   103.868    3.1    96.9    3.1    100.0
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311 (A)--V    104.341    2.6    56.8    43.2    100.0
312 (A)--V    104.661    2.0    96.4     3.6    100.0
313 (A)--V    105.279    9.5    97.9     2.1    100.0
314 (A)--V    105.515    9.6    96.6     3.4    100.0
315 (A)--V    106.931   69.6    97.2     2.8    100.0
316 (A)--V    108.129    4.2    99.1     0.9    100.0
317 (A)--V    108.805    0.7    99.2     0.8    100.0
318 (A)--V    116.386    5.8    55.2    44.8    100.0
319 (A)--V    120.502    0.1    96.9     3.1    100.0
320 (A)--V    121.024    1.0     7.4    92.6    100.0
321 (A)--V    121.435    0.0   100.0     0.0    100.0
322 (A)--V    157.547   35.4    89.4    10.6    100.0
323 (A)--V    157.893   25.7    96.8     3.2    100.0
324 (A)--V    166.645   86.8    99.3     0.7    100.0
325 (A)--V    169.132   55.8    99.6     0.4    100.0
326 (A)--V    169.281   55.7    98.2     1.8    100.0
327 (A)--V    235.784   93.4    99.8     0.2    100.0
328 (A)--V    236.410   87.2    96.2     3.8    100.0
329 (A)--V    250.448   93.9    98.8     1.2    100.0
330 (A)--V    377.742   11.5    52.8    47.2    100.0
331 (A)--V    629.124    3.9    35.0    65.0    100.0
332 (A)--V    632.721   13.0    94.0     6.0    100.0
333 (A)--V    635.610    7.6    74.1    25.9    100.0
334 (A)--V    643.915    5.9    99.1     0.9    100.0
335 (A)--V    644.508    3.1    99.3     0.7    100.0
336 (A)--V    644.995    3.2    99.6     0.4    100.0
337 (A)--V    645.497    8.7    99.0     1.0    100.0
338 (A)--V    645.944    7.4    99.8     0.2    100.0
339 (A)--V    646.410    2.0    99.5     0.5    100.0
340 (A)--V    648.750    1.7    99.7     0.3    100.0
341 (A)--V    649.851    0.6    79.8    20.2    100.0
342 (A)--V    650.108    1.0    26.0    74.0    100.0
343 (A)--V    656.935    0.1     2.1    97.9    100.0
344 (A)--V    758.915   97.7    99.9     0.1    100.0
345 (A)--V    967.474    0.0     0.4    99.6    100.0
346 (A)--V   4857.261   98.2   100.0     0.0    100.0
347 (A)--V   4857.686   96.4    99.0     1.0    100.0
348 (A)--V   4870.171   97.8    99.6     0.4    100.0
349 (A)--V  12037.816   99.5   100.0     0.0    100.0
```

Full population analysis for complex 5 (optimized geometry):

```
************************************************************************
*                         VMOdes                                       *
* Virtual Molecular Orbital description Program, Revision 7.1          *
* Cite this work as: VMOdes Program, Revision A 7.1                    *
* V. N. Nemykin, P. Basu, 2001, 2003                                   *
* Department of Chemistry, Duquesne University, Pittsburgh, PA         *
************************************************************************

Input Gaussian file:
C:\Documents and Settings\hp\My Documents\Research Dr.
Nemykin\VMOdes\VModes\FcCN3.gjf.out
Output VMOdes file: FcCN3.out

Full point group is:  C1
```

```
Number of Basis Functions = 407

    73 Alpha electrons          73 Beta electrons


Group  1  is: Fe
This group consist of  1  subunits. The Basis Functions range is:
 106          161
Group  2  is: Fc
This group consist of  1  subunits. The Basis Functions range is:
 1            263
Group  3  is: CN
This group consist of  1  subunits. The Basis Functions range is:
 264          407
Group  4  is: Total
This group consist of  1  subunits. The Basis Functions range is:
 1            407


All MO's will be printed.

Molecular Orbitals Indexes, Energies, and Group Contributions
```

	Orbital		Group Number			
Number	Index	Energy,eV	1	2	3	4
1	(A)--O	-6933.549	100.0	100.0	0.0	100.0
2	(A)--O	-803.595	99.9	100.0	0.0	100.0
3	(A)--O	-694.063	100.0	100.0	0.0	100.0
4	(A)--O	-693.717	100.0	100.0	0.0	100.0
5	(A)--O	-693.667	100.0	100.0	0.0	100.0
6	(A)--O	-381.492	0.0	0.0	100.0	100.0
7	(A)--O	-381.406	0.0	0.0	100.0	100.0
8	(A)--O	-381.203	0.0	0.0	100.0	100.0
9	(A)--O	-272.180	0.0	0.1	99.9	100.0
10	(A)--O	-272.062	0.0	0.0	100.0	100.0
11	(A)--O	-271.149	0.1	99.9	0.1	100.0
12	(A)--O	-271.031	0.0	0.1	99.9	100.0
13	(A)--O	-271.016	0.0	0.1	99.9	100.0
14	(A)--O	-270.811	0.0	0.0	100.0	100.0
15	(A)--O	-270.539	0.1	100.0	0.0	100.0
16	(A)--O	-270.515	0.1	100.0	0.0	100.0
17	(A)--O	-270.504	0.1	100.0	0.0	100.0
18	(A)--O	-270.492	0.0	100.0	0.0	100.0
19	(A)--O	-270.422	0.1	100.0	0.0	100.0
20	(A)--O	-270.403	0.1	100.0	0.0	100.0
21	(A)--O	-270.395	0.0	100.0	0.0	100.0
22	(A)--O	-270.367	0.1	100.0	0.0	100.0
23	(A)--O	-270.358	0.1	100.0	0.0	100.0
24	(A)--O	-88.846	100.0	100.0	0.0	100.0
25	(A)--O	-57.369	99.8	99.9	0.1	100.0
26	(A)--O	-56.428	99.9	100.0	0.0	100.0
27	(A)--O	-56.318	99.9	100.0	0.0	100.0
28	(A)--O	-23.676	2.0	21.5	78.5	100.0
29	(A)--O	-23.253	1.6	18.9	81.1	100.0
30	(A)--O	-23.173	3.3	38.2	61.8	100.0
31	(A)--O	-22.924	0.0	0.5	99.5	100.0

32	(A)--O	-22.817	9.1	93.1	6.9	100.0
33	(A)--O	-21.725	1.3	14.3	85.7	100.0
34	(A)--O	-19.469	1.0	46.5	53.5	100.0
35	(A)--O	-18.655	1.9	98.7	1.3	100.0
36	(A)--O	-18.442	1.8	99.7	0.3	100.0
37	(A)--O	-18.419	1.6	100.0	0.0	100.0
38	(A)--O	-17.809	0.8	52.4	47.6	100.0
39	(A)--O	-15.734	0.4	28.5	71.5	100.0
40	(A)--O	-14.776	0.4	63.4	36.6	100.0
41	(A)--O	-14.280	0.9	89.0	11.0	100.0
42	(A)--O	-14.159	0.3	97.8	2.2	100.0
43	(A)--O	-14.116	0.4	99.0	1.0	100.0
44	(A)--O	-13.958	1.9	73.3	26.7	100.0
45	(A)--O	-13.773	1.0	81.3	18.7	100.0
46	(A)--O	-13.577	0.4	38.9	61.1	100.0
47	(A)--O	-11.488	24.0	67.1	32.9	100.0
48	(A)--O	-11.293	5.8	68.2	31.8	100.0
49	(A)--O	-10.921	7.8	97.6	2.4	100.0
50	(A)--O	-10.761	21.5	63.1	36.9	100.0
51	(A)--O	-10.633	5.3	90.3	9.7	100.0
52	(A)--O	-10.599	1.7	98.9	1.1	100.0
53	(A)--O	-10.370	0.8	93.2	6.8	100.0
54	(A)--O	-10.172	0.6	88.3	11.7	100.0
55	(A)--O	-9.999	0.4	99.8	0.2	100.0
56	(A)--O	-9.998	0.2	98.2	1.8	100.0
57	(A)--O	-9.887	9.8	79.9	20.1	100.0
58	(A)--O	-9.479	2.2	17.2	82.8	100.0
59	(A)--O	-9.275	0.1	3.1	96.9	100.0
60	(A)--O	-9.217	0.2	5.0	95.0	100.0
61	(A)--O	-9.017	0.4	6.7	93.3	100.0
62	(A)--O	-8.907	0.2	6.6	93.4	100.0
63	(A)--O	-8.838	0.3	1.5	98.5	100.0
64	(A)--O	-8.782	0.1	4.3	95.7	100.0
65	(A)--O	-8.479	0.2	3.3	96.7	100.0
66	(A)--O	-8.072	13.7	57.0	43.0	100.0
67	(A)--O	-7.666	33.4	99.5	0.5	100.0
68	(A)--O	-7.438	23.2	81.4	18.6	100.0
69	(A)--O	-7.059	6.3	99.5	0.5	100.0
70	(A)--O	-6.716	5.9	54.1	45.9	100.0
71	(A)--O	-5.551	82.8	95.2	4.8	100.0
72	(A)--O	-5.350	61.2	95.9	4.1	100.0
73	(A)--O	-5.288	66.4	99.3	0.7	100.0
74	(A)--V	-4.078	13.3	25.5	74.5	100.0
75	(A)--V	-2.525	44.9	99.3	0.7	100.0
76	(A)--V	-2.492	41.0	93.7	6.3	100.0
77	(A)--V	-1.587	1.3	10.0	90.0	100.0
78	(A)--V	-1.092	1.0	30.7	69.3	100.0
79	(A)--V	-0.625	1.7	59.5	40.5	100.0
80	(A)--V	-0.251	7.3	53.1	46.9	100.0
81	(A)--V	-0.096	2.1	97.8	2.2	100.0
82	(A)--V	-0.024	5.3	94.2	5.8	100.0
83	(A)--V	0.007	12.6	96.5	3.5	100.0
84	(A)--V	0.196	27.7	56.5	43.5	100.0
85	(A)--V	0.249	38.5	85.1	14.9	100.0
86	(A)--V	0.860	4.1	47.1	52.9	100.0
87	(A)--V	1.057	18.1	90.7	9.3	100.0
88	(A)--V	1.283	1.8	93.2	6.8	100.0

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89  (A)--V    1.368    9.7    71.4   28.6   100.0
90  (A)--V    1.715    3.5    74.9   25.1   100.0
91  (A)--V    1.939    2.1    80.3   19.7   100.0
92  (A)--V    2.243   13.7    76.4   23.6   100.0
93  (A)--V    2.335   58.6    83.3   16.7   100.0
94  (A)--V    2.421    5.7    87.4   12.6   100.0
95  (A)--V    2.602    2.4    66.8   33.2   100.0
96  (A)--V    2.701    2.4    89.7   10.3   100.0
97  (A)--V    3.165   15.6    53.5   46.5   100.0
98  (A)--V    3.333    8.5    74.2   25.8   100.0
99  (A)--V    3.525   24.5    65.0   35.0   100.0
100 (A)--V    3.801   27.9    94.6    5.4   100.0
101 (A)--V    4.018   72.9    95.6    4.4   100.0
102 (A)--V    4.172   30.3    73.8   26.2   100.0
103 (A)--V    4.480   20.1    89.5   10.5   100.0
104 (A)--V    4.573   21.8    91.0    9.0   100.0
105 (A)--V    4.713   30.8    96.8    3.2   100.0
106 (A)--V    4.935   78.1    95.6    4.4   100.0
107 (A)--V    5.350    9.4    78.9   21.1   100.0
108 (A)--V    5.384    5.2    78.7   21.3   100.0
109 (A)--V    5.946    3.4    79.2   20.8   100.0
110 (A)--V    6.389    0.9    91.6    8.4   100.0
111 (A)--V    6.543    3.4    59.6   40.4   100.0
112 (A)--V    7.087   19.6    64.2   35.8   100.0
113 (A)--V    7.423   18.2    71.6   28.4   100.0
114 (A)--V    7.575   15.1    58.8   41.2   100.0
115 (A)--V    7.688   34.3    64.2   35.8   100.0
116 (A)--V    7.778   21.7    36.6   63.4   100.0
117 (A)--V    7.942    8.2    71.0   29.0   100.0
118 (A)--V    8.040   36.8    96.3    3.7   100.0
119 (A)--V    8.160   36.7    92.4    7.6   100.0
120 (A)--V    8.288   14.6    57.9   42.1   100.0
121 (A)--V    8.476   41.0    66.7   33.3   100.0
122 (A)--V    8.526   32.7    59.0   41.0   100.0
123 (A)--V    9.230    2.2    56.8   43.2   100.0
124 (A)--V    9.462   26.0    54.2   45.8   100.0
125 (A)--V    9.526   12.8    61.3   38.7   100.0
126 (A)--V    9.608   29.5    71.4   28.6   100.0
127 (A)--V    9.684    3.6    36.5   63.5   100.0
128 (A)--V   10.017    1.4    16.3   83.7   100.0
129 (A)--V   10.235   57.8    93.1    6.9   100.0
130 (A)--V   10.716   15.1    46.5   53.5   100.0
131 (A)--V   10.857   14.3    61.1   38.9   100.0
132 (A)--V   11.261   16.5    88.7   11.3   100.0
133 (A)--V   11.363    2.5    35.3   64.7   100.0
134 (A)--V   11.493    2.4    35.6   64.4   100.0
135 (A)--V   12.011    6.8    78.9   21.1   100.0
136 (A)--V   12.171   10.1    65.2   34.8   100.0
137 (A)--V   12.421    6.7    55.8   44.2   100.0
138 (A)--V   12.453   21.0    95.9    4.1   100.0
139 (A)--V   12.720   29.9    68.7   31.3   100.0
140 (A)--V   12.749   23.7    88.5   11.5   100.0
141 (A)--V   12.879   18.8    85.6   14.4   100.0
142 (A)--V   13.138   25.6    70.5   29.5   100.0
143 (A)--V   13.181   40.7    90.6    9.4   100.0
144 (A)--V   13.384   21.4    84.7   15.3   100.0
145 (A)--V   13.708   15.0    73.5   26.5   100.0
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146 (A)--V     14.059    24.3    68.2    31.8    100.0
147 (A)--V     14.154     5.1    45.2    54.8    100.0
148 (A)--V     14.274     6.8    60.5    39.5    100.0
149 (A)--V     14.506    27.8    58.9    41.1    100.0
150 (A)--V     14.650     2.2    50.7    49.3    100.0
151 (A)--V     14.851     8.5    67.4    32.6    100.0
152 (A)--V     15.006     4.9    82.9    17.1    100.0
153 (A)--V     15.182     2.3    86.7    13.3    100.0
154 (A)--V     15.399     3.0    77.4    22.6    100.0
155 (A)--V     15.664     5.3    81.2    18.8    100.0
156 (A)--V     15.993     7.3    88.8    11.2    100.0
157 (A)--V     16.035    17.9    88.4    11.6    100.0
158 (A)--V     16.156     8.1    91.4     8.6    100.0
159 (A)--V     16.245     5.3    96.8     3.2    100.0
160 (A)--V     16.370     9.4    92.1     7.9    100.0
161 (A)--V     16.495     5.9    85.9    14.1    100.0
162 (A)--V     16.564     8.7    58.5    41.5    100.0
163 (A)--V     16.743     3.2    79.2    20.8    100.0
164 (A)--V     17.046     5.9    40.4    59.6    100.0
165 (A)--V     17.181     7.1    67.2    32.8    100.0
166 (A)--V     17.905     6.1    69.3    30.7    100.0
167 (A)--V     18.024     2.2    84.3    15.7    100.0
168 (A)--V     18.202    21.1    78.3    21.7    100.0
169 (A)--V     18.447     9.2    64.6    35.4    100.0
170 (A)--V     18.580     0.3    94.4     5.6    100.0
171 (A)--V     18.712     7.5    91.8     8.2    100.0
172 (A)--V     19.047     4.8    83.4    16.6    100.0
173 (A)--V     19.464    30.4    74.1    25.9    100.0
174 (A)--V     19.556    13.0    49.8    50.2    100.0
175 (A)--V     19.918    17.3    84.5    15.5    100.0
176 (A)--V     20.023    12.1    52.6    47.4    100.0
177 (A)--V     20.056    12.1    74.3    25.7    100.0
178 (A)--V     20.247    30.9    83.8    16.2    100.0
179 (A)--V     20.756    17.5    80.4    19.6    100.0
180 (A)--V     21.072    17.3    62.7    37.3    100.0
181 (A)--V     21.449    14.5    46.9    53.1    100.0
182 (A)--V     21.989     8.8    57.8    42.2    100.0
183 (A)--V     22.133    18.6    68.0    32.0    100.0
184 (A)--V     22.713    17.8    57.7    42.3    100.0
185 (A)--V     22.946     4.2    43.0    57.0    100.0
186 (A)--V     22.982    22.0    66.8    33.2    100.0
187 (A)--V     23.483     1.3    92.4     7.6    100.0
188 (A)--V     24.129     6.2    45.0    55.0    100.0
189 (A)--V     24.443     1.9    49.3    50.7    100.0
190 (A)--V     24.549     2.3    68.1    31.9    100.0
191 (A)--V     24.576     2.2    57.7    42.3    100.0
192 (A)--V     25.392     0.8    69.2    30.8    100.0
193 (A)--V     25.637     3.3    75.3    24.7    100.0
194 (A)--V     25.895     0.5    90.9     9.1    100.0
195 (A)--V     26.166     1.9    66.2    33.8    100.0
196 (A)--V     26.671     4.0    73.5    26.5    100.0
197 (A)--V     26.812     1.5    62.2    37.8    100.0
198 (A)--V     27.160     1.9    86.8    13.2    100.0
199 (A)--V     27.548     3.2    79.7    20.3    100.0
200 (A)--V     27.668     2.2    88.0    12.0    100.0
201 (A)--V     27.758     5.0    86.5    13.5    100.0
202 (A)--V     28.064     3.2    94.2     5.8    100.0
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203 (A)--V    28.581    6.6    84.2    15.8    100.0
204 (A)--V    28.601    2.9    49.7    50.3    100.0
205 (A)--V    28.657   21.8    89.9    10.1    100.0
206 (A)--V    28.754    1.7    89.9    10.1    100.0
207 (A)--V    29.421    1.5    72.3    27.7    100.0
208 (A)--V    29.903    1.9    29.1    70.9    100.0
209 (A)--V    30.395    5.0    85.9    14.1    100.0
210 (A)--V    30.792    9.8    50.2    49.8    100.0
211 (A)--V    31.082    3.3    63.3    36.7    100.0
212 (A)--V    31.537   28.7    96.2     3.8    100.0
213 (A)--V    32.148   15.2    66.5    33.5    100.0
214 (A)--V    32.700   23.5    91.4     8.6    100.0
215 (A)--V    32.955    1.9    28.8    71.2    100.0
216 (A)--V    33.363    7.3    43.5    56.5    100.0
217 (A)--V    33.743    8.5    37.6    62.4    100.0
218 (A)--V    34.225    2.0    29.0    71.0    100.0
219 (A)--V    34.672    1.8    26.3    73.7    100.0
220 (A)--V    35.092    3.4    49.1    50.9    100.0
221 (A)--V    35.510    3.7    42.9    57.1    100.0
222 (A)--V    35.771    2.7    37.1    62.9    100.0
223 (A)--V    36.033    1.9    44.6    55.4    100.0
224 (A)--V    36.216    6.6    32.1    67.9    100.0
225 (A)--V    36.704    9.1    74.7    25.3    100.0
226 (A)--V    36.959    0.8    27.2    72.8    100.0
227 (A)--V    37.322    0.7    33.8    66.2    100.0
228 (A)--V    38.516    2.3    65.6    34.4    100.0
229 (A)--V    39.029    3.9    41.9    58.1    100.0
230 (A)--V    39.568    4.5    90.2     9.8    100.0
231 (A)--V    39.984    1.8    85.7    14.3    100.0
232 (A)--V    40.397    7.3    67.6    32.4    100.0
233 (A)--V    40.649    0.8    16.7    83.3    100.0
234 (A)--V    41.201    2.0    17.0    83.0    100.0
235 (A)--V    41.498    6.9    48.7    51.3    100.0
236 (A)--V    41.544    1.6    22.6    77.4    100.0
237 (A)--V    41.570   13.5    77.3    22.7    100.0
238 (A)--V    41.874   13.1    68.7    31.3    100.0
239 (A)--V    42.040    4.8    87.0    13.0    100.0
240 (A)--V    42.103    3.7    66.2    33.8    100.0
241 (A)--V    43.278    8.0    69.0    31.0    100.0
242 (A)--V    43.614    2.0    74.2    25.8    100.0
243 (A)--V    43.826    5.3    58.1    41.9    100.0
244 (A)--V    44.004    7.5    64.8    35.2    100.0
245 (A)--V    44.145    6.4    50.2    49.8    100.0
246 (A)--V    44.793    1.8    48.6    51.4    100.0
247 (A)--V    45.014    0.6    42.3    57.7    100.0
248 (A)--V    45.332    3.4    63.7    36.3    100.0
249 (A)--V    45.758    2.6    41.3    58.7    100.0
250 (A)--V    46.548    2.9    39.6    60.4    100.0
251 (A)--V    46.932   24.7    73.2    26.8    100.0
252 (A)--V    47.155   10.6    95.1     4.9    100.0
253 (A)--V    47.431    5.9    69.3    30.7    100.0
254 (A)--V    47.958    3.7    35.9    64.1    100.0
255 (A)--V    48.221    1.1    43.9    56.1    100.0
256 (A)--V    48.531    1.0    58.2    41.8    100.0
257 (A)--V    49.348    5.2    67.9    32.1    100.0
258 (A)--V    50.008   15.6    68.9    31.1    100.0
259 (A)--V    50.416   13.0    81.0    19.0    100.0
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260 (A)--V    50.618    21.5    86.3    13.7    100.0
261 (A)--V    51.112     5.3    43.5    56.5    100.0
262 (A)--V    51.554     3.2    50.0    50.0    100.0
263 (A)--V    51.899     4.9    77.9    22.1    100.0
264 (A)--V    52.097     2.3    88.3    11.7    100.0
265 (A)--V    53.075     0.9    79.4    20.6    100.0
266 (A)--V    53.399     1.0    27.9    72.1    100.0
267 (A)--V    53.623     1.7    55.0    45.0    100.0
268 (A)--V    54.010     9.3    46.7    53.3    100.0
269 (A)--V    54.045    22.1    68.4    31.6    100.0
270 (A)--V    54.099     1.1    19.0    81.0    100.0
271 (A)--V    54.308     1.4    36.6    63.4    100.0
272 (A)--V    54.522     1.0    31.6    68.4    100.0
273 (A)--V    54.983    23.0    68.0    32.0    100.0
274 (A)--V    55.391    32.1    65.8    34.2    100.0
275 (A)--V    55.560    41.9    85.4    14.6    100.0
276 (A)--V    55.719    30.3    71.0    29.0    100.0
277 (A)--V    55.827     6.9    72.8    27.2    100.0
278 (A)--V    56.575    22.9    85.2    14.8    100.0
279 (A)--V    56.864    29.1    83.1    16.9    100.0
280 (A)--V    57.158     2.2    99.2     0.8    100.0
281 (A)--V    57.193     0.3    99.5     0.5    100.0
282 (A)--V    57.319    17.0    95.5     4.5    100.0
283 (A)--V    57.443     9.6    77.4    22.6    100.0
284 (A)--V    57.699     9.4    79.1    20.9    100.0
285 (A)--V    58.277    16.6    83.0    17.0    100.0
286 (A)--V    58.710     0.7    59.5    40.5    100.0
287 (A)--V    58.964    14.6    65.8    34.2    100.0
288 (A)--V    59.924     1.3    72.4    27.6    100.0
289 (A)--V    60.808     9.6    63.8    36.2    100.0
290 (A)--V    60.979     4.2    91.7     8.3    100.0
291 (A)--V    61.661     0.8    69.3    30.7    100.0
292 (A)--V    62.187     0.1    92.8     7.2    100.0
293 (A)--V    64.396     3.8    20.5    79.5    100.0
294 (A)--V    64.642     5.4    51.6    48.4    100.0
295 (A)--V    65.149     6.5    50.5    49.5    100.0
296 (A)--V    65.832     0.6     4.6    95.4    100.0
297 (A)--V    66.266    27.7    86.4    13.6    100.0
298 (A)--V    66.697     1.4    14.2    85.8    100.0
299 (A)--V    66.990    11.0    60.7    39.3    100.0
300 (A)--V    67.155     7.6    53.5    46.5    100.0
301 (A)--V    67.911    11.5    40.4    59.6    100.0
302 (A)--V    67.998     1.0    32.4    67.6    100.0
303 (A)--V    69.367    12.6    60.6    39.4    100.0
304 (A)--V    70.287    18.0    77.2    22.8    100.0
305 (A)--V    71.035    24.8    92.5     7.5    100.0
306 (A)--V    71.288    47.9    72.7    27.3    100.0
307 (A)--V    72.426    18.0    58.6    41.4    100.0
308 (A)--V    72.780     9.4    21.5    78.5    100.0
309 (A)--V    73.410     5.4    18.2    81.8    100.0
310 (A)--V    74.080     4.3    46.2    53.8    100.0
311 (A)--V    74.411     0.6    54.9    45.1    100.0
312 (A)--V    74.507     1.6    83.5    16.5    100.0
313 (A)--V    74.719     4.8    62.1    37.9    100.0
314 (A)--V    74.960     1.5    21.8    78.2    100.0
315 (A)--V    75.567     0.6    21.2    78.8    100.0
316 (A)--V    76.226     1.1    32.0    68.0    100.0
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317 (A)--V    76.776    0.9    50.7    49.3    100.0
318 (A)--V    77.172    7.3    58.0    42.0    100.0
319 (A)--V    77.427    2.5    11.7    88.3    100.0
320 (A)--V    78.788    2.4    43.8    56.2    100.0
321 (A)--V    79.036    1.2    47.8    52.2    100.0
322 (A)--V    79.341    2.7    38.4    61.6    100.0
323 (A)--V    79.850    6.6    72.8    27.2    100.0
324 (A)--V    80.597    8.3    92.1     7.9    100.0
325 (A)--V    80.864   14.0    95.5     4.5    100.0
326 (A)--V    80.990   12.9    92.8     7.2    100.0
327 (A)--V    81.168   12.8    84.0    16.0    100.0
328 (A)--V    81.275    5.4    91.3     8.7    100.0
329 (A)--V    81.383   11.4    74.4    25.6    100.0
330 (A)--V    81.778   13.8    92.8     7.2    100.0
331 (A)--V    82.272    7.1    56.3    43.7    100.0
332 (A)--V    82.754    0.6    94.3     5.7    100.0
333 (A)--V    82.946    1.8    52.9    47.1    100.0
334 (A)--V    83.406    1.1    94.6     5.4    100.0
335 (A)--V    83.745    1.0    69.9    30.1    100.0
336 (A)--V    83.788    0.8    67.6    32.4    100.0
337 (A)--V    83.984    1.6    66.5    33.5    100.0
338 (A)--V    84.523    1.3    90.3     9.7    100.0
339 (A)--V    84.750    2.8    36.4    63.6    100.0
340 (A)--V    85.263    1.0    59.0    41.0    100.0
341 (A)--V    85.988    0.8     9.9    90.1    100.0
342 (A)--V    87.480    0.4    72.7    27.3    100.0
343 (A)--V    88.549    4.8    53.0    47.0    100.0
344 (A)--V    89.310    6.9    61.4    38.6    100.0
345 (A)--V    89.507   11.9    63.1    36.9    100.0
346 (A)--V    89.621    5.3    75.1    24.9    100.0
347 (A)--V    90.065    6.8    82.1    17.9    100.0
348 (A)--V    91.993    4.2    54.9    45.1    100.0
349 (A)--V    94.583    3.2    72.6    27.4    100.0
350 (A)--V    94.890    3.9    81.1    18.9    100.0
351 (A)--V    96.410    1.8    85.3    14.7    100.0
352 (A)--V    97.861    0.7    94.1     5.9    100.0
353 (A)--V    98.850    3.8    75.4    24.6    100.0
354 (A)--V    99.646    9.2    94.0     6.0    100.0
355 (A)--V    99.700    4.9    49.2    50.8    100.0
356 (A)--V   100.947    3.9    66.1    33.9    100.0
357 (A)--V   101.601   55.9    90.1     9.9    100.0
358 (A)--V   101.952   28.8    50.5    49.5    100.0
359 (A)--V   102.162    1.4    39.2    60.8    100.0
360 (A)--V   102.481    2.7    27.0    73.0    100.0
361 (A)--V   102.789    3.3    80.4    19.6    100.0
362 (A)--V   103.099    2.6    75.4    24.6    100.0
363 (A)--V   103.347    1.0    89.7    10.3    100.0
364 (A)--V   103.472    0.6    99.2     0.8    100.0
365 (A)--V   103.740    2.9    81.6    18.4    100.0
366 (A)--V   104.121    3.7    85.9    14.1    100.0
367 (A)--V   104.223    7.5    81.0    19.0    100.0
368 (A)--V   104.602    9.1    86.6    13.4    100.0
369 (A)--V   105.909    1.3    26.6    73.4    100.0
370 (A)--V   108.074   45.5    76.2    23.8    100.0
371 (A)--V   116.988    3.9    43.8    56.2    100.0
372 (A)--V   119.151    1.5    19.3    80.7    100.0
373 (A)--V   119.804    1.5    51.6    48.4    100.0
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374 (A)--V    120.101     0.0    98.8    1.2    100.0
375 (A)--V    120.390     1.4    11.8    88.2   100.0
376 (A)--V    120.863     0.7    47.1    52.9   100.0
377 (A)--V    157.342    19.4    96.3    3.7    100.0
378 (A)--V    157.607    14.3    96.6    3.4    100.0
379 (A)--V    164.501    85.8    98.4    1.6    100.0
380 (A)--V    167.235    84.9    98.7    1.3    100.0
381 (A)--V    167.373    62.6    88.7    11.3   100.0
382 (A)--V    233.565    93.5    98.4    1.6    100.0
383 (A)--V    234.452    89.6    96.4    3.6    100.0
384 (A)--V    250.219    77.9    90.8    9.2    100.0
385 (A)--V    629.406     3.1    37.1    62.9   100.0
386 (A)--V    631.736    11.9    95.2    4.8    100.0
387 (A)--V    635.646     3.3    61.7    38.3   100.0
388 (A)--V    642.932     2.4    99.3    0.7    100.0
389 (A)--V    643.386     5.3    98.3    1.7    100.0
390 (A)--V    643.817    11.0    99.2    0.8    100.0
391 (A)--V    643.986     0.8    91.4    8.6    100.0
392 (A)--V    644.731     1.7    99.3    0.7    100.0
393 (A)--V    644.806     2.5    93.3    6.7    100.0
394 (A)--V    644.966     3.9    81.7    18.3   100.0
395 (A)--V    645.309     3.2    89.9    10.1   100.0
396 (A)--V    645.785     3.1    52.2    47.8   100.0
397 (A)--V    654.467     0.6     7.1    92.9   100.0
398 (A)--V    656.121     0.2     4.3    95.7   100.0
399 (A)--V    657.858     0.1     4.7    95.3   100.0
400 (A)--V    758.480    89.3    95.8    4.2    100.0
401 (A)--V    964.417     0.0     0.6    99.4   100.0
402 (A)--V    964.763     0.0     0.4    99.6   100.0
403 (A)--V    965.206     0.0     0.7    99.3   100.0
404 (A)--V   4855.267    98.6    99.7    0.3    100.0
405 (A)--V   4855.934    97.1    99.0    1.0    100.0
406 (A)--V   4869.311    91.1    96.3    3.7    100.0
407 (A)--V  12037.293    97.6    99.0    1.0    100.0
```

