

## **Rational Redox Tuning of Transition Metal Sites: Learning from Superoxide Reductase**

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### Supporting Information

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Figure S1 (previous page): Calculated standard reduction potentials of SOR active site models with different numbers of 4-Melm (and 5-Melm) ligands. All values represent potential differences  $\Delta E^\circ$  between standard potentials of the species of interest and a model reflecting the native SOR coordination pattern, (4-Melm)<sub>1</sub>(5-Melm)<sub>3</sub>.  $\Delta E^\circ$  values were derived from gas-phase standard Gibbs free energies (left) as well as aqueous-solution standard Gibbs free energies obtained using IEFPCM<sup>1</sup> (centre) and SMD<sup>2</sup> (right) solvation models. Data in row A were derived from standard Gibbs free energies of reaction approximated as differences in total electronic energies of products and educts (ZPVE, entropic, and thermal internal energy contributions neglected), while those in row B were derived from standard Gibbs free energies obtained using the rigid-rotor-harmonic-oscillator (RRHO) model. Data in rows C and D refer to standard Gibbs free energies calculated based on *quasi*-RRHO (*q*-RRHO) approaches by Cramer & Truhlar<sup>3</sup> and Grimme<sup>4</sup>, respectively. Calculations were performed using BP86<sup>5,6</sup> (black), TPSSh<sup>7,8</sup> (red), and PBE0<sup>9</sup> (blue) density functionals. Full and dashed lines refer to values obtained from gas-phase optimized and solution-phase optimized geometries, respectively.

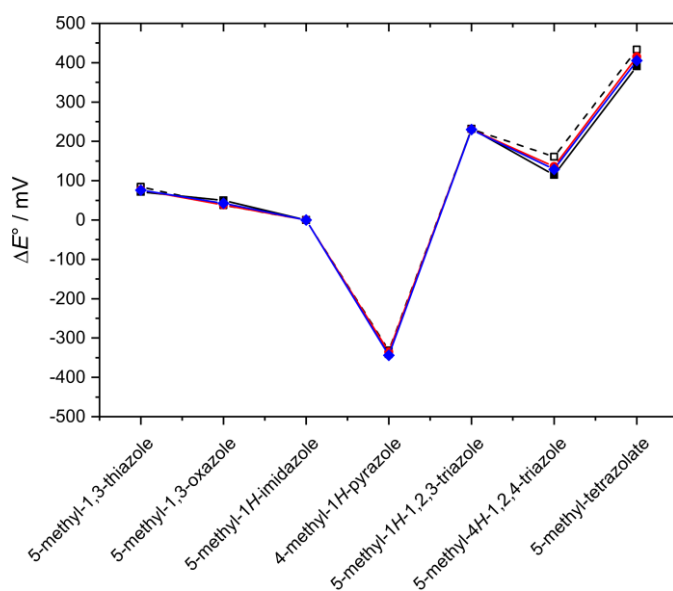


Figure S2: Calculated standard reduction potentials of SOR active site models with a non-native (4-Melm)<sub>1</sub>(5Melm)<sub>2</sub>(MeAz)<sub>1</sub> coordination pattern, where MeAz refers to the indicated methylazole ligand (see manuscript, Fig. 4). All values represent potential differences  $\Delta E^\circ$  between standard potentials of the species of interest and a model reflecting the native SOR coordination pattern, (4-Melm)<sub>1</sub>(5-Melm)<sub>3</sub>.  $\Delta E^\circ$  values were derived from gas-phase standard Gibbs free energies of reaction obtained using the TPSSh<sup>7,8</sup> density functional. These energies were approximated as differences in total electronic energies of products and educts (black dashed), obtained using the RRHO model (black full), or calculated based on *q*-RRHO approaches by Cramer & Truhlar<sup>3</sup> (red) and Grimme<sup>4</sup> (blue).

Table S1: Selected spectroscopic, structural, and thermodynamic properties calculated for Melm, protonated at either N<sub>δ</sub> (5-Melm) or N<sub>ε</sub> (4-Melm).  $\nu$ , N–H stretching frequency;  $d$ , N–H bond length;  $\Delta G^\circ$ , standard Gibbs free energy difference.

Solvation model	Density functional	$\nu / \text{cm}^{-1}$			$d / \text{Å}$			$\Delta G^\circ / \text{kcal mol}^{-1}$
		N <sub>δ</sub> –H	N <sub>ε</sub> –H	II–I	N <sub>δ</sub> –H	N <sub>ε</sub> –H	II–I	II–I
		(5-Melm: I)	(4-Melm: II)		(5-Melm: I)	(4-Melm: II)		
none ( <i>in vacuo</i> )	BP86	3555	3564	9	1.0181	1.0175	–0.0006	–0.5
	TPSSh	3641	3651	10	1.0105	1.0099	–0.0006	–0.5
	PBE0	3704	3715	10	1.0076	1.0069	–0.0007	–0.5
IEFPCM (H <sub>2</sub> O)	BP86	3549	3555	5	1.0196	1.0190	–0.0006	0.0
	TPSSh	3631	3637	6	1.0121	1.0115	–0.0006	0.1
	PBE0	3687	3693	7	1.0096	1.0089	–0.0006	0.0
SMD (H <sub>2</sub> O)	BP86	3521	3540	19	1.0214	1.0204	–0.0009	0.4
	TPSSh	3602	3622	21	1.0139	1.0130	–0.0009	0.5
	PBE0	3654	3676	21	1.0115	1.0106	–0.0009	0.4

Table S2: Energy difference between 4-Melm and 5-Melm tautomers obtained using different approaches, as indicated.  $G^\circ$ , standard Gibbs free energy;  $E$ , total electronic energy.

Solvation model	Density functional	$\Delta G^\circ / \text{kcal mol}^{-1}$						$\Delta E / \text{kcal mol}^{-1}$	
		Solution-phase geometry			Gas-phase geometry			Solution-phase geometry	Gas-phase geometry
		RRHO	Cramer & Truhlar	Grimme	RRHO	Cramer & Truhlar	Grimme		
none ( <i>in vacuo</i> )	BP86				–0.6	–0.6	–0.5		–0.5
	TPSSh				–0.5	–0.5	–0.5		–0.4
	PBE0				–0.5	–0.5	–0.5		–0.5
IEFPCM (H <sub>2</sub> O)	BP86	0.0	0.0	0.0	0.0	0.0	0.0	0.1	0.1
	TPSSh	0.1	0.1	0.1	0.1	0.1	0.1	0.2	0.1
	PBE0	0.0	0.0	0.0	0.0	0.0	0.0	0.1	0.1
SMD (H <sub>2</sub> O)	BP86	0.4	0.4	0.4	0.3	0.3	0.3	0.4	0.4
	TPSSh	0.5	0.5	0.5	0.3	0.3	0.4	0.4	0.4
	PBE0	0.4	0.4	0.4	0.3	0.3	0.3	0.4	0.4

Note that the aqueous-solution standard Gibbs free energy of 4-Melm is slightly lower than that of 5-Melm as well, as observed in the gas-phase calculations (Table S1 and Table S2).<sup>10,11</sup> However, the small energy difference is known to be not perfectly captured in calculations employing medium size basis sets due to slight inaccuracies in the total electronic energy.<sup>11</sup>

## SI2: COMPUTATIONAL METHODS

### Conceptual approach

Using the SOR active site as a model system, this study aims to demonstrate how intrinsic side-chain properties of histidine tautomers and related artificial amino acids can tune the standard reduction potentials of (bio-)catalytically relevant transition metal sites. Thus, all calculations were performed on generalized minimum models that limit interactions within or between (ligand) molecules as well as other external factors that could prohibit or distort insights into this aspect. Targeting intrinsic ligand properties, this study focusses on gas-phase calculations. However, to test the robustness of qualitative findings, implicit aqueous solvent effects were also explored as an example of external perturbations. Notably, this approach deliberately neglects *explicit* influences of the solvent and the protein matrix. It is therefore insufficient to *quantitatively* model the exact situation in a *specific* SOR but well suited to isolate side-chain effects on metal-ligand bonding and redox properties that would be otherwise inaccessible or strongly obscured by these factors.<sup>1</sup>

### Model building

To circumvent complications from conformational isomerism, steric crowding, and biologically inaccessible intramolecular hydrogen bonding, N<sub>δ</sub>-protonated and N<sub>ε</sub>-protonated histidine tautomers were modelled as 5-methylimidazole (5-Melm) and 4-methylimidazole (4-Melm), respectively. Likewise, cysteinate and glutamate ligands of the SOR active site were modelled as methanethiolate and acetate, respectively. Based on experimental data,<sup>12</sup> high-spin ground states were assumed for the ferric ( $S = 5/2$ ) and ferrous ( $S = 4$ ) forms of both native and non-native SOR active site variants, and the acetate ligand was dropped in the ferrous state models.<sup>13,14</sup> All 5-Melm and 4-Melm ligands were modelled as uncharged and single-protonated.<sup>15</sup> Starting geometries of native SOR models containing one 4-Melm and three 5-Melm ligands were obtained from slightly larger, crystal-structure-derived models employed in previous studies.<sup>14,15</sup> In contrast to the latter, no atomic coordinates were fixed to positions found in the underlying SOR from *Ignicoccus hospitalis* (PDB: 4BK8)<sup>16</sup> in order to prevent bias from structural constraints. Non-native models containing an altered number of 5-Melm and 4-Melm ligands were derived by a stepwise ligand exchange. In case of the (5-Melm)<sub>2</sub>(4-Melm)<sub>2</sub> scenario, both *cis* and *trans* configurations were considered, and reported data refer to the arithmetic mean of the two isomers. Models including non-native methylazole ligands (see manuscript, Fig. 4) as artificial amino acid mimics were built according to the following design principles in order to minimize steric and other unspecific effects: (1) All non-native methylazole congeners were included as substitutes of one of the 5-Melm ligands (modelling N<sub>ε</sub>-coordinated histidine H56 of SOR from *I. hospitalis*). (2) Methyl substitution sites and tautomeric forms of all non-native methylazole ligands were chosen to maximize spatial overlap with the native 5-Melm-containing model by ensuring (a) equal distance of the methyl substituent to the coordinating nitrogen atom, (b) if possible, preservation of the protonated nitrogen atom at its position next to the methyl substituent with the proton pointing towards the acetate ligand, and (c) avoidance of *N*-methylation. Note

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<sup>1</sup> Notably, tautomeric forms of coordinated histidines cannot be interchanged inside a real or fully modelled protein since the mode of coordination (*via* N<sub>δ</sub> or N<sub>ε</sub>) is sterically dictated by the surrounding protein matrix architecture.

that all non-native methylazole ligands have been modelled as neutral species except for tetrazole, which is likely deprotonated at neutral pH.<sup>17</sup>

### Computation of standard reduction potentials

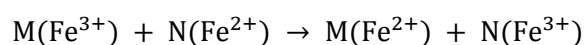
For each SOR model  $M$ , the standard reduction potential  $E^\circ(M)$  of the corresponding  $\text{Fe}^{2+}/\text{Fe}^{3+}$  couple was evaluated by calculating the potential difference

$$\Delta E^\circ = E^\circ(M) - E^\circ(N).$$

Here,  $E^\circ(N)$  represents the  $\text{Fe}^{2+}/\text{Fe}^{3+}$  standard reduction potential of an SOR model  $N$  exhibiting the enzyme's native ligand pattern (*vide supra*). In practice,  $\Delta E^\circ$  was calculated as

$$\Delta E^\circ = -\frac{\Delta G^\circ}{F}$$

where  $F$  is the Faraday constant and  $\Delta G^\circ$  is the standard Gibbs free energy change associated with the one-electron redox reaction



In contrast to  $E^\circ(M)$  and  $E^\circ(N)$ ,  $\Delta E^\circ$  is independent from the definition of a reference electrode couple so that computed values obtained by this approach can be directly compared to experimental data.

### Technical details

All calculations were performed within Gaussian 09 D.01<sup>18</sup> using density functional theory. Three generalized gradient approximation (GGA) functionals with no or few empirical parameters and different fractions of exact Hartree-Fock (HF) exchange were employed, namely PBE0<sup>9</sup> (hybrid GGA; 25 % HF exchange), TPSSH<sup>7,19</sup> (meta hybrid GGA; 10 % HF exchange), and BP86<sup>5,6</sup> (pure GGA; 0 % HF exchange). In all cases, the def2-TZVP basis set was used for the Fe atom, while all other atoms were treated using the 6-31+G(d,p) basis set.<sup>20</sup>

Numerical evaluation of two-electron integrals and their derivatives was accomplished using a pruned (99,590) grid with 99 radial shells and 590 points per radial shell and a pruned (50,194) grid, respectively. All geometries were fully optimized to stationary points of the potential energy surface (PES) by constraining residual maximum forces, root-mean-square (RMS) forces, maximum displacements, and RMS displacements to values smaller than  $1.5 \times 10^{-5}$ ,  $1.0 \times 10^{-5}$ ,  $6.0 \times 10^{-5}$ , and  $4.0 \times 10^{-5}$ , respectively (all in atomic units). Frequencies of rotational and translational modes were verified to be close to  $0 \text{ cm}^{-1}$  in all cases, and stationary points were identified as minima of the PES by the absence of negative Hessian eigenvalues.

Standard Gibbs free energies were computed at 298.15 K from total electronic and zero-point vibrational energies (ZPVE) as well as entropy and thermal internal energy contributions. Thermochemical analyses were performed within ideal-gas and rigid-rotor-harmonic-oscillator (RRHO) approximations, as implemented in Gaussian 09 D.01. Using GoodVibes v1.0.1,<sup>21</sup> two *quasi*-RRHO (*q*-RRHO) approaches by Cramer & Truhlar<sup>3</sup> and Grimme<sup>4</sup> were employed as well in order to correct for potentially erroneous entropy contributions from low-frequency vibrational modes below  $100 \text{ cm}^{-1}$ . Standard Gibbs free energies and derived properties reported in the manuscript and Table S1 refer to the *q*-RRHO approach by Grimme, while data obtained using the RRHO approximation and the *q*-RRHO approach by Cramer & Truhlar are summarized in Table S2, Fig. S1, and Fig. S2.

Effects from implicit aqueous solvation were modelled by a polarizable continuum model (PCM) based on the integral equation formalism (IEFPCM).<sup>1</sup> Where indicated, non-electrostatic contributions were included by

employing the solvation model density (SMD).<sup>2</sup> Both methods were applied using the defaults implemented in Gaussian 09 D.01. Solution-phase standard Gibbs free energies were calculated by two different approaches: (1) Solvation effects on the total electronic energy were evaluated at the gas-phase optimized geometry. This implies that dissolution-related changes of the geometry, the ZPVE, and all entropic and thermal internal energy contributions to the standard Gibbs free energy are neglected. (2) Solvation effects were evaluated at the solution-phase optimized geometry. In this case, the aforementioned contributions to the solution-phase standard Gibbs free energy are included. Solution-phase energies and derived properties reported in the manuscript refer to approach (2), while data obtained using approach (1) are summarized in Table S2 and Fig. S1 for comparison. Note that both approaches neglect the ZPVE as well as entropic and thermal internal energy contributions in cases where the standard Gibbs free energy of reaction was approximated by the difference of total electronic energies of products and educts. The latter calculations were additionally performed to evaluate the impact of these potentially error-prone quantities (ZPVE, entropic and thermal internal energy contributions) on qualitative results (Fig. S1, Fig. S2, and Table S2).

### SI3: Cartesian Coordinates and Absolute Energies of Computational Models

In the following, Cartesian coordinates (in Å) and absolute standard Gibbs free energies (in Ha) of fully optimized geometries are listed for all models discussed in the manuscript. SOR active site models are identified by the equatorial coordination pattern (as introduced in the manuscript) and the formal oxidation state of the coordinated Fe ion (ferric or ferrous). In case of the (4-Melm)<sub>2</sub>(5-Melm)<sub>2</sub> model, energies and geometries are listed for both *cis* and *trans* isomers. Solvation models and density functionals are indicated (*vide supra*). 4-Melm, 4-methyl-1*H*-imidazole; 5-Melm, 5-methyl-1*H*-imidazole; 5-Me-1,3-Th, 5-methyl-1,3-thiazole; 5-Me-1,3-Ox, 5-methyl-1,3-oxazole; 4-MePy, 4-methyl-1*H*-pyrazole; 5-Me-1,2,3-Tr, 5-methyl-1*H*-1,2,3-triazole; 5-Me-1,2,4-Tr, 5-methyl-1*H*-1,2,4-triazole; 5-MeTe<sup>-</sup>, 5-methyl-tetrazolate.

#### 5-Melm, *in vacuo*, BP86, $G^\circ = -265.491382$

C	-39.848761	-8.927242	11.705827
C	-39.676818	-9.027041	10.221556
N	-39.409040	-7.928551	9.409190
C	-39.312872	-8.377970	8.108893
N	-39.500650	-9.688737	8.032382
C	-39.726574	-10.096385	9.338220
H	-40.051672	-9.927002	12.120785
H	-40.695611	-8.273893	11.986885
H	-39.914492	-11.143022	9.578737
H	-39.106903	-7.709511	7.273344
H	-39.303597	-6.965985	9.723571
H	-38.943405	-8.537918	12.207596

#### 5-Melm, *in vacuo*, TPSSh, $G^\circ = -265.502811$

C	-39.848266	-8.927781	11.700928
C	-39.676710	-9.028111	10.219409
N	-39.410170	-7.933951	9.411888
C	-39.314598	-8.380855	8.119632
N	-39.500894	-9.682252	8.042377
C	-39.726056	-10.089738	9.342065
H	-40.049400	-9.919956	12.111553
H	-40.688285	-8.277335	11.973905
H	-39.912186	-11.128257	9.577943
H	-39.110304	-7.717465	7.291463
H	-39.305315	-6.978190	9.722694
H	-38.948212	-8.539365	12.193130

#### 5-Melm, *in vacuo*, PBE0, $G^\circ = -265.177553$

C	-39.846936	-8.927557	11.691047
C	-39.675933	-9.024968	10.216929
N	-39.411041	-7.938136	9.414068
C	-39.316115	-8.382976	8.128831
N	-39.501514	-9.677593	8.052209
C	-39.725599	-10.084558	9.343980
H	-40.048310	-9.919498	12.101953
H	-40.686973	-8.278832	11.966610

H	-39.912234	-11.122800	9.583793
H	-39.111688	-7.720311	7.298846
H	-39.306268	-6.984870	9.723037
H	-38.947785	-8.541157	12.185684

#### 4-Melm, *in vacuo*, BP86, $G^\circ = -265.492254$

C	-39.863090	-13.867417	4.043429
C	-38.400708	-13.629330	4.280783
N	-37.912619	-12.360965	4.574934
C	-36.601059	-12.503783	4.723338
N	-36.211339	-13.809105	4.539196
C	-37.356530	-14.543083	4.254393
H	-40.458094	-13.578073	4.927369
H	-40.063537	-14.929017	3.824804
H	-37.322794	-15.614113	4.065203
H	-35.263506	-14.174105	4.599371
H	-35.893894	-11.709515	4.960828
H	-40.227717	-13.264480	3.193362

#### 4-Melm, *in vacuo*, TPSSh, $G^\circ = -265.503589$

C	-39.856569	-13.866624	4.044457
C	-38.396799	-13.631324	4.280964
N	-37.910777	-12.368919	4.573722
C	-36.608273	-12.511131	4.721077
N	-36.219631	-13.807859	4.538333
C	-37.359965	-14.538521	4.254750
H	-40.443165	-13.578654	4.923341
H	-40.053832	-14.920344	3.827766
H	-37.326071	-15.600851	4.067184
H	-35.278216	-14.168374	4.598253
H	-35.907352	-11.723155	4.956661
H	-40.214236	-13.267229	3.200503

#### 4-Melm, *in vacuo*, PBE0, $G^\circ = -265.178384$

C	-39.846775	-13.866004	4.045839
C	-38.394747	-13.629242	4.281601
N	-37.909980	-12.375280	4.572603



C -36.614007 -12.517427 4.719142  
N -36.227718 -13.806846 4.537455  
C -37.361075 -14.533843 4.255519  
H -40.434823 -13.578458 4.923559  
H -40.044949 -14.919236 3.829202  
H -37.333036 -15.596630 4.067161  
H -35.288461 -14.164570 4.597722  
H -35.913261 -11.727981 4.954904  
H -40.206053 -13.267470 3.202302

**5-Melm, IEFPCM, BP86,  $G^\circ = -265.502770$**

C -39.849024 -8.929526 11.705531  
C -39.677111 -9.029076 10.221244  
N -39.409943 -7.933334 9.408992  
C -39.312476 -8.372820 8.112211  
N -39.500293 -9.690105 8.031102  
C -39.727337 -10.101721 9.340244  
H -40.053290 -9.927729 12.122669  
H -40.691274 -8.269035 11.978911  
H -39.915446 -11.147792 9.584066  
H -39.106442 -7.698851 7.281576  
H -39.304787 -6.968516 9.721312  
H -38.942974 -8.534753 12.199127

**5-Melm, IEFPCM, TPSSh,  $G^\circ = -265.514380$**

C -39.848483 -8.929566 11.700790  
C -39.676956 -9.029880 10.219036  
N -39.410971 -7.938634 9.411418  
C -39.314190 -8.375770 8.122774  
N -39.500632 -9.683612 8.041146  
C -39.726875 -10.094875 9.344096  
H -40.050612 -9.920580 12.112974  
H -40.684596 -8.273114 11.966616  
H -39.913232 -11.132960 9.583057  
H -39.109799 -7.707308 7.299144  
H -39.306257 -6.980618 9.720551  
H -38.947792 -8.536340 12.185384

**5-Melm, IEFPCM, PBE0,  $G^\circ = -265.189471$**

C -39.847165 -8.929563 11.690670  
C -39.676210 -9.027065 10.216499  
N -39.411789 -7.942901 9.413679  
C -39.315704 -8.378218 8.131751  
N -39.501364 -9.679035 8.050854  
C -39.726499 -10.089880 9.345653  
H -40.049185 -9.920170 12.103866  
H -40.683246 -8.274528 11.959208  
H -39.913467 -11.127641 9.588804  
H -39.111093 -7.709837 7.306723

H -39.307015 -6.987129 9.721535  
H -38.947658 -8.537289 12.177745

**4-Melm, IEFPCM, BP86,  $G^\circ = -265.502756$**

C -39.865959 -13.867748 4.043023  
C -38.403606 -13.624510 4.281862  
N -37.909965 -12.354773 4.577722  
C -36.592020 -12.504576 4.725176  
N -36.213854 -13.806689 4.539235  
C -37.358031 -14.537569 4.254928  
H -40.468991 -13.584180 4.924087  
H -40.057258 -14.931153 3.827400  
H -37.325220 -15.608251 4.065166  
H -35.264718 -14.172852 4.597618  
H -35.878313 -11.716591 4.962364  
H -40.236951 -13.274094 3.188429

**4-Melm, IEFPCM, TPSSh,  $G^\circ = -265.514273$**

C -39.859461 -13.867203 4.044014  
C -38.399646 -13.626885 4.282024  
N -37.908308 -12.363117 4.576607  
C -36.599436 -12.511923 4.722918  
N -36.222122 -13.805322 4.538304  
C -37.361278 -14.533257 4.255180  
H -40.453624 -13.583886 4.920051  
H -40.048213 -14.922568 3.830541  
H -37.327944 -15.595233 4.066968  
H -35.279421 -14.167376 4.596501  
H -35.892472 -11.729761 4.958230  
H -40.222961 -13.276452 3.195671

**4-Melm, IEFPCM, PBE0,  $G^\circ = -265.189417$**

C -39.849714 -13.866178 4.045455  
C -38.397611 -13.624521 4.282706  
N -37.907506 -12.369413 4.575436  
C -36.605330 -12.517916 4.720972  
N -36.230155 -13.804262 4.537508  
C -37.362542 -14.528506 4.255999  
H -40.445811 -13.584212 4.920260  
H -40.039142 -14.921252 3.831829  
H -37.334443 -15.591158 4.067104  
H -35.289369 -14.164069 4.595918  
H -35.897961 -11.734669 4.956423  
H -40.215301 -13.276830 3.197400