Full population analysis for complex *trans*-4 (optimized geometry):

```
*************************************************************************
*                         VMOdes                                       *
* Virtual Molecular Orbital description Program, Revision 7.1          *
* Cite this work as: VMOdes Program, Revision A 7.1                    *
* V. N. Nemykin, P. Basu, 2001, 2003                                  *
* Department of Chemistry, Duquesne University, Pittsburgh, PA         *
*************************************************************************


Input Gaussian file:
C:\Documents and Settings\hp\My Documents\Research Dr.
Nemykin\VMOdes\VMOdes\FcCN2-trans.gjf.out
Output VMOdes file: trans-FcCN2.out


Full point group is:  C1


Number of Basis Functions = 374

    67 Alpha electrons           67 Beta electrons
```

```
Group  1  is: Fe
This group consist of  1  subunits. The Basis Functions range is:
 106          161
Group  2  is: Fc
This group consist of  1  subunits. The Basis Functions range is:
 1            263
Group  3  is: CN
This group consist of  1  subunits. The Basis Functions range is:
 264          374
Group  4  is: Total
This group consist of  1  subunits. The Basis Functions range is:
 1            374


All MO's will be printed.

Molecular Orbitals Indexes, Energies, and Group Contributions


        Orbital                        Group Number
_____  _____

Number Index   Energy,eV   1        2        3        4

  1   (A)--O   -6933.111  100.0    100.0    0.0      100.0
  2   (A)--O   -803.156   100.0    100.0    0.0      100.0
  3   (A)--O   -693.636   100.0    100.0    0.0      100.0
  4   (A)--O   -693.264   100.0    100.0    0.0      100.0
  5   (A)--O   -693.231   100.0    100.0    0.0      100.0
  6   (A)--O   -381.139   0.0      0.0      100.0    100.0
  7   (A)--O   -380.977   0.0      0.0      100.0    100.0
  8   (A)--O   -271.608   0.0      0.1      99.9     100.0
  9   (A)--O   -270.943   0.0      0.0      100.0    100.0
 10   (A)--O   -270.694   0.0      1.2      98.8     100.0
 11   (A)--O   -270.691   0.1      98.8     1.2      100.0
 12   (A)--O   -270.567   0.0      0.0      100.0    100.0
 13   (A)--O   -270.160   0.1      100.0    0.0      100.0
 14   (A)--O   -270.135   0.1      100.0    0.0      100.0
 15   (A)--O   -270.123   0.1      100.0    0.0      100.0
 16   (A)--O   -270.105   0.0      100.0    0.0      100.0
 17   (A)--O   -270.052   0.1      100.0    0.0      100.0
 18   (A)--O   -270.047   0.1      100.0    0.0      100.0
 19   (A)--O   -270.039   0.0      100.0    0.0      100.0
 20   (A)--O   -270.019   0.0      100.0    0.0      100.0
 21   (A)--O   -270.007   0.0      100.0    0.0      100.0
 22   (A)--O   -88.406    100.0    100.0    0.0      100.0
 23   (A)--O   -56.953    99.8     100.0    0.0      100.0
 24   (A)--O   -55.959    99.9     100.0    0.0      100.0
 25   (A)--O   -55.884    99.9     100.0    0.0      100.0
 26   (A)--O   -23.174    2.5      28.0     72.0     100.0
 27   (A)--O   -22.823    2.8      32.1     67.9     100.0
 28   (A)--O   -22.778    1.6      18.2     81.8     100.0
 29   (A)--O   -22.449    9.1      93.4     6.6      100.0
 30   (A)--O   -21.130    1.4      17.6     82.4     100.0
 31   (A)--O   -18.655    1.2      58.9     41.1     100.0
 32   (A)--O   -18.246    1.8      97.7     2.3      100.0
 33   (A)--O   -18.089    1.8      99.7     0.3      100.0
 34   (A)--O   -18.072    1.6      100.0    0.0      100.0
 35   (A)--O   -17.238    0.6      38.6     61.4     100.0
 36   (A)--O   -14.659    0.7      62.1     37.9     100.0
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37	(A)--O	-14.240	0.4	76.4	23.6	100.0
38	(A)--O	-13.856	1.3	98.1	1.9	100.0
39	(A)--O	-13.808	0.2	98.5	1.5	100.0
40	(A)--O	-13.763	1.0	99.0	1.0	100.0
41	(A)--O	-13.489	1.6	98.1	1.9	100.0
42	(A)--O	-13.096	0.1	38.6	61.4	100.0
43	(A)--O	-12.249	0.9	37.9	62.1	100.0
44	(A)--O	-10.987	31.6	82.1	17.9	100.0
45	(A)--O	-10.695	5.6	61.9	38.1	100.0
46	(A)--O	-10.537	7.7	96.6	3.4	100.0
47	(A)--O	-10.313	4.2	91.4	8.6	100.0
48	(A)--O	-10.253	1.2	99.1	0.9	100.0
49	(A)--O	-10.092	14.4	56.4	43.6	100.0
50	(A)--O	-9.981	0.8	93.7	6.3	100.0
51	(A)--O	-9.773	1.0	88.3	11.7	100.0
52	(A)--O	-9.660	0.3	99.8	0.2	100.0
53	(A)--O	-9.649	0.2	97.0	3.0	100.0
54	(A)--O	-9.401	9.0	78.7	21.3	100.0
55	(A)--O	-9.042	0.5	4.5	95.5	100.0
56	(A)--O	-8.922	0.1	2.8	97.2	100.0
57	(A)--O	-8.760	0.4	7.8	92.2	100.0
58	(A)--O	-8.585	0.2	5.6	94.4	100.0
59	(A)--O	-8.316	0.4	8.9	91.1	100.0
60	(A)--O	-7.711	11.5	50.7	49.3	100.0
61	(A)--O	-7.278	33.1	99.6	0.4	100.0
62	(A)--O	-7.088	24.3	82.3	17.7	100.0
63	(A)--O	-6.694	6.1	99.6	0.4	100.0
64	(A)--O	-6.388	5.9	61.8	38.2	100.0
65	(A)--O	-5.128	85.5	97.0	3.0	100.0
66	(A)--O	-4.909	60.6	96.7	3.3	100.0
67	(A)--O	-4.860	65.5	99.2	0.8	100.0
68	(A)--V	-3.403	11.6	24.1	75.9	100.0
69	(A)--V	-2.131	44.8	99.4	0.6	100.0
70	(A)--V	-2.074	40.5	93.0	7.0	100.0
71	(A)--V	-0.715	1.1	18.9	81.1	100.0
72	(A)--V	-0.595	3.2	31.9	68.1	100.0
73	(A)--V	-0.085	2.3	80.0	20.0	100.0
74	(A)--V	0.262	3.9	97.7	2.3	100.0
75	(A)--V	0.335	5.1	97.8	2.2	100.0
76	(A)--V	0.358	19.9	96.7	3.3	100.0
77	(A)--V	0.489	38.3	83.7	16.3	100.0
78	(A)--V	0.965	0.7	26.4	73.6	100.0
79	(A)--V	1.276	4.3	51.4	48.6	100.0
80	(A)--V	1.358	17.5	72.7	27.3	100.0
81	(A)--V	1.539	1.5	94.4	5.6	100.0
82	(A)--V	1.918	5.0	76.1	23.9	100.0
83	(A)--V	1.982	3.3	78.2	21.8	100.0
84	(A)--V	2.248	3.3	87.9	12.1	100.0
85	(A)--V	2.556	4.5	50.2	49.8	100.0
86	(A)--V	2.635	64.8	95.1	4.9	100.0
87	(A)--V	2.672	3.6	95.1	4.9	100.0
88	(A)--V	2.873	6.6	81.4	18.6	100.0
89	(A)--V	3.004	6.3	78.6	21.4	100.0
90	(A)--V	3.446	6.7	69.8	30.2	100.0
91	(A)--V	3.724	23.6	73.6	26.4	100.0
92	(A)--V	4.087	27.8	86.7	13.3	100.0
93	(A)--V	4.310	72.1	96.3	3.7	100.0

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94  (A)--V    4.448   53.6   86.6   13.4   100.0
95  (A)--V    4.757   17.2   58.1   41.9   100.0
96  (A)--V    4.868   19.0   93.9    6.1   100.0
97  (A)--V    5.041   29.4   94.3    5.7   100.0
98  (A)--V    5.215   74.6   95.9    4.1   100.0
99  (A)--V    5.305   13.7   70.7   29.3   100.0
100 (A)--V    5.621    7.5   91.1    8.9   100.0
101 (A)--V    6.217    3.5   78.5   21.5   100.0
102 (A)--V    6.619    0.9   94.3    5.7   100.0
103 (A)--V    6.772    1.9   78.2   21.8   100.0
104 (A)--V    7.154   12.5   28.7   71.3   100.0
105 (A)--V    7.765   19.8   78.3   21.7   100.0
106 (A)--V    7.804   15.4   70.6   29.4   100.0
107 (A)--V    7.954   41.9   84.6   15.4   100.0
108 (A)--V    8.106   43.0   73.1   26.9   100.0
109 (A)--V    8.331   31.9   96.3    3.7   100.0
110 (A)--V    8.354   19.6   89.5   10.5   100.0
111 (A)--V    8.436   13.2   63.9   36.1   100.0
112 (A)--V    8.497   28.3   82.1   17.9   100.0
113 (A)--V    8.632   18.9   59.2   40.8   100.0
114 (A)--V    8.875   44.5   74.6   25.4   100.0
115 (A)--V    9.375   13.4   48.2   51.8   100.0
116 (A)--V    9.752    9.5   73.2   26.8   100.0
117 (A)--V    9.882   40.9   85.2   14.8   100.0
118 (A)--V   10.029    2.5   60.8   39.2   100.0
119 (A)--V   10.317   21.1   55.3   44.7   100.0
120 (A)--V   10.517   25.6   55.7   44.3   100.0
121 (A)--V   10.630   45.2   90.8    9.2   100.0
122 (A)--V   11.048   20.3   73.2   26.8   100.0
123 (A)--V   11.238   36.4   83.4   16.6   100.0
124 (A)--V   11.482    3.2   36.3   63.7   100.0
125 (A)--V   11.934    9.0   60.3   39.7   100.0
126 (A)--V   12.197    8.2   91.8    8.2   100.0
127 (A)--V   12.512   13.3   83.2   16.8   100.0
128 (A)--V   12.622   15.7   94.6    5.4   100.0
129 (A)--V   12.816   18.2   94.9    5.1   100.0
130 (A)--V   12.927    9.4   58.6   41.4   100.0
131 (A)--V   13.140   46.6   92.9    7.1   100.0
132 (A)--V   13.434   37.1   96.5    3.5   100.0
133 (A)--V   13.520   26.3   87.8   12.2   100.0
134 (A)--V   13.711   22.3   93.9    6.1   100.0
135 (A)--V   14.115   21.1   56.1   43.9   100.0
136 (A)--V   14.290   17.9   65.5   34.5   100.0
137 (A)--V   14.412   13.3   76.0   24.0   100.0
138 (A)--V   14.431   42.8   70.3   29.7   100.0
139 (A)--V   14.554    5.0   69.9   30.1   100.0
140 (A)--V   14.962   11.0   62.9   37.1   100.0
141 (A)--V   15.249    6.3   81.2   18.8   100.0
142 (A)--V   15.459    0.7   42.5   57.5   100.0
143 (A)--V   15.553    3.6   72.0   28.0   100.0
144 (A)--V   15.644    0.5   71.3   28.7   100.0
145 (A)--V   15.745    5.1   87.4   12.6   100.0
146 (A)--V   15.991   15.5   85.7   14.3   100.0
147 (A)--V   16.397   10.3   87.0   13.0   100.0
148 (A)--V   16.512    5.3   94.3    5.7   100.0
149 (A)--V   16.590    5.9   95.9    4.1   100.0
150 (A)--V   16.660    5.2   91.1    8.9   100.0
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151 (A)--V    16.751    12.9    84.5    15.5    100.0
152 (A)--V    16.904     6.9    79.0    21.0    100.0
153 (A)--V    17.178     5.6    70.7    29.3    100.0
154 (A)--V    17.611     4.5    42.8    57.2    100.0
155 (A)--V    18.004     4.3    74.6    25.4    100.0
156 (A)--V    18.206     6.1    70.1    29.9    100.0
157 (A)--V    18.496    13.8    72.6    27.4    100.0
158 (A)--V    18.839     3.4    82.0    18.0    100.0
159 (A)--V    18.907     5.7    78.4    21.6    100.0
160 (A)--V    19.052     5.5    74.1    25.9    100.0
161 (A)--V    19.281     0.8    63.0    37.0    100.0
162 (A)--V    19.627    29.5    63.1    36.9    100.0
163 (A)--V    19.892    14.4    61.7    38.3    100.0
164 (A)--V    20.159     9.0    46.0    54.0    100.0
165 (A)--V    20.286    25.9    91.4     8.6    100.0
166 (A)--V    20.497    27.1    79.3    20.7    100.0
167 (A)--V    20.948     9.1    58.3    41.7    100.0
168 (A)--V    21.275    22.5    91.5     8.5    100.0
169 (A)--V    21.722    22.3    87.1    12.9    100.0
170 (A)--V    22.117    18.8    47.1    52.9    100.0
171 (A)--V    22.797     7.7    79.1    20.9    100.0
172 (A)--V    23.231    35.2    80.8    19.2    100.0
173 (A)--V    23.552     0.5    34.8    65.2    100.0
174 (A)--V    23.613     5.2    91.0     9.0    100.0
175 (A)--V    24.354     3.3    68.7    31.3    100.0
176 (A)--V    24.895     2.1    75.0    25.0    100.0
177 (A)--V    25.414     0.6    59.8    40.2    100.0
178 (A)--V    25.533     0.3    84.4    15.6    100.0
179 (A)--V    25.800     6.8    59.9    40.1    100.0
180 (A)--V    26.172     0.6    79.0    21.0    100.0
181 (A)--V    26.394     0.7    94.8     5.2    100.0
182 (A)--V    27.175     5.7    65.2    34.8    100.0
183 (A)--V    27.442     3.3    81.0    19.0    100.0
184 (A)--V    27.499     1.5    82.4    17.6    100.0
185 (A)--V    27.964     1.7    85.3    14.7    100.0
186 (A)--V    28.120     7.7    82.2    17.8    100.0
187 (A)--V    28.351     0.2    91.0     9.0    100.0
188 (A)--V    28.446    19.2    76.4    23.6    100.0
189 (A)--V    28.694     2.5    55.2    44.8    100.0
190 (A)--V    28.905     7.0    70.0    30.0    100.0
191 (A)--V    28.973    10.3    90.6     9.4    100.0
192 (A)--V    29.284     1.6    87.6    12.4    100.0
193 (A)--V    30.201     6.8    92.5     7.5    100.0
194 (A)--V    30.644     8.5    93.3     6.7    100.0
195 (A)--V    30.725     7.8    78.9    21.1    100.0
196 (A)--V    31.369     3.8    82.2    17.8    100.0
197 (A)--V    32.055    23.3    84.6    15.4    100.0
198 (A)--V    32.112    23.8    90.0    10.0    100.0
199 (A)--V    32.941     9.3    65.4    34.6    100.0
200 (A)--V    33.389    23.4    86.2    13.8    100.0
201 (A)--V    33.928    17.9    87.9    12.1    100.0
202 (A)--V    34.659     3.6    24.2    75.8    100.0
203 (A)--V    35.353     9.5    39.1    60.9    100.0
204 (A)--V    35.407     3.7    41.8    58.2    100.0
205 (A)--V    36.018     2.9    32.9    67.1    100.0
206 (A)--V    36.235     3.5    72.7    27.3    100.0
207 (A)--V    36.713     8.3    53.8    46.2    100.0
```

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208 (A)--V    36.851    2.2    43.6    56.4    100.0
209 (A)--V    37.150    1.6    61.8    38.2    100.0
210 (A)--V    38.142    1.8    48.2    51.8    100.0
211 (A)--V    39.195    7.9    53.7    46.3    100.0
212 (A)--V    40.121    1.6    93.0     7.0    100.0
213 (A)--V    40.172    3.8    68.7    31.3    100.0
214 (A)--V    40.429    5.3    70.9    29.1    100.0
215 (A)--V    40.677    9.3    68.6    31.4    100.0
216 (A)--V    41.278   10.1    57.8    42.2    100.0
217 (A)--V    41.790   16.6    91.1     8.9    100.0
218 (A)--V    41.898   17.7    96.1     3.9    100.0
219 (A)--V    42.045   10.6    70.9    29.1    100.0
220 (A)--V    42.336    2.0    96.4     3.6    100.0
221 (A)--V    42.682    3.4    53.0    47.0    100.0
222 (A)--V    42.743    2.1    66.5    33.5    100.0
223 (A)--V    42.987    3.7    52.3    47.7    100.0
224 (A)--V    43.666   12.7    82.6    17.4    100.0
225 (A)--V    44.118   12.9    98.9     1.1    100.0
226 (A)--V    44.364   11.4    93.5     6.5    100.0
227 (A)--V    44.396    6.8    80.3    19.7    100.0
228 (A)--V    45.348    8.9    87.2    12.8    100.0
229 (A)--V    45.586    1.3    48.8    51.2    100.0
230 (A)--V    46.381    4.7    58.9    41.1    100.0
231 (A)--V    47.153   39.7    74.2    25.8    100.0
232 (A)--V    47.292    6.5    96.6     3.4    100.0
233 (A)--V    47.684    5.4    73.0    27.0    100.0
234 (A)--V    47.871   12.2    77.2    22.8    100.0
235 (A)--V    48.049    5.1    67.0    33.0    100.0
236 (A)--V    48.791    1.9    90.4     9.6    100.0
237 (A)--V    49.320    4.4    70.7    29.3    100.0
238 (A)--V    49.585   16.4    56.4    43.6    100.0
239 (A)--V    50.372    2.1    39.1    60.9    100.0
240 (A)--V    50.564   17.3    81.3    18.7    100.0
241 (A)--V    51.041   17.9    89.4    10.6    100.0
242 (A)--V    51.355   20.4    71.8    28.2    100.0
243 (A)--V    52.181   12.9    95.8     4.2    100.0
244 (A)--V    52.321    1.5    88.2    11.8    100.0
245 (A)--V    52.524    2.1    71.9    28.1    100.0
246 (A)--V    53.439    0.5    97.4     2.6    100.0
247 (A)--V    53.815    5.2    72.6    27.4    100.0
248 (A)--V    54.256    1.6    50.1    49.9    100.0
249 (A)--V    54.299    8.0    47.6    52.4    100.0
250 (A)--V    54.555    1.8    47.5    52.5    100.0
251 (A)--V    54.994   18.9    64.5    35.5    100.0
252 (A)--V    55.505   45.6    88.2    11.8    100.0
253 (A)--V    55.892   50.1    94.8     5.2    100.0
254 (A)--V    55.965   29.8    80.4    19.6    100.0
255 (A)--V    56.164    1.7    95.2     4.8    100.0
256 (A)--V    56.397    6.8    61.3    38.7    100.0
257 (A)--V    56.973   31.4    80.4    19.6    100.0
258 (A)--V    57.296   30.5    85.5    14.5    100.0
259 (A)--V    57.490    4.5    99.0     1.0    100.0
260 (A)--V    57.526    0.6    99.4     0.6    100.0
261 (A)--V    57.616    9.5    97.2     2.8    100.0
262 (A)--V    57.908   27.5    84.6    15.4    100.0
263 (A)--V    58.353    0.6    89.4    10.6    100.0
264 (A)--V    58.674   27.9    91.7     8.3    100.0
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265 (A)--V    59.231    28.0    94.5     5.5    100.0
266 (A)--V    60.171     3.9    89.0    11.0    100.0
267 (A)--V    61.049     5.8    57.6    42.4    100.0
268 (A)--V    61.322     3.9    92.0     8.0    100.0
269 (A)--V    61.803     2.5    49.5    50.5    100.0
270 (A)--V    62.270     0.1    94.6     5.4    100.0
271 (A)--V    63.924     3.2    34.3    65.7    100.0
272 (A)--V    65.134     6.0    51.6    48.4    100.0
273 (A)--V    65.763     2.3    27.0    73.0    100.0
274 (A)--V    66.524    25.5    85.4    14.6    100.0
275 (A)--V    66.750    21.4    80.7    19.3    100.0
276 (A)--V    67.235     5.8    54.0    46.0    100.0
277 (A)--V    67.600     9.2    55.2    44.8    100.0
278 (A)--V    67.744     1.1    11.7    88.3    100.0
279 (A)--V    68.073    20.8    55.9    44.1    100.0
280 (A)--V    69.185     1.9    57.8    42.2    100.0
281 (A)--V    69.889    13.8    60.2    39.8    100.0
282 (A)--V    71.434    23.1    93.0     7.0    100.0
283 (A)--V    71.548    35.0    75.6    24.4    100.0
284 (A)--V    71.817    43.9    72.0    28.0    100.0
285 (A)--V    73.344     8.8    18.4    81.6    100.0
286 (A)--V    73.626     6.9    25.8    74.2    100.0
287 (A)--V    74.486     1.2    37.0    63.0    100.0
288 (A)--V    74.941     1.9    79.3    20.7    100.0
289 (A)--V    75.010     7.8    90.3     9.7    100.0
290 (A)--V    75.836     1.5    55.4    44.6    100.0
291 (A)--V    76.321     0.7    42.5    57.5    100.0
292 (A)--V    76.738     3.0    30.7    69.3    100.0
293 (A)--V    77.999     1.1    22.7    77.3    100.0
294 (A)--V    78.628     8.4    39.8    60.2    100.0
295 (A)--V    79.005     1.2    50.0    50.0    100.0
296 (A)--V    79.331     2.5    60.9    39.1    100.0
297 (A)--V    79.848    13.8    74.1    25.9    100.0
298 (A)--V    80.474     6.2    76.5    23.5    100.0
299 (A)--V    81.192     1.9    97.5     2.5    100.0
300 (A)--V    81.426    11.3    95.3     4.7    100.0
301 (A)--V    81.466    29.0    99.3     0.7    100.0
302 (A)--V    81.826    12.0    67.0    33.0    100.0
303 (A)--V    81.967     6.9    94.1     5.9    100.0
304 (A)--V    82.492    12.4    63.9    36.1    100.0
305 (A)--V    82.629     4.0    22.4    77.6    100.0
306 (A)--V    83.157     0.4    96.2     3.8    100.0
307 (A)--V    83.714     1.3    94.7     5.3    100.0
308 (A)--V    83.991     4.1    73.2    26.8    100.0
309 (A)--V    84.115     0.6    98.4     1.6    100.0
310 (A)--V    84.371     2.2    94.0     6.0    100.0
311 (A)--V    84.727     2.7    71.3    28.7    100.0
312 (A)--V    84.952     5.1    49.5    50.5    100.0
313 (A)--V    85.619     1.8    92.0     8.0    100.0
314 (A)--V    86.956     3.0    62.3    37.7    100.0
315 (A)--V    88.342     1.1    71.0    29.0    100.0
316 (A)--V    89.324    11.8    57.4    42.6    100.0
317 (A)--V    89.813    11.2    95.3     4.7    100.0
318 (A)--V    89.925    11.8    71.7    28.3    100.0
319 (A)--V    89.983     5.6    84.4    15.6    100.0
320 (A)--V    90.481     4.1    72.0    28.0    100.0
321 (A)--V    93.485     4.0    62.1    37.9    100.0
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322 (A)--V      95.118     2.4     95.5     4.5     100.0
323 (A)--V      95.515     4.7     81.1    18.9     100.0
324 (A)--V      97.213     1.2     87.2    12.8     100.0
325 (A)--V      98.161     0.8     96.6     3.4     100.0
326 (A)--V      99.781     5.3     90.6     9.4     100.0
327 (A)--V     100.048    10.1     94.1     5.9     100.0
328 (A)--V     100.840     8.0     78.4    21.6     100.0
329 (A)--V     101.935    56.5     93.8     6.2     100.0
330 (A)--V     102.288    25.5     49.8    50.2     100.0
331 (A)--V     102.556     5.5     39.5    60.5     100.0
332 (A)--V     102.953     4.9     71.2    28.8     100.0
333 (A)--V     103.373     2.6     77.7    22.3     100.0
334 (A)--V     103.641     1.2     90.8     9.2     100.0
335 (A)--V     103.884     0.6     99.2     0.8     100.0
336 (A)--V     104.179     2.6     83.1    16.9     100.0
337 (A)--V     104.571     6.4     93.7     6.3     100.0
338 (A)--V     104.682     6.4     68.0    32.0     100.0
339 (A)--V     105.053     5.6     66.8    33.2     100.0
340 (A)--V     108.354    53.7     85.8    14.2     100.0
341 (A)--V     117.275     5.0     51.6    48.4     100.0
342 (A)--V     119.492     0.6     14.8    85.2     100.0
343 (A)--V     120.353     1.8     40.7    59.3     100.0
344 (A)--V     120.449     0.0     99.8     0.2     100.0
345 (A)--V     121.114     0.6     62.4    37.6     100.0
346 (A)--V     157.761    19.1     98.9     1.1     100.0
347 (A)--V     158.040    15.0     98.7     1.3     100.0
348 (A)--V     164.907    86.0     98.3     1.7     100.0
349 (A)--V     167.657    85.3     99.5     0.5     100.0
350 (A)--V     167.866    70.2     95.9     4.1     100.0
351 (A)--V     233.939    95.4     99.5     0.5     100.0
352 (A)--V     234.884    87.4     95.7     4.3     100.0
353 (A)--V     250.469    83.0     94.2     5.8     100.0
354 (A)--V     629.420     3.1     32.6    67.4     100.0
355 (A)--V     632.043    11.3     95.9     4.1     100.0
356 (A)--V     635.419     4.6     70.2    29.8     100.0
357 (A)--V     643.350     2.1     99.6     0.4     100.0
358 (A)--V     643.721     5.1     99.2     0.8     100.0
359 (A)--V     644.234    11.0     99.7     0.3     100.0
360 (A)--V     644.458     1.0     97.6     2.4     100.0
361 (A)--V     645.045     3.4     99.6     0.4     100.0
362 (A)--V     645.145     4.0     97.4     2.6     100.0
363 (A)--V     645.250     6.0     98.2     1.8     100.0
364 (A)--V     645.666     0.5     98.0     2.0     100.0
365 (A)--V     647.189     1.3     11.7    88.3     100.0
366 (A)--V     655.798     0.7      7.9    92.1     100.0
367 (A)--V     656.535     0.1      0.9    99.1     100.0
368 (A)--V     758.826    92.3     97.5     2.5     100.0
369 (A)--V     965.014     0.0      0.3    99.7     100.0
370 (A)--V     965.071     0.0      0.7    99.3     100.0
371 (A)--V    4855.671    98.9     99.9     0.1     100.0
372 (A)--V    4856.369    96.5     98.8     1.2     100.0
373 (A)--V    4869.646    93.5     97.8     2.2     100.0
374 (A)--V   12037.634    98.3     99.5     0.5     100.0
```

Full population analysis for complex *cis*-4 (optimized geometry):

```
************************************************************************
*                         VMOdes                                      *
* Virtual Molecular Orbital description Program, Revision 7.1          *
* Cite this work as: VMOdes Program, Revision A 7.1                    *
* V. N. Nemykin, P. Basu, 2001, 2003                                   *
* Department of Chemistry, Duquesne University, Pittsburgh, PA         *
************************************************************************


Input Gaussian file:
C:\Documents and Settings\hp\My Documents\Research Dr.
Nemykin\VMOdes\VModes\FcCN2-cis.gjf.out
Output VMOdes file: cis-FcCN2.out


Full point group is:  C1



Number of Basis Functions = 374

     67 Alpha electrons           67 Beta electrons


Group  1  is: Fe
This group consist of  1  subunits. The Basis Functions range is:
 106          161
Group  2  is: Fc
This group consist of  1  subunits. The Basis Functions range is:
 1           263
Group  3  is: CN
This group consist of  1  subunits. The Basis Functions range is:
 264          374
Group  4  is: Total
This group consist of  1  subunits. The Basis Functions range is:
 1           374


All MO's will be printed.