**5-Melm, SMD, BP86,  $G^\circ = -265.506398$**

C -39.848656 -8.930227 11.702828  
C -39.678762 -9.030473 10.220938

N -39.415231 -7.933064 9.408723  
C -39.313475 -8.372247 8.115323  
N -39.493789 -9.692384 8.030843  
C -39.722468 -10.103225 9.342874  
H -40.071809 -9.924846 12.119596  
H -40.676772 -8.251796 11.975603  
H -39.908269 -11.149144 9.586725  
H -39.109054 -7.697322 7.285777  
H -39.317727 -6.966022 9.722578  
H -38.934384 -8.552506 12.195177

**5-Melm, SMD, TPSSh,  $G^\circ = -265.518022$**

C -39.848131 -8.930189 11.698169  
C -39.678495 -9.031155 10.218706  
N -39.416197 -7.938365 9.411079  
C -39.315290 -8.375112 8.125702  
N -39.494175 -9.685869 8.040861  
C -39.721891 -10.096420 9.346616  
H -40.069749 -9.917583 12.109784  
H -40.669892 -8.255582 11.963497  
H -39.905573 -11.134442 9.585918  
H -39.112684 -7.705694 7.303022  
H -39.319171 -6.978158 9.721703  
H -38.939148 -8.554687 12.181931

**5-Melm, SMD, PBE0,  $G^\circ = -265.193461$**

C -39.846875 -8.930245 11.688267  
C -39.677668 -9.028271 10.216199  
N -39.416355 -7.942705 9.413362  
C -39.316615 -8.377668 8.134495  
N -39.495522 -9.681253 8.050488  
C -39.722131 -10.091349 9.348003  
H -40.066103 -9.917736 12.101102  
H -40.670132 -8.258727 11.956258  
H -39.906833 -11.129076 9.591428  
H -39.113545 -7.708190 7.310476  
H -39.318767 -6.984599 9.722604  
H -38.939849 -8.553438 12.174305

**4-Melm, SMD, BP86,  $G^\circ = -265.505729$**

C -39.864136 -13.868440 4.043756  
C -38.405818 -13.620539 4.285939  
N -37.909619 -12.350276 4.587125  
C -36.589656 -12.506701 4.728424  
N -36.214570 -13.805858 4.536165  
C -37.362095 -14.532860 4.253328  
H -40.475004 -13.575114 4.916609  
H -40.049341 -14.936041 3.842460  
H -37.332579 -15.602804 4.057408

H -35.263906 -14.172612 4.590980  
H -35.874225 -11.721573 4.967184  
H -40.233939 -13.290168 3.177633

**4-Melm, SMD, TPSSh,  $G^\circ = -265.517274$**

C -39.857755 -13.867960 4.044693  
C -38.401846 -13.622867 4.286042  
N -37.907960 -12.358546 4.585850  
C -36.597034 -12.513907 4.726019  
N -36.222866 -13.804432 4.535199  
C -37.365236 -14.528601 4.253532  
H -40.459619 -13.575382 4.912826  
H -40.040285 -14.927389 3.844984  
H -37.335232 -15.589928 4.059503  
H -35.278690 -14.167239 4.590349  
H -35.888087 -11.734690 4.962773  
H -40.220276 -13.292046 3.185242

**4-Melm, SMD, PBE0,  $G^\circ = -265.192768$**

C -39.848172 -13.866812 4.046088  
C -38.399774 -13.620632 4.286896  
N -37.907201 -12.364946 4.584329  
C -36.602968 -12.519727 4.723770  
N -36.230872 -13.803386 4.534561  
C -37.366416 -14.524116 4.254852  
H -40.452107 -13.577163 4.913501  
H -40.031312 -14.925711 3.844478  
H -37.341445 -15.586307 4.060649  
H -35.288395 -14.163919 4.589949  
H -35.893383 -11.739348 4.960104  
H -40.212840 -13.290919 3.187834

**(4-Melm)<sub>0</sub>(5-Melm)<sub>4</sub>, ferric, in vacuo, BP86,  $G^\circ = -2992.317863$**

C -37.415535 -12.258766 10.344219  
C -37.202093 -11.800953 8.903354  
O -36.049137 -11.800421 8.407361  
O -38.279410 -11.456847 8.244262  
C -43.447404 -14.642103 6.084181  
C -42.322239 -13.800047 6.598689  
N -41.550744 -14.149185 7.706933  
C -40.605950 -13.184691 7.910512  
N -40.728528 -12.220705 6.993098  
C -41.789149 -12.595283 6.174820  
C -40.951265 -6.304242 10.338105  
C -40.838823 -7.596898 9.592324  
N -41.653657 -8.697934 9.846294  
C -41.295527 -9.714614 9.006483  
N -40.288555 -9.329121 8.221483

C	-39.998285	-8.017206	8.575707	N	-41.253041	-14.233496	6.993490
C	-36.031441	-5.928450	5.178121	C	-40.258367	-13.358135	6.652713
C	-36.527656	-7.199498	5.793041	N	-40.690464	-12.098245	6.756508
N	-35.742320	-8.010206	6.612472	C	-42.015648	-12.184888	7.177840
C	-36.472042	-9.093334	7.005601	C	-41.697536	-6.364930	9.991408
N	-37.702011	-9.025448	6.479738	C	-41.207525	-7.647248	9.394363
C	-37.743033	-7.855500	5.723441	N	-41.160069	-8.848546	10.099961
C	-42.110862	-8.876743	5.595247	C	-40.684930	-9.827412	9.268263
S	-40.557680	-9.609955	4.944417	N	-40.415522	-9.321393	8.061905
C	-37.441850	-13.544360	2.011625	C	-40.735027	-7.968653	8.133027
C	-37.584108	-12.918795	3.363675	C	-35.245585	-6.695560	5.324532
N	-36.636303	-13.064240	4.377191	C	-36.206255	-7.631218	5.989383
C	-37.047682	-12.376636	5.480545	N	-36.238864	-7.840613	7.367243
N	-38.224377	-11.788835	5.228833	C	-37.239831	-8.728528	7.652503
C	-38.564285	-12.118156	3.920470	N	-37.854624	-9.111398	6.530837
Fe	-39.267730	-10.557984	6.692177	C	-37.216548	-8.437359	5.494200
H	-37.498076	-13.360885	10.363081	C	-42.609072	-9.064354	5.043603
H	-38.333235	-11.830774	10.776754	S	-40.819034	-9.137105	4.592033
H	-43.102539	-15.644781	5.774244	C	-37.783892	-13.385398	1.704286
H	-43.900520	-14.159096	5.205263	C	-37.840871	-12.689014	3.028260
H	-42.079861	-11.983698	5.322451	N	-36.751182	-12.600298	3.891946
H	-39.851815	-13.204701	8.693400	C	-37.126509	-11.880406	4.996722
H	-40.761466	-6.434402	11.418518	N	-38.403614	-11.503491	4.895013
H	-41.949937	-5.846672	10.222051	C	-38.854889	-12.004494	3.677283
H	-39.202854	-7.462762	8.082743	Fe	-39.688662	-10.259052	6.212929
H	-41.774609	-10.690454	8.993069	H	-44.096236	-14.785728	6.925748
H	-35.725116	-5.191408	5.942041	H	-44.432626	-13.373072	7.953142
H	-35.166826	-6.103930	4.513148	H	-42.618637	-11.292076	7.330042
H	-38.635730	-7.583739	5.163086	H	-39.267169	-13.664498	6.327033
H	-36.086727	-9.914880	7.616530	H	-41.100172	-6.062104	10.870060
H	-41.885196	-8.052975	6.291136	H	-42.753397	-6.434615	10.308948
H	-42.710970	-9.633881	6.126358	H	-40.611957	-7.324979	7.262861
H	-39.482318	-11.751355	3.465250	H	-40.563018	-10.866432	9.568232
H	-36.492871	-12.307196	6.422820	H	-35.379107	-5.654580	5.669531
H	-42.396993	-8.738807	10.542207	H	-34.194124	-6.980575	5.508428
H	-41.660419	-14.995466	8.264524	H	-37.542161	-8.558189	4.462877
H	-34.772623	-7.834275	6.872705	H	-37.490800	-9.049392	8.661305
H	-38.311473	-13.285021	1.388955	H	-42.750259	-8.683347	6.069080
H	-36.537213	-13.188730	1.486505	H	-43.077747	-10.057954	4.954931
H	-35.770868	-13.598328	4.311373	H	-39.870157	-11.804422	3.338750
H	-40.209725	-5.587889	9.953402	H	-36.453153	-11.645404	5.818502
H	-36.829375	-5.471799	4.573188	H	-41.444994	-8.979177	11.069809
H	-37.387393	-14.646335	2.069817	H	-41.174413	-15.249460	6.992838
H	-44.242370	-14.776673	6.839372	H	-35.623392	-7.400146	8.049532
H	-36.542678	-11.990087	10.958285	H	-38.766597	-13.325164	1.212523
H	-42.693083	-8.485807	4.746655	H	-37.043581	-12.922971	1.026982
<b>(4-Melm)<sub>0</sub>(5-Melm)<sub>4</sub>, ferrous, in vacuo, BP86,</b>							
<b>G° = -2763.853155</b>							
C	-43.685262	-14.149586	7.729993	H	-35.824622	-12.988774	3.722064
C	-42.393908	-13.508104	7.327965	H	-41.627195	-5.558836	9.245487
C	-43.685262	-14.149586	7.729993	H	-35.410254	-6.708008	4.236467
C	-42.393908	-13.508104	7.327965	H	-37.525086	-14.454549	1.807819
C	-43.685262	-14.149586	7.729993	H	-43.573143	-14.776703	8.632589
C	-42.393908	-13.508104	7.327965	H	-43.111485	-8.378327	4.343446

**(4-Melm)<sub>0</sub>(5-Melm)<sub>4</sub>, ferric, in vacuo, TPSSh,  
G° = -2992.199439**

C -37.445147 -12.311890 10.296530  
C -37.224503 -11.800631 8.880180  
O -36.077098 -11.773427 8.395850  
O -38.299128 -11.440192 8.239732  
C -43.418530 -14.613880 6.079689  
C -42.296017 -13.772276 6.593947  
N -41.532362 -14.118866 7.700487  
C -40.592729 -13.161639 7.902873  
N -40.709285 -12.204937 6.990051  
C -41.763910 -12.578139 6.171591  
C -40.947951 -6.307062 10.297958  
C -40.824814 -7.603102 9.564580  
N -41.616898 -8.707811 9.839609  
C -41.257667 -9.720614 9.010369  
N -40.274172 -9.332647 8.212274  
C -39.998341 -8.017957 8.547992  
C -36.045863 -5.945089 5.178867  
C -36.543620 -7.210005 5.799421  
N -35.770820 -7.998118 6.641837  
C -36.494484 -9.075067 7.032419  
N -37.706482 -9.027290 6.486443  
C -37.743029 -7.872465 5.715358  
C -42.103482 -8.905199 5.629897  
S -40.552751 -9.608420 4.957582  
C -37.461796 -13.548269 2.048578  
C -37.597530 -12.909025 3.392254  
N -36.640975 -13.032094 4.391809  
C -37.045272 -12.339851 5.483933  
N -38.222839 -11.771182 5.241723  
C -38.573284 -12.118207 3.945847  
Fe -39.262659 -10.550187 6.690471  
H -37.685700 -13.381486 10.256029  
H -38.276161 -11.791859 10.779675  
H -43.071140 -15.608152 5.777457  
H -43.864264 -14.134289 5.206156  
H -42.048735 -11.971180 5.325585  
H -39.850586 -13.182161 8.684499  
H -40.746046 -6.428370 11.368007  
H -41.948246 -5.873909 10.187355  
H -39.224993 -7.462412 8.041313  
H -41.720618 -10.694363 9.014201  
H -35.764620 -5.205183 5.936724  
H -35.172780 -6.125624 4.541767  
H -38.621610 -7.618404 5.142208  
H -36.116027 -9.875830 7.657083  
H -41.883953 -8.064275 6.291820  
H -42.662546 -9.661559 6.187292  
H -39.492833 -11.768212 3.502377

H -36.486874 -12.258859 6.411585  
H -42.344829 -8.753425 10.540698  
H -41.643606 -14.956853 8.256771  
H -34.814937 -7.812604 6.917161  
H -38.334443 -13.306573 1.438703  
H -36.571948 -13.189500 1.519194  
H -35.776739 -13.553706 4.324259  
H -40.226453 -5.591369 9.899293  
H -36.830135 -5.509144 4.557010  
H -37.394371 -14.639445 2.124269  
H -44.205270 -14.743382 6.831304  
H -36.531723 -12.200134 10.882488  
H -42.708931 -8.556160 4.790915

**(4-Melm)<sub>0</sub>(5-Melm)<sub>4</sub>, ferrous, in vacuo, TPSSh,  
G° = -2763.735802**

C -43.648602 -14.176585 7.756513  
C -42.365340 -13.528917 7.347742  
N -41.241144 -14.246811 6.968264  
C -40.256377 -13.371975 6.635685  
N -40.674040 -12.122646 6.786213  
C -41.985196 -12.213314 7.229786  
C -41.683734 -6.318234 9.915801  
C -41.205988 -7.615979 9.349038  
N -41.181650 -8.797697 10.076533  
C -40.716348 -9.792669 9.273464  
N -40.431978 -9.319894 8.068122  
C -40.731309 -7.967240 8.107313  
C -35.237828 -6.749106 5.361951  
C -36.208465 -7.671429 6.025486  
N -36.259327 -7.858246 7.399895  
C -37.259847 -8.733385 7.682862  
N -37.856044 -9.131481 6.568114  
C -37.207090 -8.476924 5.533092  
C -42.623040 -9.086339 5.075588  
S -40.853080 -9.147930 4.575411  
C -37.799161 -13.326236 1.673708  
C -37.852701 -12.652396 3.006657  
N -36.763113 -12.576089 3.862231  
C -37.132277 -11.879865 4.972438  
N -38.401395 -11.507938 4.886234  
C -38.857510 -11.985360 3.667506  
Fe -39.696269 -10.263485 6.210946  
H -44.067769 -14.785377 6.947687  
H -44.381690 -13.408500 8.010650  
H -42.574173 -11.328123 7.414989  
H -39.282064 -13.672603 6.284057  
H -41.091117 -6.012036 10.785257  
H -42.733713 -6.374361 10.224269  
H -40.596859 -7.351571 7.229474  
H -40.610406 -10.817862 9.594873

H -35.372617 -5.714116 5.695552  
H -34.199985 -7.038060 5.562797  
H -37.520389 -8.611105 4.508828  
H -37.522208 -9.034754 8.685306  
H -42.736763 -8.711455 6.097186  
H -43.083992 -10.074593 4.997669  
H -39.866611 -11.779848 3.342187  
H -36.460162 -11.660445 5.788074  
H -41.474083 -8.905333 11.039112  
H -41.167954 -15.255198 6.933634  
H -35.657400 -7.412182 8.079580  
H -38.775907 -13.256183 1.191232  
H -37.063753 -12.854527 1.012266  
H -35.842631 -12.955587 3.683352  
H -41.598776 -5.536707 9.158352  
H -35.391597 -6.774355 4.281453  
H -37.541919 -14.387733 1.764063  
H -43.516883 -14.821107 8.632890  
H -43.141938 -8.406513 4.395856

**(4-Melm)<sub>0</sub>(5-Melm)<sub>4</sub>, ferric, in vacuo, PBE0,  
*G*<sup>°</sup> = -2990.191145**

C -37.437106 -12.414009 10.243233  
C -37.239771 -11.823190 8.862652  
O -36.102826 -11.759535 8.375822  
O -38.317363 -11.440674 8.263502  
C -43.403657 -14.574953 6.082323  
C -42.284636 -13.743670 6.597871  
N -41.540607 -14.082412 7.709069  
C -40.599299 -13.136603 7.909559  
N -40.697469 -12.193656 6.990114  
C -41.740371 -12.562642 6.167915  
C -40.977671 -6.275366 10.198798  
C -40.826538 -7.583626 9.509938  
N -41.570548 -8.697599 9.833865  
C -41.194562 -9.718862 9.034744  
N -40.245205 -9.326717 8.209684  
C -40.007485 -8.000787 8.493990  
C -36.059960 -5.952258 5.213773  
C -36.550270 -7.213386 5.828957  
N -35.790499 -7.981912 6.686684  
C -36.504271 -9.060691 7.065387  
N -37.698623 -9.031759 6.496563  
C -37.735888 -7.888406 5.722053  
C -42.095504 -8.963415 5.676200  
S -40.545937 -9.606720 4.978531  
C -37.488917 -13.538285 2.074806  
C -37.607140 -12.899489 3.411579  
N -36.641646 -13.011853 4.391310  
C -37.032031 -12.321051 5.480532  
N -38.210517 -11.763657 5.254945

C -38.577578 -12.115157 3.972964  
Fe -39.251031 -10.546030 6.692192  
H -37.657317 -13.483860 10.143842  
H -38.272276 -11.939334 10.763926  
H -43.065108 -15.575795 5.792651  
H -43.836642 -14.102078 5.198732  
H -42.012706 -11.963413 5.311182  
H -39.863378 -13.153135 8.698921  
H -40.749202 -6.350979 11.267529  
H -41.993167 -5.877471 10.096434  
H -39.264090 -7.432748 7.955176  
H -41.624653 -10.707949 9.077151  
H -35.802734 -5.202777 5.970427  
H -35.173395 -6.122729 4.593053  
H -38.605805 -7.646408 5.129112  
H -36.129698 -9.856219 7.701167  
H -41.900960 -8.125467 6.350149  
H -42.635588 -9.740032 6.225243  
H -39.505111 -11.772183 3.538665  
H -36.462019 -12.233906 6.401909  
H -42.281099 -8.744311 10.548801  
H -41.664473 -14.911329 8.271441  
H -34.845493 -7.783427 6.980228  
H -38.371165 -13.304772 1.475625  
H -36.610691 -13.176526 1.528738  
H -35.777320 -13.526749 4.313368  
H -40.290441 -5.547845 9.762694  
H -36.836269 -5.528058 4.574014  
H -37.414626 -14.628830 2.149871  
H -44.201612 -14.689572 6.824176  
H -36.520945 -12.321865 10.828253  
H -42.721648 -8.615821 4.851314

**(4-Melm)<sub>0</sub>(5-Melm)<sub>4</sub>, ferrous, in vacuo, PBE0,  
*G*<sup>°</sup> = -2761.983355**

C -43.640953 -14.108217 7.828532  
C -42.373262 -13.481656 7.370419  
N -41.314865 -14.203501 6.862499  
C -40.329861 -13.345437 6.517990  
N -40.684464 -12.103190 6.782720  
C -41.955148 -12.177994 7.313130  
C -41.756436 -6.365618 9.911027  
C -41.233193 -7.642293 9.357652  
N -41.112215 -8.795711 10.103944  
C -40.628476 -9.777075 9.306661  
N -40.423818 -9.320529 8.087090  
C -40.794347 -7.993686 8.107045  
C -35.152603 -6.867929 5.330764  
C -36.167909 -7.717366 6.006705  
N -36.324325 -7.762347 7.376177  
C -37.341791 -8.602614 7.667804

N	-37.849071	-9.113841	6.563782	C	-40.824403	-6.261204	10.239532
C	-37.125672	-8.570062	5.524717	C	-40.719208	-7.596457	9.571747
C	-42.645816	-9.227881	5.103582	N	-41.444174	-8.713561	9.980744
S	-40.896463	-9.109646	4.591156	C	-41.118802	-9.769179	9.175678
C	-37.740369	-13.210690	1.649024	N	-40.219949	-9.392749	8.265927
C	-37.818522	-12.591153	2.998143	C	-39.965873	-8.047399	8.501050
N	-36.778811	-12.618097	3.903369	C	-35.984016	-6.200606	4.971160
C	-37.159794	-11.948219	5.016922	C	-36.506336	-7.413343	5.675740
N	-38.390741	-11.496494	4.884957	N	-35.780483	-8.108381	6.642738
C	-38.811496	-11.890059	3.633371	C	-36.519715	-9.164563	7.087373
Fe	-39.696554	-10.240841	6.202927	N	-37.699668	-9.190951	6.453202
H	-44.141898	-14.647635	7.017206	C	-37.697669	-8.107989	5.574838
H	-44.326307	-13.336508	8.184544	C	-42.092544	-8.867740	5.743387
H	-42.499087	-11.290127	7.600007	S	-40.611497	-9.699186	5.044227
H	-39.395180	-13.651842	6.072867	C	-39.636228	-12.484016	3.294202
H	-41.148140	-6.002655	10.746866	C	-38.392009	-12.642764	4.112664
H	-42.788303	-6.468945	10.264452	N	-38.178648	-12.047209	5.364175
H	-40.733761	-7.391438	7.210194	C	-36.959658	-12.432349	5.776034
H	-40.453141	-10.788875	9.644091	N	-36.387180	-13.240983	4.846492
H	-35.308119	-5.804517	5.543372	C	-37.273479	-13.389626	3.789175
H	-34.132938	-7.128489	5.635454	Fe	-39.291718	-10.695798	6.728443
H	-37.356449	-8.807126	4.496263	H	-36.857848	-11.941644	11.226305
H	-37.685070	-8.800364	8.672642	H	-37.642512	-13.380348	10.545571
H	-42.801331	-8.827539	6.110762	H	-43.498773	-15.528174	5.995522
H	-43.003463	-10.260864	5.071610	H	-44.269063	-13.974665	5.594259
H	-39.789254	-11.608127	3.267337	H	-42.324759	-11.907139	5.596384
H	-36.518099	-11.802858	5.874274	H	-39.800366	-13.412571	8.626199
H	-41.358107	-8.896451	11.077444	H	-40.521002	-6.306439	11.300732
H	-41.284076	-15.206072	6.752970	H	-41.852413	-5.859103	10.197832
H	-35.777099	-7.246664	8.048840	H	-39.255162	-7.492594	7.892154
H	-38.683773	-13.058499	1.121178	H	-41.540443	-10.766087	9.278361
H	-36.944788	-12.763867	1.042575	H	-35.757838	-5.379017	5.674324
H	-35.877434	-13.046152	3.753883	H	-35.062765	-6.420834	4.402554
H	-41.747617	-5.598537	9.134294	H	-38.548431	-7.915816	4.923517
H	-35.222610	-7.001878	4.249546	H	-36.174650	-9.904165	7.816782
H	-37.557534	-14.289619	1.703883	H	-42.654617	-9.548662	6.402705
H	-43.474259	-14.812973	8.650643	H	-42.737523	-8.551976	4.909055
H	-43.247401	-8.637635	4.407925	H	-39.792209	-11.438579	2.980176

**(4-Melm)<sub>1</sub>(5-Melm)<sub>3</sub>, ferric, *in vacuo*, BP86,  
G° = -2992.311366**

C	-37.642845	-12.275064	10.530982	H	-37.044019	-13.997275	2.917150
C	-37.327879	-11.795301	9.116015	H	-35.467030	-13.669572	4.927849
O	-36.134391	-11.679516	8.744209	H	-36.489477	-12.161235	6.726946
O	-38.357738	-11.567444	8.341382	H	-42.108483	-8.740269	10.753084
C	-43.745440	-14.526152	6.389729	H	-41.741057	-15.087675	8.323392
C	-42.520138	-13.773494	6.804296	H	-34.842236	-7.876003	6.966423
N	-41.647479	-14.220166	7.796223	H	-40.163952	-5.540235	9.734466
C	-40.632268	-13.317970	7.932893	H	-44.452996	-14.657522	7.227829
N	-40.801418	-12.302431	7.080512	H	-38.629280	-11.922344	10.870529
C	-41.969318	-12.578205	6.376070	H	-39.569655	-13.110020	2.390148
				H	-36.736130	-5.832619	4.256972
				H	-41.793120	-7.981276	6.325170