Molecular Orbitals Indexes, Energies, and Group Contributions
```

	Orbital			Group Number		
Number	Index	Energy,eV	1	2	3	4
1	(A)--O	-6933.177	100.0	100.0	0.0	100.0
2	(A)--O	-803.222	100.0	100.0	0.0	100.0
3	(A)--O	-693.703	100.0	100.0	0.0	100.0
4	(A)--O	-693.327	100.0	100.0	0.0	100.0
5	(A)--O	-693.299	100.0	100.0	0.0	100.0
6	(A)--O	-381.100	0.0	0.0	100.0	100.0
7	(A)--O	-380.827	0.0	0.0	100.0	100.0
8	(A)--O	-271.568	0.0	0.1	99.9	100.0
9	(A)--O	-270.958	0.0	0.0	100.0	100.0
10	(A)--O	-270.750	0.1	100.0	0.0	100.0
11	(A)--O	-270.634	0.0	0.1	99.9	100.0
12	(A)--O	-270.398	0.0	0.0	100.0	100.0
13	(A)--O	-270.295	0.1	100.0	0.0	100.0
14	(A)--O	-270.249	0.1	100.0	0.0	100.0
15	(A)--O	-270.232	0.1	100.0	0.0	100.0
16	(A)--O	-270.219	0.0	100.0	0.0	100.0

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17   (A)--O    -270.112   0.1     100.0    0.0     100.0
18   (A)--O    -270.103   0.1     100.0    0.0     100.0
19   (A)--O    -270.100   0.0     100.0    0.0     100.0
20   (A)--O    -270.094   0.0     100.0    0.0     100.0
21   (A)--O    -270.058   0.0     100.0    0.0     100.0
22   (A)--O    -88.472    100.0   100.0    0.0     100.0
23   (A)--O    -57.022    99.8    100.0    0.0     100.0
24   (A)--O    -56.018    99.9    100.0    0.0     100.0
25   (A)--O    -55.955    99.9    100.0    0.0     100.0
26   (A)--O    -23.182    4.0     46.0     54.0    100.0
27   (A)--O    -22.845    3.4     38.4     61.6    100.0
28   (A)--O    -22.615    0.1     0.7      99.3    100.0
29   (A)--O    -22.519    8.9     92.6     7.4     100.0
30   (A)--O    -21.134    1.3     17.7     82.3    100.0
31   (A)--O    -18.704    1.2     62.4     37.6    100.0
32   (A)--O    -18.369    1.8     97.4     2.6     100.0
33   (A)--O    -18.147    1.7     99.7     0.3     100.0
34   (A)--O    -18.134    1.7     99.9     0.1     100.0
35   (A)--O    -17.103    0.6     38.0     62.0    100.0
36   (A)--O    -14.962    0.5     43.3     56.7    100.0
37   (A)--O    -14.135    0.4     85.9     14.1    100.0
38   (A)--O    -13.961    1.8     95.4     4.6     100.0
39   (A)--O    -13.863    0.2     97.8     2.2     100.0
40   (A)--O    -13.841    0.5     99.4     0.6     100.0
41   (A)--O    -13.577    1.7     93.6     6.4     100.0
42   (A)--O    -13.363    0.4     55.5     44.5    100.0
43   (A)--O    -12.044    0.7     22.8     77.2    100.0
44   (A)--O    -11.050    32.0    84.0     16.0    100.0
45   (A)--O    -10.831    5.5     61.1     38.9    100.0
46   (A)--O    -10.637    7.2     95.4     4.6     100.0
47   (A)--O    -10.374    4.5     93.1     6.9     100.0
48   (A)--O    -10.328    1.4     99.4     0.6     100.0
49   (A)--O    -10.131    11.8    60.3     39.7    100.0
50   (A)--O    -10.054    1.0     95.0     5.0     100.0
51   (A)--O    -9.857     1.7     83.9     16.1    100.0
52   (A)--O    -9.720     0.3     99.7     0.3     100.0
53   (A)--O    -9.714     0.3     98.0     2.0     100.0
54   (A)--O    -9.473     8.5     77.1     22.9    100.0
55   (A)--O    -8.875     0.5     3.1      96.9    100.0
56   (A)--O    -8.824     0.2     5.2      94.8    100.0
57   (A)--O    -8.581     0.0     1.0      99.0    100.0
58   (A)--O    -8.503     0.5     7.4      92.6    100.0
59   (A)--O    -8.230     0.0     1.7      98.3    100.0
60   (A)--O    -7.758     12.6    55.3     44.7    100.0
61   (A)--O    -7.371     32.6    99.7     0.3     100.0
62   (A)--O    -7.127     23.4    82.4     17.6    100.0
63   (A)--O    -6.779     6.5     99.5     0.5     100.0
64   (A)--O    -6.390     6.2     58.4     41.6    100.0
65   (A)--O    -5.196     85.9    97.4     2.6     100.0
66   (A)--O    -4.974     59.1    96.6     3.4     100.0
67   (A)--O    -4.929     65.1    99.2     0.8     100.0
68   (A)--V    -3.381     12.4    23.8     76.2    100.0
69   (A)--V    -2.211     44.5    99.2     0.8     100.0
70   (A)--V    -2.130     39.9    92.8     7.2     100.0
71   (A)--V    -0.845     1.7     28.9     71.1    100.0
72   (A)--V    -0.219     1.3     31.4     68.6    100.0
73   (A)--V    -0.121     1.3     54.0     46.0    100.0
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74  (A)--V    0.146    6.3    95.2    4.8    100.0
75  (A)--V    0.267   21.2    96.8    3.2    100.0
76  (A)--V    0.286   15.7    97.5    2.5    100.0
77  (A)--V    0.393   39.5    93.9    6.1    100.0
78  (A)--V    0.855    4.2    48.3   51.7    100.0
79  (A)--V    1.041    9.4    57.8   42.2    100.0
80  (A)--V    1.265   14.9    91.5    8.5    100.0
81  (A)--V    1.486    2.5    87.7   12.3    100.0
82  (A)--V    1.706    4.2    70.5   29.5    100.0
83  (A)--V    2.129    5.4    80.5   19.5    100.0
84  (A)--V    2.167    2.2    79.8   20.2    100.0
85  (A)--V    2.500   15.7    83.6   16.4    100.0
86  (A)--V    2.632   64.0    92.8    7.2    100.0
87  (A)--V    2.654    6.5    86.4   13.6    100.0
88  (A)--V    2.801    3.0    83.6   16.4    100.0
89  (A)--V    3.044    3.6    63.8   36.2    100.0
90  (A)--V    3.132    4.2    74.9   25.1    100.0
91  (A)--V    3.794   24.4    70.6   29.4    100.0
92  (A)--V    4.008   31.7    95.5    4.5    100.0
93  (A)--V    4.267   75.5    98.6    1.4    100.0
94  (A)--V    4.397   22.8    65.0   35.0    100.0
95  (A)--V    4.725   24.2    94.3    5.7    100.0
96  (A)--V    4.841   22.4    94.2    5.8    100.0
97  (A)--V    4.939   25.1    98.9    1.1    100.0
98  (A)--V    5.014   55.4    83.2   16.8    100.0
99  (A)--V    5.329   42.7    82.9   17.1    100.0
100 (A)--V    5.587    0.9    84.2   15.8    100.0
101 (A)--V    6.154    5.9    77.0   23.0    100.0
102 (A)--V    6.614    0.6    88.1   11.9    100.0
103 (A)--V    6.671    2.9    81.2   18.8    100.0
104 (A)--V    7.373   30.0    83.2   16.8    100.0
105 (A)--V    7.544   12.2    74.7   25.3    100.0
106 (A)--V    7.739   34.1    84.0   16.0    100.0
107 (A)--V    7.948   48.8    91.1    8.9    100.0
108 (A)--V    8.054   10.7    37.9   62.1    100.0
109 (A)--V    8.146   17.4    64.0   36.0    100.0
110 (A)--V    8.248   23.6    76.2   23.8    100.0
111 (A)--V    8.302   37.6    94.5    5.5    100.0
112 (A)--V    8.495   16.9    72.5   27.5    100.0
113 (A)--V    8.726   17.5    40.8   59.2    100.0
114 (A)--V    8.798   58.4    90.4    9.6    100.0
115 (A)--V    9.064    8.9    70.9   29.1    100.0
116 (A)--V    9.731    7.5    80.7   19.3    100.0
117 (A)--V    9.767    4.0    94.1    5.9    100.0
118 (A)--V    9.972   59.9    86.4   13.6    100.0
119 (A)--V   10.400   61.9    86.5   13.5    100.0
120 (A)--V   10.505   18.4    69.4   30.6    100.0
121 (A)--V   10.645   15.7    54.2   45.8    100.0
122 (A)--V   11.100    4.5    49.9   50.1    100.0
123 (A)--V   11.330    8.3    64.8   35.2    100.0
124 (A)--V   11.583    1.3    33.2   66.8    100.0
125 (A)--V   11.795    0.9    26.9   73.1    100.0
126 (A)--V   12.002    7.1    61.1   38.9    100.0
127 (A)--V   12.443   16.8    96.4    3.6    100.0
128 (A)--V   12.512   10.7    72.5   27.5    100.0
129 (A)--V   12.614   16.9    94.3    5.7    100.0
130 (A)--V   12.715   15.1    88.8   11.2    100.0
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131 (A)--V    13.038   32.7   77.2   22.8   100.0
132 (A)--V    13.207   32.5   92.2    7.8   100.0
133 (A)--V    13.285   14.4   93.5    6.5   100.0
134 (A)--V    13.409   43.7   92.7    7.3   100.0
135 (A)--V    13.640   13.8   79.4   20.6   100.0
136 (A)--V    13.996   39.1   87.1   12.9   100.0
137 (A)--V    14.376   11.7   79.5   20.5   100.0
138 (A)--V    14.461    9.9   38.9   61.1   100.0
139 (A)--V    14.714    9.0   46.1   53.9   100.0
140 (A)--V    15.014   14.6   66.9   33.1   100.0
141 (A)--V    15.162    7.6   84.3   15.7   100.0
142 (A)--V    15.281    2.7   77.4   22.6   100.0
143 (A)--V    15.468    2.5   87.7   12.3   100.0
144 (A)--V    15.630    4.1   89.1   10.9   100.0
145 (A)--V    15.880    9.2   92.0    8.0   100.0
146 (A)--V    16.194    8.5   86.4   13.6   100.0
147 (A)--V    16.324    4.7   86.8   13.2   100.0
148 (A)--V    16.386    9.5   83.1   16.9   100.0
149 (A)--V    16.515    6.7   96.5    3.5   100.0
150 (A)--V    16.612    9.0   96.9    3.1   100.0
151 (A)--V    16.757   12.6   74.7   25.3   100.0
152 (A)--V    16.846   10.9   80.5   19.5   100.0
153 (A)--V    17.051    6.8   82.9   17.1   100.0
154 (A)--V    17.515    4.7   71.9   28.1   100.0
155 (A)--V    18.163    3.4   80.8   19.2   100.0
156 (A)--V    18.209    4.2   79.1   20.9   100.0
157 (A)--V    18.667    9.3   83.1   16.9   100.0
158 (A)--V    18.744    1.7   98.2    1.8   100.0
159 (A)--V    18.972    7.9   93.4    6.6   100.0
160 (A)--V    19.155    3.9   56.6   43.4   100.0
161 (A)--V    19.467   26.7   77.5   22.5   100.0
162 (A)--V    19.607    3.5   80.8   19.2   100.0
163 (A)--V    19.938   26.4   84.1   15.9   100.0
164 (A)--V    20.136   27.1   63.4   36.6   100.0
165 (A)--V    20.284   13.5   72.7   27.3   100.0
166 (A)--V    20.435   15.1   68.2   31.8   100.0
167 (A)--V    20.835   21.4   78.8   21.2   100.0
168 (A)--V    21.241   15.9   73.1   26.9   100.0
169 (A)--V    21.889   18.6   63.5   36.5   100.0
170 (A)--V    22.082    3.0   34.4   65.6   100.0
171 (A)--V    22.233    1.5   50.4   49.6   100.0
172 (A)--V    22.874   14.3   70.3   29.7   100.0
173 (A)--V    23.142   20.9   87.6   12.4   100.0
174 (A)--V    23.617   26.5   67.8   32.2   100.0
175 (A)--V    23.984    1.0   67.2   32.8   100.0
176 (A)--V    24.912    2.3   68.3   31.7   100.0
177 (A)--V    24.985    1.6   57.6   42.4   100.0
178 (A)--V    25.225    1.1   41.4   58.6   100.0
179 (A)--V    25.635    1.0   87.9   12.1   100.0
180 (A)--V    25.891    3.8   78.9   21.1   100.0
181 (A)--V    26.222    0.7   95.9    4.1   100.0
182 (A)--V    27.105    6.0   77.9   22.1   100.0
183 (A)--V    27.390    2.3   85.9   14.1   100.0
184 (A)--V    27.404    4.6   81.8   18.2   100.0
185 (A)--V    28.048    8.7   88.5   11.5   100.0
186 (A)--V    28.140    0.4   62.6   37.4   100.0
187 (A)--V    28.168    0.4   96.5    3.5   100.0
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188 (A)--V    28.388    1.9    81.3    18.7    100.0
189 (A)--V    28.566   14.9    82.4    17.6    100.0
190 (A)--V    28.783    4.5    58.6    41.4    100.0
191 (A)--V    28.973   14.9    89.3    10.7    100.0
192 (A)--V    29.641    0.7    20.6    79.4    100.0
193 (A)--V    30.336   13.4    46.5    53.5    100.0
194 (A)--V    30.541    6.9    87.2    12.8    100.0
195 (A)--V    30.794   11.9    68.7    31.3    100.0
196 (A)--V    31.183    1.8    82.5    17.5    100.0
197 (A)--V    31.675   11.3    53.6    46.4    100.0
198 (A)--V    32.072   29.1    97.6     2.4    100.0
199 (A)--V    32.526   19.6    91.7     8.3    100.0
200 (A)--V    33.456   21.2    94.1     5.9    100.0
201 (A)--V    33.783   12.8    54.6    45.4    100.0
202 (A)--V    34.307    1.9    28.3    71.7    100.0
203 (A)--V    35.222   12.2    29.8    70.2    100.0
204 (A)--V    35.405    4.8    51.8    48.2    100.0
205 (A)--V    36.073    2.0    29.3    70.7    100.0
206 (A)--V    36.183    2.3    82.3    17.7    100.0
207 (A)--V    36.290    9.4    68.6    31.4    100.0
208 (A)--V    36.642    3.5    34.2    65.8    100.0
209 (A)--V    37.175    6.8    76.3    23.7    100.0
210 (A)--V    38.359    1.0    44.7    55.3    100.0
211 (A)--V    38.935    7.3    65.4    34.6    100.0
212 (A)--V    39.948    1.6    97.7     2.3    100.0
213 (A)--V    40.245    2.3    95.1     4.9    100.0
214 (A)--V    40.507   13.8    72.8    27.2    100.0
215 (A)--V    40.811    2.5    33.7    66.3    100.0
216 (A)--V    41.297    7.1    41.2    58.8    100.0
217 (A)--V    41.696   14.3    72.7    27.3    100.0
218 (A)--V    41.823   10.8    88.9    11.1    100.0
219 (A)--V    41.894   17.6    87.5    12.5    100.0
220 (A)--V    42.054    5.8    67.7    32.3    100.0
221 (A)--V    42.393    1.6    84.4    15.6    100.0
222 (A)--V    42.770    1.4    75.2    24.8    100.0
223 (A)--V    43.477   14.6    83.7    16.3    100.0
224 (A)--V    43.795    6.5    66.5    33.5    100.0
225 (A)--V    44.147   10.4    89.8    10.2    100.0
226 (A)--V    44.665    2.8    59.6    40.4    100.0
227 (A)--V    44.899    8.9    76.6    23.4    100.0
228 (A)--V    45.123    3.1    55.4    44.6    100.0
229 (A)--V    45.619    8.9    67.1    32.9    100.0
230 (A)--V    46.125   13.3    89.3    10.7    100.0
231 (A)--V    46.236    6.3    34.4    65.6    100.0
232 (A)--V    47.196   17.8    71.7    28.3    100.0
233 (A)--V    47.259    9.1    88.7    11.3    100.0
234 (A)--V    47.579   11.3    81.7    18.3    100.0
235 (A)--V    48.038    2.6    60.6    39.4    100.0
236 (A)--V    48.730    1.8    84.7    15.3    100.0
237 (A)--V    49.235    3.2    68.6    31.4    100.0
238 (A)--V    49.757    3.9    54.0    46.0    100.0
239 (A)--V    50.000   16.2    98.0     2.0    100.0
240 (A)--V    50.665   16.0    85.7    14.3    100.0
241 (A)--V    51.140   24.9    61.4    38.6    100.0
242 (A)--V    51.825   25.8    85.0    15.0    100.0
243 (A)--V    52.091    9.7    94.9     5.1    100.0
244 (A)--V    52.285    3.6    91.7     8.3    100.0
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245 (A)--V    52.739    1.1    84.2    15.8    100.0
246 (A)--V    53.338    0.4    92.7    7.3     100.0
247 (A)--V    53.419    9.7    36.9    63.1    100.0
248 (A)--V    53.964    12.7   86.4    13.6    100.0
249 (A)--V    54.379    29.3   70.8    29.2    100.0
250 (A)--V    54.730    6.4    53.7    46.3    100.0
251 (A)--V    54.971    20.0   57.8    42.2    100.0
252 (A)--V    55.590    43.6   88.8    11.2    100.0
253 (A)--V    55.663    24.6   70.5    29.5    100.0
254 (A)--V    55.952    6.5    59.3    40.7    100.0
255 (A)--V    55.961    23.9   76.7    23.3    100.0
256 (A)--V    56.110    2.6    94.6    5.4     100.0
257 (A)--V    57.018    13.9   79.2    20.8    100.0
258 (A)--V    57.233    30.7   90.2    9.8     100.0
259 (A)--V    57.415    5.1    97.6    2.4     100.0
260 (A)--V    57.476    0.3    99.5    0.5     100.0
261 (A)--V    57.605    6.4    96.8    3.2     100.0
262 (A)--V    57.719    36.3   93.2    6.8     100.0
263 (A)--V    58.458    20.4   93.1    6.9     100.0
264 (A)--V    58.957    0.9    59.2    40.8    100.0
265 (A)--V    59.115    24.5   94.1    5.9     100.0
266 (A)--V    59.737    1.5    71.0    29.0    100.0
267 (A)--V    60.468    0.7    54.2    45.8    100.0
268 (A)--V    61.221    22.6   84.6    15.4    100.0
269 (A)--V    61.256    0.5    89.2    10.8    100.0
270 (A)--V    62.149    0.2    95.4    4.6     100.0
271 (A)--V    63.964    3.1    80.9    19.1    100.0
272 (A)--V    64.832    8.5    53.7    46.3    100.0
273 (A)--V    65.466    2.8    39.1    60.9    100.0
274 (A)--V    66.367    3.8    29.7    70.3    100.0
275 (A)--V    66.460    26.1   83.9    16.1    100.0
276 (A)--V    66.837    1.6    12.2    87.8    100.0
277 (A)--V    67.308    13.4   64.4    35.6    100.0
278 (A)--V    67.342    13.7   82.8    17.2    100.0
279 (A)--V    69.545    18.3   62.3    37.7    100.0
280 (A)--V    69.961    18.8   67.3    32.7    100.0
281 (A)--V    70.718    0.8    27.3    72.7    100.0
282 (A)--V    71.112    18.4   63.9    36.1    100.0
283 (A)--V    71.432    61.8   85.7    14.3    100.0
284 (A)--V    71.780    37.4   81.3    18.7    100.0
285 (A)--V    73.106    11.2   34.1    65.9    100.0
286 (A)--V    73.836    1.4    34.6    65.4    100.0
287 (A)--V    73.925    4.9    24.3    75.7    100.0
288 (A)--V    74.739    1.8    86.6    13.4    100.0
289 (A)--V    74.837    4.0    87.2    12.8    100.0
290 (A)--V    75.155    0.3    54.1    45.9    100.0
291 (A)--V    76.042    1.2    38.7    61.3    100.0
292 (A)--V    76.318    12.0   60.9    39.1    100.0
293 (A)--V    77.899    2.1    68.4    31.6    100.0
294 (A)--V    78.928    1.2    53.1    46.9    100.0
295 (A)--V    79.177    2.6    51.5    48.5    100.0
296 (A)--V    79.453    6.3    55.2    44.8    100.0
297 (A)--V    79.837    4.8    62.4    37.6    100.0
298 (A)--V    80.287    4.2    59.6    40.4    100.0
299 (A)--V    81.143    0.4    98.8    1.2     100.0
300 (A)--V    81.312    26.3   91.6    8.4     100.0
301 (A)--V    81.360    19.0   95.0    5.0     100.0
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302 (A)--V     81.730     6.5    97.9     2.1    100.0
303 (A)--V     81.874    18.5    86.1    13.9    100.0
304 (A)--V     82.666     5.1    73.1    26.9    100.0
305 (A)--V     82.996     1.7    88.1    11.9    100.0
306 (A)--V     83.276     0.5    77.2    22.8    100.0
307 (A)--V     83.605     2.8    67.5    32.5    100.0
308 (A)--V     84.030     0.4    94.7     5.3    100.0
309 (A)--V     84.143     0.5    72.0    28.0    100.0
310 (A)--V     84.382     3.6    53.0    47.0    100.0
311 (A)--V     84.668     0.9    62.0    38.0    100.0
312 (A)--V     84.735     0.5    44.6    55.4    100.0
313 (A)--V     85.595     1.6    63.1    36.9    100.0
314 (A)--V     86.909     6.2    83.2    16.8    100.0
315 (A)--V     87.753     0.9    75.0    25.0    100.0
316 (A)--V     89.355    16.2    69.9    30.1    100.0
317 (A)--V     89.696    13.1    90.5     9.5    100.0
318 (A)--V     89.859     4.5    87.6    12.4    100.0
319 (A)--V     89.999     7.6    62.3    37.7    100.0
320 (A)--V     90.355     5.3    80.4    19.6    100.0
321 (A)--V     94.163     2.6    57.7    42.3    100.0
322 (A)--V     94.977     2.6    90.6     9.4    100.0
323 (A)--V     95.374     2.8    59.2    40.8    100.0
324 (A)--V     96.631     1.8    85.9    14.1    100.0
325 (A)--V     98.130     0.6    95.5     4.5    100.0
326 (A)--V     99.684     6.7    93.7     6.3    100.0
327 (A)--V     99.976     9.7    96.3     3.7    100.0
328 (A)--V    100.795    11.2    85.9    14.1    100.0
329 (A)--V    101.824    59.2    96.9     3.1    100.0
330 (A)--V    102.284    19.1    36.1    63.9    100.0
331 (A)--V    102.824     4.2    31.3    68.7    100.0
332 (A)--V    103.103     2.0    61.5    38.5    100.0
333 (A)--V    103.229     2.6    89.1    10.9    100.0
334 (A)--V    103.620     1.6    94.7     5.3    100.0
335 (A)--V    103.770     0.5    98.7     1.3    100.0
336 (A)--V    103.998     1.7    87.1    12.9    100.0
337 (A)--V    104.577     6.6    94.4     5.6    100.0
338 (A)--V    104.779    10.3    93.4     6.6    100.0
339 (A)--V    105.731     1.2    24.4    75.6    100.0
340 (A)--V    108.073    60.4    90.1     9.9    100.0
341 (A)--V    116.606     4.5    53.8    46.2    100.0
342 (A)--V    119.350     2.4    24.4    75.6    100.0
343 (A)--V    120.203     0.1    51.5    48.5    100.0
344 (A)--V    120.399     0.0    98.9     1.1    100.0
345 (A)--V    120.992     0.3    41.3    58.7    100.0
346 (A)--V    157.698    19.2    96.0     4.0    100.0
347 (A)--V    157.915    14.9    98.9     1.1    100.0
348 (A)--V    164.839    86.0    98.6     1.4    100.0
349 (A)--V    167.579    84.0    97.5     2.5    100.0
350 (A)--V    167.783    68.4    94.3     5.7    100.0
351 (A)--V    233.859    95.1    99.1     0.9    100.0
352 (A)--V    234.839    88.1    95.5     4.5    100.0
353 (A)--V    250.185    88.6    97.3     2.7    100.0
354 (A)--V    629.455     3.3    39.2    60.8    100.0
355 (A)--V    631.990    11.5    95.3     4.7    100.0
356 (A)--V    635.505     4.4    65.9    34.1    100.0
357 (A)--V    643.268     2.1    99.7     0.3    100.0
358 (A)--V    643.670     4.8    99.4     0.6    100.0
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359 (A)--V     644.177    11.1    99.8     0.2    100.0
360 (A)--V     644.475     0.1    98.8     1.2    100.0
361 (A)--V     644.858     9.5    97.1     2.9    100.0
362 (A)--V     645.012     2.0    98.8     1.2    100.0
363 (A)--V     645.148     0.3    99.7     0.3    100.0
364 (A)--V     645.509     0.6    99.2     0.8    100.0
365 (A)--V     647.144     1.6     9.8    90.2    100.0
366 (A)--V     655.786     0.5     8.1    91.9    100.0
367 (A)--V     657.083     0.2     3.1    96.9    100.0
368 (A)--V     758.516    94.6    98.6     1.4    100.0
369 (A)--V     964.735     0.0     1.2    98.8    100.0
370 (A)--V     965.318     0.0     0.3    99.7    100.0
371 (A)--V    4855.598    98.9    99.8     0.2    100.0
372 (A)--V    4856.306    96.9    98.9     1.1    100.0
373 (A)--V    4869.429    95.8    99.0     1.0    100.0
374 (A)--V   12037.311    98.8    99.7     0.3    100.0
```

Full population analysis for complex *trans*-3 (optimized geometry):

```
************************************************************************
*                         VMOdes                                      *
* Virtual Molecular Orbital description Program, Revision 7.1         *
* Cite this work as: VMOdes Program, Revision A 7.1                   *
* V. N. Nemykin, P. Basu, 2001, 2003                                 *
* Department of Chemistry, Duquesne University, Pittsburgh, PA        *
************************************************************************


Input Gaussian file:
C:\Documents and Settings\hp\My Documents\Research Dr.
Nemykin\VMOdes\VMOdes\FcCN-Iodo-trans.gjf.out
Output VMOdes file: trans-FcCN-Iodo.out


Full point group is:  C1


Number of Basis Functions = 349

    64 Alpha electrons          64 Beta electrons

Group  1  is: Fe
This group consist of  1  subunits. The Basis Functions range is:
 1            56
Group  2  is: Fc
This group consist of  2  subunits. The Basis Functions range is:
 1            146
 219          335
Group  3  is: CN
This group consist of  1  subunits. The Basis Functions range is:
 183          218
Group  4  is: I
This group consist of  1  subunits. The Basis Functions range is:
 336          346
Group  5  is: Lig
This group consist of  2  subunits. The Basis Functions range is:
 147          218
 336          349
```

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Group  6  is: Total
This group consist of  1  subunits. The Basis Functions range is:
 1              349

All MO's will be printed.

Molecular Orbitals Indexes, Energies, and Group Contributions
```

	Orbital				Group Number			
Number	Index	Energy,eV	1	2	3	4	5	6
1	(A)--O	-6932.938	100.0	100.0	0.0	0.0	0.0	100.0
2	(A)--O	-802.982	100.0	100.0	0.0	0.0	0.0	100.0
3	(A)--O	-693.466	100.0	100.0	0.0	0.0	0.0	100.0
4	(A)--O	-693.084	100.0	100.0	0.0	0.0	0.0	100.0
5	(A)--O	-693.060	100.0	100.0	0.0	0.0	0.0	100.0
6	(A)--O	-380.645	0.0	0.0	99.9	0.0	100.0	100.0
7	(A)--O	-271.721	0.0	0.1	0.0	0.0	99.9	100.0
8	(A)--O	-270.546	0.0	0.9	0.0	0.0	99.1	100.0
9	(A)--O	-270.544	0.1	99.1	0.0	0.0	0.9	100.0
10	(A)--O	-270.289	0.0	0.0	99.9	0.0	100.0	100.0
11	(A)--O	-270.012	0.1	100.0	0.0	0.0	0.0	100.0
12	(A)--O	-269.988	0.1	100.0	0.0	0.0	0.0	100.0
13	(A)--O	-269.978	0.1	100.0	0.0	0.0	0.0	100.0
14	(A)--O	-269.970	0.0	100.0	0.0	0.0	0.0	100.0
15	(A)--O	-269.910	0.1	100.0	0.0	0.0	0.0	100.0
16	(A)--O	-269.902	0.0	100.0	0.0	0.0	0.0	100.0
17	(A)--O	-269.889	0.1	100.0	0.0	0.0	0.0	100.0
18	(A)--O	-269.876	0.0	100.0	0.0	0.0	0.0	100.0
19	(A)--O	-269.867	0.0	100.0	0.0	0.0	0.0	100.0
20	(A)--O	-88.231	100.0	100.0	0.0	0.0	0.0	100.0
21	(A)--O	-56.788	99.8	100.0	0.0	0.0	0.0	100.0
22	(A)--O	-55.770	99.9	100.0	0.0	0.0	0.0	100.0
23	(A)--O	-55.715	99.9	100.0	0.0	0.0	0.0	100.0
24	(A)--O	-22.798	7.3	84.0	9.6	0.2	16.0	100.0
25	(A)--O	-22.499	1.2	11.7	84.8	0.0	88.3	100.0
26	(A)--O	-22.304	8.8	90.4	8.4	0.1	9.6	100.0
27	(A)--O	-20.763	1.9	21.5	9.8	5.3	78.5	100.0
28	(A)--O	-18.420	1.1	58.1	8.3	7.1	41.9	100.0
29	(A)--O	-18.121	1.8	90.6	0.2	5.8	9.4	100.0
30	(A)--O	-17.946	1.8	99.3	0.0	0.3	0.7	100.0
31	(A)--O	-17.936	1.6	99.5	0.0	0.5	0.5	100.0
32	(A)--O	-17.732	0.8	30.9	4.1	58.0	69.1	100.0
33	(A)--O	-15.697	0.5	34.8	11.0	19.1	65.2	100.0
34	(A)--O	-13.984	0.4	66.3	11.6	0.5	33.7	100.0
35	(A)--O	-13.928	0.5	66.5	9.4	6.5	33.5	100.0
36	(A)--O	-13.717	1.5	97.3	0.7	0.1	2.7	100.0
37	(A)--O	-13.659	0.1	99.4	0.0	0.2	0.6	100.0
38	(A)--O	-13.619	0.9	98.9	0.2	0.2	1.1	100.0
39	(A)--O	-13.355	1.6	97.9	0.5	0.0	2.1	100.0
40	(A)--O	-12.141	0.8	36.2	8.8	2.5	63.8	100.0
41	(A)--O	-11.035	2.5	51.8	2.9	11.2	48.2	100.0
42	(A)--O	-10.726	36.9	91.8	0.7	0.5	8.2	100.0
43	(A)--O	-10.404	8.0	98.1	0.8	0.4	1.9	100.0
44	(A)--O	-10.214	5.8	94.0	0.9	2.1	6.0	100.0
45	(A)--O	-10.124	1.1	98.7	0.5	0.2	1.3	100.0

46	(A)--O	-9.959	1.0	71.9	5.2	5.9	28.1	100.0
47	(A)--O	-9.832	0.9	92.9	2.6	1.0	7.1	100.0
48	(A)--O	-9.638	10.1	58.8	13.1	5.2	41.2	100.0
49	(A)--O	-9.536	0.4	98.7	0.2	0.5	1.3	100.0
50	(A)--O	-9.522	0.4	99.8	0.1	0.0	0.2	100.0
51	(A)--O	-9.141	6.3	50.7	32.5	1.4	49.3	100.0
52	(A)--O	-9.093	0.9	37.7	17.6	24.2	62.3	100.0
53	(A)--O	-8.423	0.5	4.2	71.2	4.1	95.8	100.0
54	(A)--O	-8.065	0.5	8.5	75.6	3.4	91.5	100.0
55	(A)--O	-8.019	4.0	27.6	37.4	17.1	72.4	100.0
56	(A)--O	-7.134	32.2	98.0	0.2	1.6	2.0	100.0
57	(A)--O	-7.094	25.2	75.7	0.6	20.9	24.3	100.0
58	(A)--O	-6.818	1.1	18.6	0.8	69.9	81.4	100.0
59	(A)--O	-6.612	4.8	64.4	1.1	32.7	35.6	100.0
60	(A)--O	-6.486	4.2	65.3	0.2	33.5	34.7	100.0
61	(A)--O	-6.074	4.9	35.2	12.2	22.6	64.8	100.0
62	(A)--O	-4.960	86.1	97.7	0.2	0.1	2.3	100.0
63	(A)--O	-4.735	59.7	97.1	0.7	0.1	2.9	100.0
64	(A)--O	-4.689	64.6	99.0	0.0	0.5	1.0	100.0
65	(A)--V	-2.792	17.6	34.9	10.5	5.9	65.1	100.0
66	(A)--V	-2.418	1.4	7.8	2.5	38.7	92.2	100.0
67	(A)--V	-1.954	41.9	92.8	0.4	2.4	7.2	100.0
68	(A)--V	-1.757	33.1	83.7	3.6	0.7	16.3	100.0
69	(A)--V	-0.169	10.8	29.5	29.1	6.6	70.5	100.0
70	(A)--V	0.391	0.6	96.3	1.7	0.8	3.7	100.0
71	(A)--V	0.437	4.9	97.1	0.7	1.1	2.9	100.0
72	(A)--V	0.476	22.2	97.4	0.4	0.3	2.6	100.0
73	(A)--V	0.488	47.3	88.4	1.3	3.5	11.6	100.0
74	(A)--V	0.788	14.9	85.5	8.6	1.6	14.5	100.0
75	(A)--V	0.970	13.9	42.3	7.1	42.2	57.7	100.0
76	(A)--V	1.038	8.6	47.9	1.9	46.1	52.1	100.0
77	(A)--V	1.125	17.5	59.7	5.3	30.7	40.3	100.0
78	(A)--V	1.647	25.4	87.3	2.3	7.1	12.7	100.0
79	(A)--V	1.728	0.6	75.3	5.9	4.3	24.7	100.0
80	(A)--V	1.812	6.6	87.8	2.4	3.6	12.2	100.0
81	(A)--V	2.166	8.8	64.2	13.1	2.3	35.8	100.0
82	(A)--V	2.362	5.1	65.0	4.8	3.0	35.0	100.0
83	(A)--V	2.488	18.5	87.5	2.0	1.3	12.5	100.0
84	(A)--V	2.757	19.6	92.4	0.1	0.7	7.6	100.0
85	(A)--V	2.905	39.3	80.5	7.0	2.9	19.5	100.0
86	(A)--V	2.954	12.3	93.1	1.4	2.4	6.9	100.0
87	(A)--V	3.072	9.5	79.8	2.7	5.3	20.2	100.0
88	(A)--V	3.351	8.7	78.0	5.5	2.9	22.0	100.0
89	(A)--V	3.988	23.7	86.3	8.9	0.5	13.7	100.0
90	(A)--V	4.155	26.4	86.4	4.6	0.3	13.6	100.0
91	(A)--V	4.269	38.5	74.1	6.0	0.8	25.9	100.0
92	(A)--V	4.633	73.1	97.2	1.6	0.2	2.8	100.0
93	(A)--V	4.907	19.4	89.1	2.5	0.6	10.9	100.0
94	(A)--V	4.970	5.5	93.3	0.5	0.3	6.7	100.0
95	(A)--V	5.126	26.7	95.7	0.7	0.2	4.3	100.0
96	(A)--V	5.211	26.8	93.3	0.3	0.2	6.7	100.0
97	(A)--V	5.393	85.1	99.1	0.2	0.0	0.9	100.0
98	(A)--V	5.649	1.1	74.1	15.7	0.3	25.9	100.0
99	(A)--V	6.264	1.0	92.4	0.7	0.0	7.6	100.0
100	(A)--V	6.645	1.4	89.8	5.4	0.1	10.2	100.0
101	(A)--V	7.210	1.5	79.3	1.1	0.2	20.7	100.0
102	(A)--V	7.347	9.7	43.5	26.3	0.2	56.5	100.0

103 (A)--V	7.540	9.8	82.7	4.4	0.3	17.3	100.0
104 (A)--V	8.047	54.4	79.5	9.2	0.0	20.5	100.0
105 (A)--V	8.208	39.3	93.6	1.3	0.1	6.4	100.0
106 (A)--V	8.289	37.1	95.0	1.1	0.1	5.0	100.0
107 (A)--V	8.378	19.1	69.3	9.1	0.3	30.7	100.0
108 (A)--V	8.535	40.0	93.1	3.5	0.0	6.9	100.0
109 (A)--V	8.703	25.3	87.8	1.9	0.7	12.2	100.0
110 (A)--V	8.904	21.8	78.9	2.4	0.2	21.1	100.0
111 (A)--V	9.045	43.8	87.5	2.8	0.1	12.5	100.0
112 (A)--V	9.524	11.2	62.6	5.2	0.5	37.4	100.0
113 (A)--V	9.547	41.4	92.6	2.3	0.1	7.4	100.0
114 (A)--V	9.948	2.6	82.2	0.8	0.2	17.8	100.0
115 (A)--V	10.087	4.6	70.2	1.4	0.6	29.8	100.0
116 (A)--V	10.292	48.5	79.4	3.8	0.1	20.6	100.0
117 (A)--V	10.535	25.4	63.8	2.5	0.4	36.2	100.0
118 (A)--V	10.745	50.9	85.1	3.2	0.2	14.9	100.0
119 (A)--V	11.149	32.4	82.5	1.6	0.1	17.5	100.0
120 (A)--V	11.574	1.9	36.6	12.0	1.4	63.4	100.0
121 (A)--V	11.635	10.5	84.5	2.5	0.1	15.5	100.0
122 (A)--V	11.975	12.1	81.7	1.8	2.4	18.3	100.0
123 (A)--V	12.332	7.9	77.4	8.1	0.2	22.6	100.0
124 (A)--V	12.623	9.1	60.9	16.4	5.7	39.1	100.0
125 (A)--V	12.763	14.4	88.6	1.9	0.8	11.4	100.0
126 (A)--V	12.935	11.2	79.1	1.0	3.7	20.9	100.0
127 (A)--V	13.011	13.8	69.9	4.5	2.0	30.1	100.0
128 (A)--V	13.149	22.2	79.4	10.3	0.6	20.6	100.0
129 (A)--V	13.580	17.0	91.1	3.0	1.1	8.9	100.0
130 (A)--V	13.618	20.9	94.0	0.7	0.5	6.0	100.0
131 (A)--V	13.668	59.5	92.9	0.3	0.3	7.1	100.0
132 (A)--V	14.252	25.2	85.7	1.2	0.4	14.3	100.0
133 (A)--V	14.557	9.4	65.2	14.0	0.3	34.8	100.0
134 (A)--V	14.598	14.5	86.1	1.4	0.2	13.9	100.0
135 (A)--V	14.741	34.0	83.5	7.5	0.2	16.5	100.0
136 (A)--V	15.006	12.5	77.1	3.3	0.2	22.9	100.0
137 (A)--V	15.192	2.2	56.1	13.9	1.6	43.9	100.0
138 (A)--V	15.597	1.2	95.2	0.8	0.1	4.8	100.0
139 (A)--V	15.753	8.7	67.1	4.6	0.6	32.9	100.0
140 (A)--V	15.932	6.5	75.5	5.5	0.1	24.5	100.0
141 (A)--V	16.060	6.3	78.0	5.0	0.3	22.0	100.0
142 (A)--V	16.151	6.4	92.5	0.6	0.2	7.5	100.0
143 (A)--V	16.508	12.0	69.9	0.9	1.1	30.1	100.0
144 (A)--V	16.630	3.1	97.4	0.4	0.1	2.6	100.0
145 (A)--V	16.643	3.3	96.6	1.5	0.1	3.4	100.0
146 (A)--V	16.772	13.5	98.9	0.2	0.1	1.1	100.0
147 (A)--V	16.948	5.8	90.4	1.5	0.1	9.6	100.0
148 (A)--V	17.064	9.3	82.9	4.8	0.2	17.1	100.0
149 (A)--V	17.700	3.6	59.8	11.1	0.6	40.2	100.0
150 (A)--V	17.879	5.5	51.6	1.9	1.6	48.4	100.0
151 (A)--V	18.277	4.6	91.6	3.0	0.7	8.4	100.0
152 (A)--V	18.596	4.4	88.5	3.3	0.2	11.5	100.0
153 (A)--V	18.827	10.4	83.4	11.6	0.9	16.6	100.0
154 (A)--V	18.966	0.8	86.1	0.8	0.2	13.9	100.0
155 (A)--V	19.264	5.9	89.8	3.7	0.3	10.2	100.0
156 (A)--V	19.465	7.9	88.2	1.4	0.1	11.8	100.0
157 (A)--V	19.617	8.0	80.6	2.1	0.4	19.4	100.0
158 (A)--V	19.860	9.7	75.5	4.3	0.3	24.5	100.0
159 (A)--V	20.396	28.8	67.4	3.4	0.0	32.6	100.0

160 (A)--V	20.454	14.5	51.2	24.2	0.1	48.8	100.0
161 (A)--V	20.954	16.6	64.6	13.1	0.3	35.4	100.0
162 (A)--V	21.479	15.9	84.1	5.0	5.3	15.9	100.0
163 (A)--V	21.730	19.3	85.7	0.9	1.9	14.3	100.0
164 (A)--V	22.115	10.8	31.0	32.0	1.3	69.0	100.0
165 (A)--V	22.489	9.6	85.8	1.4	0.0	14.2	100.0
166 (A)--V	23.224	43.6	92.5	0.1	0.1	7.5	100.0
167 (A)--V	23.318	25.1	80.1	2.3	0.0	19.9	100.0
168 (A)--V	23.891	4.8	92.0	1.8	0.0	8.0	100.0
169 (A)--V	24.530	2.9	90.4	0.4	0.1	9.6	100.0
170 (A)--V	25.554	0.3	99.0	0.1	0.0	1.0	100.0
171 (A)--V	25.569	0.8	59.6	0.5	0.3	40.4	100.0
172 (A)--V	25.725	3.5	90.6	0.9	0.0	9.4	100.0
173 (A)--V	26.098	1.7	22.3	16.3	0.3	77.7	100.0
174 (A)--V	26.434	2.8	98.5	0.1	0.1	1.5	100.0
175 (A)--V	27.481	3.0	93.0	0.2	0.1	7.0	100.0
176 (A)--V	27.531	7.4	99.0	0.6	0.1	1.0	100.0
177 (A)--V	27.823	8.0	86.1	1.0	0.1	13.9	100.0
178 (A)--V	28.011	5.5	96.7	1.3	0.1	3.3	100.0
179 (A)--V	28.376	2.7	97.4	0.7	0.1	2.6	100.0
180 (A)--V	28.491	2.1	97.4	0.3	0.0	2.6	100.0
181 (A)--V	28.712	14.4	99.2	0.1	0.0	0.8	100.0
182 (A)--V	28.873	2.9	97.0	0.4	0.0	3.0	100.0
183 (A)--V	29.387	14.1	96.7	0.9	0.2	3.3	100.0
184 (A)--V	29.668	2.8	84.4	2.5	0.2	15.6	100.0
185 (A)--V	30.478	10.8	95.4	1.4	0.0	4.6	100.0
186 (A)--V	30.652	39.0	94.4	0.5	0.0	5.6	100.0
187 (A)--V	30.795	8.8	91.5	3.2	0.0	8.5	100.0
188 (A)--V	31.071	5.3	93.3	0.1	0.1	6.7	100.0
189 (A)--V	32.244	19.6	90.8	2.9	0.2	9.2	100.0
190 (A)--V	32.313	30.1	99.4	0.3	0.0	0.6	100.0
191 (A)--V	33.199	8.4	78.3	4.1	0.2	21.7	100.0
192 (A)--V	33.824	4.8	46.6	30.8	0.1	53.4	100.0
193 (A)--V	34.385	26.3	96.3	1.8	0.0	3.7	100.0
194 (A)--V	34.719	9.7	42.6	49.6	0.7	57.4	100.0
195 (A)--V	35.390	5.1	29.3	43.4	0.7	70.7	100.0
196 (A)--V	35.704	21.4	81.4	7.8	0.2	18.6	100.0
197 (A)--V	36.619	15.4	91.3	6.8	0.1	8.7	100.0
198 (A)--V	36.950	15.0	91.3	7.3	0.1	8.7	100.0
199 (A)--V	37.917	2.6	20.0	30.1	0.5	80.0	100.0
200 (A)--V	38.891	3.6	98.2	0.5	0.0	1.8	100.0
201 (A)--V	39.426	18.0	67.8	2.5	0.6	32.2	100.0
202 (A)--V	39.976	1.3	85.9	2.5	0.1	14.1	100.0
203 (A)--V	40.212	3.2	81.2	1.9	0.1	18.8	100.0
204 (A)--V	40.612	5.1	66.4	5.7	0.3	33.6	100.0
205 (A)--V	41.023	3.5	38.8	9.2	0.6	61.2	100.0
206 (A)--V	41.471	9.6	90.6	2.1	0.0	9.4	100.0
207 (A)--V	41.956	18.0	90.2	1.2	0.1	9.8	100.0
208 (A)--V	42.054	17.4	91.0	1.1	0.0	9.0	100.0
209 (A)--V	42.324	12.2	92.0	1.8	0.1	8.0	100.0
210 (A)--V	42.475	3.9	95.0	0.6	0.1	5.0	100.0
211 (A)--V	42.690	4.5	49.2	6.1	0.7	50.8	100.0
212 (A)--V	43.379	8.5	94.5	1.5	0.0	5.5	100.0
213 (A)--V	44.026	8.7	93.4	1.4	0.0	6.6	100.0
214 (A)--V	44.273	9.0	95.5	0.3	0.0	4.5	100.0
215 (A)--V	44.423	8.7	76.2	0.8	0.1	23.8	100.0
216 (A)--V	45.343	9.6	94.2	1.1	0.1	5.8	100.0

217 (A)--V	45.407	2.1	55.2	3.4	0.1	44.8	100.0
218 (A)--V	46.125	14.9	91.7	3.3	0.1	8.3	100.0
219 (A)--V	46.693	5.1	70.3	6.0	0.1	29.7	100.0
220 (A)--V	46.936	4.5	45.6	13.9	0.2	54.4	100.0
221 (A)--V	47.275	16.2	59.0	3.5	0.3	41.0	100.0
222 (A)--V	47.664	8.9	96.5	0.5	0.0	3.5	100.0
223 (A)--V	48.050	12.9	97.1	1.2	0.0	2.9	100.0
224 (A)--V	48.525	4.5	44.1	4.3	0.3	55.9	100.0
225 (A)--V	48.975	3.4	58.6	3.1	0.2	41.4	100.0
226 (A)--V	49.152	8.1	83.9	1.4	0.2	16.1	100.0
227 (A)--V	49.498	3.9	88.8	3.7	0.1	11.2	100.0
228 (A)--V	50.628	24.3	93.6	1.0	0.0	6.4	100.0
229 (A)--V	51.263	16.9	96.2	0.3	0.0	3.8	100.0
230 (A)--V	51.373	30.9	72.1	3.3	0.1	27.9	100.0
231 (A)--V	51.770	2.2	90.6	2.0	0.0	9.4	100.0
232 (A)--V	52.286	12.2	99.4	0.1	0.0	0.6	100.0
233 (A)--V	52.510	2.2	99.6	0.0	0.0	0.4	100.0
234 (A)--V	53.602	1.4	98.8	0.5	0.0	1.2	100.0
235 (A)--V	54.331	5.8	59.4	3.7	0.0	40.6	100.0
236 (A)--V	54.618	3.3	37.9	8.2	0.1	62.1	100.0
237 (A)--V	54.916	9.6	86.2	3.9	0.0	13.8	100.0
238 (A)--V	55.389	18.2	60.2	5.4	0.1	39.8	100.0
239 (A)--V	55.775	46.5	94.1	0.2	0.0	5.9	100.0
240 (A)--V	56.022	53.0	99.2	0.2	0.0	0.8	100.0
241 (A)--V	56.099	30.3	82.1	0.8	0.0	17.9	100.0
242 (A)--V	56.312	3.5	99.0	0.2	0.0	1.0	100.0
243 (A)--V	56.888	28.1	88.9	2.4	0.1	11.1	100.0
244 (A)--V	56.934	26.2	95.8	1.2	0.1	4.2	100.0
245 (A)--V	57.634	3.1	99.4	0.1	0.0	0.6	100.0
246 (A)--V	57.676	0.7	99.4	0.0	0.0	0.6	100.0
247 (A)--V	57.709	13.1	98.9	0.4	0.0	1.1	100.0
248 (A)--V	57.972	34.0	99.5	0.2	0.0	0.5	100.0
249 (A)--V	58.175	5.0	90.1	1.0	0.0	9.9	100.0
250 (A)--V	58.642	7.1	94.6	0.7	0.0	5.4	100.0
251 (A)--V	59.220	15.5	89.4	0.9	0.0	10.6	100.0
252 (A)--V	60.156	5.7	61.3	0.8	0.1	38.7	100.0
253 (A)--V	61.194	5.3	53.9	3.8	0.1	46.1	100.0
254 (A)--V	61.467	4.8	89.3	0.5	0.0	10.7	100.0
255 (A)--V	61.595	0.7	78.8	1.8	0.1	21.2	100.0
256 (A)--V	62.381	0.3	89.5	0.9	0.0	10.5	100.0
257 (A)--V	64.286	4.5	50.8	6.4	0.0	49.2	100.0
258 (A)--V	65.437	9.1	49.7	2.8	0.1	50.3	100.0
259 (A)--V	66.418	19.5	74.7	11.0	0.0	25.3	100.0
260 (A)--V	66.996	12.2	60.3	15.1	0.1	39.7	100.0
261 (A)--V	67.111	17.2	64.7	19.8	0.0	35.3	100.0
262 (A)--V	67.680	18.7	81.0	2.6	0.0	19.0	100.0
263 (A)--V	68.022	1.5	25.3	25.4	0.1	74.7	100.0
264 (A)--V	68.321	5.0	42.5	14.2	0.3	57.5	100.0
265 (A)--V	69.992	12.0	53.0	8.5	0.2	47.0	100.0
266 (A)--V	71.112	35.1	69.2	6.2	0.1	30.8	100.0
267 (A)--V	71.560	26.9	80.6	2.9	0.2	19.4	100.0
268 (A)--V	71.728	53.1	80.1	2.8	0.1	19.9	100.0
269 (A)--V	72.755	7.3	63.0	18.1	0.2	37.0	100.0
270 (A)--V	74.112	4.9	24.7	38.5	0.4	75.3	100.0
271 (A)--V	74.573	0.6	53.9	26.3	0.4	46.1	100.0
272 (A)--V	75.073	6.4	95.2	1.0	0.1	4.8	100.0
273 (A)--V	75.128	2.0	74.2	16.2	0.2	25.8	100.0

274 (A)--V	75.889	2.4	31.7	16.6	1.6	68.3	100.0
275 (A)--V	77.764	3.9	30.8	12.9	0.1	69.2	100.0
276 (A)--V	79.014	2.0	11.8	76.7	0.2	88.2	100.0
277 (A)--V	79.359	3.4	81.2	11.0	0.0	18.8	100.0
278 (A)--V	79.779	5.8	83.9	1.4	0.2	16.1	100.0
279 (A)--V	80.411	1.9	87.7	0.6	0.1	12.3	100.0
280 (A)--V	81.343	7.0	96.3	1.0	0.0	3.7	100.0
281 (A)--V	81.423	9.7	91.5	2.0	0.0	8.5	100.0
282 (A)--V	81.512	18.9	99.2	0.2	0.0	0.8	100.0
283 (A)--V	81.751	18.2	65.9	5.5	0.1	34.1	100.0
284 (A)--V	82.121	3.4	98.1	0.4	0.0	1.9	100.0
285 (A)--V	82.400	23.9	63.2	5.8	0.1	36.8	100.0
286 (A)--V	82.882	0.4	93.6	2.0	0.0	6.4	100.0
287 (A)--V	83.455	0.3	96.8	1.5	0.0	3.2	100.0
288 (A)--V	83.846	4.9	93.2	0.9	0.0	6.8	100.0
289 (A)--V	83.991	3.9	94.8	1.3	0.0	5.2	100.0
290 (A)--V	84.263	0.5	97.2	0.4	0.0	2.8	100.0
291 (A)--V	84.448	1.5	98.7	0.3	0.0	1.3	100.0
292 (A)--V	85.003	2.0	94.3	2.1	0.1	5.7	100.0
293 (A)--V	85.665	1.3	93.4	0.3	0.0	6.6	100.0
294 (A)--V	87.851	7.3	67.8	1.5	0.1	32.2	100.0
295 (A)--V	88.145	2.5	78.1	1.2	0.3	21.9	100.0
296 (A)--V	89.445	14.8	67.8	4.0	0.3	32.2	100.0
297 (A)--V	89.783	14.2	96.2	0.7	0.0	3.8	100.0
298 (A)--V	90.033	5.1	92.2	1.0	0.0	7.8	100.0
299 (A)--V	90.439	11.0	85.5	1.9	0.1	14.5	100.0
300 (A)--V	90.563	4.3	63.7	3.1	0.0	36.3	100.0
301 (A)--V	93.567	3.8	56.3	14.4	0.0	43.7	100.0
302 (A)--V	95.200	2.5	97.0	0.1	0.0	3.0	100.0
303 (A)--V	95.662	4.2	88.7	3.6	0.0	11.3	100.0
304 (A)--V	97.945	0.7	97.9	0.4	0.0	2.1	100.0
305 (A)--V	98.388	1.5	92.9	2.8	0.0	7.1	100.0
306 (A)--V	100.118	11.9	86.3	5.6	0.0	13.7	100.0
307 (A)--V	100.243	9.1	96.7	0.2	0.0	3.3	100.0
308 (A)--V	101.697	55.9	90.0	3.1	0.0	10.0	100.0
309 (A)--V	102.254	28.4	88.9	1.5	0.0	11.1	100.0
310 (A)--V	102.815	2.0	62.4	33.3	0.0	37.6	100.0
311 (A)--V	103.310	2.2	92.9	5.0	0.0	7.1	100.0
312 (A)--V	103.824	1.1	96.2	1.9	0.0	3.8	100.0
313 (A)--V	103.961	0.6	99.0	0.3	0.0	1.0	100.0
314 (A)--V	104.313	3.1	87.0	8.6	0.0	13.0	100.0
315 (A)--V	104.711	6.8	95.8	0.3	0.0	4.2	100.0
316 (A)--V	104.939	11.1	99.6	0.2	0.0	0.4	100.0
317 (A)--V	108.038	62.9	90.7	1.2	0.0	9.3	100.0
318 (A)--V	116.163	6.4	51.2	13.8	0.0	48.8	100.0
319 (A)--V	120.230	0.9	41.7	40.3	0.0	58.3	100.0
320 (A)--V	120.596	0.0	99.8	0.1	0.0	0.2	100.0
321 (A)--V	120.969	0.4	70.6	19.2	0.0	29.4	100.0
322 (A)--V	157.811	17.3	99.5	0.0	0.0	0.5	100.0
323 (A)--V	158.126	13.7	99.5	0.1	0.0	0.5	100.0
324 (A)--V	164.981	87.7	99.6	0.1	0.0	0.4	100.0
325 (A)--V	167.854	84.2	99.7	0.1	0.0	0.3	100.0
326 (A)--V	168.025	66.6	94.7	0.1	0.0	5.3	100.0
327 (A)--V	234.034	96.7	99.9	0.0	0.0	0.1	100.0
328 (A)--V	234.865	86.3	95.3	0.3	0.0	4.7	100.0
329 (A)--V	250.269	88.4	96.9	0.5	0.0	3.1	100.0
330 (A)--V	366.171	9.0	50.2	11.5	24.5	49.8	100.0

331 (A)--V	628.677	3.4	33.9	7.4	0.0	66.1	100.0
332 (A)--V	632.115	10.7	95.3	0.5	0.0	4.7	100.0
333 (A)--V	635.257	5.8	74.1	2.6	0.0	25.9	100.0
334 (A)--V	643.480	2.2	99.8	0.0	0.0	0.2	100.0
335 (A)--V	643.823	5.0	99.3	0.0	0.0	0.7	100.0
336 (A)--V	644.327	10.3	99.7	0.0	0.0	0.3	100.0
337 (A)--V	644.538	3.2	99.1	0.1	0.0	0.9	100.0
338 (A)--V	645.172	3.0	99.6	0.0	0.0	0.4	100.0
339 (A)--V	645.290	2.8	98.4	0.1	0.0	1.6	100.0
340 (A)--V	645.451	7.0	98.1	0.2	0.0	1.9	100.0
341 (A)--V	645.734	0.4	98.1	0.1	0.0	1.9	100.0
342 (A)--V	647.880	2.1	13.7	7.4	0.0	86.3	100.0
343 (A)--V	656.358	0.2	2.4	79.6	0.0	97.6	100.0
344 (A)--V	758.669	95.3	98.9	0.1	0.0	1.1	100.0
345 (A)--V	965.237	0.0	0.3	94.4	0.0	99.7	100.0
346 (A)--V	4855.810	99.2	100.0	0.0	0.0	0.0	100.0
347 (A)--V	4856.460	96.6	98.9	0.0	0.0	1.1	100.0
348 (A)--V	4869.608	95.8	98.9	0.1	0.0	1.1	100.0
349 (A)--V	12037.466	99.0	99.8	0.0	0.0	0.2	100.0

Full population analysis for complex *cis*-3 (optimized geometry):
```
*********************************************************************
*                         VMOdes                                   *
* Virtual Molecular Orbital description Program, Revision 7.1       *
* Cite this work as: VMOdes Program, Revision A 7.1                 *
* V. N. Nemykin, P. Basu, 2001, 2003                               *
* Department of Chemistry, Duquesne University, Pittsburgh, PA      *
*********************************************************************

Input Gaussian file:
C:\Documents and Settings\hp\My Documents\Research Dr.
Nemykin\VMOdes\VModes\FcCN-Iodo-cis.gjf.out
Output VMOdes file: cis-FcCN-Iodo


Full point group is:  C1


Number of Basis Functions = 349

    64 Alpha electrons         64 Beta electrons


Group  1  is: Fe
This group consist of  1  subunits. The Basis Functions range is:
 106         161
Group  2  is: Fc
This group consist of  1  subunits. The Basis Functions range is:
 1           263
Group  3  is: CN
This group consist of  1  subunits. The Basis Functions range is:
 300         335
Group  4  is: I
This group consist of  1  subunits. The Basis Functions range is:
 333         349
Group  5  is: Lig
This group consist of  1  subunits. The Basis Functions range is:
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 264           349
Group  6  is: Total
This group consist of  1  subunits. The Basis Functions range is:
 1             349

All MO's will be printed.

Molecular Orbitals Indexes, Energies, and Group Contributions


       Orbital                              Group Number
_____    _____

Number Index    Energy,eV    1        2        3        4        5        6

 1    (A)--O    -6932.993  100.0    100.0     0.0      0.0      0.0     100.0
 2    (A)--O    -803.037   100.0    100.0     0.0      0.0      0.0     100.0
 3    (A)--O    -693.523   100.0    100.0     0.0      0.0      0.0     100.0
 4    (A)--O    -693.136   100.0    100.0     0.0      0.0      0.0     100.0
 5    (A)--O    -693.115   100.0    100.0     0.0      0.0      0.0     100.0
 6    (A)--O    -380.540     0.0      0.0     99.9      0.0    100.0     100.0
 7    (A)--O    -271.638     0.0      0.1      0.0      0.0     99.9     100.0
 8    (A)--O    -270.577     0.1    100.0     0.0      0.0      0.0     100.0
 9    (A)--O    -270.537     0.0      0.0      0.0      0.0    100.0     100.0
10    (A)--O    -270.144     0.0      0.0     99.9      0.0    100.0     100.0
11    (A)--O    -270.139     0.1    100.0     0.0      0.0      0.0     100.0
12    (A)--O    -270.091     0.1    100.0     0.0      0.0      0.0     100.0
13    (A)--O    -270.071     0.1    100.0     0.0      0.0      0.0     100.0
14    (A)--O    -270.063     0.0    100.0     0.0      0.0      0.0     100.0
15    (A)--O    -269.965     0.1    100.0     0.0      0.0      0.0     100.0
16    (A)--O    -269.956     0.0    100.0     0.0      0.0      0.0     100.0
17    (A)--O    -269.941     0.1    100.0     0.0      0.0      0.0     100.0
18    (A)--O    -269.922     0.1    100.0     0.0      0.0      0.0     100.0
19    (A)--O    -269.912     0.0    100.0     0.0      0.0      0.0     100.0
20    (A)--O    -88.286    100.0    100.0     0.0      0.0      0.0     100.0
21    (A)--O    -56.846     99.9    100.0     0.0      0.0      0.0     100.0
22    (A)--O    -55.818     99.9    100.0     0.0      0.0      0.0     100.0
23    (A)--O    -55.772    100.0    100.0     0.0      0.0      0.0     100.0
24    (A)--O    -22.863      8.1     93.3     1.4      0.2      6.7     100.0
25    (A)--O    -22.407      5.0     50.1    45.3      0.2     49.9     100.0
26    (A)--O    -22.339      3.9     40.9    57.4      0.1     59.1     100.0
27    (A)--O    -20.762      1.9     21.5    10.4      5.5     78.5     100.0
28    (A)--O    -18.451      1.2     63.5     8.0      4.2     36.5     100.0
29    (A)--O    -18.219      1.8     92.0     1.1      4.0      8.0     100.0
30    (A)--O    -17.994      1.7     99.5     0.0      0.2      0.5     100.0
31    (A)--O    -17.989      1.7     99.6     0.0      0.3      0.4     100.0
32    (A)--O    -17.685      0.9     23.0     1.6     66.4     77.0     100.0
33    (A)--O    -15.868      0.6     38.2    14.0     14.6     61.8     100.0
34    (A)--O    -14.113      0.4     90.1     2.4      3.2      9.9     100.0
35    (A)--O    -13.826      1.4     97.3     0.6      0.4      2.7     100.0
36    (A)--O    -13.723      0.2     99.2     0.2      0.2      0.8     100.0
37    (A)--O    -13.688      0.6     99.1     0.0      0.1      0.9     100.0
38    (A)--O    -13.462      1.7     86.5     3.0      0.9     13.5     100.0
39    (A)--O    -13.266      0.7     51.7     7.0      4.0     48.3     100.0
40    (A)--O    -12.601      0.2     16.4    18.7     24.3     83.6     100.0
41    (A)--O    -11.063      2.4     57.3     1.9      6.4     42.7     100.0
42    (A)--O    -10.788     37.3     93.0     1.1      0.7      7.0     100.0
43    (A)--O    -10.492      7.6     98.1     0.2      0.5      1.9     100.0
44    (A)--O    -10.254      5.2     94.5     0.7      2.2      5.5     100.0
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45   (A)--O   -10.188   1.5   98.8   0.2   0.3   1.2   100.0
46   (A)--O   -10.037   0.9   74.4   5.9   6.8   25.6  100.0
47   (A)--O   -9.906    0.8   95.0   0.6   0.3   5.0   100.0
48   (A)--O   -9.643    10.4  66.8   8.6   5.5   33.2  100.0
49   (A)--O   -9.584    0.4   98.7   0.2   0.5   1.3   100.0
50   (A)--O   -9.571    0.5   99.6   0.1   0.0   0.4   100.0
51   (A)--O   -9.156    5.3   43.1   31.5  4.3   56.9  100.0
52   (A)--O   -9.064    1.3   36.8   8.7   30.9  63.2  100.0
53   (A)--O   -8.325    0.1   2.1    78.9  1.2   97.9  100.0
54   (A)--O   -8.008    0.1   3.5    79.4  8.0   96.5  100.0
55   (A)--O   -7.949    5.3   32.3   34.7  15.3  67.7  100.0
56   (A)--O   -7.215    31.9  99.0   0.1   0.7   1.0   100.0
57   (A)--O   -7.116    25.5  76.9   1.6   18.5  23.1  100.0
58   (A)--O   -6.716    2.0   33.1   1.6   55.5  66.9  100.0
59   (A)--O   -6.649    4.8   68.8   0.5   28.1  31.2  100.0
60   (A)--O   -6.475    2.2   37.3   0.8   58.6  62.7  100.0
61   (A)--O   -6.068    5.5   32.8   12.6  24.6  67.2  100.0
62   (A)--O   -5.019    86.3  97.9   0.2   0.1   2.1   100.0
63   (A)--O   -4.783    58.7  97.1   0.7   0.2   2.9   100.0
64   (A)--O   -4.748    64.1  98.6   0.2   0.4   1.4   100.0
65   (A)--V   -2.772    19.3  38.7   10.7  4.8   61.3  100.0
66   (A)--V   -2.212    5.4   15.8   0.9   38.7  84.2  100.0
67   (A)--V   -1.996    28.2  63.2   0.5   14.1  36.8  100.0
68   (A)--V   -1.798    31.7  82.3   2.6   1.2   17.7  100.0
69   (A)--V   -0.243    1.3   22.7   26.6  13.5  77.3  100.0
70   (A)--V   0.290     8.1   96.5   1.8   0.5   3.5   100.0
71   (A)--V   0.398     13.7  97.2   1.0   0.5   2.8   100.0
72   (A)--V   0.406     25.3  97.4   0.9   0.6   2.6   100.0
73   (A)--V   0.445     44.0  94.1   2.1   2.0   5.9   100.0
74   (A)--V   0.807     8.7   81.4   7.2   3.9   18.6  100.0
75   (A)--V   1.003     6.2   60.8   2.4   30.0  39.2  100.0
76   (A)--V   1.131     17.3  78.4   0.6   20.1  21.6  100.0
77   (A)--V   1.422     25.4  62.3   4.6   29.1  37.7  100.0
78   (A)--V   1.555     3.1   70.2   4.1   13.6  29.8  100.0
79   (A)--V   1.653     33.3  86.4   0.6   12.2  13.6  100.0
80   (A)--V   1.720     3.4   90.2   0.7   7.9   9.8   100.0
81   (A)--V   2.115     8.2   60.5   18.7  2.2   39.5  100.0
82   (A)--V   2.244     5.2   68.5   4.8   14.3  31.5  100.0
83   (A)--V   2.336     13.8  89.1   4.1   3.3   10.9  100.0
84   (A)--V   2.715     5.6   93.3   0.8   2.0   6.7   100.0
85   (A)--V   2.850     52.7  93.4   1.1   4.1   6.6   100.0
86   (A)--V   2.890     7.8   95.0   1.7   2.7   5.0   100.0
87   (A)--V   3.040     24.2  89.8   0.3   7.0   10.2  100.0
88   (A)--V   3.376     3.0   73.1   10.1  10.3  26.9  100.0
89   (A)--V   3.909     21.0  88.4   2.8   0.7   11.6  100.0
90   (A)--V   3.970     25.7  85.4   9.7   1.6   14.6  100.0
91   (A)--V   4.414     65.4  90.7   5.9   0.5   9.3   100.0
92   (A)--V   4.580     66.8  94.8   3.4   0.8   5.2   100.0
93   (A)--V   4.777     19.2  88.4   1.4   0.6   11.6  100.0
94   (A)--V   4.969     10.0  93.3   3.5   1.0   6.7   100.0
95   (A)--V   5.038     27.2  97.1   1.3   0.6   2.9   100.0
96   (A)--V   5.119     35.2  96.3   1.5   0.7   3.7   100.0
97   (A)--V   5.250     81.9  95.4   1.1   0.1   4.6   100.0
98   (A)--V   5.678     1.7   74.5   8.2   1.9   25.5  100.0
99   (A)--V   6.257     0.8   88.4   5.4   0.2   11.6  100.0
100  (A)--V   6.503     1.4   90.8   1.3   0.7   9.2   100.0
101  (A)--V   7.170     1.7   70.1   12.5  0.6   29.9  100.0
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102 (A)--V    7.326    4.1    88.4    1.0    0.5    11.6    100.0
103 (A)--V    7.580   34.6    93.4    0.3    0.8     6.6    100.0
104 (A)--V    7.736   20.8    51.5    9.7    1.2    48.5    100.0
105 (A)--V    8.116   53.2    90.4    0.5    0.5     9.6    100.0
106 (A)--V    8.197   36.3    80.9    2.7    0.4    19.1    100.0
107 (A)--V    8.309   38.8    90.5    1.9    0.3     9.5    100.0
108 (A)--V    8.500   36.3    88.7    6.1    0.3    11.3    100.0
109 (A)--V    8.613   20.7    82.3    2.3    0.7    17.7    100.0
110 (A)--V    8.741    5.6    54.8    7.9    0.8    45.2    100.0
111 (A)--V    8.892   11.0    42.5   15.8    0.4    57.5    100.0
112 (A)--V    9.022   52.9    97.6    0.6    0.6     2.4    100.0
113 (A)--V    9.777   23.5    79.9    3.3    0.3    20.1    100.0
114 (A)--V    9.878    2.2    91.7    1.7    0.4     8.3    100.0
115 (A)--V    9.980    5.6    68.9    6.8    2.5    31.1    100.0
116 (A)--V   10.346   46.4    90.6    3.3    1.1     9.4    100.0
117 (A)--V   10.560   60.7    86.5    6.6    0.4    13.5    100.0
118 (A)--V   10.801   47.6    83.7    4.1    1.3    16.3    100.0
119 (A)--V   11.077    4.7    44.0   12.2    3.2    56.0    100.0
120 (A)--V   11.340    4.2    53.4   10.4    0.8    46.6    100.0
121 (A)--V   11.865    5.2    79.2    3.2    1.9    20.8    100.0
122 (A)--V   11.884    5.0    19.9   45.2    0.9    80.1    100.0
123 (A)--V   12.233   13.6    75.5    6.8    1.7    24.5    100.0
124 (A)--V   12.622   13.8    88.9    1.5    1.8    11.1    100.0
125 (A)--V   12.780   10.1    72.5    2.8    6.3    27.5    100.0
126 (A)--V   12.844   20.4    97.9    0.5    0.4     2.1    100.0
127 (A)--V   12.970   17.3    75.7   10.7    2.8    24.3    100.0
128 (A)--V   13.021   20.0    85.7    0.7    0.3    14.3    100.0
129 (A)--V   13.268    8.0    77.2    6.3    2.7    22.8    100.0
130 (A)--V   13.580   37.5    97.7    0.3    0.4     2.3    100.0
131 (A)--V   13.603   40.6    92.9    0.2    2.1     7.1    100.0
132 (A)--V   13.786   14.7    51.0   17.5    6.2    49.0    100.0
133 (A)--V   14.086   20.8    85.6    4.1    2.0    14.4    100.0
134 (A)--V   14.406   38.3    91.5    0.9    0.7     8.5    100.0
135 (A)--V   14.746    7.6    88.3    2.1    0.3    11.7    100.0
136 (A)--V   14.929   17.9    57.0   28.4    1.8    43.0    100.0
137 (A)--V   15.099   21.2    81.9    2.8    1.0    18.1    100.0
138 (A)--V   15.399    1.5    77.1    2.4    0.9    22.9    100.0
139 (A)--V   15.623    0.3    97.4    0.2    0.1     2.6    100.0
140 (A)--V   15.697    7.6    87.9    0.8    1.5    12.1    100.0
141 (A)--V   16.044    4.7    73.4    1.0    4.4    26.6    100.0
142 (A)--V   16.245    2.0    88.7    1.1    1.5    11.3    100.0
143 (A)--V   16.330   14.8    91.7    0.9    2.2     8.3    100.0
144 (A)--V   16.591    3.2    99.0    0.3    0.1     1.0    100.0
145 (A)--V   16.637   14.9    87.4    1.7    2.7    12.6    100.0
146 (A)--V   16.714   17.5    91.7    1.2    1.4     8.3    100.0
147 (A)--V   16.915    9.7    93.8    0.5    0.2     6.2    100.0
148 (A)--V   16.964    8.9    92.3    1.0    1.0     7.7    100.0
149 (A)--V   17.482    4.8    87.5    2.6    3.0    12.5    100.0
150 (A)--V   17.991    8.9    69.6    1.4    1.7    30.4    100.0
151 (A)--V   18.212    2.3    74.1    0.9    1.2    25.9    100.0
152 (A)--V   18.545    3.1    88.1    0.4    0.8    11.9    100.0
153 (A)--V   18.809    3.7    84.1    3.3    0.7    15.9    100.0
154 (A)--V   19.074    5.2    81.4    3.2    1.0    18.6    100.0
155 (A)--V   19.308    3.7    99.4    0.1    0.1     0.6    100.0
156 (A)--V   19.435   16.5    78.5   11.4    0.6    21.5    100.0
157 (A)--V   19.577   15.3    77.1    6.0    1.3    22.9    100.0
158 (A)--V   20.049    4.1    74.0    4.4    0.3    26.0    100.0
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159 (A)--V	20.220	3.2	67.5	4.8	0.9	32.5	100.0
160 (A)--V	20.433	43.8	76.2	4.9	0.6	23.8	100.0
161 (A)--V	20.720	15.0	33.7	3.0	0.7	66.3	100.0
162 (A)--V	21.451	18.6	85.0	5.0	1.5	15.0	100.0
163 (A)--V	21.724	18.0	60.6	8.4	21.4	39.4	100.0
164 (A)--V	22.261	6.5	78.0	6.4	0.1	22.0	100.0
165 (A)--V	22.325	11.7	56.7	5.9	0.3	43.3	100.0
166 (A)--V	23.008	4.7	93.4	1.6	0.3	6.6	100.0
167 (A)--V	23.336	48.3	87.9	0.2	0.1	12.1	100.0
168 (A)--V	23.969	10.9	83.8	6.1	0.4	16.2	100.0
169 (A)--V	24.652	3.0	89.0	2.2	1.2	11.0	100.0
170 (A)--V	25.134	0.4	63.0	1.3	0.1	37.0	100.0
171 (A)--V	25.546	0.1	98.3	0.0	0.0	1.7	100.0
172 (A)--V	25.675	1.8	63.7	11.9	0.4	36.3	100.0
173 (A)--V	25.924	3.4	77.1	0.4	0.0	22.9	100.0
174 (A)--V	26.377	2.5	96.7	0.4	0.4	3.3	100.0
175 (A)--V	27.163	2.3	92.7	2.1	0.4	7.3	100.0
176 (A)--V	27.504	9.6	92.6	0.1	0.1	7.4	100.0
177 (A)--V	27.689	3.2	96.7	0.6	0.1	3.3	100.0
178 (A)--V	28.168	2.2	75.0	2.0	0.1	25.0	100.0
179 (A)--V	28.248	0.7	98.7	0.0	0.0	1.3	100.0
180 (A)--V	28.485	13.0	93.3	1.9	0.0	6.7	100.0
181 (A)--V	28.644	3.0	99.3	0.2	0.1	0.7	100.0
182 (A)--V	28.821	12.2	98.1	0.2	0.1	1.9	100.0
183 (A)--V	29.144	6.4	43.5	15.4	0.2	56.5	100.0
184 (A)--V	29.313	5.8	99.5	0.2	0.0	0.5	100.0
185 (A)--V	30.388	21.7	66.7	4.2	0.2	33.3	100.0
186 (A)--V	30.620	7.4	97.7	0.2	0.1	2.3	100.0
187 (A)--V	30.960	7.5	97.0	0.2	0.2	3.0	100.0
188 (A)--V	31.269	4.7	73.0	4.5	0.2	27.0	100.0
189 (A)--V	31.910	12.4	74.2	12.0	0.1	25.8	100.0
190 (A)--V	32.463	31.2	99.3	0.3	0.0	0.7	100.0
191 (A)--V	32.565	23.3	93.7	1.6	0.0	6.3	100.0
192 (A)--V	34.324	1.8	32.9	48.1	0.3	67.1	100.0
193 (A)--V	34.605	16.0	65.6	20.5	0.1	34.4	100.0
194 (A)--V	35.240	5.0	50.7	19.4	0.6	49.3	100.0
195 (A)--V	35.813	6.7	54.2	6.3	1.4	45.8	100.0
196 (A)--V	35.877	8.4	75.9	7.4	0.7	24.1	100.0
197 (A)--V	36.514	10.8	68.0	13.9	1.9	32.0	100.0
198 (A)--V	36.675	11.9	73.5	12.6	0.6	26.5	100.0
199 (A)--V	37.921	1.4	45.1	9.0	0.7	54.9	100.0
200 (A)--V	38.455	3.0	75.9	2.7	1.3	24.1	100.0
201 (A)--V	38.572	6.4	90.7	2.0	0.1	9.3	100.0
202 (A)--V	39.218	17.3	66.7	5.2	0.4	33.3	100.0
203 (A)--V	40.017	1.5	97.7	0.3	0.0	2.3	100.0
204 (A)--V	40.612	10.9	85.0	1.1	0.2	15.0	100.0
205 (A)--V	40.749	5.8	97.9	0.3	0.0	2.1	100.0
206 (A)--V	41.603	18.3	83.8	0.9	1.0	16.2	100.0
207 (A)--V	41.865	15.8	81.7	0.6	0.4	18.3	100.0
208 (A)--V	41.984	18.4	95.3	0.2	0.0	4.7	100.0
209 (A)--V	42.093	10.5	85.3	1.4	0.2	14.7	100.0
210 (A)--V	42.341	1.9	88.0	0.9	0.1	12.0	100.0
211 (A)--V	42.457	10.6	61.1	1.5	0.5	38.9	100.0
212 (A)--V	42.945	1.5	73.5	0.3	0.7	26.5	100.0
213 (A)--V	43.225	6.2	95.8	0.4	0.0	4.2	100.0
214 (A)--V	44.235	12.3	97.7	0.9	0.1	2.3	100.0
215 (A)--V	44.482	6.9	69.2	10.3	0.2	30.8	100.0