**(4-Melm)<sub>1</sub>(5-Melm)<sub>3</sub>, ferrous, *in vacuo*, BP86,  
G° = -2763.850933**

C -43.961031 -14.204787 7.163918  
C -42.596245 -13.593454 7.096036  
N -41.425690 -14.310559 7.333142  
C -40.356018 -13.468794 7.167716  
N -40.774287 -12.243729 6.839144  
C -42.163838 -12.311963 6.797352  
C -41.586660 -7.018729 10.632874  
C -41.109610 -8.197391 9.843000  
N -41.122289 -9.500708 10.333464  
C -40.649314 -10.341318 9.362778  
N -40.320389 -9.650575 8.267530  
C -40.602084 -8.317883 8.560572  
C -35.733519 -6.547573 4.491063  
C -36.581106 -7.400956 5.382075  
N -36.532309 -7.335382 6.773725  
C -37.437605 -8.225090 7.286834  
N -38.066718 -8.868974 6.300213  
C -37.539110 -8.364450 5.115774  
C -41.223465 -7.797166 4.809805  
S -41.042649 -9.630791 4.678976  
C -39.505008 -12.703998 3.586892  
C -38.259867 -12.588106 4.410222  
N -38.157028 -11.747190 5.525471  
C -36.908709 -11.877664 5.989517  
N -36.204678 -12.764517 5.229816  
C -37.042450 -13.221913 4.221983  
Fe -39.673382 -10.378208 6.333225  
H -44.085008 -15.018382 6.426874  
H -44.720306 -13.439114 6.944015  
H -42.753019 -11.439314 6.520105  
H -39.320107 -13.785215 7.271520  
H -41.014570 -6.887949 11.568861  
H -42.654904 -7.108167 10.899714  
H -40.441362 -7.532261 7.825057  
H -40.578720 -11.420295 9.478871  
H -35.936899 -5.471368 4.635556  
H -34.654880 -6.713671 4.662638  
H -37.897435 -8.722190 4.151643  
H -37.611334 -8.362164 8.352401  
H -40.247815 -7.305857 4.960828  
H -41.902328 -7.528975 5.635802  
H -39.805443 -11.721094 3.184676  
H -40.351840 -13.072188 4.190310  
H -36.708138 -13.933197 3.470351  
H -35.232050 -13.032057 5.369003  
H -36.485880 -11.346280 6.839627  
H -41.441524 -9.783773 11.258840  
H -41.372376 -15.300063 7.570761  
H -35.932917 -6.716253 7.318047

H -41.469277 -6.100221 10.038017  
H -44.181237 -14.618916 8.164280  
H -39.345825 -13.398010 2.746630  
H -35.945186 -6.787652 3.438144  
H -41.660406 -7.427999 3.868519

**(4-Melm)<sub>1</sub>(5-Melm)<sub>3</sub>, ferric, *in vacuo*, TPSSh,  
G° = -2992.193283**

C -37.643935 -12.510373 10.418972  
C -37.351219 -11.866319 9.070633  
O -36.172183 -11.672236 8.718630  
O -38.392494 -11.586935 8.341332  
C -43.806021 -14.396937 6.408005  
C -42.552140 -13.686463 6.802618  
N -41.669545 -14.175856 7.755605  
C -40.634374 -13.308867 7.882019  
N -40.796609 -12.276649 7.062964  
C -41.985604 -12.505815 6.387609  
C -40.945894 -6.206966 10.051862  
C -40.735997 -7.571549 9.480326  
N -41.204576 -8.728006 10.087993  
C -40.848657 -9.795458 9.329098  
N -40.177491 -9.393356 8.260823  
C -40.101965 -8.013871 8.344495  
C -35.951912 -6.224572 5.027259  
C -36.495668 -7.420538 5.739256  
N -35.835859 -8.045294 6.788620  
C -36.575554 -9.097053 7.216128  
N -37.689983 -9.190466 6.496331  
C -37.646215 -8.151009 5.575034  
C -42.099370 -8.950776 5.743807  
S -40.570070 -9.680154 5.048257  
C -39.662623 -12.554129 3.375607  
C -38.389490 -12.639197 4.155067  
N -38.163353 -12.002283 5.377262  
C -36.925162 -12.322404 5.757101  
N -36.350663 -13.127716 4.839633  
C -37.258768 -13.342291 3.819733  
Fe -39.281672 -10.689059 6.730195  
H -36.815943 -12.332997 11.106828  
H -37.737198 -13.594925 10.283258  
H -43.593888 -15.388613 5.993102  
H -44.329475 -13.818591 5.644275  
H -42.341478 -11.816045 5.638277  
H -39.796577 -13.442653 8.546649  
H -40.487953 -6.109342 11.042459  
H -42.011029 -5.967300 10.144625  
H -39.592026 -7.436680 7.588501  
H -41.080667 -10.818306 9.579146  
H -35.812528 -5.376714 5.707425  
H -34.987314 -6.441282 4.554651

H -38.441850 -8.011233 4.859162  
H -36.266380 -9.790342 7.988831  
H -42.447489 -9.516523 6.610396  
H -42.864838 -8.957253 4.964506  
H -39.854034 -11.536482 3.024305  
H -40.518803 -12.857759 3.984577  
H -37.030528 -13.958982 2.964920  
H -35.418398 -13.513414 4.904483  
H -36.447475 -12.015084 6.681909  
H -41.723596 -8.771003 10.955334  
H -41.770032 -15.045193 8.263714  
H -34.940601 -7.773183 7.173775  
H -40.490482 -5.461986 9.396567  
H -44.484464 -14.523197 7.259099  
H -38.579129 -12.137280 10.844637  
H -39.603322 -13.215688 2.507474  
H -36.647400 -5.917207 4.243879  
H -41.911289 -7.917608 6.045304

**(4-Melm)<sub>1</sub>(5-Melm)<sub>3</sub>, ferrous, *in vacuo*, TPSSH,  
*G*<sup>o</sup> = -2763.733723**

C -43.974857 -14.192347 7.097270  
C -42.609922 -13.585110 7.054540  
N -41.450473 -14.307896 7.294739  
C -40.383235 -13.474062 7.154149  
N -40.787979 -12.251188 6.842006  
C -42.171273 -12.310692 6.780457  
C -41.546215 -7.035813 10.658867  
C -41.084579 -8.213448 9.862982  
N -41.156217 -9.517941 10.327848  
C -40.684245 -10.351156 9.363922  
N -40.299918 -9.660465 8.299466  
C -40.545674 -8.329586 8.603786  
C -35.783750 -6.582392 4.404501  
C -36.613440 -7.417857 5.324800  
N -36.535139 -7.328740 6.707536  
C -37.426969 -8.201072 7.250155  
N -38.074548 -8.855106 6.296034  
C -37.573202 -8.375366 5.096736  
C -41.233179 -7.783734 4.860613  
S -41.082853 -9.608928 4.684660  
C -39.457683 -12.692322 3.630249  
C -38.221790 -12.577785 4.464124  
N -38.133444 -11.740999 5.575607  
C -36.897286 -11.863826 6.046500  
N -36.185881 -12.742118 5.300235  
C -37.008835 -13.202127 4.288954  
Fe -39.684088 -10.376493 6.333735  
H -44.084335 -14.991086 6.355125  
H -44.720803 -13.426505 6.876522  
H -42.745532 -11.437780 6.507174

H -39.358708 -13.794584 7.267248  
H -40.996620 -6.942645 11.602272  
H -42.614318 -7.102766 10.893733  
H -40.340152 -7.546598 7.889989  
H -40.652857 -11.424670 9.464329  
H -35.981672 -5.513324 4.540967  
H -34.712028 -6.751335 4.558414  
H -37.954961 -8.743168 4.155495  
H -37.574198 -8.319248 8.313122  
H -40.256075 -7.314061 5.006243  
H -41.889429 -7.528780 5.697087  
H -39.758331 -11.713187 3.244474  
H -40.296742 -13.078446 4.216925  
H -36.665359 -13.905783 3.547121  
H -35.220184 -13.001893 5.448380  
H -36.487886 -11.335081 6.893670  
H -41.511818 -9.804785 11.230453  
H -41.403174 -15.293679 7.517091  
H -35.927670 -6.707667 7.226092  
H -41.387308 -6.120896 10.084756  
H -44.202732 -14.612430 8.083503  
H -39.281674 -13.366543 2.788381  
H -36.019251 -6.837052 3.369431  
H -41.675355 -7.391934 3.941735

**(4-Melm)<sub>1</sub>(5-Melm)<sub>3</sub>, ferric, *in vacuo*, PBE0,  
*G*<sup>o</sup> = -2990.185495**

C -37.615548 -12.567742 10.352383  
C -37.348810 -11.869518 9.034310  
O -36.182489 -11.645019 8.684471  
O -38.395017 -11.579968 8.335862  
C -43.797500 -14.358760 6.439151  
C -42.545330 -13.657577 6.825716  
N -41.674209 -14.136824 7.781804  
C -40.637190 -13.281541 7.896422  
N -40.788429 -12.265750 7.065845  
C -41.971275 -12.491417 6.394095  
C -40.911260 -6.237553 10.046985  
C -40.726066 -7.590427 9.460090  
N -41.266322 -8.732832 10.011800  
C -40.914890 -9.791166 9.250768  
N -40.177748 -9.395571 8.233399  
C -40.052467 -8.029914 8.351284  
C -35.998968 -6.205547 5.060047  
C -36.527738 -7.402952 5.764336  
N -35.879690 -8.006620 6.821875  
C -36.601184 -9.067125 7.235970  
N -37.693786 -9.185673 6.499131  
C -37.656341 -8.154506 5.579682  
C -42.031500 -8.928579 5.723919  
S -40.550561 -9.715102 5.022503



C	-39.684598	-12.642258	3.445843
C	-38.396849	-12.672462	4.190077
N	-38.154529	-12.003673	5.382240
C	-36.906717	-12.286894	5.736362
N	-36.340479	-13.097903	4.830079
C	-37.262708	-13.356616	3.844365
Fe	-39.274937	-10.687450	6.716484
H	-36.784585	-12.405788	11.040406
H	-37.689306	-13.647431	10.174357
H	-43.595132	-15.357532	6.037046
H	-44.315896	-13.788214	5.666114
H	-42.319847	-11.811721	5.630714
H	-39.801034	-13.408788	8.566442
H	-40.501587	-6.175448	11.061103
H	-41.968865	-5.955292	10.090953
H	-39.483302	-7.452904	7.637212
H	-41.200081	-10.810453	9.462798
H	-35.886362	-5.351202	5.736670
H	-35.023675	-6.403305	4.601725
H	-38.441123	-8.031428	4.847824
H	-36.292699	-9.753633	8.016508
H	-42.465015	-9.532810	6.524592
H	-42.766011	-8.809697	4.923945
H	-39.924646	-11.636789	3.090136
H	-40.514799	-12.970434	4.077836
H	-37.046655	-13.988968	2.997122
H	-35.401086	-13.460612	4.882391
H	-36.414978	-11.952230	6.645244
H	-41.828998	-8.773821	10.848413
H	-41.782446	-14.995615	8.300963
H	-34.998995	-7.717035	7.220767
H	-40.395190	-5.496094	9.433998
H	-44.481312	-14.468346	7.288004
H	-38.552898	-12.230597	10.802002
H	-39.624968	-13.310159	2.582920
H	-36.686279	-5.912543	4.264022
H	-41.788347	-7.941630	6.124821

**(4-Melm)<sub>1</sub>(5-Melm)<sub>3</sub>, ferrous, *in vacuo*, PBE0,  
G° = -2761.981867**

C	-43.914257	-14.245161	7.039149
C	-42.566318	-13.618354	7.032516
N	-41.408769	-14.312876	7.312451
C	-40.359025	-13.465218	7.196899
N	-40.774229	-12.259585	6.864060
C	-42.145497	-12.341748	6.760175
C	-41.512230	-6.989375	10.625631
C	-41.080729	-8.176358	9.841794
N	-41.239365	-9.471795	10.284254
C	-40.772156	-10.314278	9.336677
N	-40.308003	-9.638018	8.304347

C	-40.496040	-8.306378	8.609218
C	-35.793409	-6.599630	4.429714
C	-36.612348	-7.432601	5.348987
N	-36.510835	-7.364441	6.722582
C	-37.400240	-8.228559	7.264690
N	-38.067827	-8.857278	6.317595
C	-37.584925	-8.371682	5.122599
C	-41.238408	-7.788894	4.922501
S	-41.093195	-9.592665	4.679566
C	-39.507859	-12.715690	3.682570
C	-38.255950	-12.582106	4.475513
N	-38.139283	-11.736336	5.565955
C	-36.894493	-11.841066	5.996295
N	-36.202703	-12.718897	5.244587
C	-37.047328	-13.197334	4.271198
Fe	-39.691348	-10.370467	6.337692
H	-43.989276	-15.053207	6.303117
H	-44.667503	-13.496532	6.786263
H	-42.729053	-11.482826	6.458721
H	-39.330982	-13.765291	7.341574
H	-40.999195	-6.929458	11.591807
H	-42.591019	-7.000940	10.815901
H	-40.222768	-7.525274	7.914910
H	-40.801310	-11.390224	9.423041
H	-35.975207	-5.529851	4.580738
H	-34.720951	-6.781949	4.559798
H	-37.986754	-8.719230	4.180640
H	-37.533755	-8.359725	8.329223
H	-40.258795	-7.312076	5.027249
H	-41.847080	-7.555972	5.800847
H	-39.836878	-11.741399	3.306548
H	-40.325011	-13.116010	4.290359
H	-36.725240	-13.907262	3.524839
H	-35.232606	-12.965726	5.365145
H	-36.463698	-11.294473	6.822760
H	-41.649049	-9.747748	11.164108
H	-41.350584	-15.293207	7.544167
H	-35.889207	-6.759377	7.238054
H	-41.284685	-6.077589	10.069894
H	-44.168770	-14.658314	8.021501
H	-39.348928	-13.384490	2.833358
H	-36.048567	-6.836176	3.394957
H	-41.732205	-7.363376	4.045470

***cis*-(4-Melm)<sub>2</sub>(5-Melm)<sub>2</sub>, ferric, *in vacuo*, BP86,  
G° = -2992.306085**

C	-37.662480	-12.396442	10.410828
C	-37.362382	-11.836794	9.021637
O	-36.176020	-11.661579	8.652317
O	-38.412958	-11.549646	8.292738
C	-42.483836	-13.866402	6.933630

N -41.307240 -14.472303 7.351983  
 C -40.327426 -13.528668 7.364422  
 N -40.810227 -12.343925 6.969656  
 C -42.170137 -12.539346 6.692365  
 C -41.149360 -6.387718 10.155169  
 C -40.935774 -7.702102 9.472135  
 N -41.485105 -8.898847 9.930028  
 C -41.103534 -9.909267 9.094901  
 N -40.337339 -9.427937 8.114090  
 C -40.224678 -8.061318 8.340487  
 C -35.855321 -6.195480 5.098292  
 C -36.457243 -7.364769 5.812592  
 N -35.923368 -7.904058 6.982931  
 C -36.686666 -8.962515 7.377475  
 N -37.699006 -9.140770 6.518986  
 C -37.561850 -8.152115 5.545283  
 C -41.420165 -8.309253 5.143631  
 S -40.374748 -9.769142 4.759105  
 C -39.709869 -12.854380 3.484160  
 C -38.386440 -12.794540 4.184052  
 N -38.137916 -12.049042 5.345701  
 C -36.852145 -12.253231 5.676787  
 N -36.270066 -13.089845 4.778969  
 C -37.218740 -13.445662 3.829644  
 Fe -39.286003 -10.680413 6.638594  
 H -36.778679 -12.907871 10.818858  
 H -38.527767 -13.078767 10.391492  
 H -39.298884 -13.714072 7.661238  
 H -40.770651 -6.396296 11.192808  
 H -42.217657 -6.108515 10.186905  
 H -39.633382 -7.426201 7.684486  
 H -41.372721 -10.953593 9.232618  
 H -35.833024 -5.290481 5.731579  
 H -34.821002 -6.402751 4.770145  
 H -38.252111 -8.097350 4.705535  
 H -36.442688 -9.613848 8.216273  
 H -42.005928 -8.467205 6.061809  
 H -42.100546 -8.138024 4.295180  
 H -39.965712 -11.891053 3.011634  
 H -40.524450 -13.097920 4.186542  
 H -36.991952 -14.112721 3.001422  
 H -35.304261 -13.410799 4.816080  
 H -36.357898 -11.866141 6.574319  
 H -42.071509 -9.005093 10.756849  
 H -41.193350 -15.451937 7.606581  
 H -35.082099 -7.581194 7.459612  
 H -40.614301 -5.594747 9.611095  
 H -37.920839 -11.559957 11.084876  
 H -39.684819 -13.627531 2.699943  
 H -36.448647 -5.961861 4.201333  
 H -40.790773 -7.413240 5.274729  
 H -43.419972 -14.412956 6.846441

C -43.091557 -11.457432 6.221750  
 H -43.121103 -10.613351 6.932654  
 H -42.760434 -11.054422 5.249193  
 H -44.114997 -11.849439 6.112755

*cis*-(4-Melm)<sub>2</sub>(5-Melm)<sub>2</sub>, ferrous, *in vacuo*, BP86,  
 $G^\circ = -2763.847929$

C -42.475457 -13.696997 7.256840  
 N -41.244094 -14.331697 7.332089  
 C -40.279123 -13.407690 7.053050  
 N -40.826319 -12.211176 6.806643  
 C -42.212148 -12.375281 6.934266  
 C -41.647981 -6.943037 10.503539  
 C -41.165200 -8.129237 9.728557  
 N -41.127130 -9.419294 10.251810  
 C -40.660470 -10.272083 9.288214  
 N -40.387041 -9.601472 8.165039  
 C -40.693953 -8.269388 8.433986  
 C -35.572667 -6.581383 4.733914  
 C -36.487600 -7.437661 5.552717  
 N -36.501039 -7.424969 6.946412  
 C -37.458522 -8.301267 7.383688  
 N -38.061935 -8.886780 6.345588  
 C -37.462688 -8.357606 5.206173  
 C -41.142830 -7.730494 4.683549  
 S -40.847750 -9.535212 4.427621  
 C -39.572813 -12.697996 3.488835  
 C -38.321951 -12.571417 4.301918  
 N -38.212847 -11.722215 5.411104  
 C -36.956795 -11.839446 5.859011  
 N -36.255898 -12.726899 5.097084  
 C -37.102383 -13.197723 4.102987  
 Fe -39.714971 -10.344137 6.232022  
 H -39.217049 -13.639588 7.017864  
 H -41.050575 -6.774315 11.417339  
 H -42.704628 -7.052398 10.806515  
 H -40.570577 -7.497918 7.676641  
 H -40.556051 -11.345260 9.430293  
 H -35.748120 -5.504884 4.909542  
 H -34.508966 -6.789450 4.947896  
 H -37.790167 -8.666734 4.214506  
 H -37.686455 -8.469746 8.434225  
 H -40.213294 -7.210640 4.970060  
 H -41.913047 -7.562480 5.453951  
 H -39.829394 -11.738482 3.007070  
 H -40.433266 -12.980976 4.117883  
 H -36.771728 -13.910666 3.351269  
 H -35.278966 -12.984515 5.224682  
 H -36.528013 -11.298299 6.699762  
 H -41.408554 -9.686621 11.194139  
 H -41.088092 -15.317172 7.535994

H -35.907739 -6.847435 7.540734  
H -41.572752 -6.037488 9.882627  
H -39.445187 -13.460728 2.704651  
H -35.742563 -6.775937 3.664164  
H -41.503418 -7.305260 3.733748  
C -43.192841 -11.264157 6.718222  
H -44.224184 -11.645095 6.785458  
H -43.067784 -10.465971 7.470482  
H -43.040538 -10.798408 5.729333  
H -43.410879 -14.226249 7.423479

***cis*-(4-Melm)<sub>2</sub>(5-Melm)<sub>2</sub>, ferric, *in vacuo*, TPSSh,  
 $G^\circ = -2992.188546$**

C -37.116938 -12.214985 10.137578  
C -37.168197 -11.557484 8.762834  
O -36.127374 -11.131961 8.235018  
O -38.363958 -11.476391 8.239112  
C -42.519714 -13.711733 7.250722  
N -41.307821 -14.365402 7.383241  
C -40.322538 -13.458630 7.211103  
N -40.834687 -12.255187 6.968779  
C -42.222617 -12.395262 6.992244  
C -42.570521 -7.064638 10.128085  
C -41.678104 -8.136446 9.591792  
N -41.161368 -9.157922 10.377642  
C -40.393025 -9.963222 9.602376  
N -40.382132 -9.519746 8.351642  
C -41.180902 -8.387506 8.335949  
C -35.131967 -7.163865 4.861590  
C -36.161276 -7.856880 5.693650  
N -36.242318 -7.713367 7.072823  
C -37.267712 -8.466500 7.532008  
N -37.870405 -9.082401 6.525419  
C -37.188097 -8.710873 5.377119  
C -40.363784 -7.770675 4.849914  
S -40.671977 -9.568309 5.009616  
C -40.001740 -12.679351 3.565240  
C -38.621746 -12.599598 4.136157  
N -38.293918 -11.901167 5.300811  
C -36.983008 -12.054651 5.491230  
N -36.457627 -12.815326 4.506463  
C -37.476086 -13.173405 3.641558  
Fe -39.404859 -10.596321 6.687887  
H -36.108354 -12.574008 10.347049  
H -37.836741 -13.034794 10.211907  
H -39.270130 -13.682586 7.276846  
H -42.073175 -6.477336 10.908035  
H -43.491222 -7.480805 10.551946  
H -41.355174 -7.836304 7.425869  
H -39.871243 -10.841140 9.948581  
H -35.209984 -6.074293 4.947467

H -34.116647 -7.455709 5.152277  
H -37.486862 -9.080941 4.408173  
H -37.529370 -8.554676 8.573528  
H -41.323543 -7.248424 4.889191  
H -39.904824 -7.573177 3.878024  
H -40.364729 -11.689910 3.271703  
H -40.711678 -13.086513 4.291736  
H -37.303967 -13.787946 2.772020  
H -35.484852 -13.079636 4.429182  
H -36.422098 -11.638753 6.323696  
H -41.333482 -9.287786 11.366276  
H -41.177420 -15.348529 7.580076  
H -35.609309 -7.175467 7.650065  
H -42.850276 -6.383686 9.321974  
H -37.376547 -11.471466 10.901425  
H -40.000896 -13.327239 2.685121  
H -35.270775 -7.428365 3.811485  
H -39.704863 -7.406197 5.639671  
H -43.462983 -14.225278 7.349063  
C -43.182908 -11.269856 6.775229  
H -44.205182 -11.623719 6.930999  
H -42.987747 -10.447707 7.469693  
H -43.101479 -10.865717 5.762303

***cis*-(4-Melm)<sub>2</sub>(5-Melm)<sub>2</sub>, ferrous, *in vacuo*,  
TPSSh,  $G^\circ = -2763.730800$**

C -42.494577 -13.675948 7.253129  
N -41.273930 -14.322309 7.303436  
C -40.309393 -13.408165 7.037348  
N -40.841752 -12.209123 6.824515  
C -42.221748 -12.360207 6.958285  
C -41.606375 -6.954063 10.522032  
C -41.130541 -8.139077 9.745616  
N -41.121815 -9.427860 10.257836  
C -40.656321 -10.274230 9.301912  
N -40.355040 -9.606385 8.196551  
C -40.644849 -8.277247 8.466724  
C -35.621251 -6.618635 4.646289  
C -36.522305 -7.455811 5.495265  
N -36.516771 -7.408917 6.882167  
C -37.461468 -8.269962 7.349227  
N -38.074168 -8.876886 6.342360  
C -37.494180 -8.377993 5.186510  
C -41.147486 -7.739860 4.701330  
S -40.863760 -9.531922 4.398552  
C -39.544738 -12.708144 3.527447  
C -38.296767 -12.573104 4.340037  
N -38.196074 -11.719517 5.438283  
C -36.947450 -11.819466 5.882059  
N -36.241534 -12.700110 5.133152  
C -37.080412 -13.185537 4.147295