216 (A)--V	44.767	14.8	97.1	1.1	0.3	2.9	100.0
217 (A)--V	45.614	6.9	86.0	1.5	0.1	14.0	100.0
218 (A)--V	45.798	14.5	91.6	1.3	0.1	8.4	100.0
219 (A)--V	46.064	6.9	88.6	0.9	0.3	11.4	100.0
220 (A)--V	47.177	8.0	71.1	0.5	0.3	28.9	100.0
221 (A)--V	47.297	16.1	89.9	1.8	0.1	10.1	100.0
222 (A)--V	47.517	9.2	95.0	1.2	0.1	5.0	100.0
223 (A)--V	47.801	13.7	82.0	2.8	0.1	18.0	100.0
224 (A)--V	48.796	1.8	85.5	2.8	0.2	14.5	100.0
225 (A)--V	49.197	3.5	87.1	5.0	0.1	12.9	100.0
226 (A)--V	49.718	1.9	47.5	4.8	0.8	52.5	100.0
227 (A)--V	49.936	9.7	87.0	1.2	0.2	13.0	100.0
228 (A)--V	50.815	16.1	74.5	2.3	0.0	25.5	100.0
229 (A)--V	51.287	30.8	83.1	0.9	0.2	16.9	100.0
230 (A)--V	51.560	11.6	68.0	14.0	0.3	32.0	100.0
231 (A)--V	52.073	18.2	92.2	3.4	0.1	7.8	100.0
232 (A)--V	52.292	5.9	97.0	1.0	0.2	3.0	100.0
233 (A)--V	52.451	1.8	94.0	2.4	0.1	6.0	100.0
234 (A)--V	53.264	3.2	83.7	0.9	0.6	16.3	100.0
235 (A)--V	53.561	2.0	97.5	0.7	0.1	2.5	100.0
236 (A)--V	54.586	30.0	73.8	10.9	4.6	26.2	100.0
237 (A)--V	54.939	4.1	33.1	13.8	4.0	66.9	100.0
238 (A)--V	55.418	33.2	81.8	7.1	1.4	18.2	100.0
239 (A)--V	55.719	43.8	89.6	1.4	0.2	10.4	100.0
240 (A)--V	55.950	42.4	94.3	0.9	0.1	5.7	100.0
241 (A)--V	56.042	28.4	82.3	2.3	0.4	17.7	100.0
242 (A)--V	56.262	3.1	99.8	0.0	0.0	0.2	100.0
243 (A)--V	56.788	20.1	95.6	0.7	0.4	4.4	100.0
244 (A)--V	57.174	24.7	84.7	2.3	0.5	15.3	100.0
245 (A)--V	57.599	1.2	99.6	0.0	0.0	0.4	100.0
246 (A)--V	57.603	0.7	99.4	0.0	0.0	0.6	100.0
247 (A)--V	57.817	16.2	92.6	0.3	0.4	7.4	100.0
248 (A)--V	57.874	37.9	93.0	0.3	0.3	7.0	100.0
249 (A)--V	58.150	0.8	64.2	0.4	0.1	35.8	100.0
250 (A)--V	58.399	9.9	83.0	1.5	0.8	17.0	100.0
251 (A)--V	58.912	20.4	89.9	0.5	0.2	10.1	100.0
252 (A)--V	59.331	2.9	73.6	1.3	1.2	26.4	100.0
253 (A)--V	60.328	3.3	50.7	0.5	0.8	49.3	100.0
254 (A)--V	61.206	7.8	98.7	0.0	0.1	1.3	100.0
255 (A)--V	61.418	4.2	86.8	0.3	0.0	13.2	100.0
256 (A)--V	61.775	0.3	96.8	0.6	0.0	3.2	100.0
257 (A)--V	64.085	5.1	65.0	2.4	3.9	35.0	100.0
258 (A)--V	65.154	14.6	85.6	1.2	0.9	14.4	100.0
259 (A)--V	66.320	11.0	55.3	8.4	0.3	44.7	100.0
260 (A)--V	66.571	22.5	73.3	11.0	0.1	26.7	100.0
261 (A)--V	67.119	2.9	41.5	29.3	0.5	58.5	100.0
262 (A)--V	67.436	8.1	46.6	13.5	0.3	53.4	100.0
263 (A)--V	67.563	11.8	63.9	12.7	0.1	36.1	100.0
264 (A)--V	69.002	1.7	45.1	26.4	0.4	54.9	100.0
265 (A)--V	69.805	17.0	65.8	2.4	0.2	34.2	100.0
266 (A)--V	70.978	26.6	86.0	4.6	0.3	14.0	100.0
267 (A)--V	71.364	70.8	89.7	0.4	0.1	10.3	100.0
268 (A)--V	71.411	31.1	89.7	1.3	0.0	10.3	100.0
269 (A)--V	73.553	5.9	25.7	62.4	2.0	74.3	100.0
270 (A)--V	73.653	1.6	12.7	65.7	2.7	87.3	100.0
271 (A)--V	74.614	2.7	82.0	3.4	0.2	18.0	100.0
272 (A)--V	74.921	1.8	91.8	3.3	0.2	8.2	100.0

273 (A)--V	75.370	2.9	75.5	3.7	0.2	24.5	100.0
274 (A)--V	76.754	2.7	50.1	12.5	4.9	49.9	100.0
275 (A)--V	77.757	6.6	31.9	15.2	1.5	68.1	100.0
276 (A)--V	78.938	1.2	27.6	62.1	1.4	72.4	100.0
277 (A)--V	79.140	4.0	70.2	20.4	0.9	29.8	100.0
278 (A)--V	79.828	7.2	84.4	6.5	0.8	15.6	100.0
279 (A)--V	80.058	2.6	88.8	0.8	0.2	11.2	100.0
280 (A)--V	81.218	2.0	99.2	0.3	0.1	0.8	100.0
281 (A)--V	81.375	9.2	99.3	0.1	0.0	0.7	100.0
282 (A)--V	81.467	32.4	98.5	0.1	0.0	1.5	100.0
283 (A)--V	81.656	15.5	92.2	1.7	0.5	7.8	100.0
284 (A)--V	82.042	32.2	97.6	0.8	0.0	2.4	100.0
285 (A)--V	82.451	0.8	97.5	0.9	0.3	2.5	100.0
286 (A)--V	83.068	0.8	93.5	1.1	0.0	6.5	100.0
287 (A)--V	83.468	0.7	76.0	5.1	0.2	24.0	100.0
288 (A)--V	83.703	9.6	95.7	1.0	0.2	4.3	100.0
289 (A)--V	83.968	0.7	69.3	8.7	0.3	30.7	100.0
290 (A)--V	84.225	0.4	91.7	2.4	0.1	8.3	100.0
291 (A)--V	84.388	1.5	93.2	1.3	0.1	6.8	100.0
292 (A)--V	84.887	1.0	69.2	9.1	0.1	30.8	100.0
293 (A)--V	85.324	1.3	77.6	4.3	0.4	22.4	100.0
294 (A)--V	87.024	6.8	83.7	1.0	2.8	16.3	100.0
295 (A)--V	88.029	1.9	83.1	0.9	0.6	16.9	100.0
296 (A)--V	89.302	8.5	84.9	1.2	0.5	15.1	100.0
297 (A)--V	89.731	15.1	97.0	0.4	0.2	3.0	100.0
298 (A)--V	89.864	13.4	89.4	3.6	0.4	10.6	100.0
299 (A)--V	90.083	3.1	74.5	1.6	1.1	25.5	100.0
300 (A)--V	90.498	4.8	84.3	2.0	0.2	15.7	100.0
301 (A)--V	94.010	3.5	73.3	7.8	0.9	26.7	100.0
302 (A)--V	95.148	2.4	97.2	0.2	0.1	2.8	100.0
303 (A)--V	95.906	3.4	88.5	2.7	0.1	11.5	100.0
304 (A)--V	97.963	0.7	98.1	0.3	0.0	1.9	100.0
305 (A)--V	98.524	2.2	88.0	4.5	0.0	12.0	100.0
306 (A)--V	100.056	11.4	83.8	5.4	0.1	16.2	100.0
307 (A)--V	100.191	9.8	97.6	0.3	0.1	2.4	100.0
308 (A)--V	101.627	53.1	87.8	2.9	0.0	12.2	100.0
309 (A)--V	102.181	29.8	89.6	1.5	0.0	10.4	100.0
310 (A)--V	102.820	0.6	17.9	80.5	0.3	82.1	100.0
311 (A)--V	103.354	2.6	99.6	0.1	0.0	0.4	100.0
312 (A)--V	103.672	1.9	41.1	41.0	0.9	58.9	100.0
313 (A)--V	103.825	1.6	99.1	0.2	0.0	0.9	100.0
314 (A)--V	103.960	0.5	99.6	0.1	0.0	0.4	100.0
315 (A)--V	104.683	6.8	92.8	0.6	0.1	7.2	100.0
316 (A)--V	104.859	11.2	99.6	0.2	0.0	0.4	100.0
317 (A)--V	107.807	69.0	94.4	0.3	0.0	5.6	100.0
318 (A)--V	115.531	5.9	52.8	11.6	0.3	47.2	100.0
319 (A)--V	120.006	0.7	13.9	60.7	0.7	86.1	100.0
320 (A)--V	120.545	0.0	99.7	0.2	0.0	0.3	100.0
321 (A)--V	120.645	0.2	95.7	2.1	0.0	4.3	100.0
322 (A)--V	157.732	17.7	98.4	0.1	0.0	1.6	100.0
323 (A)--V	158.026	13.5	99.5	0.0	0.0	0.5	100.0
324 (A)--V	164.929	87.0	99.2	0.3	0.0	0.8	100.0
325 (A)--V	167.771	84.3	99.0	0.1	0.0	1.0	100.0
326 (A)--V	167.988	61.7	93.1	1.2	0.0	6.9	100.0
327 (A)--V	233.977	96.5	99.8	0.0	0.0	0.2	100.0
328 (A)--V	234.754	88.0	95.7	0.1	0.0	4.3	100.0
329 (A)--V	250.050	91.9	98.7	0.2	0.0	1.3	100.0

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330 (A)--V    365.108   10.7   58.2    3.0    27.8   41.8   100.0
331 (A)--V    628.949    3.4   35.4    7.2     0.1   64.6   100.0
332 (A)--V    632.069   10.7   95.1    0.5     0.0    4.9   100.0
333 (A)--V    635.180    5.8   72.3    2.9     0.0   27.7   100.0
334 (A)--V    643.394    2.2   99.8    0.0     0.0    0.2   100.0
335 (A)--V    643.777    4.9   99.4    0.0     0.0    0.6   100.0
336 (A)--V    644.277   10.7   99.9    0.0     0.0    0.1   100.0
337 (A)--V    644.571    1.6   99.0    0.0     0.0    1.0   100.0
338 (A)--V    645.044    7.3   98.1    0.0     0.0    1.9   100.0
339 (A)--V    645.207    4.6   97.7    0.2     0.0    2.3   100.0
340 (A)--V    645.309    1.4   99.9    0.0     0.0    0.1   100.0
341 (A)--V    645.569    0.3   98.5    0.1     0.0    1.5   100.0
342 (A)--V    647.879    2.0   13.5    8.0     0.0   86.5   100.0
343 (A)--V    657.016    0.1    3.1   76.7     0.2   96.9   100.0
344 (A)--V    758.395   96.8   99.5    0.0     0.0    0.5   100.0
345 (A)--V    965.333    0.0    0.4   94.1     0.1   99.6   100.0
346 (A)--V   4855.753   99.2  100.0    0.0     0.0    0.0   100.0
347 (A)--V   4856.364   97.1   99.0    0.0     0.0    1.0   100.0
348 (A)--V   4869.443   97.1   99.6    0.0     0.0    0.4   100.0
349 (A)--V  12037.182   99.3   99.9    0.0     0.0    0.1   100.0
```

Full population analysis for complex *trans*-2 (optimized geometry):
```
**********************************************************************
*                        VMOdes                                      *
* Virtual Molecular Orbital description Program, Revision 7.1        *
* Cite this work as: VMOdes Program, Revision A 7.1                  *
* V. N. Nemykin, P. Basu, 2001, 2003                                 *
* Department of Chemistry, Duquesne University, Pittsburgh, PA       *
**********************************************************************


Input Gaussian file:
C:\Documents and Settings\hp\My Documents\Research Dr.
Nemykin\VMOdes\VModes\FcI2-trans.gjf.out
Output VMOdes file: trans-FcI2.out


Full point group is:  C1


Number of Basis Functions = 324

   61 Alpha electrons          61 Beta electrons

Group  1  is: Fe
This group consist of  1  subunits. The Basis Functions range is:
 106         161
Group  2  is: Fc
This group consist of  1  subunits. The Basis Functions range is:
 1           263
Group  3  is: I
This group consist of  2  subunits. The Basis Functions range is:
 300         310
 314         324
Group  4  is: Lig
This group consist of  1  subunits. The Basis Functions range is:
 264         324
```

```
Group  5  is: Total
This group consist of  1  subunits. The Basis Functions range is:
 1              324

All MO's will be printed.

Molecular Orbitals Indexes, Energies, and Group Contributions
```

	Orbital		Group Number				
Number	Index	Energy,eV	1	2	3	4	5
1	(A)--O	-6932.698	100.0	100.0	0.0	0.0	100.0
2	(A)--O	-802.741	100.0	100.0	0.0	0.0	100.0
3	(A)--O	-693.232	100.0	100.0	0.0	0.0	100.0
4	(A)--O	-692.835	100.0	100.0	0.0	0.0	100.0
5	(A)--O	-692.821	100.0	100.0	0.0	0.0	100.0
6	(A)--O	-271.266	0.0	0.0	0.0	100.0	100.0
7	(A)--O	-270.777	0.0	0.0	0.0	100.0	100.0
8	(A)--O	-270.326	0.1	100.0	0.0	0.0	100.0
9	(A)--O	-269.821	0.1	100.0	0.0	0.0	100.0
10	(A)--O	-269.798	0.1	100.0	0.0	0.0	100.0
11	(A)--O	-269.791	0.1	100.0	0.0	0.0	100.0
12	(A)--O	-269.784	0.0	100.0	0.0	0.0	100.0
13	(A)--O	-269.719	0.1	100.0	0.0	0.0	100.0
14	(A)--O	-269.706	0.1	100.0	0.0	0.0	100.0
15	(A)--O	-269.690	0.1	100.0	0.0	0.0	100.0
16	(A)--O	-269.656	0.1	100.0	0.0	0.0	100.0
17	(A)--O	-269.648	0.0	100.0	0.0	0.0	100.0
18	(A)--O	-87.990	100.0	100.0	0.0	0.0	100.0
19	(A)--O	-56.560	99.9	100.0	0.0	0.0	100.0
20	(A)--O	-55.511	99.9	100.0	0.0	0.0	100.0
21	(A)--O	-55.478	99.9	100.0	0.0	0.0	100.0
22	(A)--O	-22.563	8.3	96.4	0.2	3.6	100.0
23	(A)--O	-22.112	9.8	98.3	0.1	1.7	100.0
24	(A)--O	-20.435	1.9	23.9	9.6	76.1	100.0
25	(A)--O	-18.296	0.8	41.3	37.6	58.7	100.0
26	(A)--O	-17.911	1.7	94.8	3.4	5.2	100.0
27	(A)--O	-17.747	1.8	98.2	1.5	1.8	100.0
28	(A)--O	-17.741	1.7	98.8	1.1	1.2	100.0
29	(A)--O	-17.595	0.9	42.2	52.7	57.8	100.0
30	(A)--O	-16.680	0.3	6.0	76.4	94.0	100.0
31	(A)--O	-14.831	0.6	49.8	9.9	50.2	100.0
32	(A)--O	-13.761	0.5	96.8	1.5	3.2	100.0
33	(A)--O	-13.534	1.3	99.0	0.2	1.0	100.0
34	(A)--O	-13.469	0.1	99.5	0.1	0.5	100.0
35	(A)--O	-13.424	0.8	99.5	0.2	0.5	100.0
36	(A)--O	-13.174	1.7	98.3	0.2	1.7	100.0
37	(A)--O	-12.302	0.8	38.2	9.5	61.8	100.0
38	(A)--O	-11.057	3.3	21.8	33.0	78.2	100.0
39	(A)--O	-10.546	7.5	61.2	8.8	38.8	100.0
40	(A)--O	-10.401	29.1	79.7	7.6	20.3	100.0
41	(A)--O	-10.203	8.0	99.5	0.3	0.5	100.0
42	(A)--O	-9.983	3.6	96.5	1.3	3.5	100.0
43	(A)--O	-9.929	1.0	99.7	0.3	0.3	100.0
44	(A)--O	-9.638	2.0	85.9	4.7	14.1	100.0
45	(A)--O	-9.624	2.0	88.4	1.8	11.6	100.0

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 46 (A)--O   -9.340   0.6   99.4   0.1    0.6   100.0
 47 (A)--O   -9.327   0.3   99.8   0.0    0.2   100.0
 48 (A)--O   -9.198   8.4   82.8   5.7   17.2   100.0
 49 (A)--O   -8.427   4.4   24.8  42.4   75.2   100.0
 50 (A)--O   -8.256   1.4   23.1  37.2   76.9   100.0
 51 (A)--O   -6.980  16.2   53.2  40.5   46.8   100.0
 52 (A)--O   -6.951  27.7   89.3   8.6   10.7   100.0
 53 (A)--O   -6.830  10.7   38.4  58.4   61.6   100.0
 54 (A)--O   -6.615   1.6   21.8  69.3   78.2   100.0
 55 (A)--O   -6.578   3.7   25.7  61.6   74.3   100.0
 56 (A)--O   -6.292   3.4   57.7  38.2   42.3   100.0
 57 (A)--O   -6.191   3.1   47.1  51.4   52.9   100.0
 58 (A)--O   -5.675   3.9   20.3  54.0   79.7   100.0
 59 (A)--O   -4.731  86.1   97.7   0.4    2.3   100.0
 60 (A)--O   -4.476  58.1   96.8   1.1    3.2   100.0
 61 (A)--O   -4.462  63.6   98.7   0.7    1.3   100.0
 62 (A)--V   -2.836   1.7    4.3  50.4   95.7   100.0
 63 (A)--V   -2.042  27.9   57.8   8.6   42.2   100.0
 64 (A)--V   -1.755  43.0   96.2   1.2    3.8   100.0
 65 (A)--V   -1.269  10.3   36.3   9.7   63.7   100.0
 66 (A)--V   -1.092   2.9   13.5  27.6   86.5   100.0
 67 (A)--V    0.549   2.3   93.3   3.7    6.7   100.0
 68 (A)--V    0.595  51.1   89.7   6.4   10.3   100.0
 69 (A)--V    0.642   6.8   95.1   3.6    4.9   100.0
 70 (A)--V    0.675   6.6   91.3   3.9    8.7   100.0
 71 (A)--V    0.867   9.0   54.4  39.8   45.6   100.0
 72 (A)--V    1.052   6.6   48.2  48.5   51.8   100.0
 73 (A)--V    1.170  22.2   58.1  36.1   41.9   100.0
 74 (A)--V    1.216   3.9   74.7   9.8   25.3   100.0
 75 (A)--V    1.450  18.6   58.6  36.3   41.4   100.0
 76 (A)--V    1.610  10.7   55.3  41.7   44.7   100.0
 77 (A)--V    1.672  11.8   37.2  48.5   62.8   100.0
 78 (A)--V    1.865  16.8   88.6  10.2   11.4   100.0
 79 (A)--V    2.033   9.1   91.3   6.9    8.7   100.0
 80 (A)--V    2.118   4.4   80.9  14.4   19.1   100.0
 81 (A)--V    2.695   4.9   86.6   7.9   13.4   100.0
 82 (A)--V    2.845   8.4   90.7   3.0    9.3   100.0
 83 (A)--V    3.060   2.0   86.5   3.6   13.5   100.0
 84 (A)--V    3.100  61.9   95.7   0.7    4.3   100.0
 85 (A)--V    3.229  25.8   92.2   4.7    7.8   100.0
 86 (A)--V    3.304   4.7   77.4   5.8   22.6   100.0
 87 (A)--V    3.504   5.2   52.7   7.2   47.3   100.0
 88 (A)--V    4.159  22.9   91.4   1.2    8.6   100.0
 89 (A)--V    4.359  26.5   96.7   1.1    3.3   100.0
 90 (A)--V    4.807  73.7   95.2   0.1    4.8   100.0
 91 (A)--V    5.020   7.3   93.3   0.3    6.7   100.0
 92 (A)--V    5.195  11.3   96.7   0.3    3.3   100.0
 93 (A)--V    5.294  30.0   99.3   0.4    0.7   100.0
 94 (A)--V    5.407  36.4   94.8   0.3    5.2   100.0
 95 (A)--V    5.666  83.4   99.4   0.2    0.6   100.0
 96 (A)--V    5.912   9.0   86.3   0.7   13.7   100.0
 97 (A)--V    6.499   1.6   80.2   0.2   19.8   100.0
 98 (A)--V    6.662   2.3   86.5   0.3   13.5   100.0
 99 (A)--V    7.125   1.5   44.5   0.6   55.5   100.0
100 (A)--V    7.433   4.3   82.3   0.3   17.7   100.0
101 (A)--V    7.686   0.4   92.6   0.2    7.4   100.0
102 (A)--V    8.114  50.7   96.4   0.2    3.6   100.0
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103 (A)--V	8.400	56.4	97.3	0.2	2.7	100.0
104 (A)--V	8.435	38.8	92.2	0.3	7.8	100.0
105 (A)--V	8.537	56.5	97.6	0.1	2.4	100.0
106 (A)--V	8.690	41.8	98.0	0.2	2.0	100.0
107 (A)--V	8.910	22.9	96.5	0.2	3.5	100.0
108 (A)--V	9.144	23.3	88.5	0.4	11.5	100.0
109 (A)--V	9.261	49.2	98.1	0.4	1.9	100.0
110 (A)--V	9.740	46.2	93.6	0.4	6.4	100.0
111 (A)--V	9.939	17.9	91.9	0.5	8.1	100.0
112 (A)--V	10.152	1.0	97.4	0.2	2.6	100.0
113 (A)--V	10.435	52.7	92.5	0.4	7.5	100.0
114 (A)--V	10.624	16.5	70.9	1.0	29.1	100.0
115 (A)--V	10.840	52.3	96.6	0.3	3.4	100.0
116 (A)--V	11.345	5.7	60.7	1.1	39.3	100.0
117 (A)--V	11.469	31.4	81.9	0.3	18.1	100.0
118 (A)--V	11.957	6.0	78.7	0.3	21.3	100.0
119 (A)--V	12.325	8.2	89.7	0.2	10.3	100.0
120 (A)--V	12.741	10.8	70.5	0.7	29.5	100.0
121 (A)--V	12.860	5.4	41.5	13.5	58.5	100.0
122 (A)--V	13.018	16.3	87.2	0.9	12.8	100.0
123 (A)--V	13.124	18.5	85.4	0.3	14.6	100.0
124 (A)--V	13.193	18.7	84.9	1.5	15.1	100.0
125 (A)--V	13.557	11.6	86.9	1.2	13.1	100.0
126 (A)--V	13.829	7.5	95.6	1.0	4.4	100.0
127 (A)--V	13.943	62.9	93.0	0.6	7.0	100.0
128 (A)--V	14.120	18.4	77.2	3.4	22.8	100.0
129 (A)--V	14.494	15.1	71.0	5.0	29.0	100.0
130 (A)--V	14.645	19.4	74.9	3.8	25.1	100.0
131 (A)--V	14.956	23.9	89.2	1.3	10.8	100.0
132 (A)--V	15.101	23.0	94.9	0.9	5.1	100.0
133 (A)--V	15.726	1.1	97.8	0.2	2.2	100.0
134 (A)--V	15.908	8.9	89.6	0.8	10.4	100.0
135 (A)--V	16.023	5.0	89.7	0.3	10.3	100.0
136 (A)--V	16.181	5.9	92.9	0.7	7.1	100.0
137 (A)--V	16.667	10.2	80.1	2.2	19.9	100.0
138 (A)--V	16.731	3.1	97.3	0.3	2.7	100.0
139 (A)--V	16.781	5.4	93.3	0.7	6.7	100.0
140 (A)--V	16.838	7.9	98.9	0.2	1.1	100.0
141 (A)--V	16.929	24.0	92.0	0.4	8.0	100.0
142 (A)--V	17.266	7.4	89.7	0.8	10.3	100.0
143 (A)--V	17.367	7.3	92.9	0.3	7.1	100.0
144 (A)--V	17.618	10.0	74.5	2.0	25.5	100.0
145 (A)--V	18.237	3.9	53.5	4.0	46.5	100.0
146 (A)--V	18.477	1.7	68.9	0.6	31.1	100.0
147 (A)--V	18.906	3.6	82.7	0.7	17.3	100.0
148 (A)--V	19.104	1.3	95.0	0.2	5.0	100.0
149 (A)--V	19.428	7.0	95.5	0.6	4.5	100.0
150 (A)--V	19.672	9.1	94.6	0.4	5.4	100.0
151 (A)--V	19.886	6.5	91.8	1.4	8.2	100.0
152 (A)--V	20.287	4.2	64.7	2.1	35.3	100.0
153 (A)--V	20.655	30.1	65.7	1.3	34.3	100.0
154 (A)--V	20.871	36.8	78.4	1.7	21.6	100.0
155 (A)--V	21.115	16.8	65.2	9.4	34.8	100.0
156 (A)--V	21.370	18.6	76.4	4.0	23.6	100.0
157 (A)--V	22.046	12.5	86.1	10.8	13.9	100.0
158 (A)--V	22.463	11.2	83.9	1.8	16.1	100.0
159 (A)--V	22.778	9.6	89.8	0.7	10.2	100.0

160 (A)--V	23.284	33.4	81.6	0.5	18.4	100.0
161 (A)--V	23.594	4.8	88.9	0.4	11.1	100.0
162 (A)--V	24.072	30.8	97.9	1.2	2.1	100.0
163 (A)--V	24.632	16.7	83.9	0.4	16.1	100.0
164 (A)--V	25.262	2.2	86.8	0.6	13.2	100.0
165 (A)--V	25.792	1.0	98.6	0.0	1.4	100.0
166 (A)--V	26.144	5.2	96.0	0.7	4.0	100.0
167 (A)--V	26.433	1.0	94.1	0.2	5.9	100.0
168 (A)--V	27.703	7.3	95.5	0.2	4.5	100.0
169 (A)--V	27.794	5.5	97.9	0.0	2.1	100.0
170 (A)--V	28.025	13.0	98.9	0.2	1.1	100.0
171 (A)--V	28.218	2.9	95.8	0.1	4.2	100.0
172 (A)--V	28.464	2.8	95.1	0.1	4.9	100.0
173 (A)--V	28.650	0.4	98.2	0.0	1.8	100.0
174 (A)--V	28.784	20.6	99.8	0.0	0.2	100.0
175 (A)--V	29.340	18.0	96.6	0.1	3.4	100.0
176 (A)--V	29.703	9.4	99.4	0.1	0.6	100.0
177 (A)--V	30.258	20.5	94.4	0.1	5.6	100.0
178 (A)--V	30.911	3.9	72.5	0.4	27.5	100.0
179 (A)--V	30.954	5.5	93.6	0.2	6.4	100.0
180 (A)--V	31.511	11.9	98.2	0.1	1.8	100.0
181 (A)--V	31.925	1.3	88.4	0.5	11.6	100.0
182 (A)--V	32.754	30.7	99.0	0.0	1.0	100.0
183 (A)--V	33.189	30.6	97.6	0.1	2.4	100.0
184 (A)--V	33.214	22.4	94.4	0.7	5.6	100.0
185 (A)--V	34.946	9.7	91.3	1.5	8.7	100.0
186 (A)--V	35.716	7.9	72.6	1.4	27.4	100.0
187 (A)--V	36.093	23.8	82.2	0.4	17.8	100.0
188 (A)--V	36.879	17.7	95.4	0.3	4.6	100.0
189 (A)--V	37.125	15.8	98.0	0.3	2.0	100.0
190 (A)--V	39.002	4.6	85.6	0.2	14.4	100.0
191 (A)--V	39.362	7.1	79.2	0.4	20.8	100.0
192 (A)--V	39.870	1.8	97.2	0.1	2.8	100.0
193 (A)--V	40.425	1.0	97.7	0.0	2.3	100.0
194 (A)--V	40.546	10.6	65.1	0.5	34.9	100.0
195 (A)--V	41.310	6.7	72.5	0.2	27.5	100.0
196 (A)--V	41.627	6.0	58.6	0.6	41.4	100.0
197 (A)--V	42.113	18.8	90.3	0.2	9.7	100.0
198 (A)--V	42.271	10.6	83.3	0.2	16.7	100.0
199 (A)--V	42.483	11.2	92.0	0.2	8.0	100.0
200 (A)--V	42.585	8.0	95.5	0.0	4.5	100.0
201 (A)--V	42.873	9.3	95.5	0.1	4.5	100.0
202 (A)--V	43.063	11.8	96.6	0.2	3.4	100.0
203 (A)--V	43.894	6.3	96.5	0.0	3.5	100.0
204 (A)--V	44.508	13.1	97.3	0.0	2.7	100.0
205 (A)--V	44.563	6.7	78.3	0.2	21.7	100.0
206 (A)--V	45.322	11.0	87.7	0.1	12.3	100.0
207 (A)--V	45.850	7.5	89.0	0.0	11.0	100.0
208 (A)--V	46.239	11.2	79.3	0.5	20.7	100.0
209 (A)--V	46.831	2.8	71.7	0.4	28.3	100.0
210 (A)--V	47.517	24.3	94.7	0.0	5.3	100.0
211 (A)--V	47.833	13.2	92.0	0.1	8.0	100.0
212 (A)--V	48.133	16.0	83.7	0.2	16.3	100.0
213 (A)--V	49.018	7.2	90.5	0.1	9.5	100.0
214 (A)--V	49.146	12.4	92.6	0.0	7.4	100.0
215 (A)--V	49.673	3.9	89.3	0.1	10.7	100.0
216 (A)--V	50.589	6.8	97.7	0.1	2.3	100.0

217 (A)--V	50.911	21.7	94.9	0.1	5.1	100.0
218 (A)--V	51.399	36.0	84.1	0.1	15.9	100.0
219 (A)--V	51.506	15.7	92.4	0.0	7.6	100.0
220 (A)--V	52.411	17.6	98.3	0.0	1.7	100.0
221 (A)--V	52.652	2.6	99.7	0.0	0.3	100.0
222 (A)--V	53.787	0.8	98.6	0.0	1.4	100.0
223 (A)--V	53.894	4.3	96.2	0.1	3.8	100.0
224 (A)--V	54.231	8.2	45.4	0.1	54.6	100.0
225 (A)--V	55.978	50.5	96.9	0.0	3.1	100.0
226 (A)--V	56.098	53.3	97.4	0.0	2.6	100.0
227 (A)--V	56.359	34.2	83.2	0.1	16.8	100.0
228 (A)--V	56.515	3.0	99.7	0.0	0.3	100.0
229 (A)--V	56.618	15.8	92.7	0.1	7.3	100.0
230 (A)--V	57.115	18.6	93.5	0.0	6.5	100.0
231 (A)--V	57.444	22.0	89.9	0.1	10.1	100.0
232 (A)--V	57.694	3.4	91.9	0.1	8.1	100.0
233 (A)--V	57.878	0.4	99.5	0.0	0.5	100.0
234 (A)--V	57.941	0.9	99.5	0.0	0.5	100.0
235 (A)--V	58.136	41.8	98.8	0.1	1.2	100.0
236 (A)--V	58.893	6.8	93.8	0.1	6.2	100.0
237 (A)--V	59.112	19.0	90.3	0.1	9.7	100.0
238 (A)--V	59.867	3.6	72.4	0.1	27.6	100.0
239 (A)--V	60.607	2.7	82.3	0.0	17.7	100.0
240 (A)--V	61.361	0.7	96.4	0.0	3.6	100.0
241 (A)--V	61.630	0.4	97.6	0.0	2.4	100.0
242 (A)--V	61.807	8.5	90.2	0.0	9.8	100.0
243 (A)--V	64.569	1.1	75.0	0.1	25.0	100.0
244 (A)--V	65.264	19.1	77.0	0.1	23.0	100.0
245 (A)--V	66.720	31.7	99.5	0.0	0.5	100.0
246 (A)--V	67.503	25.4	89.1	0.1	10.9	100.0
247 (A)--V	67.617	21.0	98.0	0.1	2.0	100.0
248 (A)--V	68.815	10.0	63.4	0.1	36.6	100.0
249 (A)--V	70.156	20.9	79.4	0.6	20.6	100.0
250 (A)--V	70.482	11.4	70.3	0.5	29.7	100.0
251 (A)--V	71.632	55.7	91.0	0.1	9.0	100.0
252 (A)--V	71.784	53.2	88.8	0.0	11.2	100.0
253 (A)--V	72.121	42.1	84.0	0.2	16.0	100.0
254 (A)--V	74.935	2.6	78.6	0.4	21.4	100.0
255 (A)--V	75.117	1.2	73.3	0.5	26.7	100.0
256 (A)--V	75.901	7.0	49.9	0.5	50.1	100.0
257 (A)--V	76.203	3.9	74.6	0.4	25.4	100.0
258 (A)--V	79.646	5.0	93.9	0.2	6.1	100.0
259 (A)--V	80.181	4.2	82.4	0.3	17.6	100.0
260 (A)--V	80.464	5.0	91.6	0.2	8.4	100.0
261 (A)--V	81.222	6.4	95.9	0.2	4.1	100.0
262 (A)--V	81.595	1.7	99.5	0.0	0.5	100.0
263 (A)--V	81.738	29.3	97.9	0.0	2.1	100.0
264 (A)--V	82.164	15.8	89.2	0.5	10.8	100.0
265 (A)--V	82.327	40.5	98.1	0.1	1.9	100.0
266 (A)--V	82.459	3.4	98.8	0.0	1.2	100.0
267 (A)--V	83.353	0.3	99.3	0.0	0.7	100.0
268 (A)--V	83.904	1.1	98.0	0.0	2.0	100.0
269 (A)--V	84.142	25.6	93.2	0.1	6.8	100.0
270 (A)--V	84.497	0.2	97.8	0.1	2.2	100.0
271 (A)--V	84.605	1.5	99.2	0.0	0.8	100.0
272 (A)--V	84.970	2.0	95.8	0.1	4.2	100.0
273 (A)--V	85.623	1.2	86.6	0.0	13.4	100.0

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274 (A)--V      86.949      4.4     92.6      0.2     7.4     100.0
275 (A)--V      87.722      1.6     69.2      0.0    30.8     100.0
276 (A)--V      89.419     13.0     82.1      0.1    17.9     100.0
277 (A)--V      89.916     14.0     98.4      0.0     1.6     100.0
278 (A)--V      90.171     13.9     98.8      0.0     1.2     100.0
279 (A)--V      90.492      7.8     77.1      0.0    22.9     100.0
280 (A)--V      90.663      5.8     81.0      0.0    19.0     100.0
281 (A)--V      94.957      3.2     81.2      0.0    18.8     100.0
282 (A)--V      95.380      2.6     95.7      0.0     4.3     100.0
283 (A)--V      96.783      2.5     91.7      0.0     8.3     100.0
284 (A)--V      98.369      0.7     98.5      0.0     1.5     100.0
285 (A)--V     100.173     10.6     95.5      0.0     4.5     100.0
286 (A)--V     100.455     11.6     99.0      0.0     1.0     100.0
287 (A)--V     100.842     27.0     93.7      0.0     6.3     100.0
288 (A)--V     102.274     50.0     97.0      0.0     3.0     100.0
289 (A)--V     103.612      2.5     99.8      0.0     0.2     100.0
290 (A)--V     103.985      1.7     99.7      0.0     0.3     100.0
291 (A)--V     104.278      0.7     99.8      0.0     0.2     100.0
292 (A)--V     104.930      6.3     97.6      0.0     2.4     100.0
293 (A)--V     105.163     11.4     99.9      0.0     0.1     100.0
294 (A)--V     107.903     67.3     96.1      0.0     3.9     100.0
295 (A)--V     113.606     12.1     71.8      0.1    28.2     100.0
296 (A)--V     120.799      0.0    100.0      0.0     0.0     100.0
297 (A)--V     120.877      0.1     99.6      0.0     0.4     100.0
298 (A)--V     158.008     17.6     99.5      0.0     0.5     100.0
299 (A)--V     158.375     13.1     98.4      0.0     1.6     100.0
300 (A)--V     165.146     87.9     99.7      0.0     0.3     100.0
301 (A)--V     168.057     84.4     99.7      0.0     0.3     100.0
302 (A)--V     168.306     61.0     93.7      0.0     6.3     100.0
303 (A)--V     234.270     96.5     99.9      0.0     0.1     100.0
304 (A)--V     235.046     88.4     96.4      0.0     3.6     100.0
305 (A)--V     250.386     90.7     98.3      0.0     1.7     100.0
306 (A)--V     342.251      5.8     38.6     49.5    61.4     100.0
307 (A)--V     366.837     10.8     61.0     30.5    39.0     100.0
308 (A)--V     627.419      3.3     26.1      0.0    73.9     100.0
309 (A)--V     632.242      9.7     95.6      0.0     4.4     100.0
310 (A)--V     634.864      7.5     83.4      0.0    16.6     100.0
311 (A)--V     643.683      2.2     99.8      0.0     0.2     100.0
312 (A)--V     644.044      5.2     99.4      0.0     0.6     100.0
313 (A)--V     644.542     10.8     99.8      0.0     0.2     100.0
314 (A)--V     644.867      0.5     99.4      0.0     0.6     100.0
315 (A)--V     645.356      2.7     99.8      0.0     0.2     100.0
316 (A)--V     645.590      9.1     98.4      0.0     1.6     100.0
317 (A)--V     645.602      1.2    100.0      0.0     0.0     100.0
318 (A)--V     645.862      0.4     99.1      0.0     0.9     100.0
319 (A)--V     650.002      0.7      4.8      0.0    95.2     100.0
320 (A)--V     758.793     96.5     99.5      0.0     0.5     100.0
321 (A)--V    4856.058     99.2    100.0      0.0     0.0     100.0
322 (A)--V    4856.683     97.0     99.1      0.0     0.9     100.0
323 (A)--V    4869.788     96.6     99.3      0.0     0.7     100.0
324 (A)--V   12037.585     99.3     99.9      0.0     0.1     100.0
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Full population analysis for complex *cis*-2 (optimized geometry):
```
*********************************************************************
*                          VMOdes                                   *
```

```
* Virtual Molecular Orbital description Program, Revision 7.1      *
* Cite this work as: VMOdes Program, Revision A 7.1                *
* V. N. Nemykin, P. Basu, 2001, 2003                              *
* Department of Chemistry, Duquesne University, Pittsburgh, PA     *
*****************************************************************

Input Gaussian file:
C:\Documents and Settings\hp\My Documents\Research Dr.
Nemykin\VMOdes\VModes\FcI2-cis.gjf.out
Output VMOdes file: cis-FcI2.out


Full point group is:  C1



Number of Basis Functions = 324

     61 Alpha electrons          61 Beta electrons


Group  1  is: Fe
This group consist of  1  subunits. The Basis Functions range is:
 106          161
Group  2  is: Fc
This group consist of  1  subunits. The Basis Functions range is:
 1            263
Group  3  is: I
This group consist of  2  subunits. The Basis Functions range is:
 300          310
 314          324
Group  4  is: Lig
This group consist of  1  subunits. The Basis Functions range is:
 264          324
Group  5  is: Total
This group consist of  1  subunits. The Basis Functions range is:
 1            324


All MO's will be printed.

Molecular Orbitals Indexes, Energies, and Group Contributions
```

	Orbital		Group Number				
Number	Index	Energy,eV	1	2	3	4	5
1	(A)--O	-6932.685	100.0	100.0	0.0	0.0	100.0
2	(A)--O	-802.729	100.0	100.0	0.0	0.0	100.0
3	(A)--O	-693.221	100.0	100.0	0.0	0.0	100.0
4	(A)--O	-692.821	100.0	100.0	0.0	0.0	100.0
5	(A)--O	-692.808	100.0	100.0	0.0	0.0	100.0
6	(A)--O	-271.170	0.0	0.1	0.0	99.9	100.0
7	(A)--O	-270.703	0.0	0.0	0.0	100.0	100.0
8	(A)--O	-270.320	0.1	100.0	0.0	0.0	100.0
9	(A)--O	-269.848	0.1	100.0	0.0	0.0	100.0
10	(A)--O	-269.809	0.1	100.0	0.0	0.0	100.0
11	(A)--O	-269.788	0.1	100.0	0.0	0.0	100.0
12	(A)--O	-269.774	0.0	100.0	0.0	0.0	100.0
13	(A)--O	-269.709	0.1	100.0	0.0	0.0	100.0
14	(A)--O	-269.696	0.1	100.0	0.0	0.0	100.0

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15   (A)--O   -269.682   0.1    100.0   0.0    0.0    100.0
16   (A)--O   -269.656   0.1    100.0   0.0    0.0    100.0
17   (A)--O   -269.644   0.0    100.0   0.0    0.0    100.0
18   (A)--O    -87.978  100.0   100.0   0.0    0.0    100.0
19   (A)--O    -56.549   99.9   100.0   0.0    0.0    100.0
20   (A)--O    -55.496   99.9   100.0   0.0    0.0    100.0
21   (A)--O    -55.466   99.9   100.0   0.0    0.0    100.0
22   (A)--O    -22.567    8.3    95.8   0.2    4.2    100.0
23   (A)--O    -22.107    9.6    98.2   0.1    1.8    100.0
24   (A)--O    -20.450    1.9    21.6  10.2   78.4    100.0
25   (A)--O    -18.335    0.8    41.5  41.1   58.5    100.0
26   (A)--O    -17.950    1.8    92.7   6.5    7.3    100.0
27   (A)--O    -17.735    1.8    99.5   0.4    0.5    100.0
28   (A)--O    -17.732    1.7    99.4   0.5    0.6    100.0
29   (A)--O    -17.491    0.9    37.0  58.5   63.0    100.0
30   (A)--O    -16.841    0.4    20.6  58.2   79.4    100.0
31   (A)--O    -14.459    0.4    47.0  19.9   53.0    100.0
32   (A)--O    -13.714    0.5    94.6   2.4    5.4    100.0
33   (A)--O    -13.527    1.7    97.8   0.8    2.2    100.0
34   (A)--O    -13.459    0.2    99.1   0.3    0.9    100.0
35   (A)--O    -13.429    0.7    99.5   0.1    0.5    100.0
36   (A)--O    -13.160    1.6    97.6   0.8    2.4    100.0
37   (A)--O    -12.690    0.3    26.6  14.2   73.4    100.0
38   (A)--O    -10.843    4.8    62.6   8.9   37.4    100.0
39   (A)--O    -10.622   13.7    50.8  19.8   49.2    100.0
40   (A)--O    -10.361   19.9    65.7  15.9   34.3    100.0
41   (A)--O    -10.209    7.8    98.9   0.4    1.1    100.0
42   (A)--O     -9.986    4.2    98.0   0.7    2.0    100.0
43   (A)--O     -9.927    1.0    99.5   0.3    0.5    100.0
44   (A)--O     -9.630    0.8    95.3   0.5    4.7    100.0
45   (A)--O     -9.460    5.8    73.4  10.0   26.6    100.0
46   (A)--O     -9.332    0.8    99.0   0.2    1.0    100.0
47   (A)--O     -9.318    0.5    99.5   0.1    0.5    100.0
48   (A)--O     -9.129    5.2    73.4  13.9   26.6    100.0
49   (A)--O     -8.590    1.7    19.1  45.2   80.9    100.0
50   (A)--O     -8.348    3.5    31.7  25.7   68.3    100.0
51   (A)--O     -7.015   14.8    50.8  41.5   49.2    100.0
52   (A)--O     -6.930   31.5    98.3   1.3    1.7    100.0
53   (A)--O     -6.843    0.5     9.8  78.2   90.2    100.0
54   (A)--O     -6.763   11.8    44.3  52.0   55.7    100.0
55   (A)--O     -6.382    5.7    87.5   9.8   12.5    100.0
56   (A)--O     -6.335    2.6    37.4  57.3   62.6    100.0
57   (A)--O     -6.089    0.6    12.2  76.2   87.8    100.0
58   (A)--O     -5.638    5.5    28.0  45.6   72.0    100.0
59   (A)--O     -4.723   86.4    97.9   0.5    2.1    100.0
60   (A)--O     -4.460   59.1    96.9   1.1    3.1    100.0
61   (A)--O     -4.449   62.3    98.2   0.9    1.8    100.0
62   (A)--V     -2.464    3.5     8.4  45.1   91.6    100.0
63   (A)--V     -1.963   23.9    52.2  13.3   47.8    100.0
64   (A)--V     -1.757   42.1    94.4   2.3    5.6    100.0
65   (A)--V     -1.280   10.2    35.7  15.7   64.3    100.0
66   (A)--V     -1.136    2.1     9.6  34.7   90.4    100.0
67   (A)--V      0.532    5.5    90.9   2.6    9.1    100.0
68   (A)--V      0.630   35.8    88.7   8.0   11.3    100.0
69   (A)--V      0.652    4.7    74.0  22.9   26.0    100.0
70   (A)--V      0.670   20.4    95.5   3.1    4.5    100.0
71   (A)--V      0.772   24.0    67.3  22.6   32.7    100.0
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72	(A)--V	1.205	8.1	54.9	40.8	45.1	100.0
73	(A)--V	1.243	31.5	69.6	24.2	30.4	100.0
74	(A)--V	1.310	22.1	64.7	26.9	35.3	100.0
75	(A)--V	1.524	16.9	62.8	29.8	37.2	100.0
76	(A)--V	1.606	32.3	71.8	24.6	28.2	100.0
77	(A)--V	1.678	2.8	59.5	26.3	40.5	100.0
78	(A)--V	1.896	6.1	88.0	11.1	12.0	100.0
79	(A)--V	2.027	9.1	70.9	26.5	29.1	100.0
80	(A)--V	2.204	0.6	57.3	37.1	42.7	100.0
81	(A)--V	2.558	9.3	86.8	3.5	13.2	100.0
82	(A)--V	2.755	13.3	81.4	8.7	18.6	100.0
83	(A)--V	2.940	4.6	91.1	1.9	8.9	100.0
84	(A)--V	3.093	53.6	95.5	1.6	4.5	100.0
85	(A)--V	3.236	8.1	87.1	11.2	12.9	100.0
86	(A)--V	3.340	25.0	84.1	6.9	15.9	100.0
87	(A)--V	3.610	13.1	72.2	2.4	27.8	100.0
88	(A)--V	4.166	22.9	84.9	1.2	15.1	100.0
89	(A)--V	4.312	29.5	95.8	0.4	4.2	100.0
90	(A)--V	4.768	75.7	98.1	0.1	1.9	100.0
91	(A)--V	4.972	11.6	78.3	0.4	21.7	100.0
92	(A)--V	5.206	2.0	98.5	0.3	1.5	100.0
93	(A)--V	5.292	27.1	97.8	0.6	2.2	100.0
94	(A)--V	5.393	29.3	97.9	0.4	2.1	100.0
95	(A)--V	5.570	77.4	96.7	0.2	3.3	100.0
96	(A)--V	5.733	7.3	84.3	0.8	15.7	100.0
97	(A)--V	6.550	3.0	81.6	0.3	18.4	100.0
98	(A)--V	6.705	1.4	80.8	0.5	19.2	100.0
99	(A)--V	6.984	2.1	64.8	0.4	35.2	100.0
100	(A)--V	7.522	3.1	92.4	0.2	7.6	100.0
101	(A)--V	7.847	24.5	91.0	0.2	9.0	100.0
102	(A)--V	7.923	18.6	91.7	0.1	8.3	100.0
103	(A)--V	8.372	64.2	96.3	0.1	3.7	100.0
104	(A)--V	8.431	38.3	95.4	0.2	4.6	100.0
105	(A)--V	8.550	45.1	96.6	0.1	3.4	100.0
106	(A)--V	8.810	39.0	87.9	0.2	12.1	100.0
107	(A)--V	8.903	16.2	93.2	0.4	6.8	100.0
108	(A)--V	9.073	36.6	86.7	0.7	13.3	100.0
109	(A)--V	9.247	46.9	96.7	0.4	3.3	100.0
110	(A)--V	9.816	36.9	92.8	0.3	7.2	100.0
111	(A)--V	10.038	22.7	85.2	0.3	14.8	100.0
112	(A)--V	10.146	4.4	98.4	0.1	1.6	100.0
113	(A)--V	10.417	4.5	72.8	1.3	27.2	100.0
114	(A)--V	10.753	40.6	86.5	0.8	13.5	100.0
115	(A)--V	10.888	60.1	93.1	0.3	6.9	100.0
116	(A)--V	11.340	8.8	66.7	1.9	33.3	100.0
117	(A)--V	11.698	11.2	75.5	1.2	24.5	100.0
118	(A)--V	11.898	9.0	53.3	4.8	46.7	100.0
119	(A)--V	12.204	13.6	87.0	1.0	13.0	100.0
120	(A)--V	12.585	8.6	88.0	0.8	12.0	100.0
121	(A)--V	12.881	16.1	89.7	2.2	10.3	100.0
122	(A)--V	13.048	15.9	90.8	2.1	9.2	100.0
123	(A)--V	13.109	22.3	90.7	1.0	9.3	100.0
124	(A)--V	13.309	16.0	82.2	1.7	17.8	100.0
125	(A)--V	13.332	16.7	77.5	4.4	22.5	100.0
126	(A)--V	13.761	4.5	93.0	2.1	7.0	100.0
127	(A)--V	13.863	66.2	97.8	0.3	2.2	100.0
128	(A)--V	14.015	10.4	57.6	9.2	42.4	100.0

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129 (A)--V    14.538    26.8    80.5     4.4    19.5    100.0
130 (A)--V    14.622    21.0    70.5     6.4    29.5    100.0
131 (A)--V    14.792    13.0    93.6     0.2     6.4    100.0
132 (A)--V    15.248    28.2    88.6     0.9    11.4    100.0
133 (A)--V    15.803     2.0    95.7     0.7     4.3    100.0
134 (A)--V    15.892     1.1    89.1     1.3    10.9    100.0
135 (A)--V    15.980     2.2    87.0     0.1    13.0    100.0
136 (A)--V    16.090     7.7    90.1     0.8     9.9    100.0
137 (A)--V    16.558     3.9    91.7     1.0     8.3    100.0
138 (A)--V    16.719    13.5    92.0     1.0     8.0    100.0
139 (A)--V    16.814     4.0    98.0     0.1     2.0    100.0
140 (A)--V    16.915    19.9    93.5     0.2     6.5    100.0
141 (A)--V    16.988     4.7    95.4     0.4     4.6    100.0
142 (A)--V    17.088    11.2    96.3     0.2     3.7    100.0
143 (A)--V    17.275    10.0    95.3     0.1     4.7    100.0
144 (A)--V    17.883     4.6    66.4     1.2    33.6    100.0
145 (A)--V    18.307     4.1    94.7     1.9     5.3    100.0
146 (A)--V    18.627     2.9    90.3     0.3     9.7    100.0
147 (A)--V    19.031     2.2    98.4     0.3     1.6    100.0
148 (A)--V    19.172     6.0    88.8     1.1    11.2    100.0
149 (A)--V    19.502     5.4    98.7     0.8     1.3    100.0
150 (A)--V    19.653    17.7    92.1     1.9     7.9    100.0
151 (A)--V    19.943     7.2    87.7     4.4    12.3    100.0
152 (A)--V    20.345    10.6    82.5     4.4    17.5    100.0
153 (A)--V    20.467    19.6    52.2     2.0    47.8    100.0
154 (A)--V    20.744    22.4    64.4     2.5    35.6    100.0
155 (A)--V    20.847    14.3    64.0    10.1    36.0    100.0
156 (A)--V    21.208    23.6    96.0     1.8     4.0    100.0
157 (A)--V    22.344     5.4    49.0     3.5    51.0    100.0
158 (A)--V    22.490     6.9    58.2     3.4    41.8    100.0
159 (A)--V    22.803    12.3    96.0     0.3     4.0    100.0
160 (A)--V    23.034    15.5    75.6     1.2    24.4    100.0
161 (A)--V    23.529    35.2    97.8     0.6     2.2    100.0
162 (A)--V    23.772    45.6    95.4     0.7     4.6    100.0
163 (A)--V    24.467    13.9    89.3     0.2    10.7    100.0
164 (A)--V    25.257     0.8    84.8     0.6    15.2    100.0
165 (A)--V    25.747     0.3    99.3     0.0     0.7    100.0
166 (A)--V    26.114     1.5    91.0     0.1     9.0    100.0
167 (A)--V    26.464     2.8    93.1     0.1     6.9    100.0
168 (A)--V    27.641    11.3    93.5     0.8     6.5    100.0
169 (A)--V    27.768     7.9    96.7     0.1     3.3    100.0
170 (A)--V    28.068     9.6    98.8     0.1     1.2    100.0
171 (A)--V    28.312     1.8    96.3     0.1     3.7    100.0
172 (A)--V    28.526     0.2    98.4     0.0     1.6    100.0
173 (A)--V    28.579     2.3    97.9     0.0     2.1    100.0
174 (A)--V    28.806    23.6    99.9     0.0     0.1    100.0
175 (A)--V    29.291    17.5    98.4     0.1     1.6    100.0
176 (A)--V    29.782    14.0    99.4     0.1     0.6    100.0
177 (A)--V    30.369    29.2    92.5     0.1     7.5    100.0
178 (A)--V    30.684     8.3    78.7     0.7    21.3    100.0
179 (A)--V    30.989     4.1    98.0     0.1     2.0    100.0
180 (A)--V    31.471    13.7    95.6     0.2     4.4    100.0
181 (A)--V    32.762    29.4    97.5     0.1     2.5    100.0
182 (A)--V    32.973    31.8    99.1     0.0     0.9    100.0
183 (A)--V    33.184     9.3    92.3     0.6     7.7    100.0
184 (A)--V    33.563    11.5    90.4     0.5     9.6    100.0
185 (A)--V    34.962    18.1    89.7     1.6    10.3    100.0
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186 (A)--V    35.862    26.4    84.6    0.7    15.4    100.0
187 (A)--V    36.557     9.5    77.6    1.1    22.4    100.0
188 (A)--V    36.974    14.2    97.4    0.2     2.6    100.0
189 (A)--V    37.670     4.1    76.4    0.8    23.6    100.0
190 (A)--V    39.262    26.9    90.7    0.5     9.3    100.0
191 (A)--V    39.367     4.0    85.3    0.2    14.7    100.0
192 (A)--V    39.683     2.8    94.6    0.1     5.4    100.0
193 (A)--V    40.378     2.8    89.5    0.2    10.5    100.0
194 (A)--V    40.644     5.7    99.1    0.1     0.9    100.0
195 (A)--V    41.243     6.2    83.0    0.2    17.0    100.0
196 (A)--V    41.710     8.2    72.6    1.1    27.4    100.0
197 (A)--V    42.077    17.1    91.1    0.1     8.9    100.0
198 (A)--V    42.237    16.2    92.4    0.1     7.6    100.0
199 (A)--V    42.496    11.7    90.0    0.2    10.0    100.0
200 (A)--V    42.632     6.6    98.3    0.0     1.7    100.0
201 (A)--V    42.925     6.7    97.3    0.1     2.7    100.0
202 (A)--V    43.024    13.2    95.7    0.5     4.3    100.0
203 (A)--V    43.914     6.9    98.7    0.0     1.3    100.0
204 (A)--V    44.526    13.2    99.3    0.0     0.7    100.0
205 (A)--V    44.923    13.9    94.7    0.0     5.3    100.0
206 (A)--V    45.348     2.4    59.3    0.2    40.7    100.0
207 (A)--V    45.869    11.0    97.6    0.0     2.4    100.0
208 (A)--V    46.636     4.6    79.8    0.5    20.2    100.0
209 (A)--V    46.937     5.7    64.9    0.3    35.1    100.0
210 (A)--V    47.482    17.5    92.6    0.1     7.4    100.0
211 (A)--V    47.740    22.4    95.1    0.1     4.9    100.0
212 (A)--V    48.273    15.9    97.3    0.1     2.7    100.0
213 (A)--V    49.051     4.6    95.7    0.1     4.3    100.0
214 (A)--V    49.324    12.3    92.1    0.2     7.9    100.0
215 (A)--V    49.600     5.1    74.8    0.2    25.2    100.0
216 (A)--V    50.432     9.8    93.5    0.2     6.5    100.0
217 (A)--V    50.996    15.9    96.0    0.0     4.0    100.0
218 (A)--V    51.504    28.5    73.7    0.2    26.3    100.0
219 (A)--V    51.597    24.5    90.7    0.1     9.3    100.0
220 (A)--V    52.409    27.7    98.9    0.0     1.1    100.0
221 (A)--V    52.605     1.0    99.6    0.0     0.4    100.0
222 (A)--V    53.422     1.5    90.3    0.1     9.7    100.0
223 (A)--V    53.807     2.0    98.9    0.0     1.1    100.0
224 (A)--V    54.411    20.3    66.5    0.2    33.5    100.0
225 (A)--V    55.797    35.7    82.6    0.1    17.4    100.0
226 (A)--V    56.138    50.3    94.6    0.0     5.4    100.0
227 (A)--V    56.215    49.0    99.2    0.0     0.8    100.0
228 (A)--V    56.518     2.7    99.9    0.0     0.1    100.0
229 (A)--V    56.900    23.7    95.0    0.1     5.0    100.0
230 (A)--V    57.098    22.4    77.5    0.2    22.5    100.0
231 (A)--V    57.562    30.7    90.9    0.1     9.1    100.0
232 (A)--V    57.818     0.2    94.4    0.0     5.6    100.0
233 (A)--V    57.889     0.2   100.0    0.0     0.0    100.0
234 (A)--V    57.973     1.1    88.2    0.1    11.8    100.0
235 (A)--V    58.117    33.3    95.7    0.0     4.3    100.0
236 (A)--V    58.600    15.7    87.6    0.1    12.4    100.0
237 (A)--V    59.102    29.5    94.6    0.1     5.4    100.0
238 (A)--V    59.437     1.7    81.7    0.0    18.3    100.0
239 (A)--V    60.368     6.9    68.0    0.1    32.0    100.0
240 (A)--V    61.411     3.0    99.0    0.0     1.0    100.0
241 (A)--V    61.657     7.0    94.8    0.0     5.2    100.0
242 (A)--V    61.724     0.4    99.2    0.0     0.8    100.0
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243 (A)--V    64.085    12.7    74.8    0.2    25.2    100.0
244 (A)--V    65.784    15.5    71.8    0.1    28.2    100.0
245 (A)--V    66.815    32.1    99.4    0.0    0.6     100.0
246 (A)--V    67.266    13.7    84.8    0.2    15.2    100.0
247 (A)--V    67.612    18.3    91.0    0.1    9.0     100.0
248 (A)--V    68.032    14.1    65.8    0.2    34.2    100.0
249 (A)--V    69.634    8.6     79.3    0.4    20.7    100.0
250 (A)--V    70.283    18.1    86.7    0.1    13.3    100.0
251 (A)--V    71.595    77.7    97.0    0.1    3.0     100.0
252 (A)--V    71.664    49.7    93.9    0.0    6.1     100.0
253 (A)--V    71.914    25.9    92.1    0.1    7.9     100.0
254 (A)--V    75.003    1.4     90.2    0.0    9.8     100.0
255 (A)--V    75.415    3.4     98.1    0.1    1.9     100.0
256 (A)--V    76.191    1.8     59.7    0.3    40.3    100.0
257 (A)--V    76.483    4.9     53.5    0.9    46.5    100.0
258 (A)--V    79.576    3.4     96.7    0.0    3.3     100.0
259 (A)--V    80.075    4.9     92.4    0.2    7.6     100.0
260 (A)--V    80.297    1.9     93.6    0.0    6.4     100.0
261 (A)--V    81.545    6.6     98.8    0.0    1.2     100.0
262 (A)--V    81.611    8.3     99.2    0.1    0.8     100.0
263 (A)--V    81.723    32.4    99.5    0.0    0.5     100.0
264 (A)--V    82.270    28.1    99.4    0.0    0.6     100.0
265 (A)--V    82.399    5.0     99.6    0.0    0.4     100.0
266 (A)--V    82.775    5.2     75.6    1.2    24.4    100.0
267 (A)--V    83.408    0.7     99.6    0.0    0.4     100.0
268 (A)--V    83.845    4.3     99.2    0.0    0.8     100.0
269 (A)--V    84.029    3.2     95.8    0.0    4.2     100.0
270 (A)--V    84.473    0.3     98.9    0.1    1.1     100.0
271 (A)--V    84.576    1.2     99.1    0.0    0.9     100.0
272 (A)--V    84.935    2.0     96.8    0.1    3.2     100.0
273 (A)--V    85.362    1.2     78.7    0.0    21.3    100.0
274 (A)--V    87.059    3.7     75.7    0.1    24.3    100.0
275 (A)--V    87.706    4.5     88.7    0.4    11.3    100.0
276 (A)--V    89.621    23.0    87.6    0.2    12.4    100.0
277 (A)--V    89.968    15.1    99.2    0.0    0.8     100.0
278 (A)--V    90.249    7.1     95.5    0.1    4.5     100.0
279 (A)--V    90.613    6.3     84.0    0.1    16.0    100.0
280 (A)--V    90.776    8.2     82.2    0.2    17.8    100.0
281 (A)--V    94.863    2.6     79.6    0.0    20.4    100.0
282 (A)--V    95.433    2.3     96.7    0.1    3.3     100.0
283 (A)--V    96.591    2.3     91.9    0.0    8.1     100.0
284 (A)--V    98.261    0.7     98.0    0.0    2.0     100.0
285 (A)--V    100.071   9.8     95.9    0.0    4.1     100.0
286 (A)--V    100.470   10.7    98.7    0.0    1.3     100.0
287 (A)--V    100.926   27.5    94.2    0.0    5.8     100.0
288 (A)--V    102.223   54.3    98.3    0.0    1.7     100.0
289 (A)--V    103.607   2.6     99.9    0.0    0.1     100.0
290 (A)--V    104.001   1.8     99.7    0.0    0.3     100.0
291 (A)--V    104.239   0.5     99.9    0.0    0.1     100.0
292 (A)--V    104.884   5.8     97.9    0.0    2.1     100.0
293 (A)--V    105.121   11.2    100.0   0.0    0.0     100.0
294 (A)--V    107.938   71.5    96.8    0.0    3.2     100.0
295 (A)--V    114.290   8.9     71.2    0.0    28.8    100.0
296 (A)--V    120.800   0.0     100.0   0.0    0.0     100.0
297 (A)--V    120.869   0.1     99.8    0.0    0.2     100.0
298 (A)--V    158.039   17.7    98.8    0.0    1.2     100.0
299 (A)--V    158.337   13.2    99.3    0.0    0.7     100.0
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300 (A)--V      165.182    88.4    99.7     0.0      0.3     100.0
301 (A)--V      168.070    84.4    99.2     0.0      0.8     100.0
302 (A)--V      168.305    64.9    96.6     0.0      3.4     100.0
303 (A)--V      234.271    96.7   100.0     0.0      0.0     100.0
304 (A)--V      234.977    91.1    97.4     0.0      2.6     100.0
305 (A)--V      250.196    93.6    99.5     0.0      0.5     100.0
306 (A)--V      335.877     3.1    46.6    27.5     53.4     100.0
307 (A)--V      367.229     9.8    61.0    34.5     39.0     100.0
308 (A)--V      627.763     3.4    27.1     0.1     72.9     100.0
309 (A)--V      632.238     9.6    95.9     0.0      4.1     100.0
310 (A)--V      634.809     7.5    82.4     0.0     17.6     100.0
311 (A)--V      643.692     2.1    99.9     0.0      0.1     100.0
312 (A)--V      644.017     4.4    99.3     0.0      0.7     100.0
313 (A)--V      644.569    10.4    99.9     0.0      0.1     100.0
314 (A)--V      644.823     2.6    99.0     0.0      1.0     100.0
315 (A)--V      645.234     8.9    98.6     0.0      1.4     100.0
316 (A)--V      645.415     4.2    98.9     0.0      1.1     100.0
317 (A)--V      645.552     0.5    99.9     0.0      0.1     100.0
318 (A)--V      645.789     0.3    99.3     0.0      0.7     100.0
319 (A)--V      649.298     1.4     9.8     0.0     90.2     100.0
320 (A)--V      758.659    97.2    99.7     0.0      0.3     100.0
321 (A)--V     4856.055    99.2   100.0     0.0      0.0     100.0
322 (A)--V     4856.638    97.6    99.3     0.0      0.7     100.0
323 (A)--V     4869.684    97.5    99.7     0.0      0.3     100.0
324 (A)--V    12037.443    99.4    99.9     0.0      0.1     100.0
```

Full TDDFT analysis for complex *trans*-4 (X-ray geometry):

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SWizard program: Copyright (c) S. I. Gorelsky, 1999-2007.
This software is provided under written license and may be used, copied,
transmitted, or stored only in accord with that license.
****************************************************************
 Use of this program should be acknowledged in publications as:
  S.I. Gorelsky, SWizard program, http://www.sg-chem.net/
****************************************************************
The file SWizard.txt was created on 03-15-2007 from the Gaussian 98/03 output
file (TRANS-~1.OUT)
Framework group  C1[X(C14H10FeN2)]
bpw91/gen td=(nstates=40) test geom=connectivity