Fe -39.733000 -10.351166 6.225652  
 H -39.258546 -13.648187 6.989819  
 H -41.019074 -6.804761 11.434973  
 H -42.658734 -7.057070 10.808978  
 H -40.499723 -7.511516 7.720155  
 H -40.570717 -11.340937 9.438668  
 H -35.796815 -5.548586 4.804119  
 H -34.564394 -6.822640 4.852047  
 H -37.837383 -8.706974 4.216341  
 H -37.670380 -8.413071 8.398503  
 H -40.221888 -7.237131 4.997221  
 H -41.909299 -7.589695 5.471135  
 H -39.790840 -11.762154 3.034618  
 H -40.399021 -12.978246 4.155120  
 H -36.744111 -13.894706 3.407382  
 H -35.269076 -12.944307 5.262602  
 H -36.527201 -11.272892 6.712242  
 H -41.420447 -9.696864 11.186397  
 H -41.126343 -15.306240 7.483079  
 H -35.921576 -6.821334 7.451433  
 H -41.513190 -6.054477 9.910561  
 H -39.414851 -13.478287 2.763074  
 H -35.807188 -6.836620 3.592912  
 H -41.503828 -7.294270 3.769863  
 C -43.186174 -11.232976 6.769862  
 H -43.052640 -10.464835 7.539039  
 H -43.026681 -10.753100 5.799160  
 H -44.212911 -11.603191 6.827131  
 H -43.425470 -14.196432 7.414918

***cis*-(4-Melm)<sub>2</sub>(5-Melm)<sub>2</sub>, ferric, *in vacuo*, PBE0,  
*G*<sup>o</sup> = -2990.181020**

C -37.112567 -12.156402 10.130222  
 C -37.170746 -11.538813 8.745613  
 O -36.136294 -11.136599 8.205054  
 O -38.360698 -11.466054 8.233935  
 C -42.496668 -13.685490 7.222551  
 N -41.294725 -14.340034 7.358618  
 C -40.310508 -13.439881 7.204575  
 N -40.813454 -12.238634 6.969132  
 C -42.193477 -12.371431 6.980353  
 C -42.595262 -7.093722 10.071359  
 C -41.688033 -8.148762 9.548983  
 N -41.158269 -9.149060 10.337833  
 C -40.379300 -9.942504 9.573549  
 N -40.373745 -9.510065 8.326098  
 C -41.186981 -8.397906 8.298895  
 C -35.101965 -7.199437 4.892227  
 C -36.137392 -7.878949 5.713555  
 N -36.232238 -7.729121 7.082346  
 C -37.261003 -8.471231 7.531265

N -37.851911 -9.086505 6.526689  
 C -37.160897 -8.727141 5.389295  
 C -40.321237 -7.777225 4.889211  
 S -40.628165 -9.565535 4.989931  
 C -40.016181 -12.686883 3.608132  
 C -38.636443 -12.610259 4.160500  
 N -38.288181 -11.903083 5.303540  
 C -36.982965 -12.065599 5.478442  
 N -36.479782 -12.840494 4.503473  
 C -37.505868 -13.199687 3.661027  
 Fe -39.389368 -10.585524 6.675176  
 H -36.100610 -12.497281 10.352726  
 H -37.822619 -12.982046 10.227118  
 H -39.258088 -13.667753 7.276175  
 H -42.111622 -6.489046 10.846363  
 H -43.510379 -7.519723 10.497070  
 H -41.373596 -7.854859 7.385373  
 H -39.842525 -10.811229 9.924258  
 H -35.173270 -6.108992 4.969884  
 H -34.090418 -7.494808 5.191674  
 H -37.449681 -9.098066 4.416643  
 H -37.536074 -8.553334 8.571199  
 H -41.279417 -7.250664 4.916148  
 H -39.836390 -7.546272 3.937183  
 H -40.374406 -11.700015 3.300515  
 H -40.724768 -13.074322 4.346670  
 H -37.355257 -13.827185 2.796024  
 H -35.512786 -13.113628 4.419459  
 H -36.408996 -11.646355 6.301838  
 H -41.329368 -9.274524 11.324536  
 H -41.168375 -15.322706 7.546597  
 H -35.605069 -7.191928 7.662065  
 H -42.887044 -6.423381 9.260584  
 H -37.382754 -11.397320 10.874447  
 H -40.032789 -13.349034 2.739127  
 H -35.230135 -7.466612 3.841447  
 H -39.683232 -7.426503 5.702473  
 H -43.445582 -14.192208 7.307947  
 C -43.144886 -11.246414 6.775170  
 H -42.975950 -10.449167 7.505117  
 H -43.031508 -10.801896 5.782566  
 H -44.171393 -11.604554 6.884546

***cis*-(4-Melm)<sub>2</sub>(5-Melm)<sub>2</sub>, ferrous, *in vacuo*, PBE0,  
*G*<sup>o</sup> = -2761.979704**

C -42.491412 -13.671826 7.224191  
 N -41.280206 -14.320106 7.266555  
 C -40.316610 -13.412060 7.015898  
 N -40.840426 -12.214153 6.820614  
 C -42.212541 -12.357293 6.948288  
 C -41.634203 -6.957565 10.476991

C -41.154212 -8.141567 9.717143  
 N -41.178736 -9.423930 10.221803  
 C -40.698114 -10.269020 9.282825  
 N -40.355257 -9.605687 8.195891  
 C -40.633223 -8.280852 8.456804  
 C -35.625188 -6.628143 4.692656  
 C -36.521858 -7.464518 5.533018  
 N -36.515913 -7.428322 6.911508  
 C -37.458068 -8.285630 7.369582  
 N -38.068946 -8.879968 6.364009  
 C -37.493458 -8.378535 5.217021  
 C -41.133958 -7.747913 4.737186  
 S -40.862363 -9.517885 4.382550  
 C -39.539637 -12.711012 3.547924  
 C -38.292007 -12.569524 4.346260  
 N -38.184724 -11.721616 5.436562  
 C -36.937871 -11.812028 5.865144  
 N -36.237430 -12.683917 5.114347  
 C -37.077473 -13.173182 4.142474  
 Fe -39.733660 -10.355068 6.218768  
 H -39.265379 -13.655308 6.964127  
 H -41.072360 -6.813981 11.406476  
 H -42.695542 -7.044725 10.733902  
 H -40.457298 -7.512486 7.718109  
 H -40.632737 -11.338825 9.416449  
 H -35.797041 -5.558456 4.855630  
 H -34.567929 -6.834642 4.892584  
 H -37.838317 -8.696049 4.242321  
 H -37.669998 -8.435702 8.418540  
 H -40.203329 -7.246200 5.021328  
 H -41.875956 -7.609062 5.528920  
 H -39.815530 -11.757422 3.085676  
 H -40.382499 -13.020810 4.172981  
 H -36.748251 -13.880063 3.396294  
 H -35.264202 -12.918948 5.233617  
 H -36.513214 -11.259228 6.690520  
 H -41.509420 -9.690802 11.137189  
 H -41.136836 -15.304513 7.431421  
 H -35.921176 -6.847393 7.483310  
 H -41.513502 -6.057165 9.871508  
 H -39.402856 -13.453552 2.758262  
 H -35.811826 -6.836593 3.637423  
 H -41.514104 -7.271429 3.830316  
 C -43.166025 -11.228322 6.774129  
 H -44.195696 -11.592568 6.805706  
 H -43.043466 -10.477677 7.562288  
 H -42.989960 -10.724569 5.817793  
 H -43.428011 -14.186259 7.376238

*trans*-(4-Melm)<sub>2</sub>(5-Melm)<sub>2</sub>, ferric, in vacuo, BP86,  
*G*<sup>o</sup> = -2992.306044

C -37.712814 -12.104483 10.640394  
 C -37.372149 -11.734355 9.199287  
 O -36.174356 -11.662111 8.834951  
 O -38.388472 -11.496090 8.406926  
 C -43.643013 -14.495090 6.192797  
 C -42.432442 -13.744202 6.651408  
 N -41.525553 -14.249958 7.581313  
 C -40.539059 -13.328412 7.784020  
 N -40.759015 -12.243862 7.034672  
 C -41.929803 -12.496026 6.327088  
 C -41.015939 -7.734273 9.800597  
 N -41.363599 -8.993449 10.267795  
 C -40.845301 -9.917493 9.412848  
 N -40.184642 -9.316231 8.418179  
 C -40.280175 -7.939182 8.645480  
 C -35.589207 -6.638391 4.567072  
 C -36.228911 -7.686596 5.422348  
 N -35.590107 -8.281516 6.510406  
 C -36.430012 -9.190720 7.082505  
 N -37.593154 -9.212873 6.418108  
 C -37.474018 -8.285393 5.385199  
 C -42.215281 -8.950675 5.922841  
 S -40.615437 -9.492587 5.199115  
 C -39.607430 -12.242820 3.298026  
 C -38.397829 -12.507120 4.140967  
 N -38.183249 -11.964667 5.414953  
 C -37.001388 -12.433067 5.844495  
 N -36.452655 -13.247870 4.904431  
 C -37.317240 -13.310327 3.821056  
 Fe -39.268278 -10.577825 6.794757  
 H -36.906781 -12.709910 11.080374  
 H -38.675224 -12.636460 10.713972  
 H -43.375365 -15.451908 5.709973  
 H -44.197037 -13.893494 5.456427  
 H -42.327408 -11.772517 5.618918  
 H -39.687282 -13.464457 8.445461  
 H -40.956507 -10.991340 9.536186  
 H -35.321868 -5.737936 5.148638  
 H -34.670456 -7.010175 4.079091  
 H -38.293989 -8.104075 4.693031  
 H -36.156802 -9.853815 7.907708  
 H -42.532581 -9.618273 6.738398  
 H -42.975096 -8.946746 5.125560  
 H -39.710791 -11.173184 3.050935  
 H -40.532584 -12.546009 3.816079  
 H -37.100133 -13.902751 2.935443  
 H -35.560289 -13.730394 4.992870  
 H -36.536009 -12.205989 6.808815  
 H -41.911384 -9.193532 11.102624

H -41.579641 -15.164875 8.027563  
H -34.643340 -8.080367 6.830007  
H -44.330878 -14.718540 7.027780  
H -37.799583 -11.175383 11.232029  
H -39.537592 -12.809884 2.356145  
H -36.286533 -6.329151 3.773845  
H -42.119558 -7.927245 6.319894  
H -41.305472 -6.822707 10.317988  
C -39.639887 -6.903682 7.773693  
H -38.540149 -6.941448 7.850722  
H -39.892611 -7.059948 6.711669  
H -39.971355 -5.896743 8.072130

***trans*-(4-Melm)<sub>2</sub>(5-Melm)<sub>2</sub>, ferrous, *in vacuo*,  
BP86,  $G^\circ = -2763.848245$**

C -44.200836 -13.790469 7.293786  
C -42.800002 -13.291672 7.122406  
N -41.677177 -14.101145 7.272894  
C -40.558580 -13.346270 7.030330  
N -40.899671 -12.090164 6.733279  
C -42.288831 -12.047691 6.792570  
C -40.931101 -8.719949 10.203240  
N -40.218786 -9.853309 10.563729  
C -39.731596 -10.423147 9.422633  
N -40.088554 -9.708980 8.348072  
C -40.848045 -8.632352 8.822996  
C -35.522737 -6.684748 4.397392  
C -36.485025 -7.419259 5.277669  
N -36.789134 -7.017629 6.577484  
C -37.707739 -7.885090 7.101693  
N -38.014986 -8.832377 6.211875  
C -37.259339 -8.549545 5.077985  
C -40.761291 -7.773234 4.234090  
S -41.073127 -9.538892 4.671533  
C -39.452271 -12.690449 3.581413  
C -38.237023 -12.578512 4.449033  
N -38.163450 -11.726286 5.559035  
C -36.937485 -11.874099 6.076632  
N -36.220074 -12.781902 5.356047  
C -37.023819 -13.235363 4.319194  
Fe -39.663674 -10.297410 6.290457  
H -44.442916 -14.594259 6.575570  
H -44.910144 -12.966822 7.121737  
H -42.829373 -11.130675 6.564608  
H -39.546818 -13.745971 7.056663  
H -39.153614 -11.344855 9.414974  
H -35.849327 -5.646745 4.207034  
H -34.509126 -6.645307 4.834944  
H -37.332970 -9.169373 4.186137  
H -38.119235 -7.797770 8.105273  
H -39.686041 -7.535136 4.262531

H -41.301660 -7.096413 4.915818  
H -39.815642 -11.691711 3.284501  
H -40.283787 -13.181664 4.115479  
H -36.672297 -13.962031 3.590455  
H -35.257922 -13.062937 5.536263  
H -36.537552 -11.333030 6.931699  
H -40.094401 -10.207921 11.510102  
H -41.686433 -15.092559 7.507616  
H -36.399809 -6.204949 7.053927  
H -44.380341 -14.180767 8.311698  
H -39.225377 -13.278538 2.678267  
H -35.447461 -7.193175 3.424263  
H -41.135793 -7.606312 3.211827  
C -41.459996 -7.610271 7.915337  
H -42.060323 -8.098772 7.128312  
H -42.106350 -6.925107 8.485851  
H -40.689172 -7.007101 7.403472  
H -41.432800 -8.093387 10.936997

***trans*-(4-Melm)<sub>2</sub>(5-Melm)<sub>2</sub>, ferric, *in vacuo*,  
TPSSh,  $G^\circ = -2992.187750$**

C -37.685940 -12.253822 10.527596  
C -37.382565 -11.762075 9.119230  
O -36.203547 -11.608426 8.751882  
O -38.423289 -11.510761 8.375428  
C -43.723360 -14.399398 6.301586  
C -42.474034 -13.683636 6.701070  
N -41.518502 -14.235298 7.542948  
C -40.511194 -13.342542 7.708255  
N -40.759823 -12.234708 7.020299  
C -41.976470 -12.441714 6.388861  
C -41.062243 -7.762548 9.690972  
N -41.355840 -9.017053 10.191258  
C -40.818760 -9.935376 9.357286  
N -40.198776 -9.338789 8.344782  
C -40.338994 -7.966148 8.540041  
C -35.600648 -6.624797 4.651399  
C -36.263864 -7.651708 5.510493  
N -35.719609 -8.112248 6.702286  
C -36.552970 -9.032964 7.243962  
N -37.619297 -9.193430 6.466283  
C -37.444705 -8.338949 5.385491  
C -42.165720 -8.956532 5.777861  
S -40.568895 -9.552634 5.105564  
C -39.666390 -12.435739 3.390526  
C -38.402037 -12.557083 4.179702  
N -38.168102 -11.924443 5.402047  
C -36.941266 -12.274031 5.791101  
N -36.380928 -13.096099 4.878926  
C -37.286963 -13.289194 3.852783  
Fe -39.274556 -10.590309 6.761000

H -36.816984 -12.763501 10.945520  
H -38.557932 -12.914135 10.544510  
H -43.501557 -15.332086 5.771086  
H -44.311200 -13.765675 5.634787  
H -42.404696 -11.694190 5.740454  
H -39.630843 -13.513931 8.305802  
H -40.883940 -11.000744 9.506506  
H -35.467407 -5.676669 5.184405  
H -34.616165 -6.961489 4.307676  
H -38.185446 -8.269106 4.603908  
H -36.328830 -9.603197 8.133783  
H -42.399033 -9.434654 6.730697  
H -42.949590 -9.174735 5.048318  
H -39.829486 -11.411148 3.044868  
H -40.535434 -12.720256 3.990411  
H -37.067676 -13.911534 2.999662  
H -35.458671 -13.504130 4.949981  
H -36.462878 -11.972426 6.717958  
H -41.880373 -9.216254 11.032308  
H -41.556270 -15.158091 7.956545  
H -34.835004 -7.826090 7.101593  
H -44.345312 -14.642714 7.170225  
H -37.915716 -11.387957 11.159487  
H -39.616861 -13.092472 2.518107  
H -36.216044 -6.431881 3.770581  
H -42.119330 -7.874229 5.921403  
C -39.741286 -6.932893 7.639510  
H -40.177700 -5.953633 7.851496  
H -38.658607 -6.863800 7.785815  
H -39.911842 -7.180132 6.588492  
H -41.378252 -6.858353 10.186809

***trans*-(4-Melm)<sub>2</sub>(5-Melm)<sub>2</sub>, ferrous, *in vacuo*,  
TPSSH,  $G^\circ = -2763.730951$**

C -44.229375 -13.753174 7.257477  
C -42.826507 -13.264970 7.093858  
N -41.716896 -14.084566 7.233870  
C -40.598978 -13.342543 7.002576  
N -40.923154 -12.088153 6.725502  
C -42.305824 -12.030925 6.782784  
C -40.882367 -8.738794 10.205438  
N -40.188442 -9.878529 10.561938  
C -39.712354 -10.446321 9.426680  
N -40.055320 -9.730319 8.362067  
C -40.797648 -8.650345 8.835266  
C -35.538738 -6.714539 4.364344  
C -36.498859 -7.435513 5.254043  
N -36.768518 -7.039932 6.556542  
C -37.691862 -7.885435 7.085845  
N -38.034444 -8.811718 6.201422  
C -37.295991 -8.538715 5.060820

C -40.807323 -7.760480 4.255378  
S -41.117471 -9.530062 4.646596  
C -39.401110 -12.697080 3.621326  
C -38.195941 -12.574728 4.498674  
N -38.141331 -11.719808 5.599605  
C -36.926255 -11.849536 6.122731  
N -36.197103 -12.748850 5.420634  
C -36.983875 -13.215423 4.384049  
Fe -39.676942 -10.293364 6.265870  
H -44.469918 -14.540183 6.533935  
H -44.923588 -12.926474 7.095170  
H -42.829414 -11.112018 6.565222  
H -39.599537 -13.749855 7.027585  
H -39.147886 -11.366273 9.417756  
H -35.848757 -5.677545 4.193802  
H -34.527118 -6.701447 4.785290  
H -37.401503 -9.144324 4.173074  
H -38.079693 -7.795400 8.089062  
H -39.755518 -7.497754 4.390336  
H -41.425614 -7.113546 4.883265  
H -39.773472 -11.708645 3.335156  
H -40.218726 -13.209397 4.138372  
H -36.619593 -13.936170 3.668999  
H -35.240362 -13.015244 5.610118  
H -36.542031 -11.304057 6.971179  
H -40.068778 -10.235155 11.500318  
H -41.734913 -15.071916 7.452834  
H -36.355049 -6.247439 7.030712  
H -44.406671 -14.150712 8.263248  
H -39.153485 -13.264938 2.721012  
H -35.493600 -7.213951 3.394637  
H -41.082032 -7.594055 3.211295  
H -41.371563 -8.113676 10.935761  
C -41.396757 -7.625849 7.925565  
H -40.622931 -7.073913 7.381346  
H -42.037359 -8.104078 7.177747  
H -41.990178 -6.910101 8.499572

***trans*-(4-Melm)<sub>2</sub>(5-Melm)<sub>2</sub>, ferric, *in vacuo*, PBE0,  
 $G^\circ = -2990.180275$**

C -37.521900 -12.567236 10.307496  
C -37.336265 -11.818504 9.002529  
O -36.199972 -11.534917 8.609217  
O -38.430176 -11.546237 8.365792  
C -43.789014 -14.288315 6.367809  
C -42.532337 -13.599806 6.762339  
N -41.628438 -14.130053 7.658930  
C -40.598012 -13.271243 7.800192  
N -40.783493 -12.204423 7.043373  
C -41.982622 -12.401484 6.391907  
C -41.005702 -7.716857 9.632728

N -41.275061 -8.949446 10.177016  
 C -40.749004 -9.885035 9.367985  
 N -40.158139 -9.320921 8.328434  
 C -40.304934 -7.951372 8.478461  
 C -35.537400 -6.687448 4.757454  
 C -36.251694 -7.665772 5.618498  
 N -35.862192 -7.964047 6.909249  
 C -36.703548 -8.884311 7.420357  
 N -37.627874 -9.196989 6.530242  
 C -37.355571 -8.444566 5.405337  
 C -42.111497 -8.967041 5.764251  
 S -40.536920 -9.575833 5.086992  
 C -39.751749 -12.593593 3.510816  
 C -38.434452 -12.577163 4.201907  
 N -38.165549 -11.888827 5.377150  
 C -36.896403 -12.128971 5.683827  
 N -36.342020 -12.932784 4.763946  
 C -37.293851 -13.229310 3.817303  
 Fe -39.273027 -10.601231 6.756239  
 H -36.626665 -12.481683 10.924543  
 H -37.679734 -13.630807 10.091750  
 H -43.589983 -15.257705 5.897854  
 H -44.334841 -13.675742 5.647619  
 H -42.363797 -11.681543 5.684100  
 H -39.741877 -13.431619 8.437083  
 H -40.800684 -10.946634 9.553590  
 H -35.532457 -5.684802 5.199003  
 H -34.497443 -6.984413 4.582420  
 H -37.980301 -8.498040 4.526123  
 H -36.581287 -9.337546 8.391541  
 H -42.367113 -9.463247 6.702721  
 H -42.900478 -9.147395 5.029528  
 H -40.059334 -11.590504 3.203533  
 H -40.536358 -12.987941 4.163290  
 H -37.091125 -13.862034 2.967015  
 H -35.390274 -13.265343 4.781496  
 H -36.385262 -11.766689 6.571573  
 H -41.778500 -9.125359 11.032847  
 H -41.713041 -15.021504 8.124638  
 H -35.059904 -7.583775 7.389028  
 H -44.446726 -14.458048 7.227313  
 H -38.395594 -12.203122 10.854673  
 H -39.693176 -13.228105 2.623010  
 H -36.032437 -6.621050 3.786694  
 H -42.053000 -7.890021 5.941579  
 H -41.320288 -6.796262 10.099872  
 C -39.740482 -6.942427 7.540605  
 H -38.665222 -6.811595 7.700956  
 H -39.874812 -7.248515 6.500185  
 H -40.223723 -5.974318 7.693659

***trans*-(4-Melm)<sub>2</sub>(5-Melm)<sub>2</sub>, ferrous, *in vacuo*,  
PBE0,  $G^\circ = -2761.979933$**

C -44.198238 -13.759359 7.273071  
 C -42.803933 -13.273457 7.102093  
 N -41.700186 -14.091446 7.209173  
 C -40.590886 -13.349951 6.978252  
 N -40.915723 -12.096921 6.733027  
 C -42.288958 -12.036935 6.809540  
 C -40.882711 -8.746965 10.198020  
 N -40.210377 -9.890724 10.553230  
 C -39.729992 -10.453974 9.426879  
 N -40.048918 -9.731266 8.368565  
 C -40.780263 -8.651945 8.833338  
 C -35.541238 -6.729311 4.399082  
 C -36.503248 -7.441993 5.279989  
 N -36.793842 -7.035805 6.565080  
 C -37.713881 -7.877931 7.087536  
 N -38.034159 -8.812058 6.214205  
 C -37.286144 -8.550455 5.087336  
 C -40.768669 -7.777602 4.248170  
 S -41.153661 -9.512879 4.658984  
 C -39.398621 -12.692988 3.643114  
 C -38.194505 -12.566551 4.508737  
 N -38.134303 -11.717600 5.602320  
 C -36.921703 -11.840955 6.114073  
 N -36.197710 -12.733242 5.411969  
 C -36.984397 -13.201423 4.386568  
 Fe -39.682724 -10.292504 6.260537  
 H -44.452620 -14.529674 6.536709  
 H -44.894556 -12.929584 7.137382  
 H -42.817948 -11.114367 6.616271  
 H -39.589882 -13.757503 6.979515  
 H -39.176874 -11.382193 9.417666  
 H -35.856184 -5.697743 4.207081  
 H -34.535314 -6.700670 4.832170  
 H -37.369772 -9.166271 4.202987  
 H -38.117922 -7.780933 8.085076  
 H -39.691721 -7.599762 4.192418  
 H -41.203872 -7.089888 4.978908  
 H -39.789530 -11.706902 3.372152  
 H -40.207427 -13.221802 4.157485  
 H -36.626132 -13.920719 3.666057  
 H -35.240812 -12.993578 5.594843  
 H -36.534317 -11.291035 6.959727  
 H -40.107673 -10.254939 11.487863  
 H -41.716693 -15.080565 7.406989  
 H -36.394285 -6.236955 7.034771  
 H -44.366046 -14.177153 8.271965  
 H -39.154246 -13.244905 2.732381  
 H -35.475587 -7.239803 3.436293  
 H -41.206528 -7.554841 3.272239



H -41.376305 -8.117633 10.922698  
C -41.354502 -7.619974 7.928049  
H -40.570012 -7.045573 7.423489  
H -41.959778 -8.089197 7.145183  
H -41.978204 -6.921933 8.491237

**(4-Melm)<sub>3</sub>(5-Melm)<sub>1</sub>, ferric, in vacuo, BP86,  
G° = -2992.299053**

C -37.783602 -12.125253 10.520918  
C -37.405962 -11.724065 9.097842  
O -36.205231 -11.695215 8.737438  
O -38.410701 -11.413306 8.314491  
C -42.326373 -13.929314 6.847845  
N -41.130839 -14.474015 7.294628  
C -40.203247 -13.479588 7.335026  
N -40.736788 -12.319319 6.933509  
C -42.076076 -12.586621 6.619362  
C -41.217156 -7.836283 9.647866  
N -41.668397 -9.106923 9.973344  
C -41.131546 -9.986581 9.084864  
N -40.360098 -9.344512 8.200103  
C -40.396904 -7.987817 8.542503  
C -35.473912 -6.530146 4.784714  
C -36.169860 -7.583344 5.588363  
N -35.656404 -8.102955 6.776779  
C -36.516635 -9.042584 7.262805  
N -37.573656 -9.158074 6.447999  
C -37.362994 -8.256800 5.406274  
C -41.742370 -8.388859 5.261250  
S -40.400616 -9.577094 4.859653  
C -39.684513 -12.573841 3.386873  
C -38.396062 -12.636225 4.148510  
N -38.144062 -11.941463 5.340058  
C -36.896556 -12.258689 5.722784  
N -36.341213 -13.118959 4.829366  
C -37.268688 -13.371429 3.827963  
Fe -39.266033 -10.554333 6.669624  
H -36.920364 -12.566008 11.039590  
H -38.629235 -12.833011 10.520130  
H -39.173775 -13.615676 7.654227  
H -41.301241 -11.059891 9.107201  
H -35.340702 -5.594687 5.357143  
H -34.476591 -6.863405 4.446015  
H -38.084304 -8.160540 4.597116  
H -36.311869 -9.662866 8.134820  
H -41.980590 -8.391138 6.335119  
H -42.639963 -8.659836 4.682826  
H -39.857328 -11.573056 2.956927  
H -40.545156 -12.799191 4.038474  
H -37.056992 -14.032402 2.990873  
H -35.405952 -13.515896 4.899463

H -36.410579 -11.931069 6.648069  
H -42.293297 -9.343398 10.742071  
H -40.971473 -15.447536 7.548312  
H -34.770545 -7.843033 7.209117  
H -38.111795 -11.228017 11.075255  
H -39.669341 -13.306521 2.564421  
H -36.068033 -6.292672 3.889342  
H -41.433079 -7.376282 4.954973  
H -43.229721 -14.523994 6.733655  
C -43.040172 -11.555706 6.120507  
H -43.089919 -10.685814 6.797265  
H -42.738831 -11.181181 5.127424  
H -44.050332 -11.987166 6.039674  
H -41.503980 -6.954715 10.216205  
C -39.623233 -6.923401 7.827081  
H -38.542981 -7.007768 8.034972  
H -39.749335 -6.995647 6.735713  
H -39.958261 -5.926280 8.153119

**(4-Melm)<sub>3</sub>(5-Melm)<sub>1</sub>, ferrous, in vacuo, BP86,  
G° = -2763.844101**

C -42.681919 -13.496685 7.289249  
N -41.505530 -14.222957 7.181059  
C -40.507018 -13.354096 6.848456  
N -40.979436 -12.106423 6.740796  
C -42.350223 -12.178888 7.020313  
C -40.978134 -8.495533 10.075093  
N -40.459861 -9.719216 10.471878  
C -40.043788 -10.381980 9.353026  
N -40.259538 -9.641742 8.258583  
C -40.851305 -8.450074 8.696206  
C -35.446124 -6.756711 4.543835  
C -36.446732 -7.480948 5.389258  
N -36.681141 -7.171568 6.728081  
C -37.661236 -7.998737 7.204862  
N -38.073435 -8.833407 6.247250  
C -37.322512 -8.518748 5.118627  
C -40.729821 -7.709559 4.128598  
S -41.007109 -9.501285 4.476871  
C -39.475793 -12.611742 3.451540  
C -38.287776 -12.508998 4.356734  
N -38.254928 -11.688021 5.493115  
C -37.041078 -11.838845 6.038293  
N -36.294130 -12.718305 5.312146  
C -37.064475 -13.149878 4.241451  
Fe -39.769507 -10.267120 6.228152  
H -39.477771 -13.660549 6.676850  
H -39.621572 -11.384452 9.371683  
H -35.687239 -5.682763 4.449763  
H -34.422867 -6.838700 4.952019  
H -37.472998 -9.051139 4.181035

H -38.040302 -7.960784 8.224316  
H -39.717569 -7.391465 4.424657  
H -41.475001 -7.090732 4.653811  
H -39.785546 -11.614633 3.094382  
H -40.346689 -13.040252 3.976819  
H -36.685949 -13.851734 3.501970  
H -35.334513 -12.995224 5.511200  
H -36.671536 -11.323287 6.922185  
H -40.416197 -10.071003 11.426592  
H -41.407386 -15.228989 7.304057  
H -36.208939 -6.441409 7.260061  
H -39.242935 -13.251611 2.585928  
H -35.437338 -7.185386 3.530285  
H -40.849728 -7.551226 3.045229  
C -43.259884 -10.989120 7.000454  
H -44.305861 -11.306185 7.137147  
H -43.007586 -10.279480 7.807620  
H -43.171096 -10.444329 6.045197  
H -43.632307 -13.965575 7.533581  
H -41.395180 -7.785296 10.785354  
C -41.289003 -7.373711 7.751511  
H -42.002906 -7.773447 7.011005  
H -41.773555 -6.550925 8.300020  
H -40.437452 -6.959115 7.184818

**(4-Melm)<sub>3</sub>(5-Melm)<sub>1</sub>, ferric, in vacuo, TPSSh,  
*G*<sup>o</sup> = -2992.183372**

C -37.121333 -12.084024 10.062481  
C -37.195661 -11.443268 8.681705  
O -36.181902 -10.942143 8.166463  
O -38.380485 -11.465436 8.129827  
C -42.535187 -13.720850 7.355172  
N -41.310476 -14.363094 7.387670  
C -40.347898 -13.440497 7.174837  
N -40.888089 -12.237363 7.000291  
C -42.269967 -12.394702 7.112055  
C -41.549175 -8.225694 9.837240  
N -41.221139 -9.433525 10.425155  
C -40.532609 -10.166322 9.521924  
N -40.404195 -9.496805 8.379274  
C -41.042895 -8.269672 8.560043  
C -35.076805 -7.152566 5.057482  
C -36.197190 -7.811426 5.793921  
N -36.434688 -7.613303 7.146670  
C -37.506080 -8.349658 7.516216  
N -37.996189 -9.005409 6.472381  
C -37.183817 -8.679203 5.396943  
C -40.245444 -8.307665 4.048549  
S -40.926213 -9.696712 5.023298  
C -40.014167 -12.701468 3.509364  
C -38.639855 -12.563568 4.083020

N -38.335264 -11.835185 5.236171  
C -37.022176 -11.957659 5.436907  
N -36.473398 -12.723191 4.468901  
C -37.478440 -13.120882 3.605704  
Fe -39.484116 -10.564139 6.637443  
H -36.084044 -12.289868 10.329391  
H -37.712067 -13.003865 10.099940  
H -39.290657 -13.651442 7.168308  
H -40.132896 -11.151288 9.703464  
H -35.159801 -6.060509 5.088964  
H -34.103337 -7.432115 5.475295  
H -37.357982 -9.091098 4.415433  
H -37.884310 -8.400012 8.524196  
H -41.082489 -7.762071 3.608291  
H -39.617513 -8.695140 3.241560  
H -40.404044 -11.738606 3.167477  
H -40.719489 -13.084237 4.252832  
H -37.288042 -13.751074 2.751247  
H -35.494711 -12.968439 4.403103  
H -36.474590 -11.514412 6.264504  
H -41.449143 -9.719908 11.367752  
H -41.157223 -15.349550 7.548379  
H -35.864888 -7.058788 7.772104  
H -37.537921 -11.391947 10.804464  
H -39.992383 -13.393131 2.663266  
H -35.094897 -7.460146 4.010087  
H -39.655773 -7.636351 4.675051  
H -43.464277 -14.248221 7.503026  
C -43.253271 -11.274839 6.984091  
H -44.248579 -11.623268 7.270921  
H -42.978404 -10.434425 7.627697  
H -43.298386 -10.899640 5.957706  
H -42.097594 -7.460478 10.363707  
C -41.130991 -7.214671 7.504910  
H -40.141365 -6.972098 7.105941  
H -41.750644 -7.551461 6.668119  
H -41.568856 -6.304645 7.922528

**(4-Melm)<sub>3</sub>(5-Melm)<sub>1</sub>, ferrous, in vacuo, TPSSh,  
*G*<sup>o</sup> = -2763.727504**

C -42.700934 -13.470406 7.268942  
N -41.538482 -14.205128 7.135539  
C -40.539120 -13.345466 6.821682  
N -40.992700 -12.098288 6.750843  
C -42.356549 -12.159968 7.034011  
C -40.955331 -8.501084 10.067052  
N -40.433583 -9.714695 10.472420  
C -40.012187 -10.376044 9.366850  
N -40.225662 -9.650343 8.275220  
C -40.824136 -8.465341 8.698178  
C -35.471639 -6.811745 4.491967

C	-36.469209	-7.514751	5.354501	N	-41.304380	-14.344683	7.356805
N	-36.680487	-7.191435	6.687239	C	-40.342787	-13.429943	7.152170
C	-37.660065	-7.995718	7.179893	N	-40.873397	-12.227647	6.995603
N	-38.093741	-8.827278	6.242851	C	-42.247005	-12.375475	7.112720
C	-37.356206	-8.535364	5.106194	C	-41.548356	-8.231047	9.802724
C	-40.743598	-7.716319	4.124832	N	-41.224815	-9.430927	10.390907
S	-41.033544	-9.505583	4.435513	C	-40.529104	-10.158658	9.500376
C	-39.434842	-12.632238	3.480613	N	-40.391839	-9.493541	8.363841
C	-38.253647	-12.517402	4.390453	C	-41.030258	-8.274584	8.534516
N	-38.234326	-11.689705	5.514156	C	-35.053450	-7.186975	5.107583
C	-37.029302	-11.820751	6.059789	C	-36.185908	-7.828144	5.824814
N	-36.274194	-12.694432	5.352176	N	-36.446588	-7.619384	7.162608
C	-37.032672	-13.143238	4.287293	C	-37.524560	-8.341649	7.514567
Fe	-39.785484	-10.273973	6.206455	N	-37.996437	-8.999095	6.472286
H	-39.522314	-13.657293	6.640551	C	-37.166832	-8.689670	5.415236
H	-39.583253	-11.366046	9.394870	C	-40.200913	-8.355707	4.049430
H	-35.701510	-5.744573	4.397782	S	-40.921961	-9.703297	5.026812
H	-34.454505	-6.905821	4.888637	C	-40.019163	-12.701389	3.537081
H	-37.528750	-9.068757	4.183165	C	-38.647255	-12.558712	4.095814
H	-38.020991	-7.942507	8.195796	N	-38.329765	-11.824417	5.231531
H	-39.756459	-7.402146	4.471842	C	-37.021770	-11.949978	5.420132
H	-41.510223	-7.114783	4.619506	N	-36.487713	-12.722476	4.460064
H	-39.743123	-11.646363	3.119584	C	-37.495716	-13.122941	3.614495
H	-40.296919	-13.064101	3.999239	Fe	-39.476754	-10.556795	6.625407
H	-36.645264	-13.841978	3.562578	H	-36.075280	-12.205670	10.320427
H	-35.319455	-12.956332	5.557331	H	-37.678037	-12.974132	10.094081
H	-36.671179	-11.296871	6.932793	H	-39.285561	-13.646749	7.137771
H	-40.390238	-10.057903	11.422553	H	-40.126900	-11.143417	9.685449
H	-41.451716	-15.207880	7.230050	H	-35.126006	-6.094123	5.128669
H	-36.194734	-6.470049	7.204437	H	-34.088927	-7.471397	5.542080
H	-39.189974	-13.269934	2.627599	H	-37.321690	-9.105603	4.431278
H	-35.484171	-7.246325	3.490591	H	-37.923773	-8.382142	8.516295
H	-40.810676	-7.546137	3.047924	H	-41.015077	-7.815641	3.561148
C	-43.244759	-10.957046	7.048799	H	-39.543387	-8.758636	3.273800
H	-42.997732	-10.295544	7.886078	H	-40.417846	-11.741350	3.198060
H	-43.128996	-10.383674	6.124018	H	-40.719256	-13.084424	4.285560
H	-44.288800	-11.263241	7.152620	H	-37.320394	-13.761677	2.762414
H	-43.647133	-13.931970	7.503906	H	-35.512904	-12.970888	4.389434
C	-41.266269	-7.405915	7.740129	H	-36.465837	-11.503240	6.241887
H	-41.988376	-7.813644	7.025682	H	-41.460412	-9.717468	11.328753
H	-41.732176	-6.576918	8.278208	H	-41.155376	-15.331224	7.503753
H	-40.423918	-7.015272	7.160545	H	-35.886859	-7.064918	7.792990
H	-41.375249	-7.795464	10.766597	H	-37.559887	-11.349141	10.773585

**(4-Melm)<sub>3</sub>(5-Melm)<sub>1</sub>, ferric, in vacuo, PBE0,  
G° = -2990.176266**

C	-37.116594	-12.037006	10.043722	H	-40.004638	-13.394206	2.692069
C	-37.206364	-11.423265	8.659909	H	-35.053507	-7.499458	4.061488
O	-36.205413	-10.923656	8.135994	H	-39.632360	-7.664485	4.674595
O	-38.385154	-11.467948	8.121791	H	-43.453297	-14.218372	7.485481
C	-42.518637	-13.699144	7.339317	C	-43.220897	-11.254677	7.010929
				H	-42.949635	-10.431882	7.678878
				H	-43.259531	-10.848483	5.996221
				H	-44.219888	-11.604975	7.281315
				H	-42.104139	-7.463318	10.318999

C -41.109091 -7.223173 7.485549  
H -40.116223 -6.971295 7.100515  
H -41.711810 -7.562289 6.637502  
H -41.559341 -6.316070 7.895722

**(4-Melm)<sub>3</sub>(5-Melm)<sub>1</sub>, ferrous, *in vacuo*, PBE0,  
G° = -2761.976998**

C -42.688826 -13.464456 7.259235  
N -41.538942 -14.198675 7.096983  
C -40.544460 -13.344292 6.786477  
N -40.988862 -12.099929 6.745058  
C -42.340410 -12.155924 7.043318  
C -41.009884 -8.513148 10.037190  
N -40.492181 -9.716561 10.451900  
C -40.040102 -10.369700 9.363174  
N -40.230079 -9.648698 8.273064  
C -40.844937 -8.475836 8.675833  
C -35.448694 -6.827278 4.577225  
C -36.457084 -7.524205 5.418004  
N -36.712129 -7.183910 6.729420  
C -37.691289 -7.988403 7.202484  
N -38.083201 -8.836347 6.272205  
C -37.320278 -8.557126 5.159307  
C -40.680730 -7.723047 4.112532  
S -41.062759 -9.476892 4.441371  
C -39.430755 -12.619023 3.481867  
C -38.250363 -12.505989 4.380832  
N -38.225348 -11.690784 5.502036  
C -37.024203 -11.821648 6.038370  
N -36.274945 -12.685640 5.326941  
C -37.032443 -13.127922 4.268811  
Fe -39.786975 -10.274829 6.195647  
H -39.530534 -13.657716 6.585622  
H -39.604466 -11.357829 9.400295  
H -35.688146 -5.765272 4.454775  
H -34.441857 -6.899726 5.003021  
H -37.454135 -9.105542 4.237452  
H -38.085595 -7.924240 8.206591  
H -39.647663 -7.472342 4.366276  
H -41.353018 -7.065711 4.670590  
H -39.778838 -11.628987 3.170287  
H -40.273817 -13.104163 3.984890  
H -36.651146 -13.821636 3.535116  
H -35.320805 -12.944398 5.525725  
H -36.663061 -11.298909 6.912271  
H -40.470584 -10.060406 11.399765  
H -41.456390 -15.200787 7.171224  
H -36.252584 -6.450018 7.247754  
H -39.177486 -13.207115 2.596605  
H -35.423832 -7.277604 3.583018  
H -40.830732 -7.534337 3.046858

C -43.217470 -10.954794 7.091012  
H -44.263015 -11.254418 7.196072  
H -42.961768 -10.310681 7.939120  
H -43.107432 -10.361025 6.177967  
H -43.637449 -13.920347 7.498297  
H -41.454620 -7.807972 10.722709  
C -41.270495 -7.424055 7.713392  
H -40.416840 -7.006129 7.170215  
H -41.950076 -7.843050 6.964052  
H -41.779245 -6.610292 8.235284

**(4-Melm)<sub>4</sub>(5-Melm)<sub>0</sub>, ferric, *in vacuo*, BP86,  
G° = -2992.293425**

C -37.422654 -12.183004 10.296617  
C -37.292714 -11.709656 8.848742  
O -36.167748 -11.598694 8.313659  
O -38.435121 -11.438698 8.254201  
C -42.355675 -13.940842 6.955451  
N -41.128471 -14.478419 7.317103  
C -40.210174 -13.474940 7.312315  
N -40.780072 -12.315147 6.961143  
C -42.133518 -12.593018 6.729630  
C -41.289780 -7.797617 9.599643  
N -41.551875 -9.079513 10.061466  
C -40.965958 -9.965167 9.210937  
N -40.342281 -9.315476 8.220626  
C -40.529835 -7.947064 8.450824  
C -35.941271 -7.728707 6.060813  
N -36.032526 -7.892859 7.436190  
C -37.062429 -8.739748 7.691451  
N -37.651077 -9.121424 6.551882  
C -36.955332 -8.491701 5.509159  
C -41.991565 -8.435882 5.326421  
S -40.576263 -9.527036 4.902661  
C -39.974341 -12.580808 3.422225  
C -38.609730 -12.541387 4.039095  
N -38.283020 -11.828865 5.203414  
C -36.980609 -12.051349 5.450675  
N -36.463213 -12.867955 4.496946  
C -37.470741 -13.189684 3.596693  
Fe -39.352220 -10.539367 6.632392  
H -36.441788 -12.476159 10.696921  
H -38.122940 -13.032923 10.365354  
H -39.162203 -13.602027 7.568031  
H -40.993563 -11.045113 9.330982  
H -37.350032 -9.057791 8.688607  
H -42.197079 -8.432287 6.407181  
H -42.883543 -8.784497 4.782122  
H -40.283424 -11.589121 3.051801  
H -40.733943 -12.904325 4.153575  
H -37.300604 -13.834415 2.737722

H -35.499279 -13.195660 4.466406  
H -36.436116 -11.692556 6.333404  
H -42.091702 -9.318895 10.891514  
H -40.943567 -15.452932 7.548617  
H -35.403923 -7.496928 8.132651  
H -37.842059 -11.372581 10.918972  
H -39.982762 -13.287383 2.577232  
H -41.766278 -7.410598 4.991783  
H -43.258928 -14.543183 6.892288  
C -43.136688 -11.566834 6.305214  
H -43.146780 -10.702818 6.990828  
H -42.907179 -11.184824 5.296059  
H -44.146785 -12.005614 6.289596  
H -41.650988 -6.910656 10.114898  
C -39.934175 -6.868682 7.594313  
H -38.925960 -6.587295 7.946560  
H -39.830787 -7.205746 6.552317  
H -40.560298 -5.962533 7.617943  
H -35.183417 -7.099857 5.599885  
C -37.284316 -8.648647 4.056737  
H -37.219189 -9.702690 3.738421  
H -38.311497 -8.311645 3.837650  
H -36.581728 -8.059377 3.446681

**(4-Melm)<sub>4</sub>(5-Melm)<sub>0</sub>, ferrous, in vacuo, BP86,  
*G*<sup>o</sup> = -2763.840100**

C -42.713987 -13.471514 7.344050  
N -41.546509 -14.212021 7.240020  
C -40.543711 -13.360740 6.875093  
N -41.004477 -12.111408 6.741236  
C -42.372358 -12.163946 7.038903  
C -40.953213 -8.526618 10.042478  
N -40.425926 -9.750377 10.426282  
C -40.005329 -10.398680 9.301139  
N -40.226317 -9.648528 8.213879  
C -40.827637 -8.465639 8.664179  
C -36.425124 -7.389497 5.457582  
N -36.708471 -7.166237 6.797392  
C -37.680933 -8.044657 7.172738  
N -38.036233 -8.825734 6.145090  
C -37.250454 -8.426706 5.055092  
C -40.810502 -7.722705 4.132006  
S -41.052581 -9.522439 4.474424  
C -39.525233 -12.696787 3.494863  
C -38.329425 -12.588521 4.389070  
N -38.279107 -11.743003 5.506247  
C -37.062999 -11.892210 6.046502  
N -36.329986 -12.793761 5.333871  
C -37.112958 -13.243132 4.279403  
Fe -39.754956 -10.272916 6.185484  
H -39.519666 -13.682882 6.701116

H -39.578050 -11.399048 9.309373  
H -38.105065 -8.081701 8.173864  
H -39.826174 -7.370699 4.479992  
H -41.600073 -7.128114 4.618700  
H -39.841002 -11.701669 3.137600  
H -40.390115 -13.127118 4.028322  
H -36.746406 -13.964987 3.553279  
H -35.371745 -13.076218 5.532707  
H -36.681274 -11.358915 6.914555  
H -40.380030 -10.112113 11.377198  
H -41.456865 -15.215862 7.385432  
H -36.280645 -6.457228 7.390600  
H -39.298113 -13.337176 2.628217  
H -40.881547 -7.565787 3.044079  
C -43.273369 -10.967789 7.005259  
H -44.320053 -11.274816 7.158632  
H -43.008667 -10.244980 7.796726  
H -43.190147 -10.441356 6.039450  
H -43.666085 -13.924323 7.611115  
H -41.374977 -7.826601 10.760020  
C -41.272852 -7.381316 7.732503  
H -41.985527 -7.777003 6.988802  
H -41.761548 -6.568065 8.291365  
H -40.424984 -6.953851 7.169762  
H -35.685715 -6.802895 4.917051  
C -37.337744 -9.066617 3.702910  
H -36.830602 -10.047373 3.685077  
H -38.390348 -9.239834 3.422406  
H -36.862844 -8.426652 2.942623

**(4-Melm)<sub>4</sub>(5-Melm)<sub>0</sub>, ferric, in vacuo, TPSSh,  
*G*<sup>o</sup> = -2992.176255**

C -37.118742 -12.029293 10.062215  
C -37.167826 -11.434300 8.660155  
O -36.138417 -10.986116 8.130042  
O -38.352841 -11.436274 8.105071  
C -42.549343 -13.663846 7.367111  
N -41.336410 -14.325990 7.426604  
C -40.357889 -13.430265 7.175999  
N -40.875881 -12.225263 6.952548  
C -42.260708 -12.353306 7.071426  
C -41.570672 -8.295718 9.809930  
N -41.209434 -9.501932 10.380636  
C -40.501301 -10.202451 9.467296  
N -40.390011 -9.514716 8.333128  
C -41.063903 -8.309541 8.532554  
C -36.198264 -7.710732 5.808597  
N -36.484793 -7.563088 7.151348  
C -37.514271 -8.377653 7.453447  
N -37.919184 -9.036534 6.370644  
C -37.093074 -8.632880 5.321586