  #  (nm  1000 cm-1  eV)   (f)  (Assignment; H=HOMO,L=LUMO,L+1=LUMO+1,etc.)
  1  719.6  13.9   1.72 0.0001 S H-1->L+0(+62%)  H-0->L+0(35%)
  2  671.3  14.9   1.85 0.0061 S H-0->L+0(+40%)  H-1->L+0(+26%)
                                 H-2->L+0(+26%)
  3  593.0  16.9   2.09 0.0309 S H-2->L+0(+66%)  H-0->L+0(13%)
                                 H-1->L+0(6%)
  4  413.8  24.2   3.00 0.0002 S H-0->L+1(+54%)  H-1->L+2(36%)
  5  412.8  24.2   3.00 0.0005 S H-1->L+1(+49%)  H-0->L+2(+43%)
  6  392.5  25.5   3.16 0.0003 S H-2->L+1(+40%)  H-2->L+2(20%)
                                 H-1->L+2(16%)   H-0->L+2(12%)
                                 H-1->L+1(+6%)
  7  388.1  25.8   3.19 0.0005 S H-2->L+1(+48%)  H-2->L+2(+31%)
                                 H-0->L+2(+12%)  H-1->L+1(8%)
  8  356.9  28.0   3.47 0.0001 S H-4->L+0(+98%)
  9  338.6  29.5   3.66 0.1126 S H-3->L+0(+57%)  H-5->L+0(26%)
 10  330.4  30.3   3.75 0.0186 S H-1->L+2(+27%)  H-0->L+1(+19%)
                                 H-1->L+1(+11%)  H-0->L+2(9%)
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                                  H-3->L+0(+5%)
11  324.7  30.8   3.82 0.0004 S H-2->L+2(+37%)  H-1->L+1(+11%)
                                  H-0->L+2(11%)   H-6->L+0(7%)
                                  H-0->L+1(6%)
12  302.7  33.0   4.10 0.0002 S H-0->L+3(+77%)  H-6->L+0(+15%)
13  300.7  33.3   4.12 0.0125 S H-1->L+3(+72%)  H-5->L+0(+10%)
                                  H-0->L+3(+8%)
14  298.3  33.5   4.16 0.0045 S H-6->L+0(+74%)  H-0->L+3(9%)
15  296.2  33.8   4.19 0.0824 S H-5->L+0(+43%)  H-1->L+3(20%)
                                  H-7->L+0(13%)   H-3->L+0(+9%)
16  286.4  34.9   4.33 0.0014 S H-2->L+3(+99%)
17  280.9  35.6   4.41 0.0022 S H-0->L+4(+99%)
18  278.6  35.9   4.45 0.0021 S H-1->L+4(+98%)
19  268.1  37.3   4.62 0.0002 S H-3->L+2(+87%)  H-4->L+1(+9%)
20  267.6  37.4   4.63 0.0113 S H-3->L+1(+74%)  H-4->L+2(+10%)
                                  H-7->L+0(+6%)
21  266.7  37.5   4.65 0.0012 S H-2->L+4(+97%)
22  259.9  38.5   4.77 0.0006 S H-4->L+1(+89%)  H-3->L+2(8%)
23  248.0  40.3   5.00 0.0143 S H-4->L+2(+44%)  H-0->L+5(+38%)
24  245.8  40.7   5.04 0.0005 S H-1->L+5(+94%)
25  241.5  41.4   5.13 0.0808 S H-0->L+5(+30%)  H-7->L+0(+18%)
                                  H-5->L+1(+12%)  H-4->L+2(7%)
                                  H-1->L+6(7%)   H-2->L+5(+6%)
26  237.9  42.0   5.21 0.0008 S H-8->L+0(+97%)
27  236.9  42.2   5.23 0.0385 S H-1->L+6(+41%)  H-7->L+0(+16%)
                                  H-5->L+1(+8%)   H-0->L+6(7%)
                                  H-0->L+5(7%)
28  235.9  42.4   5.26 0.0208 S H-2->L+5(+83%)
29  234.7  42.6   5.28 0.0013 S H-0->L+6(+76%)  H-5->L+2(+12%)
                                  H-1->L+6(+7%)
30  234.4  42.7   5.29 0.0005 S H-5->L+2(+59%)  H-6->L+1(19%)
                                  H-0->L+6(12%)
31  230.9  43.3   5.37 0.0006 S H-0->L+7(+88%)
32  228.3  43.8   5.43 0.0060 S H-0->L+8(+46%)  H-6->L+1(+19%)
                                  H-2->L+7(9%)   H-1->L+7(7%)
                                  H-5->L+1(+5%)   H-5->L+2(+5%)
33  227.4  44.0   5.45 0.0260 S H-1->L+7(+28%)  H-1->L+8(+20%)
                                  H-5->L+1(+16%)  H-7->L+0(6%)
34  227.2  44.0   5.46 0.0116 S H-1->L+8(+53%)  H-0->L+8(+22%)
35  226.8  44.1   5.47 0.0028 S H-6->L+1(32%)  H-0->L+8(+18%)
                                  H-2->L+7(+8%)   H-5->L+1(+7%)
                                  H-1->L+8(5%)
36  225.7  44.3   5.49 0.0054 S H-2->L+6(+90%)
37  223.5  44.7   5.55 0.0120 S H-0->L+9(+45%)  H-1->L+7(+17%)
                                  H-1->L+8(8%)   H-5->L+1(6%)
38  221.4  45.2   5.60 0.0010 S H-9->L+0(+64%)  H-10->L+0(21%)
                                  H-3->L+3(5%)
39  220.9  45.3   5.61 0.0056 S H-1->L+9(+79%)
40  218.5  45.8   5.67 0.0026 S H-2->L+8(+68%)  H-2->L+7(+16%)
                                  H-2->L+9(+6%)
```

Full TDDFT analysis for complex *cis*-4 (X-ray geometry):

```
    The file SWizard.txt was created on 03-15-2007 from the Gaussian 98/03 output
    file (CIS-CN~1.OUT)
    Framework group  C1[X(C14H10FeN2)]
    bpw91/gen td=(nstates=40) test geom=connectivity

      #  (nm  1000 cm-1  eV)   (f)   (Assignment; H=HOMO,L=LUMO,L+1=LUMO+1,etc.)
      1  674.5   14.8   1.84 0.0002 S H-0->L+0(+92%)
      2  653.7   15.3   1.90 0.0003 S H-1->L+0(+86%)   H-2->L+0(6%)
      3  555.3   18.0   2.23 0.0393 S H-2->L+0(+78%)
      4  403.8   24.8   3.07 0.0001 S H-1->L+1(+47%)   H-0->L+1(+39%)
                                      H-0->L+2(+11%)
      5  399.9   25.0   3.10 0.0001 S H-1->L+2(+37%)   H-0->L+1(25%)
                                      H-1->L+1(+20%)   H-0->L+2(+9%)
      6  394.4   25.4   3.14 0.0002 S H-1->L+2(+33%)   H-0->L+2(32%)
                                      H-2->L+1(22%)
      7  383.1   26.1   3.24 0.0018 S H-2->L+2(+55%)   H-2->L+1(32%)
                                      H-1->L+2(6%)
      8  343.4   29.1   3.61 0.0048 S H-4->L+0(+89%)   H-3->L+0(+9%)
      9  323.4   30.9   3.83 0.0336 S H-0->L+2(+18%)   H-1->L+1(17%)
                                      H-1->L+2(+12%)   H-3->L+0(12%)
                                      H-0->L+1(+9%)   H-5->L+0(+6%)
     10  318.3   31.4   3.89 0.1558 S H-3->L+0(+37%)   H-2->L+2(+12%)
                                      H-5->L+0(10%)   H-0->L+1(+8%)
     11  317.4   31.5   3.91 0.0415 S H-2->L+1(28%)   H-0->L+2(+18%)
                                      H-2->L+2(15%)   H-3->L+0(+9%)
     12  281.6   35.5   4.40 0.0012 S H-0->L+3(+99%)
     13  280.1   35.7   4.43 0.0003 S H-1->L+3(+98%)
     14  273.6   36.6   4.53 0.0028 S H-0->L+4(+95%)
     15  272.1   36.8   4.56 0.0009 S H-2->L+3(+88%)   H-3->L+1(+5%)
     16  271.4   36.8   4.57 0.0162 S H-1->L+4(+59%)   H-3->L+1(19%)
                                      H-0->L+5(+7%)   H-2->L+3(+5%)
     17  270.6   36.9   4.58 0.0062 S H-3->L+1(+50%)   H-1->L+4(+30%)
                                      H-5->L+0(+6%)
     18  268.0   37.3   4.63 0.0382 S H-3->L+2(+40%)   H-1->L+5(25%)
                                      H-5->L+0(12%)   H-3->L+1(+6%)
     19  266.2   37.6   4.66 0.0063 S H-1->L+5(+60%)   H-0->L+5(+13%)
                                      H-3->L+2(+7%)   H-3->L+1(+7%)
     20  264.8   37.8   4.68 0.0017 S H-2->L+4(+71%)   H-0->L+5(+20%)
     21  261.8   38.2   4.74 0.0460 S H-5->L+0(16%)   H-0->L+6(+15%)
                                      H-3->L+2(14%)   H-2->L+5(+10%)
                                      H-7->L+0(10%)   H-6->L+0(9%)
                                      H-0->L+5(7%)
     22  260.0   38.5   4.77 0.0058 S H-0->L+6(+51%)   H-2->L+5(21%)
                                      H-6->L+0(+19%)
     23  259.6   38.5   4.78 0.0304 S H-2->L+5(+41%)   H-0->L+6(+17%)
                                      H-1->L+6(+17%)   H-5->L+0(+6%)
     24  257.7   38.8   4.81 0.0181 S H-1->L+6(+24%)   H-4->L+1(+24%)
                                      H-6->L+0(14%)   H-3->L+2(9%)
                                      H-0->L+6(8%)   H-7->L+0(5%)
     25  256.2   39.0   4.84 0.0026 S H-6->L+0(+39%)   H-2->L+5(+18%)
                                      H-4->L+2(16%)   H-1->L+6(10%)
     26  255.3   39.2   4.86 0.0001 S H-1->L+6(25%)   H-4->L+1(+22%)
                                      H-0->L+7(+12%)   H-2->L+6(+11%)
```

```
                                 H-0->L+5(+8%)
27  251.2  39.8  4.94 0.0062 S H-2->L+6(+46%)  H-0->L+7(42%)
28  250.8  39.9  4.94 0.0038 S H-1->L+7(+49%)  H-4->L+2(28%)
                                 H-4->L+1(+6%)  H-2->L+6(+5%)
29  249.4  40.1  4.97 0.0016 S H-1->L+7(+36%)  H-4->L+2(+36%)
                                 H-6->L+0(+7%)  H-4->L+1(6%)
30  247.9  40.3  5.00 0.0019 S H-0->L+8(+58%)  H-2->L+6(+14%)
                                 H-0->L+7(+9%)
31  245.7  40.7  5.05 0.0003 S H-1->L+8(+63%)  H-0->L+8(21%)
32  243.8  41.0  5.09 0.0016 S H-2->L+7(+90%)
33  241.4  41.4  5.14 0.0017 S H-2->L+8(+47%)  H-1->L+8(20%)
                                 H-0->L+8(9%)  H-1->L+9(+5%)
34  237.7  42.1  5.22 0.0071 S H-8->L+0(+89%)
35  235.9  42.4  5.26 0.0607 S H-7->L+0(32%)  H-0->L+9(+10%)
                                 H-2->L+8(+9%)  H-8->L+0(+9%)
                                 H-1->L+9(6%)  H-5->L+0(+6%)
36  234.9  42.6  5.28 0.0083 S H-1->L+9(+40%)  H-2->L+8(16%)
                                 H-7->L+0(11%)  H-5->L+2(6%)
37  234.3  42.7  5.29 0.0044 S H-0->L+9(+84%)  H-1->L+9(+8%)
38  230.1  43.5  5.39 0.0011 S H-2->L+9(+54%)  H-1->L+9(28%)
39  226.9  44.1  5.46 0.0038 S H-9->L+0(+90%)
40  223.7  44.7  5.54 0.0040 S H-10->L+0(+67%)  H-11->L+0(13%)
                                 H-5->L+1(7%)
```

Full TDDFT analysis for complex *trans*-3 (X-ray geometry):

```
SWizard program: Copyright (c) S. I. Gorelsky, 1999-2007.
This software is provided under written license and may be used, copied,
transmitted, or stored only in accord with that license.
*****************************************************************
 Use of this program should be acknowledged in publications as:
  S.I. Gorelsky, SWizard program, http://www.sg-chem.net/
*****************************************************************
The file SWizard.txt was created on 03-15-2007 from the Gaussian 98/03 output
file (TRANS-~1.OUT)
Framework group  C1[X(C13H10FeIN)]
bpw91/gen td=(nstates=40) test pseudo=read geom=connectivity

  #  (nm  1000 cm-1  eV)   (f)  (Assignment; H=HOMO,L=LUMO,L+1=LUMO+1,etc.)
  1  564.7  17.7  2.20 0.0003 S H-1->L+0(+63%)  H-0->L+0(29%)
  2  561.0  17.8  2.21 0.0006 S H-0->L+0(+52%)  H-1->L+0(+32%)
                                 H-2->L+0(10%)
  3  498.2  20.1  2.49 0.0288 S H-2->L+0(+73%)  H-0->L+0(+9%)
  4  470.4  21.3  2.64 0.0006 S H-0->L+1(+99%)
  5  459.7  21.8  2.70 0.0045 S H-1->L+1(+97%)
  6  441.7  22.6  2.81 0.0012 S H-2->L+1(+98%)
  7  398.4  25.1  3.11 0.0001 S H-0->L+2(+75%)  H-0->L+3(+11%)
                                 H-1->L+3(+10%)
  8  392.8  25.5  3.16 0.0013 S H-1->L+2(+50%)  H-0->L+3(43%)
  9  384.8  26.0  3.22 0.0007 S H-1->L+3(+43%)  H-2->L+2(+24%)
                                 H-0->L+3(18%)  H-2->L+3(+7%)
                                 H-1->L+2(7%)
 10  373.5  26.8  3.32 0.0051 S H-2->L+3(+54%)  H-2->L+2(34%)
 11  324.6  30.8  3.82 0.0032 S H-4->L+0(+75%)  H-3->L+0(12%)
 12  320.4  31.2  3.87 0.0000 S H-0->L+3(+18%)  H-1->L+2(+17%)
                                 H-1->L+3(+16%)  H-0->L+2(13%)
```

```
                          H-4->L+0(11%)
13  314.2   31.8    3.95 0.0005 S H-2->L+2(+26%)  H-2->L+3(+24%)
                          H-1->L+3(18%)  H-1->L+2(+7%)
14  306.3   32.6    4.05 0.0781 S H-3->L+0(37%)  H-3->L+1(+35%)
                          H-4->L+0(7%)
15  296.5   33.7    4.18 0.0275 S H-5->L+0(+55%)  H-6->L+0(+38%)
16  293.4   34.1    4.23 0.0292 S H-6->L+0(+35%)  H-3->L+1(+32%)
                          H-5->L+0(11%)  H-3->L+0(+7%)
17  291.1   34.4    4.26 0.1242 S H-6->L+0(24%)  H-5->L+0(+23%)
                          H-3->L+1(+21%)  H-3->L+0(+12%)
18  284.9   35.1    4.35 0.0007 S H-4->L+1(+98%)
19  273.8   36.5    4.53 0.0024 S H-3->L+2(+52%)  H-3->L+3(+32%)
                          H-0->L+4(9%)
20  271.1   36.9    4.57 0.0002 S H-0->L+4(+84%)  H-3->L+2(6%)
21  265.9   37.6    4.66 0.0407 S H-3->L+3(+42%)  H-1->L+4(17%)
                          H-3->L+2(15%)  H-7->L+0(5%)
22  263.8   37.9    4.70 0.0030 S H-0->L+5(+51%)  H-2->L+4(30%)
23  262.3   38.1    4.73 0.0016 S H-1->L+4(+30%)  H-0->L+5(14%)
                          H-0->L+6(+11%)  H-3->L+3(+6%)
                          H-4->L+2(5%)
24  261.2   38.3    4.75 0.0016 S H-2->L+4(+47%)  H-0->L+6(+23%)
                          H-0->L+5(+18%)
25  260.5   38.4    4.76 0.0015 S H-5->L+1(+81%)
26  260.0   38.5    4.77 0.0007 S H-0->L+6(+46%)  H-1->L+5(16%)
                          H-2->L+4(10%)  H-0->L+5(7%)
                          H-1->L+6(+7%)
27  258.4   38.7    4.80 0.0010 S H-1->L+6(+78%)  H-1->L+5(+11%)
28  256.0   39.1    4.84 0.0025 S H-0->L+7(+67%)  H-1->L+5(+14%)
                          H-4->L+2(+7%)
29  254.9   39.2    4.86 0.0016 S H-0->L+8(+46%)  H-2->L+5(+15%)
                          H-1->L+5(+11%)  H-0->L+7(6%)
                          H-1->L+7(+5%)
30  254.6   39.3    4.87 0.0045 S H-4->L+2(+50%)  H-4->L+3(17%)
31  254.0   39.4    4.88 0.0002 S H-2->L+5(+57%)  H-0->L+7(+7%)
                          H-0->L+8(7%)  H-1->L+7(+7%)
                          H-2->L+6(+6%)
32  252.7   39.6    4.91 0.0035 S H-1->L+7(+52%)  H-0->L+8(17%)
                          H-1->L+8(9%)  H-2->L+6(7%)
33  251.8   39.7    4.92 0.0005 S H-2->L+6(+58%)  H-0->L+8(+10%)
                          H-1->L+7(+9%)  H-1->L+8(9%)
                          H-2->L+5(6%)
34  251.2   39.8    4.94 0.0014 S H-1->L+8(+66%)  H-1->L+7(+16%)
                          H-4->L+3(+6%)  H-2->L+5(5%)
35  248.2   40.3    5.00 0.0015 S H-2->L+7(+73%)
36  246.7   40.5    5.03 0.0023 S H-2->L+8(+56%)  H-6->L+1(9%)
                          H-8->L+0(9%)
37  246.4   40.6    5.03 0.0035 S H-5->L+2(+34%)  H-8->L+0(22%)
                          H-6->L+1(+13%)  H-4->L+3(+9%)
38  246.2   40.6    5.04 0.0005 S H-6->L+1(+54%)  H-2->L+8(+13%)
                          H-5->L+2(8%)  H-6->L+2(6%)
39  244.0   41.0    5.08 0.0533 S H-7->L+0(+44%)  H-8->L+0(8%)
                          H-5->L+2(8%)  H-2->L+8(+7%)
40  242.1   41.3    5.12 0.0079 S H-5->L+3(+38%)  H-8->L+0(27%)
                          H-6->L+2(7%)  H-2->L+8(7%)
                          H-4->L+3(6%)
```

Full TDDFT analysis for complex *cis*-3 (X-ray geometry):
```
SWizard program: Copyright (c) S. I. Gorelsky, 1999-2007.
This software is provided under written license and may be used, copied,
transmitted, or stored only in accord with that license.
*****************************************************************
 Use of this program should be acknowledged in publications as:
  S.I. Gorelsky, SWizard program, http://www.sg-chem.net/
*****************************************************************
The file SWizard.txt was created on 03-15-2007 from the Gaussian 98/03 output
file (CIS-I-~1.OUT)
Framework group  C1[X(C13H10FeIN)]
bpw91/gen td=(nstates=40) test pseudo=read geom=connectivity

   #  (nm  1000 cm-1  eV)   (f)  (Assignment; H=HOMO,L=LUMO,L+1=LUMO+1,etc.)
   1  548.7   18.2   2.26 0.0003 S H-0->L+0(+88%)   H-1->L+0(6%)
   2  531.8   18.8   2.33 0.0001 S H-1->L+0(+73%)   H-2->L+0(+16%)
   3  479.7   20.8   2.58 0.0387 S H-2->L+0(+70%)   H-1->L+0(11%)
   4  424.5   23.6   2.92 0.0002 S H-0->L+1(+52%)   H-1->L+1(+41%)
   5  421.2   23.7   2.94 0.0011 S H-1->L+1(+55%)   H-0->L+1(31%)
                                 H-0->L+2(7%)
   6  404.4   24.7   3.07 0.0003 S H-2->L+1(+75%)   H-0->L+3(+17%)
   7  397.7   25.1   3.12 0.0004 S H-1->L+2(+43%)   H-0->L+2(+41%)
                                 H-1->L+3(12%)
   8  394.2   25.4   3.14 0.0039 S H-1->L+2(+38%)   H-0->L+2(21%)
                                 H-1->L+3(+18%)   H-0->L+3(+17%)
   9  388.7   25.7   3.19 0.0004 S H-2->L+2(+51%)   H-0->L+3(28%)
                                 H-1->L+2(+10%)   H-1->L+3(+8%)
  10  374.9   26.7   3.31 0.0075 S H-2->L+3(+89%)
  11  325.3   30.7   3.81 0.0002 S H-1->L+3(+36%)   H-0->L+2(+17%)
                                 H-0->L+1(9%)   H-0->L+3(+6%)
  12  322.3   31.0   3.85 0.0019 S H-2->L+2(+33%)   H-0->L+3(+19%)
                                 H-2->L+1(14%)   H-1->L+3(5%)
  13  311.7   32.1   3.98 0.0283 S H-4->L+0(+63%)   H-3->L+0(+25%)
  14  304.5   32.8   4.07 0.0044 S H-5->L+0(+85%)   H-6->L+0(+5%)
  15  299.0   33.4   4.15 0.0617 S H-6->L+0(+27%)   H-3->L+0(+23%)
                                 H-4->L+0(22%)   H-3->L+3(7%)
                                 H-3->L+1(+6%)
  16  291.1   34.3   4.26 0.1211 S H-6->L+0(+56%)   H-3->L+1(14%)
                                 H-5->L+0(9%)
  17  287.4   34.8   4.31 0.0569 S H-3->L+1(+70%)   H-3->L+0(5%)
  18  276.5   36.2   4.48 0.0099 S H-3->L+2(+89%)
  19  271.5   36.8   4.57 0.0230 S H-1->L+4(+45%)   H-0->L+4(+23%)
                                 H-3->L+3(+19%)
  20  270.1   37.0   4.59 0.0239 S H-3->L+3(+41%)   H-1->L+4(40%)
  21  266.2   37.6   4.66 0.0025 S H-0->L+4(+34%)   H-4->L+1(+19%)
                                 H-3->L+3(9%)   H-1->L+5(7%)
                                 H-2->L+4(+7%)
  22  264.8   37.8   4.68 0.0015 S H-2->L+4(+56%)   H-0->L+5(+36%)
  23  264.3   37.8   4.69 0.0008 S H-0->L+5(+55%)   H-2->L+4(29%)
                                 H-4->L+1(+6%)
  24  261.3   38.3   4.75 0.0009 S H-1->L+5(+69%)   H-4->L+1(+11%)
                                 H-1->L+6(+6%)
  25  259.7   38.5   4.77 0.0077 S H-4->L+1(+32%)   H-0->L+6(19%)
                                 H-4->L+2(+14%)   H-0->L+4(6%)
  26  257.6   38.8   4.81 0.0000 S H-5->L+1(+62%)   H-5->L+2(18%)
```

```
                                        H-4->L+2(10%)
  27  256.7   39.0   4.83 0.0050 S H-0->L+6(+49%)  H-2->L+5(25%)
  28  255.0   39.2   4.86 0.0003 S H-1->L+6(+32%)  H-2->L+5(24%)
                                        H-6->L+1(23%)  H-6->L+2(+6%)
  29  254.8   39.3   4.87 0.0018 S H-1->L+6(+40%)  H-0->L+7(21%)
                                        H-2->L+5(+20%)
  30  254.6   39.3   4.87 0.0018 S H-6->L+1(+44%)  H-4->L+2(18%)
                                        H-2->L+5(11%)  H-1->L+6(+6%)
  31  250.9   39.9   4.94 0.0003 S H-1->L+7(+65%)  H-0->L+8(+10%)
                                        H-0->L+7(+10%)
  32  250.5   39.9   4.95 0.0003 S H-5->L+3(+49%)  H-4->L+3(+38%)
  33  250.1   40.0   4.96 0.0012 S H-2->L+6(+47%)  H-0->L+8(+28%)
                                        H-1->L+7(11%)  H-0->L+7(+7%)
  34  249.6   40.1   4.97 0.0027 S H-0->L+8(+57%)  H-2->L+6(23%)
                                        H-0->L+7(10%)
  35  248.7   40.2   4.99 0.0009 S H-1->L+8(+23%)  H-5->L+3(17%)
                                        H-4->L+2(11%)  H-6->L+3(+8%)
                                        H-4->L+3(+7%)  H-2->L+6(6%)
                                        H-6->L+1(5%)
  36  247.8   40.3   5.00 0.0050 S H-1->L+8(+48%)  H-5->L+3(+20%)
                                        H-4->L+3(13%)  H-2->L+6(5%)
  37  245.5   40.7   5.05 0.0015 S H-2->L+7(+72%)  H-6->L+3(+10%)
                                        H-8->L+0(9%)
  38  244.9   40.8   5.06 0.0057 S H-6->L+3(+40%)  H-2->L+7(20%)
                                        H-4->L+3(14%)
  39  243.3   41.1   5.10 0.0022 S H-2->L+8(+77%)
  40  243.0   41.2   5.10 0.0095 S H-6->L+2(+58%)  H-5->L+2(13%)
                                        H-7->L+0(8%)  H-6->L+1(+7%)
```

Full TDDFT analysis for complex 5 (optimized geometry):
The file SWizard.txt was created on 02-18-2007 from the Gaussian 98/03 output
file (FCCN3-~1.OUT)
Framework group C1[X(C15H9FeN3)]
bpw91 td=(nstates=40) geom=connectivity gen test

```
   #  (nm  1000 cm-1  eV)    (f)  (Assignment; H=HOMO,L=LUMO,L+1=LUMO+1,etc.)
   1  986.8   10.1   1.26 0.0001 S H-0->L+0(+95%)
   2  840.8   11.9   1.47 0.0031 S H-1->L+0(+52%)  H-2->L+0(38%)
   3  700.5   14.3   1.77 0.0387 S H-2->L+0(+49%)  H-1->L+0(+25%)
                                        H-3->L+0(6%)
   4  438.9   22.8   2.82 0.0003 S H-0->L+1(+56%)  H-1->L+2(+37%)
   5  438.4   22.8   2.83 0.0000 S H-1->L+1(+52%)  H-0->L+2(42%)
   6  418.2   23.9   2.97 0.0000 S H-2->L+1(+51%)  H-1->L+1(22%)
                                        H-0->L+2(22%)
   7  411.6   24.3   3.01 0.0011 S H-4->L+0(+95%)
   8  403.8   24.8   3.07 0.0069 S H-2->L+2(+83%)  H-3->L+0(6%)
   9  385.4   25.9   3.22 0.1955 S H-3->L+0(+46%)  H-5->L+0(31%)
```

```
                                 H-2->L+2(+8%)
 10   351.0   28.5   3.53 0.0006 S H-6->L+0(+49%)  H-2->L+1(22%)
                                 H-0->L+2(12%)  H-1->L+1(7%)
 11   347.1   28.8   3.57 0.0705 S H-1->L+2(+36%)  H-0->L+1(21%)
                                 H-5->L+0(+7%)  H-3->L+0(+6%)
 12   335.2   29.8   3.70 0.0042 S H-0->L+3(+91%)
 13   332.6   30.1   3.73 0.1179 S H-5->L+0(+41%)  H-3->L+0(+10%)
                                 H-7->L+0(7%)  H-0->L+3(+5%)
 14   329.8   30.3   3.76 0.0052 S H-6->L+0(45%)  H-2->L+1(17%)
                                 H-0->L+2(10%)  H-1->L+1(7%)
 15   329.0   30.4   3.77 0.0044 S H-1->L+3(+96%)
 16   312.4   32.0   3.97 0.0054 S H-2->L+3(+99%)
 17   295.3   33.9   4.20 0.0006 S H-0->L+4(+97%)
 18   292.4   34.2   4.24 0.0005 S H-3->L+1(+88%)
 19   290.8   34.4   4.26 0.0006 S H-1->L+4(+94%)
 20   287.8   34.7   4.31 0.0121 S H-3->L+2(+55%)  H-7->L+0(25%)
                                 H-4->L+1(+6%)
 21   279.4   35.8   4.44 0.0015 S H-8->L+0(+97%)
 22   277.8   36.0   4.46 0.0024 S H-2->L+4(+98%)
 23   271.0   36.9   4.58 0.0638 S H-7->L+0(+40%)  H-3->L+2(+15%)
                                 H-4->L+1(+14%)
 24   267.7   37.4   4.63 0.0008 S H-4->L+2(+91%)
 25   264.6   37.8   4.69 0.0018 S H-0->L+5(+91%)
 26   261.3   38.3   4.74 0.0087 S H-1->L+5(+74%)  H-4->L+1(+15%)
 27   260.0   38.5   4.77 0.0007 S H-9->L+0(+96%)
 28   253.5   39.4   4.89 0.0012 S H-11->L+0(+84%)  H-12->L+0(+6%)
 29   252.5   39.6   4.91 0.0262 S H-2->L+5(+26%)  H-4->L+1(+19%)
                                 H-1->L+6(+9%)  H-0->L+7(+9%)
                                 H-1->L+5(7%)  H-11->L+0(+5%)
 30   250.9   39.9   4.94 0.0118 S H-2->L+5(+53%)  H-10->L+0(25%)
                                 H-1->L+6(7%)
 31   248.7   40.2   4.99 0.0008 S H-5->L+1(+81%)  H-6->L+2(+8%)
 32   247.1   40.5   5.02 0.0011 S H-12->L+0(+89%)  H-11->L+0(6%)
 33   246.1   40.6   5.04 0.0021 S H-0->L+6(+78%)  H-10->L+0(+10%)
 34   244.3   40.9   5.07 0.0285 S H-10->L+0(+29%)  H-0->L+7(19%)
                                 H-0->L+6(19%)  H-2->L+5(+8%)
 35   240.7   41.5   5.15 0.0011 S H-1->L+6(41%)  H-3->L+3(+27%)
                                 H-5->L+2(13%)  H-10->L+0(+5%)
 36   240.3   41.6   5.16 0.0014 S H-3->L+3(+71%)  H-1->L+6(+16%)
 37   237.5   42.1   5.22 0.0139 S H-5->L+2(+34%)  H-0->L+7(+14%)
                                 H-0->L+8(12%)  H-1->L+6(8%)
                                 H-6->L+1(+8%)  H-2->L+6(+6%)
                                 H-2->L+9(5%)
 38   235.5   42.5   5.26 0.0002 S H-6->L+2(+37%)  H-1->L+7(+31%)
                                 H-13->L+0(16%)
 39   235.3   42.5   5.27 0.0010 S H-13->L+0(+63%)  H-14->L+0(+12%)
                                 H-1->L+7(+10%)  H-6->L+2(+7%)
 40   234.0   42.7   5.30 0.0018 S H-0->L+9(+34%)  H-1->L+8(29%)
                                 H-1->L+7(+19%)  H-6->L+2(9%)
```

Full TDDFT analysis for complex *trans*-4 (optimized geometry):

```
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****************************************************************
```

****
The file SWizard.txt was created on 03-11-2007 from the Gaussian 98/03 output
file (FCCN2-~1.OUT)
Framework group C1[X(C14H10FeN2)]
bpw91/gen geom=connectivity test td=(nstates=40)

```
  #  (nm  1000 cm-1  eV)   (f)  (Assignment; MO# -> MO#)
  1  826.1   12.1   1.50 0.0001 S 67->68(+96%)
  2  722.5   13.8   1.72 0.0058 S 66->68(+54%)   65->68(37%)
  3  649.0   15.4   1.91 0.0271 S 65->68(+55%)   66->68(+27%)
  4  443.4   22.6   2.80 0.0000 S 66->69(+51%)   67->70(39%)
                                67->69(+6%)
  5  443.0   22.6   2.80 0.0009 S 67->69(+53%)   66->70(+36%)
  6  419.8   23.8   2.95 0.0000 S 65->69(+59%)   67->70(22%)
                                66->69(17%)
  7  405.4   24.7   3.06 0.0005 S 65->70(+83%)   66->70(+10%)
  8  373.6   26.8   3.32 0.0006 S 63->68(+96%)
  9  355.2   28.2   3.49 0.1125 S 64->68(+46%)   62->68(+30%)
 10  345.4   29.0   3.59 0.0132 S 65->69(+20%)   67->70(+17%)
                                66->69(+13%)  66->70(+10%)
                                67->69(7%)   61->68(+5%)
 11  344.8   29.0   3.60 0.0261 S 66->70(+24%)   67->69(16%)
                                65->69(12%)   65->70(6%)
                                64->68(6%)   67->70(6%)
 12  313.7   31.9   3.95 0.0001 S 61->68(+88%)
 13  308.1   32.5   4.02 0.1320 S 62->68(+51%)   60->68(15%)
                                64->68(14%)
 14  298.7   33.5   4.15 0.0051 S 67->71(+98%)
 15  295.4   33.9   4.20 0.0001 S 66->71(+100%)
 16  290.3   34.5   4.27 0.0039 S 67->72(+99%)
 17  288.1   34.7   4.30 0.0012 S 64->69(+92%)
 18  286.9   34.9   4.32 0.0000 S 66->72(+97%)
 19  280.8   35.6   4.41 0.0002 S 65->71(+100%)
 20  279.6   35.8   4.43 0.0057 S 64->70(+70%)   63->69(12%)
                                60->68(+10%)
 21  273.2   36.6   4.54 0.0016 S 65->72(+100%)
 22  264.7   37.8   4.68 0.0017 S 63->70(+92%)
 23  259.5   38.5   4.78 0.0224 S 63->69(+44%)   66->73(31%)
 24  258.5   38.7   4.80 0.0023 S 67->73(+88%)   66->73(+7%)
 25  252.7   39.6   4.91 0.0926 S 66->73(+32%)   60->68(+30%)
                                62->70(9%)
 26  250.1   40.0   4.96 0.0016 S 59->68(+98%)
 27  247.1   40.5   5.02 0.0115 S 62->69(+64%)   65->73(+11%)
 28  246.0   40.7   5.04 0.0281 S 67->74(+37%)   62->69(+19%)
                                66->73(+10%)  60->68(7%)
                                63->69(+5%)
 29  244.9   40.8   5.06 0.0019 S 65->73(+79%)   67->74(+9%)
 30  238.7   41.9   5.20 0.0014 S 66->74(+88%)   67->74(5%)
 31  237.3   42.1   5.22 0.0002 S 67->76(+49%)   67->75(22%)
                                66->75(20%)
 32  236.9   42.2   5.23 0.0025 S 58->68(+75%)   62->70(+6%)
                                67->76(+6%)
 33  235.6   42.4   5.26 0.0144 S 66->76(+20%)   67->76(14%)
                                67->75(14%)   62->70(14%)
                                58->68(+13%)  61->69(+6%)
```

```
34  235.0   42.6    5.28 0.0010 S 66->75(+52%)  61->70(+18%)
                                   67->76(+15%)
35  234.1   42.7    5.30 0.0202 S 66->76(+28%)  67->75(18%)
                                   62->70(+16%)  61->69(9%)
                                   65->76(+8%)
36  233.1   42.9    5.32 0.0010 S 61->70(+49%)  66->75(14%)
                                   65->75(11%)   65->74(+7%)
37  232.2   43.1    5.34 0.0021 S 67->77(+88%)
38  230.2   43.4    5.39 0.0003 S 66->77(+82%)
39  229.7   43.5    5.40 0.0006 S 65->74(+85%)  65->75(+10%)
40  226.3   44.2    5.48 0.0173 S 61->69(+23%)  66->76(+13%)
                                   62->70(+13%)  66->77(10%)
                                   67->75(+8%)   65->76(6%)
```

Full TDDFT analysis for complex *cis*-4 (optimized geometry):

```
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transmitted, or stored only in accord with that license.
*****************************************************************
 Use of this program should be acknowledged in publications as:
  S.I. Gorelsky, SWizard program, http://www.sg-chem.net/
*****************************************************************
The file SWizard.txt was created on 12-01-2006 from the Gaussian 98/03 output
file (FCCN2-~1.OUT)
Framework group  C1[X(C14H10FeN2)]
bpw91/gen geom=connectivity test td=(nstates=40)

   #  (nm  1000 cm-1  eV)    (f)   (Assignment; H=HOMO,L=LUMO,L+1=LUMO+1,etc.)
   1  778.4   12.8    1.59 0.0001 S H-0->L+0(+96%)
   2  684.6   14.6    1.81 0.0076 S H-1->L+0(+52%)  H-2->L+0(+39%)
   3  623.8   16.0    1.99 0.0327 S H-2->L+0(+55%)  H-1->L+0(29%)
   4  443.9   22.5    2.79 0.0000 S H-1->L+1(+58%)  H-0->L+2(+41%)
   5  443.1   22.6    2.80 0.0013 S H-0->L+1(+59%)  H-1->L+2(39%)
   6  420.1   23.8    2.95 0.0000 S H-2->L+1(+62%)  H-0->L+2(23%)
                                   H-1->L+1(+13%)
   7  404.6   24.7    3.06 0.0007 S H-2->L+2(+79%)  H-1->L+2(13%)
   8  362.3   27.6    3.42 0.0027 S H-4->L+0(+93%)
   9  349.7   28.6    3.55 0.0942 S H-3->L+0(+29%)  H-5->L+0(+24%)
                                   H-1->L+2(+11%)  H-0->L+1(+9%)
                                   H-2->L+2(+8%)
  10  345.4   28.9    3.59 0.0044 S H-2->L+1(+28%)  H-0->L+2(+23%)
                                   H-1->L+1(17%)
  11  342.9   29.2    3.62 0.0981 S H-1->L+2(22%)   H-3->L+0(+21%)
                                   H-0->L+1(13%)   H-5->L+0(+8%)
                                   H-2->L+2(7%)
  12  306.3   32.7    4.05 0.0268 S H-6->L+0(+65%)  H-5->L+0(+15%)
  13  303.8   32.9    4.08 0.0469 S H-0->L+3(+50%)  H-6->L+0(19%)
                                   H-5->L+0(+14%)
  14  302.8   33.0    4.09 0.0928 S H-0->L+3(47%)   H-5->L+0(+21%)
                                   H-3->L+0(7%)    H-6->L+0(7%)
                                   H-7->L+0(+6%)
  15  299.9   33.3    4.13 0.0074 S H-1->L+3(+97%)
  16  293.0   34.1    4.23 0.0087 S H-3->L+1(+92%)
  17  284.8   35.1    4.35 0.0037 S H-2->L+3(+99%)
  18  282.3   35.4    4.39 0.0057 S H-3->L+2(+71%)  H-7->L+0(11%)
```

```
                                                  H-4->L+1(10%)
 19  263.2   38.0   4.71 0.0045 S H-4->L+2(+80%)  H-0->L+4(9%)
                                                  H-4->L+1(5%)
 20  262.7   38.1   4.72 0.0008 S H-0->L+4(+90%)  H-4->L+2(+8%)
 21  260.7   38.4   4.76 0.0060 S H-1->L+4(+61%)  H-4->L+1(+23%)
 22  258.1   38.7   4.80 0.0158 S H-0->L+5(+26%)  H-1->L+4(22%)
                                                  H-4->L+1(+20%)  H-1->L+5(18%)
 23  256.3   39.0   4.84 0.0066 S H-0->L+5(+58%)  H-1->L+5(+29%)
 24  253.4   39.5   4.89 0.0102 S H-8->L+0(+81%)  H-1->L+5(9%)
 25  252.6   39.6   4.91 0.0611 S H-1->L+5(+27%)  H-7->L+0(22%)
                                                  H-8->L+0(+16%)  H-5->L+2(7%)
 26  248.9   40.2   4.98 0.0030 S H-5->L+1(+63%)  H-2->L+4(+11%)
                                                  H-0->L+6(+6%)
 27  248.4   40.3   4.99 0.0075 S H-2->L+4(+83%)  H-5->L+1(8%)
 28  247.5   40.4   5.01 0.0188 S H-0->L+6(+37%)  H-5->L+1(16%)
                                                  H-1->L+5(+8%)   H-7->L+0(+7%)
                                                  H-4->L+1(+7%)
 29  243.6   41.0   5.09 0.0017 S H-2->L+5(+92%)
 30  241.2   41.5   5.14 0.0034 S H-1->L+6(+80%)  H-0->L+6(16%)
 31  239.8   41.7   5.17 0.0003 S H-9->L+0(+83%)  H-10->L+0(+9%)
 32  237.6   42.1   5.22 0.0001 S H-0->L+8(+48%)  H-0->L+7(+33%)
                                                  H-1->L+7(16%)
 33  236.4   42.3   5.24 0.0115 S H-5->L+2(+32%)  H-6->L+1(+12%)
                                                  H-0->L+7(12%)   H-2->L+8(+8%)
                                                  H-1->L+8(+7%)   H-7->L+0(6%)
 34  235.3   42.5   5.27 0.0028 S H-1->L+7(+64%)  H-0->L+8(+25%)
 35  234.9   42.6   5.28 0.0049 S H-1->L+8(+44%)  H-0->L+7(15%)
                                                  H-0->L+9(12%)
 36  233.2   42.9   5.32 0.0044 S H-0->L+9(+63%)  H-1->L+8(+16%)
                                                  H-1->L+9(+8%)
 37  232.9   42.9   5.32 0.0011 S H-2->L+6(+45%)  H-6->L+2(42%)
 38  231.6   43.2   5.35 0.0016 S H-1->L+9(+66%)  H-0->L+9(16%)
                                                  H-0->L+7(+7%)
 39  230.9   43.3   5.37 0.0033 S H-10->L+0(+87%) H-9->L+0(9%)
 40  230.9   43.3   5.37 0.0012 S H-2->L+6(+47%)  H-6->L+2(+22%)
                                                  H-2->L+7(18%)
```

Full TDDFT analysis for complex *trans*-3 (optimized geometry):

```
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transmitted, or stored only in accord with that license.
****************************************************************
 Use of this program should be acknowledged in publications as:
  S.I. Gorelsky, SWizard program, http://www.sg-chem.net/
****************************************************************
The file SWizard.txt was created on 12-01-2006 from the Gaussian 98/03 output
file (FCCN-I~1.OUT)
Framework group  C1[X(C13H10FeIN)]
bpw91 td=(nstates=40) geom=connectivity gen pseudo=read test

  #  (nm  1000 cm-1  eV)   (f)  (Assignment; H=HOMO,L=LUMO,L+1=LUMO+1,etc.)
  1  628.3   15.9   1.97 0.0004 S H-0->L+0(+93%)
  2  568.3   17.6   2.18 0.0105 S H-1->L+0(+70%)  H-2->L+0(+10%)
                                                  H-0->L+2(+5%)
  3  551.9   18.1   2.25 0.0027 S H-2->L+0(+73%)  H-0->L+1(18%)
```

```
 4   535.3   18.7   2.32 0.0092 S H-0->L+1(+59%)   H-1->L+1(+29%)
                                  H-2->L+0(+5%)
 5   531.3   18.8   2.33 0.0068 S H-1->L+1(+67%)   H-0->L+1(16%)
                                  H-2->L+0(7%)   H-1->L+0(+5%)
 6   484.7   20.6   2.56 0.0023 S H-2->L+1(+97%)
 7   434.3   23.0   2.85 0.0001 S H-1->L+2(+67%)   H-0->L+3(+27%)
 8   428.8   23.3   2.89 0.0048 S H-0->L+2(+61%)   H-1->L+3(30%)
 9   412.6   24.2   3.01 0.0000 S H-2->L+2(+60%)   H-0->L+3(35%)
10   386.5   25.9   3.21 0.0020 S H-2->L+3(+73%)   H-1->L+3(17%)
11   342.0   29.2   3.62 0.0004 S H-2->L+2(+22%)   H-0->L+3(+18%)
                                  H-1->L+3(14%)   H-1->L+2(12%)
                                  H-0->L+2(8%)
12   340.4   29.4   3.64 0.0011 S H-1->L+3(+21%)   H-2->L+3(+18%)
                                  H-0->L+2(+12%)   H-0->L+3(+10%)
                                  H-1->L+2(7%)   H-2->L+2(+6%)
13   335.3   29.8   3.70 0.0240 S H-3->L+1(+62%)   H-3->L+0(19%)
                                  H-4->L+0(9%)
14   330.1   30.3   3.76 0.0090 S H-4->L+0(+78%)   H-3->L+1(+11%)
                                  H-5->L+0(8%)
15   316.8   31.6   3.91 0.1043 S H-5->L+0(+54%)   H-3->L+0(13%)
                                  H-4->L+0(+8%)   H-6->L+0(7%)
                                  H-3->L+1(5%)
16   311.7   32.1   3.98 0.0843 S H-5->L+0(+29%)   H-3->L+0(+27%)
                                  H-3->L+1(+12%)   H-3->L+3(11%)
17   304.3   32.9   4.07 0.0387 S H-6->L+0(+86%)
18   300.8   33.2   4.12 0.0003 S H-4->L+1(+80%)   H-5->L+1(14%)
19   298.6   33.5   4.15 0.0020 S H-3->L+2(+95%)
20   287.6   34.8   4.31 0.0006 S H-5->L+1(+74%)   H-4->L+1(+12%)
21   280.5   35.7   4.42 0.0011 S H-8->L+0(+92%)
22   276.6   36.2   4.48 0.0239 S H-7->L+0(+53%)   H-3->L+3(+29%)
23   274.0   36.5   4.52 0.0015 S H-0->L+4(+92%)
24   271.3   36.9   4.57 0.0007 S H-1->L+4(+97%)
25   270.5   37.0   4.58 0.1122 S H-4->L+2(+25%)   H-3->L+3(21%)
                                  H-7->L+0(+19%)   H-0->L+4(6%)
                                  H-3->L+0(6%)
26   268.2   37.3   4.62 0.0250 S H-5->L+2(+27%)   H-4->L+2(+23%)
                                  H-3->L+3(+15%)   H-6->L+1(7%)
                                  H-4->L+3(+6%)
27   265.7   37.6   4.67 0.0034 S H-6->L+1(+55%)   H-8->L+1(+14%)
                                  H-7->L+1(+7%)   H-4->L+2(+7%)
                                  H-5->L+2(+6%)
28   260.9   38.3   4.75 0.0062 S H-8->L+1(+77%)   H-7->L+1(8%)
29   260.4   38.4   4.76 0.0046 S H-7->L+1(+53%)   H-5->L+2(12%)
                                  H-6->L+2(+9%)   H-6->L+1(7%)
30   258.7   38.7   4.79 0.0041 S H-2->L+4(+85%)   H-4->L+3(+6%)
31   258.3   38.7   4.80 0.0209 S H-4->L+3(+36%)   H-5->L+2(21%)
                                  H-7->L+1(15%)   H-2->L+4(15%)
32   256.1   39.0   4.84 0.0066 S H-4->L+3(+32%)   H-6->L+2(14%)
                                  H-5->L+3(10%)   H-4->L+2(8%)
                                  H-6->L+1(6%)   H-5->L+2(+6%)
                                  H-0->L+5(6%)
33   252.0   39.7   4.92 0.0028 S H-6->L+2(+66%)   H-5->L+3(15%)
34   248.7   40.2   4.99 0.0124 S H-5->L+3(+52%)   H-0->L+5(+20%)
                                  H-1->L+6(7%)
35   244.0   41.0   5.08 0.0048 S H-6->L+3(+88%)   H-0->L+5(8%)
36   241.7   41.4   5.13 0.0011 S H-0->L+6(+50%)   H-1->L+5(+31%)
                                  H-0->L+5(13%)
```

```
37   240.0   41.7   5.17 0.0003 S H-1->L+5(+53%)  H-0->L+6(33%)
                                   H-0->L+8(6%)
38   239.5   41.7   5.18 0.0002 S H-0->L+8(+79%)  H-1->L+5(+8%)
                                   H-0->L+7(+7%)
39   238.9   41.9   5.19 0.0026 S H-1->L+6(+58%)  H-0->L+5(+16%)
                                   H-1->L+8(8%)  H-0->L+7(+6%)
40   238.2   42.0   5.21 0.0004 S H-7->L+2(+79%)  H-2->L+7(+6%)
                                   H-8->L+3(+6%)
```

Full TDDFT analysis for complex _cis_-3 (optimized geometry):

```
SWizard program: Copyright (c) S. I. Gorelsky, 1999-2006.
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transmitted, or stored only in accord with that license.
*****************************************************************
 Use of this program should be acknowledged in publications as:
  S.I. Gorelsky, SWizard program, http://www.sg-chem.net/
*****************************************************************
The file SWizard.txt was created on 11-27-2006 from the Gaussian 98/03 output
file (FCCN-I~1.OUT)
Framework group  C1[X(C13H10FeIN)]
bpw91 td=(nstates=40) geom=connectivity gen pseudo=read test

  #  (nm  1000 cm-1  eV)   (f)  (Assignment; H=HOMO,L=LUMO,L+1=LUMO+1,etc.)
  1  603.8   16.6   2.05 0.0003 S H-0->L+0(+92%)
  2  549.6   18.2   2.26 0.0170 S H-1->L+0(+72%)  H-2->L+0(10%)
                                   H-0->L+2(6%)
  3  531.5   18.8   2.33 0.0104 S H-2->L+0(+84%)  H-1->L+0(+8%)
  4  481.4   20.8   2.58 0.0043 S H-0->L+1(+92%)
  5  477.9   20.9   2.59 0.0003 S H-1->L+1(+94%)
  6  440.1   22.7   2.82 0.0005 S H-2->L+1(+80%)  H-1->L+2(+16%)
  7  432.1   23.1   2.87 0.0001 S H-1->L+2(+52%)  H-0->L+3(29%)
                                   H-2->L+1(12%)
  8  426.0   23.5   2.91 0.0082 S H-0->L+2(+58%)  H-1->L+3(+27%)
  9  410.0   24.4   3.02 0.0002 S H-2->L+2(+65%)  H-0->L+3(31%)
 10  385.2   26.0   3.22 0.0023 S H-2->L+3(+70%)  H-1->L+3(+19%)
 11  342.5   29.2   3.62 0.0001 S H-0->L+3(+22%)  H-2->L+2(+22%)
                                   H-1->L+2(13%)  H-1->L+3(9%)
 12  340.1   29.4   3.65 0.0009 S H-1->L+3(+25%)  H-2->L+3(23%)
                                   H-0->L+2(13%)  H-0->L+3(+7%)
 13  329.2   30.4   3.77 0.0041 S H-4->L+0(+89%)  H-5->L+0(+5%)
 14  323.3   30.9   3.83 0.1209 S H-3->L+0(+41%)  H-3->L+1(+26%)
                                   H-6->L+0(+13%)
 15  314.4   31.8   3.94 0.0068 S H-5->L+0(+48%)  H-6->L+0(30%)
                                   H-3->L+1(+17%)
 16  310.9   32.2   3.99 0.0143 S H-5->L+0(+37%)  H-3->L+1(32%)
                                   H-6->L+0(+12%)
 17  304.9   32.8   4.07 0.1465 S H-6->L+0(+41%)  H-3->L+0(15%)
                                   H-3->L+1(+12%)  H-3->L+2(5%)
 18  300.6   33.3   4.12 0.0043 S H-3->L+2(+86%)
 19  283.0   35.3   4.38 0.0085 S H-4->L+1(+73%)  H-5->L+1(+5%)
 20  277.5   36.0   4.47 0.0055 S H-3->L+3(+31%)  H-5->L+1(+23%)
                                   H-7->L+0(+10%)  H-8->L+0(10%)
                                   H-4->L+2(+9%)
 21  276.8   36.1   4.48 0.0052 S H-4->L+2(26%)  H-5->L+1(23%)
                                   H-7->L+0(+20%)  H-3->L+3(+15%)
```

```
                                      H-6->L+1(+8%)
   22  274.7   36.4   4.51 0.0001 S H-0->L+4(+93%)
   23  274.3   36.5   4.52 0.0032 S H-8->L+0(+77%)
   24  272.6   36.7   4.55 0.0011 S H-1->L+4(+87%)
   25  271.1   36.9   4.57 0.0462 S H-5->L+1(+26%)   H-4->L+2(24%)
                                      H-6->L+1(+13%)   H-7->L+0(11%)
                                      H-1->L+4(6%)
   26  267.8   37.3   4.63 0.1261 S H-7->L+0(30%)   H-3->L+3(+16%)
                                      H-6->L+2(+10%)   H-5->L+1(8%)
                                      H-3->L+0(+6%)   H-9->L+0(5%)
   27  266.1   37.6   4.66 0.0016 S H-5->L+2(+28%)   H-6->L+1(23%)
                                      H-6->L+2(+13%)   H-4->L+2(12%)
                                      H-4->L+3(+12%)   H-4->L+1(5%)
   28  261.8   38.2   4.74 0.0216 S H-4->L+3(+66%)   H-5->L+2(21%)
   29  259.4   38.6   4.78 0.0011 S H-2->L+4(+99%)
   30  256.3   39.0   4.84 0.0194 S H-6->L+1(+24%)   H-5->L+2(+22%)
                                      H-5->L+3(+16%)   H-4->L+2(+9%)
                                      H-0->L+5(+6%)   H-4->L+3(+6%)
   31  254.2   39.3   4.88 0.0063 S H-6->L+2(+51%)   H-6->L+3(12%)
                                      H-6->L+1(+10%)   H-5->L+3(8%)
   32  249.7   40.0   4.96 0.0043 S H-6->L+3(+42%)   H-5->L+3(38%)
                                      H-7->L+1(7%)
   33  249.2   40.1   4.97 0.0071 S H-0->L+5(23%)   H-5->L+3(+20%)
                                      H-7->L+1(19%)   H-6->L+3(+17%)
   34  247.3   40.4   5.01 0.0117 S H-7->L+1(+59%)   H-6->L+3(+15%)
   35  245.4   40.7   5.05 0.0078 S H-8->L+1(+85%)   H-8->L+2(+9%)
   36  243.2   41.1   5.10 0.0016 S H-1->L+5(+88%)   H-0->L+5(+5%)
   37  240.3   41.6   5.16 0.0006 S H-0->L+6(+68%)   H-1->L+7(14%)
                                      H-0->L+8(11%)
   38  239.6   41.7   5.18 0.0002 S H-0->L+7(+46%)   H-0->L+8(+39%)
                                      H-0->L+6(+6%)
   39  238.8   41.9   5.19 0.0016 S H-7->L+2(+82%)
   40  238.5   41.9   5.20 0.0041 S H-1->L+7(+59%)   H-1->L+8(+14%)
                                      H-0->L+6(+13%)   H-0->L+5(+8%)
```

Full TDDFT analysis for complex *trans*-2 (optimized geometry):

```
SWizard program: Copyright (c) S. I. Gorelsky, 1999-2006.
This software is provided under written license and may be used, copied,
transmitted, or stored only in accord with that license.
******************************************************************
 Use of this program should be acknowledged in publications as:
  S.I. Gorelsky, SWizard program, http://www.sg-chem.net/
******************************************************************
The file SWizard.txt was created on 12-01-2006 from the Gaussian 98/03 output
file (FCI2-T~1.OUT)
Framework group  C1[X(C12H10FeI2)]
bpw91/gen geom=connectivity test pseudo=read td=(nstates=40)

   #  (nm  1000 cm-1  eV)   (f)   (Assignment; H=HOMO,L=LUMO,L+1=LUMO+1,etc.)
   1  754.1   13.3   1.64 0.0006 S H-0->L+0(+78%)   H-1->L+0(+21%)
   2  724.6   13.8   1.71 0.0089 S H-1->L+0(+74%)   H-0->L+0(20%)
   3  648.7   15.4   1.91 0.0002 S H-2->L+0(+99%)
   4  493.5   20.3   2.51 0.0002 S H-0->L+1(+79%)   H-1->L+2(15%)
   5  482.5   20.7   2.57 0.0060 S H-1->L+1(+70%)   H-0->L+2(+24%)
   6  454.7   22.0   2.73 0.0013 S H-2->L+1(+84%)   H-0->L+2(10%)
```

```
 7   429.6   23.3   2.89 0.0007 S H-1->L+2(+46%)   H-2->L+2(41%)
 8   412.4   24.2   3.01 0.0081 S H-3->L+0(+89%)
 9   403.7   24.8   3.07 0.0018 S H-0->L+2(+28%)   H-0->L+3(23%)
                                  H-1->L+3(+14%)   H-1->L+1(8%)
                                  H-2->L+1(+6%)
10   390.6   25.6   3.17 0.0091 S H-0->L+3(+29%)   H-2->L+2(26%)
                                  H-1->L+3(+15%)   H-0->L+2(+7%)
                                  H-0->L+4(5%)
11   371.3   26.9   3.34 0.0006 S H-1->L+4(+42%)   H-1->L+3(+18%)
                                  H-0->L+3(14%)   H-2->L+3(+7%)
                                  H-0->L+4(7%)
12   369.6   27.1   3.35 0.0029 S H-0->L+4(+59%)   H-1->L+4(+14%)
                                  H-1->L+3(+10%)   H-0->L+3(+8%)
13   359.9   27.8   3.44 0.0008 S H-4->L+0(+77%)   H-5->L+0(+17%)
14   355.8   28.1   3.49 0.0075 S H-2->L+3(+54%)   H-1->L+4(19%)
                                  H-0->L+4(+9%)   H-1->L+3(+5%)
15   350.7   28.5   3.54 0.0051 S H-5->L+0(+76%)   H-4->L+0(16%)
16   344.3   29.0   3.60 0.0001 S H-2->L+4(+50%)   H-1->L+3(12%)
                                  H-1->L+4(+9%)   H-0->L+2(+5%)
17   338.3   29.6   3.66 0.0002 S H-0->L+3(+15%)   H-0->L+4(14%)
                                  H-2->L+2(+13%)   H-2->L+4(+13%)
                                  H-1->L+2(+12%)   H-2->L+3(+8%)
18   331.0   30.2   3.75 0.0003 S H-2->L+4(+35%)   H-2->L+3(15%)
                                  H-1->L+3(+9%)   H-1->L+4(9%)
                                  H-0->L+2(7%)
19   322.0   31.1   3.85 0.0000 S H-6->L+0(+90%)
20   316.9   31.6   3.91 0.0723 S H-3->L+1(+61%)   H-7->L+0(+8%)
                                  H-3->L+3(+5%)
21   313.2   31.9   3.96 0.0003 S H-3->L+2(+92%)
22   310.8   32.2   3.99 0.0298 S H-7->L+0(+67%)   H-3->L+1(8%)
                                  H-8->L+0(+8%)
23   300.8   33.2   4.12 0.0014 S H-8->L+0(+55%)   H-9->L+0(+26%)
                                  H-7->L+0(7%)   H-10->L+0(+6%)
24   297.8   33.6   4.16 0.0081 S H-9->L+0(+59%)   H-8->L+0(25%)
                                  H-10->L+0(+5%)
25   295.0   33.9   4.20 0.0036 S H-4->L+1(+76%)   H-10->L+0(8%)
                                  H-5->L+1(+7%)
26   289.9   34.5   4.28 0.0109 S H-10->L+0(+57%)   H-5->L+1(+25%)
27   285.1   35.1   4.35 0.0388 S H-5->L+1(+58%)   H-10->L+0(11%)
                                  H-4->L+1(11%)
28   276.2   36.2   4.49 0.0045 S H-4->L+2(+74%)   H-5->L+2(18%)
29   270.8   36.9   4.58 0.0026 S H-6->L+1(+88%)   H-7->L+1(+6%)
30   269.8   37.1   4.60 0.0006 S H-7->L+1(+68%)   H-5->L+2(21%)
31   264.2   37.8   4.69 0.0459 S H-5->L+2(+34%)   H-3->L+4(14%)
                                  H-6->L+2(+12%)   H-7->L+1(+9%)
                                  H-4->L+2(+5%)
32   263.2   38.0   4.71 0.0154 S H-3->L+4(+57%)   H-3->L+3(+15%)
                                  H-5->L+2(+6%)
33   259.2   38.6   4.78 0.0878 S H-3->L+3(+49%)   H-3->L+4(16%)
                                  H-6->L+2(+7%)
34   254.4   39.3   4.87 0.0143 S H-7->L+2(+77%)   H-6->L+2(13%)
35   253.8   39.4   4.88 0.0021 S H-8->L+1(+60%)   H-6->L+2(+22%)
36   251.3   39.8   4.93 0.0060 S H-6->L+2(+25%)   H-4->L+3(13%)
                                  H-0->L+5(+13%)   H-8->L+1(10%)
                                  H-9->L+1(10%)   H-7->L+2(+9%)
37   249.0   40.2   4.98 0.0059 S H-4->L+3(+72%)   H-0->L+5(+11%)
38   248.6   40.2   4.99 0.0010 S H-9->L+1(+51%)   H-10->L+1(+21%)
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39  245.9   40.7   5.04 0.0005 S H-1->L+5(+80%)  H-0->L+6(+9%)
                                 H-5->L+3(6%)
40  245.4   40.8   5.05 0.0008 S H-0->L+6(+82%)  H-5->L+3(+6%)
```

Full TDDFT analysis for complex *cis*-2 (optimized geometry):

```
SWizard program: Copyright (c) S. I. Gorelsky, 1999-2007.
This software is provided under written license and may be used, copied,
transmitted, or stored only in accord with that license.
*****************************************************************
 Use of this program should be acknowledged in publications as:
  S.I. Gorelsky, SWizard program, http://www.sg-chem.net/
*****************************************************************
The file SWizard.txt was created on 03-15-2007 from the Gaussian 98/03 output
file (FCI2-C~2.OUT)
Framework group  C1[X(C12H10FeI2)]
bpw91 geom=connectivity gen test pseudo=read td=(nstates=40)

  #  (nm  1000 cm-1  eV)   (f)  (Assignment; H=HOMO,L=LUMO,L+1=LUMO+1,etc.)
  1  614.4   16.3   2.02 0.0009 S H-1->L+0(+53%)  H-0->L+0(44%)
  2  596.8   16.8   2.08 0.0143 S H-0->L+0(+51%)  H-1->L+0(+41%)
  3  542.4   18.4   2.29 0.0021 S H-2->L+0(+98%)
  4  484.6   20.6   2.56 0.0003 S H-0->L+1(+78%)  H-1->L+2(+18%)
  5  476.2   21.0   2.60 0.0058 S H-1->L+1(+67%)  H-0->L+2(29%)
  6  445.5   22.4   2.78 0.0018 S H-2->L+1(+83%)  H-1->L+2(+8%)
                                 H-0->L+2(5%)
  7  431.5   23.2   2.87 0.0008 S H-2->L+2(+40%)  H-1->L+2(+35%)
                                 H-0->L+2(+11%)
  8  400.8   25.0   3.09 0.0041 S H-0->L+3(+21%)  H-0->L+2(17%)
                                 H-1->L+3(+11%)  H-1->L+2(+11%)
                                 H-2->L+2(7%)   H-2->L+1(7%)
                                 H-1->L+1(6%)
  9  395.7   25.3   3.13 0.0047 S H-0->L+3(+36%)  H-2->L+2(23%)
                                 H-1->L+3(17%)   H-0->L+2(+10%)
 10  377.0   26.5   3.29 0.0029 S H-1->L+4(+51%)  H-3->L+0(+21%)
                                 H-0->L+4(9%)   H-1->L+3(+7%)
                                 H-0->L+3(6%)
 11  376.6   26.6   3.29 0.0008 S H-0->L+4(+53%)  H-1->L+3(+24%)
                                 H-1->L+4(+10%)   H-0->L+3(+7%)
 12  372.0   26.9   3.33 0.0175 S H-3->L+0(+63%)  H-0->L+4(+12%)
                                 H-1->L+4(6%)
 13  358.6   27.9   3.46 0.0066 S H-2->L+3(+63%)  H-1->L+4(+11%)
                                 H-1->L+3(8%)
 14  348.0   28.7   3.56 0.0082 S H-2->L+4(+48%)  H-0->L+3(+10%)
                                 H-0->L+4(9%)   H-1->L+2(6%)
                                 H-2->L+2(+5%)
 15  340.3   29.4   3.64 0.0010 S H-1->L+4(+14%)  H-2->L+2(+12%)
                                 H-1->L+3(10%)   H-2->L+4(10%)
                                 H-0->L+2(8%)   H-0->L+3(+7%)
                                 H-2->L+3(5%)
 16  333.3   30.0   3.72 0.0008 S H-2->L+4(+34%)  H-2->L+3(17%)
                                 H-1->L+3(8%)   H-0->L+4(+6%)
                                 H-0->L+2(5%)
 17  329.1   30.4   3.77 0.0014 S H-4->L+0(+88%)
 18  315.7   31.7   3.93 0.0004 S H-3->L+2(+90%)
 19  315.3   31.7   3.93 0.0206 S H-5->L+0(+54%)  H-3->L+1(+21%)
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                              H-6->L+0(13%)
20  313.1   31.9   3.96 0.0068 S H-6->L+0(+76%)   H-3->L+1(+7%)
21  305.4   32.7   4.06 0.1188 S H-3->L+1(+36%)   H-5->L+0(32%)
                              H-3->L+3(+6%)
22  297.1   33.7   4.17 0.0053 S H-4->L+1(+93%)
23  284.7   35.1   4.36 0.0048 S H-4->L+2(+89%)
24  282.5   35.4   4.39 0.0204 S H-7->L+0(+73%)   H-5->L+1(+12%)
25  279.7   35.8   4.43 0.0018 S H-6->L+1(+53%)   H-5->L+1(37%)
26  276.4   36.2   4.49 0.0118 S H-8->L+0(+36%)   H-6->L+1(18%)
                              H-5->L+1(16%)   H-3->L+3(6%)
27  275.6   36.3   4.50 0.0046 S H-8->L+0(+25%)   H-6->L+1(+22%)
                              H-5->L+1(+18%)   H-9->L+0(+11%)
                              H-3->L+4(9%)
28  275.4   36.3   4.50 0.0059 S H-9->L+0(+78%)   H-8->L+0(9%)
29  269.4   37.1   4.60 0.0063 S H-5->L+2(+52%)   H-10->L+0(+13%)
                              H-3->L+3(10%)   H-3->L+4(9%)
                              H-8->L+0(7%)
30  268.5   37.2   4.62 0.0016 S H-5->L+2(+37%)   H-3->L+4(+18%)
                              H-10->L+0(11%)   H-3->L+3(+11%)
                              H-8->L+0(+11%)
31  264.7   37.8   4.68 0.0293 S H-10->L+0(+59%)   H-3->L+4(+11%)
                              H-3->L+3(+10%)
32  259.0   38.6   4.79 0.1394 S H-6->L+2(26%)   H-4->L+3(+22%)
                              H-3->L+4(+17%)   H-3->L+3(13%)
33  255.4   39.2   4.85 0.0108 S H-6->L+2(+27%)   H-0->L+5(+17%)
                              H-4->L+3(+16%)   H-7->L+1(+11%)
                              H-4->L+4(6%)
34  253.8   39.4   4.88 0.0561 S H-4->L+3(+46%)   H-7->L+1(12%)
                              H-3->L+4(11%)   H-3->L+3(+11%)
35  252.5   39.6   4.91 0.0036 S H-8->L+1(+56%)   H-7->L+1(+10%)
                              H-4->L+4(9%)   H-4->L+3(+6%)
36  250.1   40.0   4.96 0.0432 S H-7->L+1(+38%)   H-8->L+1(25%)
                              H-7->L+2(+6%)   H-0->L+5(6%)
                              H-9->L+1(+5%)
37  247.7   40.4   5.01 0.0028 S H-1->L+5(+67%)   H-9->L+1(11%)
                              H-0->L+5(+7%)   H-7->L+2(7%)
38  247.2   40.4   5.01 0.0010 S H-9->L+1(+39%)   H-7->L+2(+18%)
                              H-1->L+5(14%)   H-0->L+5(+11%)
39  244.8   40.9   5.07 0.0037 S H-5->L+3(+21%)   H-7->L+2(18%)
                              H-8->L+2(+17%)   H-4->L+4(+17%)
                              H-0->L+6(8%)
40  244.5   40.9   5.07 0.0018 S H-0->L+6(+34%)   H-7->L+2(21%)
                              H-9->L+1(+14%)   H-0->L+5(7%)
```