C -40.388401 -8.072425 4.227293  
 S -40.843150 -9.698278 4.933342  
 C -40.035381 -12.810101 3.535142  
 C -38.663253 -12.716443 4.122446  
 N -38.341307 -11.964356 5.254773  
 C -37.036000 -12.129328 5.473751  
 N -36.508586 -12.947490 4.536992  
 C -37.519934 -13.333931 3.676345  
 Fe -39.436237 -10.578279 6.575778  
 H -36.087717 -12.240970 10.347792  
 H -37.722147 -12.939920 10.122069  
 H -39.305075 -13.661973 7.175962  
 H -40.073915 -11.177723 9.636015  
 H -37.934473 -8.479477 8.440486  
 H -41.261341 -7.417504 4.277074  
 H -40.118125 -8.206981 3.177249  
 H -40.377729 -11.838208 3.168289  
 H -40.765065 -13.147695 4.277198  
 H -37.346235 -13.998864 2.844959  
 H -35.539527 -13.232582 4.489830  
 H -36.475496 -11.669629 6.283760  
 H -41.428345 -9.807882 11.319229  
 H -41.200767 -15.308175 7.625067  
 H -35.982080 -6.981675 7.808192  
 H -37.534912 -11.308270 10.776308  
 H -40.033499 -13.519442 2.703717  
 H -39.555543 -7.618997 4.766361  
 H -43.487914 -14.168263 7.534038  
 C -43.227468 -11.224821 6.901587  
 H -44.231326 -11.556136 7.178958  
 H -42.953348 -10.374032 7.531586  
 H -43.249374 -10.871233 5.867000  
 H -42.139544 -7.552654 10.346357  
 C -41.190559 -7.245772 7.491298  
 H -40.216819 -6.994315 7.061173  
 H -41.839946 -7.576623 6.675335  
 H -41.618922 -6.341470 7.930554  
 H -35.404426 -7.161173 5.328080  
 C -37.192970 -9.172413 3.926721  
 H -36.429119 -9.935691 3.743697  
 H -38.167991 -9.633388 3.761901  
 H -37.048521 -8.374157 3.193313

**(4-Melm)<sub>4</sub>(5-Melm)<sub>0</sub>, ferrous, *in vacuo*, TPSSh,  
G° = -2763.723796**

C -42.707149 -13.459897 7.345424  
 N -41.549686 -14.201852 7.213929  
 C -40.554212 -13.354259 6.856048  
 N -41.005052 -12.108368 6.753508  
 C -42.363839 -12.158159 7.063766  
 C -40.952459 -8.519481 10.028710

N -40.429851 -9.736317 10.422465  
 C -40.000823 -10.383702 9.311882  
 N -40.209545 -9.645570 8.227064  
 C -40.814271 -8.466960 8.661142  
 C -36.438139 -7.428729 5.433827  
 N -36.709842 -7.193275 6.768104  
 C -37.685290 -8.051115 7.151253  
 N -38.053619 -8.830019 6.138692  
 C -37.272635 -8.451122 5.046666  
 C -40.803971 -7.728426 4.120691  
 S -41.109027 -9.511307 4.460131  
 C -39.504669 -12.696408 3.517184  
 C -38.310821 -12.588152 4.411033  
 N -38.265291 -11.744052 5.521337  
 C -37.055801 -11.882347 6.055184  
 N -36.321629 -12.776017 5.351008  
 C -37.099673 -13.231790 4.302952  
 Fe -39.773566 -10.276505 6.164774  
 H -39.541780 -13.676045 6.668465  
 H -39.571541 -11.373683 9.330548  
 H -38.100648 -8.074200 8.146838  
 H -39.825800 -7.408476 4.488183  
 H -41.580687 -7.117133 4.586649  
 H -39.820849 -11.707470 3.171469  
 H -40.357929 -13.136706 4.042973  
 H -36.730449 -13.946830 3.584683  
 H -35.368463 -13.049219 5.549591  
 H -36.679368 -11.349263 6.914798  
 H -40.391551 -10.091060 11.368601  
 H -41.463500 -15.201516 7.337176  
 H -36.273716 -6.491154 7.350643  
 H -39.270336 -13.323060 2.653206  
 H -40.844935 -7.574657 3.039938  
 C -43.253981 -10.956360 7.063040  
 H -42.985453 -10.266658 7.870353  
 H -43.167261 -10.412186 6.118054  
 H -44.293470 -11.261752 7.207467  
 H -43.650307 -13.910463 7.611975  
 C -41.254269 -7.395998 7.715221  
 H -41.973370 -7.795985 6.993501  
 H -41.722649 -6.574641 8.262702  
 H -40.410729 -6.995643 7.143778  
 H -41.377969 -7.823070 10.734054  
 H -35.700876 -6.858743 4.890417  
 C -37.381595 -9.100522 3.702891  
 H -36.844590 -10.055050 3.676841  
 H -38.429407 -9.303014 3.461044  
 H -36.954914 -8.452285 2.933279

**(4-Melm)<sub>4</sub>(5-Melm)<sub>0</sub>, ferric, *in vacuo*, PBE0,  
G° = -2990.169644**

C -37.129929 -11.988364 10.056486  
 C -37.185389 -11.419905 8.651808  
 O -36.164845 -10.972163 8.121225  
 O -38.360412 -11.444793 8.101688  
 C -42.538615 -13.640534 7.346377  
 N -41.337776 -14.309652 7.384282  
 C -40.358912 -13.422953 7.143109  
 N -40.864824 -12.215901 6.944612  
 C -42.241204 -12.331398 7.072491  
 C -41.567689 -8.300667 9.776694  
 N -41.208343 -9.497093 10.350036  
 C -40.493068 -10.193295 9.450167  
 N -40.375218 -9.512229 8.320247  
 C -41.050797 -8.316085 8.507718  
 C -36.188766 -7.739307 5.809319  
 N -36.484293 -7.577567 7.140392  
 C -37.516546 -8.377273 7.439738  
 N -37.914848 -9.041551 6.366161  
 C -37.082728 -8.657801 5.325586  
 C -40.355152 -8.095991 4.245339  
 S -40.830085 -9.708424 4.932223  
 C -40.017756 -12.803582 3.551215  
 C -38.651945 -12.706585 4.133854  
 N -38.327813 -11.960543 5.259067  
 C -37.028949 -12.127450 5.474480  
 N -36.506719 -12.940556 4.541220  
 C -37.513488 -13.322854 3.686076  
 Fe -39.428241 -10.575370 6.567359  
 H -36.097141 -12.177132 10.351379  
 H -37.718038 -12.907493 10.131181  
 H -39.306971 -13.663695 7.130545  
 H -40.062085 -11.167486 9.624073  
 H -37.947160 -8.465790 8.424982  
 H -41.219311 -7.428342 4.285529  
 H -40.073625 -8.220351 3.196635  
 H -40.367085 -11.833058 3.187844  
 H -40.747304 -13.144995 4.291848  
 H -37.346984 -13.987267 2.852024  
 H -35.540481 -13.225893 4.494158  
 H -36.466507 -11.669373 6.285805  
 H -41.432967 -9.801641 11.284896  
 H -41.208338 -15.293583 7.563887  
 H -35.985401 -6.994643 7.794800  
 H -37.561129 -11.263789 10.757545  
 H -40.016956 -13.510639 2.718132  
 H -39.524344 -7.646217 4.791064  
 H -43.483376 -14.135116 7.511880  
 C -43.196473 -11.198241 6.938462  
 H -42.928436 -10.373241 7.604919  
 H -43.205622 -10.800704 5.919916  
 H -44.205415 -11.533394 7.190674  
 H -42.144721 -7.554959 10.301882

C -41.173534 -7.259333 7.469596  
 H -40.198395 -6.998035 7.048560  
 H -41.809597 -7.595764 6.645687  
 H -41.614425 -6.357422 7.900803  
 H -35.388362 -7.201493 5.324977  
 C -37.170210 -9.201878 3.939604  
 H -36.431836 -9.994047 3.776858  
 H -38.155549 -9.629498 3.749595  
 H -36.979821 -8.415601 3.204129

**(4-Melm)<sub>4</sub>(5-Melm)<sub>6</sub>, ferrous, *in vacuo*, PBE0,  
 $G^\circ = -2761.974111$**

C -42.717961 -13.445189 7.313888  
 N -41.577543 -14.195000 7.160466  
 C -40.578672 -13.358770 6.814469  
 N -41.010898 -12.111792 6.740313  
 C -42.359409 -12.146753 7.056057  
 C -40.988108 -8.537983 10.003773  
 N -40.479651 -9.750167 10.403607  
 C -40.028468 -10.391702 9.307924  
 N -40.209333 -9.654442 8.226623  
 C -40.818652 -8.483090 8.643696  
 C -36.431152 -7.449437 5.468175  
 N -36.713703 -7.212038 6.791604  
 C -37.690668 -8.061057 7.164690  
 N -38.049971 -8.836721 6.155795  
 C -37.263493 -8.466628 5.076464  
 C -40.762511 -7.732779 4.123988  
 S -41.109789 -9.497460 4.440365  
 C -39.463657 -12.693491 3.530508  
 C -38.281769 -12.581265 4.427501  
 N -38.248729 -11.753181 5.538709  
 C -37.046560 -11.881665 6.073265  
 N -36.303430 -12.756249 5.368848  
 C -37.066792 -13.209384 4.319279  
 Fe -39.775276 -10.282659 6.154343  
 H -39.570125 -13.689201 6.614186  
 H -39.601801 -11.384050 9.332663  
 H -38.116896 -8.081574 8.157102  
 H -39.777381 -7.432604 4.491041  
 H -41.520520 -7.101118 4.594713  
 H -39.807721 -11.703700 3.213354  
 H -40.308507 -13.172370 4.035994  
 H -36.690714 -13.913755 3.593073  
 H -35.350439 -13.018824 5.569185  
 H -36.679519 -11.349392 6.938935  
 H -40.464338 -10.107445 11.346659  
 H -41.503524 -15.195320 7.262441  
 H -36.282489 -6.512536 7.376251  
 H -39.213457 -13.285806 2.647279  
 H -40.799556 -7.557712 3.045998

C -43.228205 -10.938845 7.084675  
H -44.273455 -11.229576 7.215030  
H -42.955580 -10.273727 7.911081  
H -43.129603 -10.369529 6.155203  
H -43.668260 -13.883985 7.577178  
H -41.430594 -7.839214 10.697246  
C -41.235617 -7.415490 7.695221  
H -40.379818 -6.998578 7.154538  
H -41.922328 -7.818762 6.943911  
H -41.734386 -6.602943 8.228422  
H -35.687643 -6.885553 4.925666  
C -37.360768 -9.110574 3.737396  
H -36.862208 -10.085758 3.723975  
H -38.407580 -9.274021 3.462810  
H -36.889259 -8.481832 2.978196

**(4-Melm)<sub>0</sub>(5-Melm)<sub>4</sub>, ferric, IEFPCM, BP86,  
*G*<sup>o</sup> = -2992.385684**

C -37.406549 -12.261894 10.296400  
C -37.121616 -11.816644 8.862874  
O -35.945316 -11.863412 8.408940  
O -38.152519 -11.431052 8.169043  
C -43.482177 -14.570070 6.228576  
C -42.317999 -13.747916 6.683014  
N -41.555832 -14.059123 7.806061  
C -40.574851 -13.126844 7.948327  
N -40.660166 -12.214084 6.971490  
C -41.741034 -12.594320 6.180356  
C -40.945360 -6.404265 10.352151  
C -40.843995 -7.668948 9.559401  
N -41.731133 -8.731194 9.700340  
C -41.368074 -9.728059 8.846522  
N -40.281795 -9.367764 8.152863  
C -39.949648 -8.088424 8.589031  
C -36.106271 -5.802230 5.344802  
C -36.564338 -7.124703 5.873733  
N -35.753379 -7.968038 6.629200  
C -36.456332 -9.086356 6.959051  
N -37.695248 -9.014893 6.451188  
C -37.768174 -7.799587 5.772939  
C -42.043638 -8.844509 5.501668  
S -40.513181 -9.633253 4.857379  
C -37.487447 -13.679351 2.007959  
C -37.593446 -12.998086 3.335786  
N -36.608701 -13.081842 4.317130  
C -36.996642 -12.359037 5.403850  
N -38.194931 -11.803262 5.175014  
C -38.573024 -12.195260 3.893776  
Fe -39.241771 -10.565542 6.643527  
H -37.600108 -13.350076 10.301071  
H -38.293467 -11.756061 10.708214

H -43.181607 -15.607279 5.997900  
H -43.914618 -14.129233 5.317686  
H -42.021351 -12.021380 5.298622  
H -39.833354 -13.131893 8.742013  
H -40.857346 -6.595993 11.436038  
H -41.908611 -5.892851 10.179336  
H -39.094477 -7.553697 8.182465  
H -41.902016 -10.670208 8.757014  
H -35.813815 -5.117196 6.160168  
H -35.237290 -5.911985 4.672189  
H -38.675929 -7.500248 5.253013  
H -36.049085 -9.925688 7.526310  
H -41.791032 -8.044844 6.215622  
H -42.677993 -9.587843 6.010783  
H -39.518368 -11.876959 3.458742  
H -36.416776 -12.257750 6.325273  
H -42.526045 -8.764231 10.338704  
H -41.701140 -14.857964 8.423631  
H -34.784512 -7.786727 6.892054  
H -38.384481 -13.465003 1.407519  
H -36.605525 -13.331315 1.441651  
H -35.734776 -13.602183 4.240641  
H -40.136755 -5.717276 10.060230  
H -36.920128 -5.327600 4.776044  
H -37.403161 -14.774975 2.118146  
H -44.273993 -14.613813 6.997069  
H -36.532001 -12.076369 10.938685  
H -42.600212 -8.415357 4.654121

**(4-Melm)<sub>0</sub>(5-Melm)<sub>4</sub>, ferrous, IEFPCM, BP86,  
*G*<sup>o</sup> = -2763.924456**

C -43.414773 -14.415269 7.703513  
C -42.199388 -13.635527 7.310277  
N -40.928286 -14.194170 7.223652  
C -40.047346 -13.228301 6.831574  
N -40.680285 -12.061481 6.664666  
C -42.019622 -12.307445 6.959920  
C -41.564561 -6.316669 10.075436  
C -41.213538 -7.585785 9.364214  
N -41.332553 -8.844707 9.946673  
C -40.942580 -9.786906 9.040152  
N -40.574907 -9.207291 7.892296  
C -40.738674 -7.838892 8.087922  
C -35.139778 -6.763124 5.548844  
C -36.204312 -7.662212 6.094531  
N -36.284690 -8.021187 7.437054  
C -37.362960 -8.837091 7.611795  
N -37.990573 -9.031606 6.446709  
C -37.275585 -8.306431 5.498020  
C -42.704130 -8.669367 5.048873  
S -41.049852 -9.206928 4.405505



C -37.914795 -13.680952 1.799087  
 C -37.955983 -12.785004 2.997732  
 N -36.841440 -12.504126 3.780249  
 C -37.213601 -11.652226 4.783394  
 N -38.515522 -11.362118 4.693126  
 C -38.984097 -12.066293 3.587519  
 Fe -39.799365 -10.183226 6.086969  
 H -43.609132 -15.247211 7.003720  
 H -44.295622 -13.755466 7.701290  
 H -42.769358 -11.520722 6.900516  
 H -38.986202 -13.407975 6.676113  
 H -40.961287 -6.181899 10.990666  
 H -42.628662 -6.295456 10.370459  
 H -40.501991 -7.123104 7.302459  
 H -40.943141 -10.854894 9.245854  
 H -35.168243 -5.764801 6.020147  
 H -34.130722 -7.181399 5.711491  
 H -37.575796 -8.292368 4.452197  
 H -37.653858 -9.251800 8.574238  
 H -42.608438 -8.202237 6.042129  
 H -43.391205 -9.528395 5.124389  
 H -40.026875 -12.003585 3.281245  
 H -36.523224 -11.272716 5.533045  
 H -41.656699 -9.036141 10.894779  
 H -40.688349 -15.166672 7.415988  
 H -35.643742 -7.725803 8.173480  
 H -38.918492 -13.748622 1.352226  
 H -37.222994 -13.299644 1.027065  
 H -35.900471 -12.869053 3.633999  
 H -41.377373 -5.456812 9.414381  
 H -35.283907 -6.632641 4.465588  
 H -37.589528 -14.702877 2.063396  
 H -43.312926 -14.846012 8.715287  
 H -43.140778 -7.935764 4.351380

**(4-Melm)<sub>0</sub>(5-Melm)<sub>4</sub>, ferric, IEFPCM, TPSSh,  
G° = -2992.268237**

C -37.449936 -12.273693 10.254917  
 C -37.148078 -11.799935 8.840103  
 O -35.973686 -11.831519 8.406360  
 O -38.167123 -11.405506 8.146943  
 C -43.448247 -14.548716 6.210307  
 C -42.290171 -13.723691 6.667705  
 N -41.536435 -14.031105 7.789555  
 C -40.564867 -13.102375 7.934580  
 N -40.646042 -12.195800 6.964096  
 C -41.718064 -12.577580 6.170086  
 C -40.912917 -6.428057 10.348821  
 C -40.815827 -7.686857 9.550551  
 N -41.700080 -8.743425 9.690462  
 C -41.345205 -9.729753 8.835410

N -40.269679 -9.371218 8.141321  
 C -39.933730 -8.099198 8.580433  
 C -36.123270 -5.816222 5.343841  
 C -36.583439 -7.135101 5.873429  
 N -35.781815 -7.966516 6.640391  
 C -36.480463 -9.077574 6.966902  
 N -37.705524 -9.015413 6.448568  
 C -37.775182 -7.809320 5.763490  
 C -42.040375 -8.864070 5.526409  
 S -40.513477 -9.629672 4.861830  
 C -37.508489 -13.700679 2.057936  
 C -37.609590 -12.997626 3.372114  
 N -36.617033 -13.051783 4.338683  
 C -36.999676 -12.319419 5.409527  
 N -38.198770 -11.785511 5.187239  
 C -38.586025 -12.203010 3.922313  
 Fe -39.240346 -10.555174 6.635848  
 H -37.659696 -13.349723 10.229518  
 H -38.325081 -11.764885 10.665196  
 H -43.141196 -15.575279 5.983288  
 H -43.874152 -14.110362 5.305711  
 H -41.992039 -12.008578 5.295006  
 H -39.835620 -13.106882 8.727014  
 H -40.821178 -6.628391 11.421677  
 H -41.870132 -5.922979 10.180948  
 H -39.086862 -7.569150 8.174579  
 H -41.877502 -10.662548 8.746018  
 H -35.844768 -5.135560 6.155636  
 H -35.253600 -5.930894 4.687809  
 H -38.672081 -7.520476 5.237922  
 H -36.079860 -9.902610 7.541313  
 H -41.790391 -8.057636 6.219140  
 H -42.646481 -9.609322 6.047196  
 H -39.532762 -11.905368 3.498624  
 H -36.416614 -12.200206 6.315032  
 H -42.486154 -8.779586 10.327914  
 H -41.680781 -14.823389 8.403662  
 H -34.823937 -7.782274 6.912764  
 H -38.409230 -13.510506 1.471057  
 H -36.644026 -13.350290 1.483603  
 H -35.743723 -13.558717 4.263042  
 H -40.110420 -5.747767 10.057274  
 H -36.927245 -5.352602 4.768873  
 H -37.407361 -14.783228 2.191047  
 H -44.232862 -14.592849 6.973286  
 H -36.583731 -12.117223 10.900937  
 H -42.611521 -8.459164 4.688097

**(4-Melm)<sub>0</sub>(5-Melm)<sub>4</sub>, ferrous, IEFPCM, TPSSh,  
G° = -2763.810660**

C -43.413110 -14.420824 7.707575

C -42.201315 -13.642745 7.309311  
 N -40.944869 -14.210495 7.176395  
 C -40.068415 -13.248887 6.796868  
 N -40.685237 -12.078512 6.680275  
 C -42.014887 -12.316303 6.997574  
 C -41.539991 -6.305525 10.057645  
 C -41.201152 -7.578613 9.352759  
 N -41.321751 -8.826719 9.943020  
 C -40.944406 -9.770801 9.046295  
 N -40.584335 -9.206585 7.899217  
 C -40.739466 -7.841411 8.084341  
 C -35.134522 -6.807233 5.536912  
 C -36.210269 -7.682117 6.093330  
 N -36.313892 -7.992065 7.440197  
 C -37.390286 -8.793405 7.622895  
 N -37.994868 -9.026889 6.463492  
 C -37.265452 -8.339381 5.505630  
 C -42.718882 -8.695953 5.069635  
 S -41.092979 -9.239841 4.387343  
 C -37.898493 -13.633078 1.792251  
 C -37.947528 -12.754922 3.000562  
 N -36.843323 -12.492656 3.793530  
 C -37.218355 -11.659657 4.798622  
 N -38.508491 -11.363664 4.703065  
 C -38.969863 -12.044604 3.587411  
 Fe -39.795635 -10.190356 6.102606  
 H -43.625813 -15.222696 6.992304  
 H -44.278407 -13.756034 7.743526  
 H -42.748724 -11.524734 6.978245  
 H -39.021833 -13.434757 6.614149  
 H -40.930662 -6.172668 10.958252  
 H -42.593142 -6.283069 10.358323  
 H -40.507124 -7.139923 7.296873  
 H -40.947340 -10.828255 9.259855  
 H -35.169954 -5.803265 5.973497  
 H -34.140333 -7.223865 5.731571  
 H -37.546641 -8.362520 4.463808  
 H -37.696511 -9.170001 8.586307  
 H -42.592201 -8.194534 6.032088  
 H -43.386626 -9.551911 5.202374  
 H -40.001672 -11.971101 3.278032  
 H -36.538009 -11.298392 5.553825  
 H -41.637640 -9.009621 10.887621  
 H -40.712592 -15.183950 7.331061  
 H -35.690048 -7.675810 8.172471  
 H -38.890642 -13.686000 1.339216  
 H -37.200143 -13.245082 1.042589  
 H -35.908940 -12.855884 3.651914  
 H -41.356218 -5.459445 9.392418  
 H -35.261373 -6.715115 4.456449  
 H -37.584268 -14.650808 2.048603  
 H -43.288672 -14.876176 8.696027

H -43.184906 -7.999546 4.367079

**(4-Melm)<sub>0</sub>(5-Melm)<sub>4</sub>, ferric, IEFPCM, PBE0,  
G° = -2990.260656**

C -37.425697 -12.435218 10.168965  
 C -37.148597 -11.832169 8.807428  
 O -35.983562 -11.801745 8.371088  
 O -38.175761 -11.401188 8.168455  
 C -43.443370 -14.496087 6.242418  
 C -42.281688 -13.685169 6.690036  
 N -41.537990 -13.985237 7.809830  
 C -40.560286 -13.071620 7.943641  
 N -40.628766 -12.181400 6.966539  
 C -41.697821 -12.556136 6.178704  
 C -40.939867 -6.401439 10.258900  
 C -40.823032 -7.670297 9.494771  
 N -41.684588 -8.731323 9.656062  
 C -41.313105 -9.725745 8.829089  
 N -40.247518 -9.367624 8.132960  
 C -39.933663 -8.087645 8.539457  
 C -36.154185 -5.810943 5.378020  
 C -36.601867 -7.126655 5.904112  
 N -35.814581 -7.930084 6.699551  
 C -36.497814 -9.045877 7.012720  
 N -37.700314 -9.012665 6.457763  
 C -37.773216 -7.821595 5.762143  
 C -42.017213 -8.897778 5.550137  
 S -40.500529 -9.635752 4.868302  
 C -37.532185 -13.717665 2.104030  
 C -37.613608 -13.000152 3.402738  
 N -36.603319 -13.018261 4.339392  
 C -36.972219 -12.279359 5.401487  
 N -38.180542 -11.775573 5.201479  
 C -38.590020 -12.218496 3.960630  
 Fe -39.224185 -10.550352 6.636046  
 H -37.640206 -13.503182 10.043576  
 H -38.292510 -11.968787 10.642527  
 H -43.150939 -15.528909 6.025555  
 H -43.865040 -14.063950 5.332850  
 H -41.965558 -11.995844 5.295023  
 H -39.831559 -13.072074 8.738254  
 H -40.847287 -6.573215 11.336451  
 H -41.903333 -5.913184 10.078774  
 H -39.095421 -7.548910 8.124789  
 H -41.830951 -10.669683 8.758874  
 H -35.911791 -5.116476 6.189449  
 H -35.264377 -5.912791 4.747696  
 H -38.658546 -7.553443 5.205342  
 H -36.099858 -9.860790 7.605398  
 H -41.779421 -8.093222 6.250045  
 H -42.620375 -9.649418 6.066315

H	-39.552105	-11.946447	3.552533
H	-36.370663	-12.136235	6.292638
H	-42.469976	-8.766056	10.290770
H	-41.692362	-14.765683	8.432717
H	-34.872040	-7.725168	7.000277
H	-38.451355	-13.558436	1.536821
H	-36.692358	-13.358585	1.499630
H	-35.724687	-13.509024	4.251516
H	-40.148010	-5.714260	9.954617
H	-36.948327	-5.365709	4.775506
H	-37.403492	-14.795591	2.248714
H	-44.230250	-14.523415	7.003579
H	-36.549478	-12.346192	10.813765
H	-42.601178	-8.488031	4.722454

**(4-Melm)<sub>0</sub>(5-Melm)<sub>4</sub>, ferrous, IEFPCM, PBE0,  
G° = -2762.060908**

C	-43.398673	-14.399340	7.771462
C	-42.198048	-13.638161	7.338164
N	-40.969806	-14.221887	7.123526
C	-40.098299	-13.270406	6.733001
N	-40.692121	-12.091557	6.686504
C	-42.001622	-12.309888	7.060988
C	-41.539555	-6.311810	10.029775
C	-41.205060	-7.583515	9.337172
N	-41.294093	-8.817835	9.941312
C	-40.927889	-9.762909	9.051244
N	-40.605786	-9.211329	7.895234
C	-40.772684	-7.853806	8.064369
C	-35.124063	-6.870198	5.531844
C	-36.213510	-7.711592	6.092349
N	-36.353927	-7.966237	7.438739
C	-37.435301	-8.748739	7.622574
N	-38.007676	-9.022628	6.464071
C	-37.254155	-8.382371	5.503745
C	-42.729692	-8.736393	5.088820
S	-41.130250	-9.268871	4.376106
C	-37.840149	-13.540577	1.756374
C	-37.917676	-12.707885	2.985449
N	-36.853421	-12.516618	3.836387
C	-37.246451	-11.708028	4.844698
N	-38.511054	-11.361286	4.695860
C	-38.939531	-11.980450	3.542282
Fe	-39.804810	-10.200801	6.103183
H	-43.667294	-15.172922	7.044271
H	-44.247488	-13.720411	7.874093
H	-42.721813	-11.505469	7.104784
H	-39.065310	-13.469682	6.489575
H	-40.910831	-6.158460	10.913402
H	-42.584844	-6.295130	10.356418
H	-40.568275	-7.155308	7.265236

H	-40.911541	-10.819086	9.276979
H	-35.158530	-5.850752	5.930520
H	-34.137180	-7.286170	5.761067
H	-37.504543	-8.443352	4.454615
H	-37.771682	-9.084874	8.592296
H	-42.588231	-8.191848	6.025917
H	-43.377752	-9.596110	5.283644
H	-39.951213	-11.857055	3.182827
H	-36.592675	-11.396680	5.646210
H	-41.584430	-8.992793	10.892970
H	-40.751297	-15.202061	7.234055
H	-35.748988	-7.626320	8.172919
H	-38.809015	-13.543558	1.252697
H	-37.093737	-13.153755	1.054221
H	-35.929589	-12.910517	3.729460
H	-41.382641	-5.470758	9.351416
H	-35.224671	-6.813654	4.446158
H	-37.574655	-14.577590	1.988331
H	-43.236078	-14.889772	8.737104
H	-43.242608	-8.079196	4.380812

**(4-Melm)<sub>1</sub>(5-Melm)<sub>3</sub>, ferric, IEFPCM, BP86,  
G° = -2992.378958**

C	-37.567204	-12.393064	10.411435
C	-37.205954	-11.843729	9.031492
O	-35.993997	-11.738721	8.695025
O	-38.205595	-11.538058	8.257649
C	-43.839519	-14.356231	6.691545
C	-42.539243	-13.674444	6.977934
N	-41.615306	-14.149781	7.905287
C	-40.542817	-13.313175	7.931924
N	-40.718314	-12.309123	7.062753
C	-41.957494	-12.527796	6.465122
C	-40.852333	-6.430972	10.286558
C	-40.778691	-7.715446	9.523114
N	-41.675029	-8.763626	9.704849
C	-41.338590	-9.784588	8.868635
N	-40.261446	-9.452914	8.147208
C	-39.907230	-8.167829	8.546648
C	-36.110116	-6.017794	5.171104
C	-36.581235	-7.295586	5.790786
N	-35.846697	-7.998248	6.742464
C	-36.538078	-9.111984	7.108488
N	-37.697447	-9.174060	6.435989
C	-37.729241	-8.047549	5.614930
C	-41.802219	-8.644409	5.483549
S	-40.512647	-9.803645	4.871411
C	-39.741062	-12.826009	3.435204
C	-38.416007	-12.808452	4.134571
N	-38.139085	-12.080262	5.300993
C	-36.860739	-12.342380	5.623696

N -36.312099 -13.192282 4.719716  
 C -37.274239 -13.501639 3.771229  
 Fe -39.255856 -10.719001 6.665585  
 H -36.785877 -12.138484 11.144025  
 H -37.624829 -13.495397 10.354588  
 H -43.685207 -15.383123 6.315873  
 H -44.393593 -13.792132 5.926156  
 H -42.341380 -11.852626 5.703036  
 H -39.676863 -13.443787 8.573982  
 H -40.750230 -6.597857 11.373327  
 H -41.811763 -5.911671 10.115814  
 H -39.055218 -7.651638 8.110949  
 H -41.882859 -10.723416 8.812029  
 H -35.957206 -5.229854 5.929652  
 H -35.155072 -6.154701 4.633714  
 H -38.571142 -7.861227 4.951349  
 H -36.171623 -9.861019 7.813699  
 H -42.517694 -9.169440 6.136010  
 H -42.338636 -8.231543 4.615303  
 H -39.996213 -11.839378 3.012854  
 H -40.555317 -13.103924 4.125237  
 H -37.075059 -14.173915 2.940265  
 H -35.357835 -13.549221 4.747241  
 H -36.339998 -11.977426 6.511254  
 H -42.458018 -8.773228 10.358543  
 H -41.719395 -14.989332 8.475494  
 H -34.932452 -7.730384 7.106957  
 H -40.039911 -5.761491 9.966010  
 H -44.472039 -14.421386 7.594306  
 H -38.544117 -12.017703 10.753048  
 H -39.715847 -13.559064 2.613199  
 H -36.858612 -5.656209 4.449906  
 H -41.341716 -7.822086 6.053633

**(4-Melm)<sub>1</sub>(5-Melm)<sub>3</sub>, ferrous, IEFPCM, BP86,  
G° = -2763.922305**

C -43.969442 -14.194473 7.428060  
 C -42.630786 -13.570409 7.184935  
 N -41.430230 -14.248309 7.362625  
 C -40.399823 -13.404320 7.051251  
 N -40.870150 -12.209974 6.677324  
 C -42.255911 -12.304460 6.762166  
 C -41.599345 -7.171260 10.727312  
 C -41.127011 -8.294233 9.857923  
 N -40.925689 -9.588538 10.325484  
 C -40.507412 -10.372292 9.289059  
 N -40.418392 -9.650503 8.166037  
 C -40.802963 -8.356862 8.512416  
 C -35.583377 -6.592882 4.616579  
 C -36.551648 -7.402900 5.420467  
 N -36.642600 -7.326543 6.807562

C -37.620726 -8.178345 7.231302  
 N -38.174481 -8.808798 6.190175  
 C -37.513348 -8.333060 5.061649  
 C -41.142059 -7.691506 4.562794  
 S -41.186550 -9.544673 4.600275  
 C -39.470035 -12.749010 3.499286  
 C -38.261002 -12.575383 4.366817  
 N -38.217603 -11.686228 5.446394  
 C -36.993723 -11.793798 5.982780  
 N -36.253858 -12.707216 5.300396  
 C -37.034050 -13.211956 4.271186  
 Fe -39.751424 -10.340045 6.230473  
 H -44.135386 -15.071938 6.778114  
 H -44.763811 -13.461692 7.219337  
 H -42.893223 -11.460142 6.504819  
 H -39.352589 -13.693869 7.100972  
 H -40.898364 -6.976392 11.558147  
 H -42.589056 -7.385554 11.167889  
 H -40.826329 -7.554245 7.777864  
 H -40.290498 -11.433459 9.386008  
 H -35.752605 -5.509103 4.745376  
 H -34.538054 -6.804469 4.903263  
 H -37.769206 -8.688851 4.064955  
 H -37.895563 -8.305513 8.275868  
 H -40.110831 -7.320896 4.678263  
 H -41.766472 -7.268660 5.367181  
 H -39.816118 -11.778497 3.104127  
 H -40.310482 -13.182318 4.068688  
 H -36.659023 -13.957744 3.574512  
 H -35.290853 -12.968039 5.508983  
 H -36.618808 -11.233189 6.836045  
 H -41.067374 -9.905499 11.284268  
 H -41.330218 -15.214937 7.671776  
 H -36.074742 -6.732509 7.411689  
 H -41.684372 -6.250503 10.130403  
 H -44.080321 -14.528661 8.474962  
 H -39.240446 -13.417174 2.654196  
 H -35.698218 -6.830697 3.548085  
 H -41.539243 -7.341964 3.595687

**(4-Melm)<sub>1</sub>(5-Melm)<sub>3</sub>, ferric, IEFPCM, TPSSh,  
G° = -2992.261762**

C -37.602101 -12.474373 10.332241  
 C -37.233598 -11.834358 9.000314  
 O -36.028473 -11.677344 8.697543  
 O -38.224838 -11.507066 8.235970  
 C -43.854493 -14.308554 6.782416  
 C -42.532252 -13.653740 7.014688  
 N -41.558741 -14.185000 7.846501  
 C -40.485088 -13.363890 7.847630  
 N -40.703556 -12.318727 7.054486

C -41.977432 -12.493493 6.530568  
 C -40.875972 -6.496739 10.299812  
 C -40.797905 -7.767310 9.518325  
 N -41.687356 -8.815653 9.684673  
 C -41.351882 -9.815687 8.837682  
 N -40.284467 -9.473277 8.122839  
 C -39.933190 -8.198602 8.541036  
 C -36.160826 -6.047432 5.125150  
 C -36.637975 -7.307152 5.771161  
 N -35.945023 -7.947975 6.786284  
 C -36.627361 -9.053812 7.159697  
 N -37.739173 -9.172020 6.435160  
 C -37.750472 -8.086714 5.567887  
 C -41.582961 -8.466365 5.420090  
 S -40.525980 -9.852323 4.851459  
 C -39.750325 -12.904119 3.525256  
 C -38.415581 -12.832062 4.196525  
 N -38.141180 -12.062203 5.328704  
 C -36.858270 -12.272528 5.633016  
 N -36.302354 -13.127921 4.752896  
 C -37.267718 -13.496352 3.837227  
 Fe -39.267706 -10.721588 6.656004  
 H -36.849747 -12.236805 11.087287  
 H -37.617830 -13.563797 10.208122  
 H -43.733634 -15.306408 6.347220  
 H -44.445858 -13.702981 6.092921  
 H -42.395672 -11.778672 5.838740  
 H -39.589934 -13.539129 8.419654  
 H -40.775514 -6.682894 11.374447  
 H -41.830264 -5.985342 10.134141  
 H -39.090799 -7.677722 8.114814  
 H -41.889066 -10.747596 8.770427  
 H -36.066976 -5.235889 5.854778  
 H -35.183574 -6.187914 4.650724  
 H -38.550243 -7.951770 4.856579  
 H -36.284279 -9.757557 7.906049  
 H -42.291364 -8.811839 6.175915  
 H -42.131563 -8.083839 4.556651  
 H -40.011618 -11.956751 3.044125  
 H -40.541452 -13.137497 4.243452  
 H -37.062559 -14.183333 3.031721  
 H -35.343570 -13.450873 4.773909  
 H -36.338442 -11.863888 6.489508  
 H -42.463557 -8.838656 10.334716  
 H -41.632506 -15.047497 8.372325  
 H -35.063670 -7.647802 7.184477  
 H -40.070411 -5.827833 9.990891  
 H -44.416530 -14.414360 7.716517  
 H -38.590391 -12.153399 10.668213  
 H -39.731226 -13.685510 2.761210  
 H -36.872776 -5.737441 4.357738  
 H -40.971980 -7.666086 5.843834

**(4-Melm)<sub>1</sub>(5-Melm)<sub>3</sub>, ferrous, IEFPCM, TPSSH,  
 $G^\circ = -2763.808824$**

C -43.960789 -14.198790 7.399659  
 C -42.624818 -13.571247 7.166431  
 N -41.429867 -14.246680 7.344466  
 C -40.406240 -13.404710 7.047442  
 N -40.871140 -12.216056 6.683574  
 C -42.251495 -12.310852 6.758153  
 C -41.594626 -7.174143 10.735612  
 C -41.129380 -8.296435 9.865783  
 N -40.968181 -9.593476 10.323464  
 C -40.545590 -10.370277 9.296030  
 N -40.416162 -9.647118 8.189644  
 C -40.778687 -8.353804 8.537050  
 C -35.596077 -6.626097 4.581497  
 C -36.562013 -7.422491 5.397166  
 N -36.649395 -7.324310 6.776768  
 C -37.620646 -8.164060 7.212369  
 N -38.173728 -8.806475 6.190443  
 C -37.517826 -8.351131 5.057377  
 C -41.130769 -7.669560 4.601126  
 S -41.236639 -9.511316 4.628935  
 C -39.463935 -12.752965 3.529233  
 C -38.250315 -12.571227 4.384544  
 N -38.204422 -11.681846 5.455912  
 C -36.983055 -11.777837 5.977570  
 N -36.246689 -12.682394 5.298113  
 C -37.028753 -13.194992 4.281871  
 Fe -39.744016 -10.347084 6.244540  
 H -44.114798 -15.066745 6.749227  
 H -44.747704 -13.471288 7.190438  
 H -42.880914 -11.470617 6.505794  
 H -39.367579 -13.691713 7.100977  
 H -40.908022 -7.005740 11.572361  
 H -42.587849 -7.375937 11.151009  
 H -40.767593 -7.552512 7.813941  
 H -40.354546 -11.427785 9.388287  
 H -35.767529 -5.550222 4.696340  
 H -34.560527 -6.834191 4.871780  
 H -37.776226 -8.719548 4.075653  
 H -37.889173 -8.274445 8.251346  
 H -40.095228 -7.337074 4.706889  
 H -41.727533 -7.236015 5.408649  
 H -39.818203 -11.790865 3.146618  
 H -40.285191 -13.198920 4.099541  
 H -36.656108 -13.934566 3.591122  
 H -35.286732 -12.932208 5.498350  
 H -36.608051 -11.215371 6.818299  
 H -41.137934 -9.915152 11.268286  
 H -41.330040 -15.208870 7.643235  
 H -36.084467 -6.726292 7.367070

H -41.649631 -6.255491 10.148145  
H -44.070575 -14.533194 8.437140  
H -39.232153 -13.407320 2.685093  
H -35.712985 -6.879989 3.526009  
H -41.523299 -7.305048 3.647831

**(4-Melm)<sub>1</sub>(5-Melm)<sub>3</sub>, ferric, IEFPCM, PBE0,  
G° = -2990.254823**

C -37.560292 -12.618758 10.231023  
C -37.232369 -11.863643 8.958637  
O -36.044777 -11.647210 8.658615  
O -38.240491 -11.507758 8.246573  
C -43.858657 -14.251090 6.820593  
C -42.533765 -13.614871 7.038237  
N -41.563458 -14.152007 7.855584  
C -40.486615 -13.346883 7.844147  
N -40.700820 -12.306545 7.055221  
C -41.974600 -12.464894 6.546606  
C -40.900234 -6.497285 10.244501  
C -40.812368 -7.768127 9.479810  
N -41.694387 -8.811592 9.644901  
C -41.348225 -9.812561 8.814718  
N -40.280225 -9.474682 8.111620  
C -39.937982 -8.202340 8.518577  
C -36.203222 -6.050634 5.146498  
C -36.671548 -7.302335 5.796285  
N -36.013419 -7.898322 6.849360  
C -36.678020 -9.009337 7.213334  
N -37.746402 -9.172684 6.446200  
C -37.749040 -8.113425 5.559250  
C -41.473385 -8.428695 5.396302  
S -40.511446 -9.871837 4.845167  
C -39.769149 -12.987950 3.636594  
C -38.421042 -12.856678 4.253270  
N -38.131297 -12.058077 5.350563  
C -36.839286 -12.221876 5.612186  
N -36.291044 -13.075419 4.736916  
C -37.269780 -13.491809 3.868876  
Fe -39.262987 -10.721899 6.656778  
H -36.773319 -12.477774 10.974266  
H -37.613628 -13.689849 10.002250  
H -43.755583 -15.250106 6.383942  
H -44.452266 -13.640621 6.137361  
H -42.393001 -11.747851 5.855853  
H -39.587114 -13.527922 8.409755  
H -40.809230 -6.671186 11.321853  
H -41.853323 -5.988249 10.066365  
H -39.094271 -7.677008 8.098056  
H -41.882617 -10.747647 8.749123  
H -36.161810 -5.220552 5.859658  
H -35.203571 -6.172346 4.715996

H -38.517122 -8.014691 4.807115  
H -36.348561 -9.690943 7.986747  
H -42.181884 -8.708461 6.179359  
H -42.027606 -8.041578 4.537891  
H -40.098300 -12.050270 3.179296  
H -40.520569 -13.269150 4.380125  
H -37.075913 -14.190728 3.069965  
H -35.324473 -13.366787 4.731829  
H -36.302355 -11.778287 6.441240  
H -42.475403 -8.831814 10.285571  
H -41.641177 -15.010105 8.383513  
H -35.161417 -7.566924 7.279426  
H -40.094384 -5.827222 9.938772  
H -44.413834 -14.351261 7.759192  
H -38.525923 -12.311857 10.638833  
H -39.743712 -13.758355 2.861993  
H -36.888166 -5.774193 4.342550  
H -40.820392 -7.640502 5.779513

**(4-Melm)<sub>1</sub>(5-Melm)<sub>3</sub>, ferrous, IEFPCM, PBE0,  
G° = -2762.059131**

C -43.919701 -14.263535 7.293279  
C -42.596717 -13.608697 7.118978  
N -41.402241 -14.244639 7.366450  
C -40.393020 -13.384315 7.108339  
N -40.867533 -12.220974 6.704030  
C -42.238796 -12.348532 6.709313  
C -41.525073 -7.124212 10.728814  
C -41.108296 -8.261233 9.867503  
N -41.084686 -9.567410 10.301046  
C -40.671423 -10.354608 9.287453  
N -40.417874 -9.629299 8.213060  
C -40.687568 -8.322915 8.564061  
C -35.628891 -6.640577 4.558328  
C -36.575622 -7.430046 5.388660  
N -36.613535 -7.358012 6.763329  
C -37.579970 -8.184659 7.213543  
N -38.176730 -8.792703 6.204764  
C -37.556722 -8.331425 5.064046  
C -41.141331 -7.681273 4.666250  
S -41.248229 -9.508124 4.652647  
C -39.494904 -12.770051 3.596805  
C -38.267489 -12.569255 4.414735  
N -38.199231 -11.673607 5.467933  
C -36.969935 -11.752896 5.954651  
N -36.248016 -12.654474 5.270118  
C -37.047597 -13.182704 4.286520  
Fe -39.737663 -10.346754 6.276976  
H -44.021937 -15.142320 6.647522  
H -44.714919 -13.560445 7.037277  
H -42.879339 -11.530654 6.411319

H -39.349469 -13.642009 7.216486  
H -40.881771 -7.031577 11.610326  
H -42.556326 -7.242460 11.078141  
H -40.567612 -7.509793 7.862824  
H -40.575797 -11.427366 9.364600  
H -35.776696 -5.563856 4.694529  
H -34.587583 -6.869347 4.809135  
H -37.853028 -8.674575 4.082743  
H -37.815426 -8.311540 8.260070  
H -40.101969 -7.344311 4.705703  
H -41.675040 -7.262495 5.524654  
H -39.878655 -11.813864 3.227612  
H -40.293273 -13.232086 4.186471  
H -36.690987 -13.927176 3.591456  
H -35.282822 -12.891797 5.446645  
H -36.577337 -11.175784 6.778936  
H -41.337929 -9.889550 11.224360  
H -41.292491 -15.196830 7.685116  
H -36.019390 -6.782802 7.343331  
H -41.462901 -6.192131 10.163659  
H -44.074128 -14.589318 8.327582  
H -39.277775 -13.416796 2.743196  
H -35.782818 -6.873023 3.502655  
H -41.599628 -7.283662 3.756227

***cis*-(4-Melm)<sub>2</sub>(5-Melm)<sub>2</sub>, ferric, IEFPCM, BP86,  
*G*<sup>o</sup> = -2992.374318**

C -37.206037 -12.250002 10.229307  
C -37.113328 -11.762107 8.781595  
O -35.993509 -11.573330 8.242160  
O -38.268812 -11.571512 8.201563  
C -42.523877 -13.747601 7.054521  
N -41.367260 -14.389178 7.470494  
C -40.348030 -13.493781 7.433124  
N -40.788489 -12.300591 7.006179  
C -42.160999 -12.442979 6.763019  
C -41.499459 -6.503519 10.097657  
C -41.163301 -7.808046 9.446962  
N -41.581776 -9.039988 9.942255  
C -41.114521 -10.026301 9.129814  
N -40.409181 -9.498930 8.121279  
C -40.433518 -8.119935 8.313056  
C -35.406546 -6.564511 5.252111  
C -36.279714 -7.530144 5.989329  
N -36.253967 -7.678750 7.374628  
C -37.156495 -8.630806 7.733632  
N -37.778038 -9.111287 6.650504  
C -37.239525 -8.430501 5.561342  
C -41.160440 -8.198133 4.983860  
S -40.257526 -9.767288 4.670857  
C -39.992849 -13.119249 3.715451

C -38.584764 -12.851661 4.154969  
N -38.234010 -12.042075 5.245033  
C -36.894911 -12.079605 5.343010  
N -36.376498 -12.868243 4.367538  
C -37.423073 -13.366826 3.606078  
Fe -39.303904 -10.685481 6.642681  
H -36.207328 -12.458937 10.640319  
H -37.827548 -13.159673 10.286348  
H -39.324068 -13.718721 7.717330  
H -41.109208 -6.451240 11.129325  
H -42.590814 -6.341664 10.143431  
H -39.922520 -7.439739 7.636418  
H -41.293603 -11.084984 9.296746  
H -35.591103 -5.523286 5.570594  
H -34.335329 -6.779043 5.413476  
H -37.583586 -8.630651 4.548607  
H -37.331800 -8.935692 8.761294  
H -41.838781 -8.294486 5.845274  
H -41.743538 -7.945544 4.084431  
H -40.517332 -12.188392 3.441263  
H -40.579989 -13.600816 4.515934  
H -37.260134 -14.033981 2.763102  
H -35.386312 -13.068551 4.232947  
H -36.314013 -11.611443 6.141479  
H -42.145756 -9.187316 10.779487  
H -41.291520 -15.363000 7.762189  
H -35.658541 -7.160058 8.020356  
H -41.055764 -5.676873 9.522488  
H -37.700535 -11.481555 10.848911  
H -39.988720 -13.789495 2.841284  
H -35.608849 -6.631593 4.172420  
H -40.443312 -7.383886 5.179569  
H -43.483222 -14.256932 7.006489  
C -43.041821 -11.332740 6.280389  
H -43.054192 -10.488732 6.991880  
H -42.683746 -10.937205 5.313902  
H -44.074415 -11.695689 6.157633

***cis*-(4-Melm)<sub>2</sub>(5-Melm)<sub>2</sub>, ferrous, IEFPCM, BP86,  
*G*<sup>o</sup> = -2763.918593**

C -42.180077 -13.804807 7.467276  
N -40.883867 -14.273247 7.609329  
C -40.033490 -13.288604 7.208637  
N -40.717134 -12.204575 6.815713  
C -42.073213 -12.512214 6.978077  
C -41.614651 -6.770186 10.395785  
C -41.217768 -7.982321 9.612491  
N -41.189013 -9.264148 10.150436  
C -40.796194 -10.140504 9.178989  
N -40.564337 -9.493797 8.030676  
C -40.821425 -8.150196 8.295525

C	-35.408942	-6.596046	5.128879	N	-41.310093	-14.403445	7.313358
C	-36.413546	-7.481279	5.797344	C	-40.325416	-13.512549	7.089481
N	-36.495926	-7.633950	7.178308	N	-40.829964	-12.288878	6.928392
C	-37.516532	-8.492460	7.466422	C	-42.214026	-12.406555	7.062571
N	-38.102243	-8.914410	6.339815	C	-42.404033	-7.009962	10.104202
C	-37.420723	-8.290890	5.298237	C	-41.568534	-8.124677	9.565446
C	-41.144175	-7.609085	4.608061	N	-41.086278	-9.160026	10.351393
S	-40.923101	-9.432083	4.357369	C	-40.367285	-10.002492	9.575703
C	-39.842517	-12.819169	3.475738	N	-40.355653	-9.572319	8.317329
C	-38.517312	-12.608690	4.142507	C	-41.104441	-8.404739	8.302822
N	-38.319195	-11.674429	5.165108	C	-35.173995	-7.072965	4.984433
C	-37.026080	-11.756172	5.507353	C	-36.226235	-7.789974	5.765613
N	-36.389309	-12.695141	4.756831	N	-36.489523	-7.528377	7.101793
C	-37.314240	-13.245174	3.882121	C	-37.491804	-8.334560	7.517480
Fe	-39.763520	-10.303332	6.160120	N	-37.899851	-9.109694	6.519407
H	-38.951559	-13.395388	7.206925	C	-37.118519	-8.777252	5.423970
H	-40.955634	-6.614374	11.268224	C	-40.257713	-7.819612	4.750157
H	-42.651138	-6.847148	10.769386	S	-40.708019	-9.580268	4.994965
H	-40.705668	-7.386607	7.529298	C	-40.022133	-12.692550	3.515780
H	-40.698158	-11.210973	9.341390	C	-38.642706	-12.622045	4.089732
H	-35.526897	-5.541380	5.434637	N	-38.311420	-11.933690	5.259321
H	-34.374512	-6.899859	5.368177	C	-37.003669	-12.114520	5.455251
H	-37.700689	-8.462195	4.260228	N	-36.485116	-12.876325	4.470919
H	-37.796575	-8.775730	8.478341	C	-37.502479	-13.211479	3.598822
H	-40.201458	-7.142160	4.937806	Fe	-39.411789	-10.639282	6.659428
H	-41.928844	-7.405743	5.354880	H	-36.203153	-12.565186	10.446691
H	-40.204743	-11.886777	3.008240	H	-37.918994	-13.028467	10.220293
H	-40.608774	-13.136306	4.203728	H	-39.278411	-13.765596	7.057753
H	-37.043057	-14.017615	3.166346	H	-41.868380	-6.447087	10.876205
H	-35.402778	-12.942490	4.823154	H	-43.333587	-7.385549	10.545315
H	-36.530719	-11.162296	6.271762	H	-41.269415	-7.851984	7.391837
H	-41.418927	-9.514920	11.111905	H	-39.878981	-10.893561	9.933729
H	-40.610319	-15.194900	7.947733	H	-35.370135	-5.996017	4.946020
H	-35.897718	-7.176929	7.866463	H	-34.181636	-7.219108	5.424348
H	-41.549139	-5.877040	9.755962	H	-37.252757	-9.262696	4.469667
H	-39.759711	-13.592489	2.695552	H	-37.882705	-8.337003	8.522002
H	-35.535717	-6.650133	4.036942	H	-41.177175	-7.243635	4.619812
H	-41.446432	-7.152415	3.651651	H	-39.647107	-7.721644	3.849277
C	-43.176289	-11.550066	6.656047	H	-40.390592	-11.697244	3.249737
H	-44.153972	-12.052919	6.726180	H	-40.730021	-13.122606	4.231351
H	-43.177111	-10.694195	7.354032	H	-37.333840	-13.827585	2.729874
H	-43.055832	-11.135159	5.640821	H	-35.515767	-13.156410	4.394697
H	-43.045534	-14.414314	7.716228	H	-36.440650	-11.717308	6.292769

***cis*-(4-Melm)<sub>2</sub>(5-Melm)<sub>2</sub>, ferric, IEFPCM, TPSSh,  
G° = -2992.257860**

C	-37.194941	-12.211707	10.158623	H	-41.182886	-15.395611	7.467378
C	-37.167645	-11.612854	8.756212	H	-36.014304	-6.845595	7.679239
O	-36.084631	-11.237542	8.258603	H	-42.661425	-6.322785	9.295853
O	-38.326025	-11.532237	8.176933	H	-37.504233	-11.437160	10.870543
C	-42.513979	-13.726467	7.301628	H	-40.014722	-13.318084	2.619490
				H	-35.154938	-7.454257	3.961628
				H	-39.698147	-7.433913	5.603416
				H	-43.454795	-14.228258	7.462368



C -43.168240 -11.259221 6.965918  
H -44.185877 -11.614752 7.146346  
H -42.932688 -10.485924 7.702953  
H -43.128806 -10.790399 5.978378

***cis*-(4-Melm)<sub>2</sub>(5-Melm)<sub>2</sub>, ferrous, IEFPCM, TPSSh,  
G° = -2763.804677**

C -42.176154 -13.794673 7.493822  
N -40.885087 -14.269810 7.603239  
C -40.044596 -13.292477 7.195920  
N -40.724423 -12.207738 6.830938  
C -42.072427 -12.507959 7.017183  
C -41.609985 -6.798265 10.422600  
C -41.212263 -8.001110 9.630176  
N -41.178770 -9.280593 10.157800  
C -40.786293 -10.142578 9.186658  
N -40.559479 -9.494048 8.049901  
C -40.819982 -8.158548 8.321051  
C -35.402109 -6.662467 5.041205  
C -36.424440 -7.503905 5.733735  
N -36.531063 -7.583489 7.113084  
C -37.553984 -8.416930 7.424057  
N -38.119420 -8.891096 6.319593  
C -37.420095 -8.327824 5.263185  
C -41.122594 -7.587540 4.630140  
S -40.950764 -9.400094 4.335183  
C -39.833273 -12.818223 3.504268  
C -38.509527 -12.601823 4.166503  
N -38.316483 -11.665687 5.179766  
C -37.030968 -11.737293 5.517516  
N -36.392840 -12.669872 4.776609  
C -37.311854 -13.228009 3.909762  
Fe -39.773346 -10.307422 6.159197  
H -38.972280 -13.404102 7.171952  
H -40.949153 -6.649950 11.283601  
H -42.635445 -6.887250 10.797476  
H -40.707638 -7.397580 7.564368  
H -40.684636 -11.204800 9.342283  
H -35.511628 -5.604201 5.302068  
H -34.384712 -6.970329 5.306116  
H -37.683285 -8.549976 4.239812  
H -37.848988 -8.644787 8.436276  
H -40.179466 -7.161808 4.983395  
H -41.906778 -7.384405 5.364211  
H -40.189511 -11.896615 3.032338  
H -40.590327 -13.128802 4.231211  
H -37.038188 -13.996323 3.204013  
H -35.411819 -12.908654 4.843529  
H -36.542345 -11.141956 6.272554  
H -41.405736 -9.537832 11.110490  
H -40.610538 -15.189050 7.925099

H -35.947844 -7.097858 7.783338  
H -41.552986 -5.909554 9.790884  
H -39.747678 -13.592382 2.737423  
H -35.518757 -6.762124 3.960196  
H -41.394250 -7.102981 3.688645  
C -43.172651 -11.537800 6.722401  
H -43.137807 -10.682312 7.405524  
H -43.084380 -11.144702 5.705157  
H -44.143327 -12.028030 6.832975  
H -43.031835 -14.397508 7.753938

***cis*-(4-Melm)<sub>2</sub>(5-Melm)<sub>2</sub>, ferric, IEFPCM, PBE0,  
G° = -2990.251471**

C -37.189621 -12.149595 10.152668  
C -37.171533 -11.590771 8.742203  
O -36.097709 -11.232993 8.232366  
O -38.325974 -11.525065 8.174259  
C -42.498129 -13.696534 7.264992  
N -41.307508 -14.381001 7.268551  
C -40.318320 -13.500096 7.070416  
N -40.807190 -12.274619 6.932249  
C -42.184388 -12.378494 7.057932  
C -42.426082 -7.031173 10.037700  
C -41.577757 -8.133155 9.514838  
N -41.092796 -9.153441 10.303528  
C -40.362808 -9.986747 9.540582  
N -40.346803 -9.563653 8.287091  
C -41.103544 -8.410893 8.260092  
C -35.153599 -7.104483 5.010325  
C -36.206169 -7.814162 5.782585  
N -36.473137 -7.555371 7.109650  
C -37.475128 -8.354307 7.517045  
N -37.879229 -9.122008 6.521065  
C -37.097295 -8.794361 5.434648  
C -40.224511 -7.824227 4.792977  
S -40.657867 -9.584165 4.965247  
C -40.029899 -12.715472 3.561649  
C -38.650678 -12.638709 4.116129  
N -38.302445 -11.939275 5.263982  
C -36.999319 -12.120884 5.444312  
N -36.498751 -12.893786 4.469651  
C -37.522058 -13.236585 3.620177  
Fe -39.393425 -10.634865 6.648705  
H -36.193652 -12.478315 10.454215  
H -37.900615 -12.975610 10.236763  
H -39.272722 -13.763677 7.036043  
H -41.905108 -6.456505 10.810775  
H -43.355359 -7.413248 10.473345  
H -41.273636 -7.862489 7.346559  
H -39.865999 -10.872368 9.904368  
H -35.343612 -6.026661 4.970967

H	-34.162900	-7.254254	5.452306
H	-37.227316	-9.275239	4.476399
H	-37.872693	-8.356367	8.520424
H	-41.144216	-7.245439	4.673938
H	-39.603688	-7.679480	3.905214
H	-40.400974	-11.724480	3.284312
H	-40.732653	-13.133138	4.289576
H	-37.371075	-13.865249	2.756145
H	-35.533435	-13.177101	4.386554
H	-36.425177	-11.716387	6.272155
H	-41.253995	-9.264098	11.294827
H	-41.190049	-15.375154	7.400108
H	-35.999352	-6.876773	7.689068
H	-42.686329	-6.349893	9.225262
H	-37.514447	-11.362605	10.843386
H	-40.035671	-13.354316	2.675055
H	-35.129863	-7.482905	3.986544
H	-39.677165	-7.457769	5.663016
H	-43.447531	-14.188157	7.410669
C	-43.121861	-11.224584	6.998930
H	-42.932546	-10.518137	7.813155
H	-43.014956	-10.670998	6.062002
H	-44.151044	-11.581567	7.084826

***cis*-(4-Melm)<sub>2</sub>(5-Melm)<sub>2</sub>, ferrous, IEFPCM, PBE0,  
G° = -2762.056099**

C	-42.450240	-13.656452	7.359342
N	-41.220592	-14.266572	7.367575
C	-40.304615	-13.359306	6.985058
N	-40.875898	-12.192144	6.731826
C	-42.229551	-12.360107	6.967061
C	-41.580000	-6.996593	10.523860
C	-41.147091	-8.156893	9.702009
N	-41.053425	-9.438543	10.194635
C	-40.640486	-10.255378	9.203772
N	-40.456060	-9.573676	8.087749
C	-40.766747	-8.264294	8.388608
C	-35.488576	-6.666130	4.836056
C	-36.492403	-7.465355	5.586281
N	-36.586923	-7.460578	6.959753
C	-37.597178	-8.277328	7.326556
N	-38.165416	-8.817859	6.264520
C	-37.482903	-8.320554	5.175742
C	-41.176002	-7.698962	4.630952
S	-40.951728	-9.477128	4.262884
C	-39.539839	-12.788610	3.489996
C	-38.304872	-12.581645	4.295356
N	-38.228527	-11.672688	5.336498
C	-36.992111	-11.740200	5.805009
N	-36.274054	-12.648394	5.122498
C	-37.084555	-13.192697	4.157082

Fe	-39.773880	-10.330567	6.142907
H	-39.251104	-13.579008	6.896916
H	-40.910375	-6.835639	11.375504
H	-42.592604	-7.137727	10.916556
H	-40.697203	-7.479602	7.649397
H	-40.495774	-11.318092	9.329045
H	-35.604485	-5.593658	5.026030
H	-34.465650	-6.945321	5.110559
H	-37.750786	-8.604426	4.167846
H	-37.882387	-8.445934	8.354449
H	-40.235977	-7.244473	4.957120
H	-41.930146	-7.546885	5.408387
H	-39.847330	-11.860085	2.997575
H	-40.373871	-13.114738	4.119499
H	-36.734404	-13.944596	3.466630
H	-35.306200	-12.880868	5.290252
H	-36.591794	-11.153549	6.618657
H	-41.256913	-9.726376	11.141310
H	-41.031822	-15.227938	7.610655
H	-36.002631	-6.933061	7.592636
H	-41.575914	-6.091391	9.913385
H	-39.368299	-13.547642	2.722872
H	-35.610011	-6.835608	3.764231
H	-41.511306	-7.185105	3.725985
C	-43.224326	-11.264474	6.802689
H	-44.239832	-11.657607	6.895926
H	-43.086054	-10.487409	7.562298
H	-43.113045	-10.783553	5.825837
H	-43.356040	-14.180652	7.623242

***trans*-(4-Melm)<sub>2</sub>(5-Melm)<sub>2</sub>, ferric, IEFPCM, BP86,  
G° = -2992.373289**

C	-38.083954	-11.175391	10.671317
C	-37.381495	-11.326233	9.326020
O	-36.127078	-11.310613	9.254346
O	-38.146903	-11.470637	8.272500
C	-43.344479	-14.826873	6.325266
C	-42.220056	-13.961393	6.798989
N	-41.402004	-14.295080	7.874335
C	-40.478125	-13.310810	8.050086
N	-40.656134	-12.342509	7.141832
C	-41.735274	-12.741294	6.358953
C	-40.982340	-7.913557	9.941138
N	-41.589004	-9.130858	10.200797
C	-41.122650	-10.035970	9.301730
N	-40.240370	-9.462811	8.471635
C	-40.142651	-8.121224	8.858302
C	-35.739210	-6.749180	4.315308
C	-36.329814	-7.823532	5.172668
N	-35.578310	-8.593955	6.057225
C	-36.396752	-9.478734	6.688572

N	-37.657978	-9.317739	6.259470	C	-40.809653	-8.730125	10.197679
C	-37.622686	-8.294247	5.314896	N	-40.128728	-9.903859	10.476481
C	-42.357255	-9.129477	6.151949	C	-39.753535	-10.466314	9.295632
S	-40.786987	-9.572760	5.307205	N	-40.154151	-9.707190	8.265642
C	-38.766465	-11.129258	2.986736	C	-40.823206	-8.609047	8.817069
C	-38.190246	-12.129927	3.941263	C	-35.465332	-6.712645	4.434962
N	-38.327942	-12.058391	5.332402	C	-36.485101	-7.423718	5.268261
C	-37.674334	-13.114555	5.835617	N	-36.747143	-7.098261	6.595779
N	-37.130309	-13.858339	4.837872	C	-37.725153	-7.926322	7.066102
C	-37.442980	-13.254542	3.630318	N	-38.118618	-8.775493	6.110960
Fe	-39.295992	-10.634371	6.809058	C	-37.350802	-8.469067	4.991102
H	-37.369731	-11.305650	11.497674	C	-40.862775	-7.708445	4.192287
H	-38.912478	-11.894620	10.774246	S	-41.178298	-9.486107	4.607345
H	-42.985506	-15.823139	6.012275	C	-39.357754	-12.744857	3.523551
H	-43.838136	-14.354978	5.462340	C	-38.200628	-12.581012	4.461009
H	-42.080911	-12.133931	5.524765	N	-38.210491	-11.685982	5.536548
H	-39.703273	-13.327994	8.811569	C	-37.025274	-11.809290	6.151630
H	-41.438389	-11.074921	9.277441	N	-36.259999	-12.738979	5.523076
H	-35.265613	-5.958250	4.923333	C	-36.980748	-13.237943	4.448685
H	-34.970469	-7.151257	3.631981	Fe	-39.725477	-10.274497	6.220034
H	-38.527477	-7.959558	4.811478	H	-44.431059	-14.722547	6.704084
H	-36.065738	-10.202571	7.437856	H	-44.949605	-13.080413	7.169252
H	-42.771471	-9.997074	6.689248	H	-42.959715	-11.199939	6.453270
H	-43.078382	-8.793690	5.390716	H	-39.566026	-13.659694	7.010946
H	-38.395295	-10.111426	3.197888	H	-39.211360	-11.406430	9.224251
H	-39.867397	-11.093761	3.048941	H	-35.696385	-5.637039	4.337940
H	-37.115456	-13.661433	2.676683	H	-34.452696	-6.799307	4.867159
H	-36.581766	-14.708240	4.962511	H	-37.464899	-9.018870	4.058362
H	-37.571536	-13.341212	6.893416	H	-38.111286	-7.883106	8.081967
H	-42.269171	-9.321154	10.935856	H	-39.781740	-7.498590	4.157904
H	-41.477186	-15.139279	8.442134	H	-41.329477	-7.043013	4.937228
H	-34.573737	-8.511841	6.214160	H	-39.721073	-11.764252	3.172094
H	-44.102665	-14.976610	7.114018	H	-40.208343	-13.242980	4.021153
H	-38.521881	-10.163827	10.735594	H	-36.574181	-13.994840	3.782426
H	-38.484299	-11.390691	1.954559	H	-35.316347	-13.013295	5.793764
H	-36.528562	-6.284291	3.705490	H	-36.696054	-11.245999	7.021689
H	-42.182537	-8.313766	6.871404	H	-39.945890	-10.287877	11.402780
H	-41.191424	-7.024086	10.530342	H	-41.632225	-15.056047	7.579958
C	-39.267326	-7.115992	8.175482	H	-36.286773	-6.363458	7.132758
H	-38.203048	-7.399688	8.229284	H	-44.328657	-14.205103	8.406810
H	-39.525620	-7.021689	7.107118	H	-39.062213	-13.352690	2.653842
H	-39.388453	-6.129722	8.650399	H	-35.442704	-7.148484	3.424556
<b><i>trans</i>-(4-Melm)<sub>2</sub>(5-Melm)<sub>2</sub>, ferrous, IEFPCM, BP86, <i>G</i><sup>o</sup> = -2763.919484</b>							
C	-44.203310	-13.865940	7.363164	H	-41.301197	-7.488061	3.205064
C	-42.828452	-13.327238	7.116769	C	-41.433215	-7.526010	7.980257
N	-41.672839	-14.082119	7.280659	H	-42.096387	-7.952337	7.207849
C	-40.592679	-13.302909	6.969093	H	-42.018349	-6.838538	8.611031
N	-40.986808	-12.078096	6.607736	H	-40.661105	-6.934801	7.456290
C	-42.375322	-12.084783	6.700174	H	-41.219797	-8.099542	10.982709

***trans*-(4-Melm)<sub>2</sub>(5-Melm)<sub>2</sub>, ferric, IEFPCM, TPSSh,  
*G*<sup>o</sup> = -2992.257178**

C -37.376556 -12.389693 10.263622  
C -37.196059 -11.814894 8.863181  
O -36.051960 -11.628879 8.398490  
O -38.305254 -11.545441 8.244944  
C -43.921099 -14.133154 6.739469  
C -42.567175 -13.530318 6.926254  
N -41.509423 -14.206199 7.515146  
C -40.428691 -13.394302 7.540542  
N -40.723476 -12.218528 6.993367  
C -42.052828 -12.296940 6.606581  
C -41.167820 -7.862380 9.569031  
N -41.389778 -9.122518 10.087373  
C -40.826935 -10.023613 9.258972  
N -40.249780 -9.410198 8.225765  
C -40.452330 -8.041356 8.408550  
C -35.282975 -6.733092 5.060591  
C -36.142973 -7.670246 5.843927  
N -36.031134 -7.834597 7.217332  
C -36.938936 -8.750019 7.624070  
N -37.643841 -9.190092 6.588590  
C -37.155601 -8.522119 5.475685  
C -42.038165 -8.891969 5.389272  
S -40.424017 -9.606345 4.888361  
C -39.883892 -12.855499 3.628954  
C -38.495736 -12.665908 4.152533  
N -38.167468 -11.877322 5.258243  
C -36.848928 -11.989612 5.433056  
N -36.320235 -12.799579 4.495162  
C -37.341634 -13.238553 3.674855  
Fe -39.268383 -10.622743 6.682993  
H -36.414359 -12.667678 10.696801  
H -38.033785 -13.264294 10.233188  
H -43.875705 -15.027452 6.108674  
H -44.580514 -13.407933 6.258758  
H -42.550188 -11.472311 6.122645  
H -39.472498 -13.669563 7.953068  
H -40.846552 -11.088221 9.423804  
H -35.401708 -5.699898 5.404433  
H -34.223348 -6.996908 5.146794  
H -37.567877 -8.692762 4.493330  
H -37.054007 -9.061703 8.648371  
H -42.192436 -8.982603 6.465692  
H -42.838328 -9.413084 4.856840  
H -40.320540 -11.907417 3.302320  
H -40.543006 -13.268380 4.398570  
H -37.165388 -13.905531 2.845955  
H -35.342523 -13.048807 4.418820  
H -36.291890 -11.551897 6.251418  
H -41.893352 -9.338690 10.938267

H -41.533570 -15.153284 7.872860  
H -35.377473 -7.353706 7.822969  
H -44.366073 -14.419654 7.698422  
H -37.859677 -11.642983 10.903057  
H -39.862402 -13.546984 2.782579  
H -35.561937 -6.777010 4.005957  
H -42.064162 -7.836345 5.108069  
C -39.925779 -6.988120 7.484042  
H -40.522422 -6.076965 7.577013  
H -38.886173 -6.736405 7.720383  
H -39.952700 -7.330996 6.447070  
H -41.526193 -6.970871 10.058543

***trans*-(4-Melm)<sub>2</sub>(5-Melm)<sub>2</sub>, ferrous, IEFPCM,  
TPSSh, *G*<sup>o</sup> = -2763.805797**

C -44.201733 -13.890040 7.306570  
C -42.832743 -13.336094 7.077254  
N -41.677665 -14.081975 7.234759  
C -40.609510 -13.294572 6.944756  
N -41.006295 -12.075009 6.604671  
C -42.389620 -12.092416 6.687381  
C -40.768951 -8.723960 10.216312  
N -40.116562 -9.910772 10.480761  
C -39.762318 -10.465725 9.300706  
N -40.147121 -9.695334 8.285733  
C -40.785528 -8.592190 8.846851  
C -35.470232 -6.781650 4.372502  
C -36.495172 -7.464969 5.218159  
N -36.713147 -7.148171 6.549168  
C -37.704158 -7.940379 7.028536  
N -38.148101 -8.756729 6.080391  
C -37.398478 -8.467060 4.950954  
C -40.929358 -7.673137 4.235787  
S -41.288016 -9.433959 4.645989  
C -39.272998 -12.697838 3.520144  
C -38.156153 -12.557013 4.505022  
N -38.203578 -11.672552 5.579536  
C -37.052523 -11.806055 6.235724  
N -36.272902 -12.731459 5.638543  
C -36.950590 -13.218386 4.538120  
Fe -39.748132 -10.263347 6.216311  
H -44.409776 -14.733222 6.638717  
H -44.946086 -13.113708 7.117896  
H -42.972769 -11.213988 6.454588  
H -39.589142 -13.642311 6.987698  
H -39.243398 -11.408155 9.219813  
H -35.666299 -5.706516 4.297282  
H -34.462407 -6.911452 4.781683  
H -37.553792 -8.997815 4.023359  
H -38.061370 -7.895363 8.045476  
H -39.852798 -7.498099 4.173830

H -41.352713 -7.005440 4.991207  
H -39.548123 -11.725270 3.100920  
H -40.167918 -13.112470 3.995631  
H -36.525216 -13.969095 3.891327  
H -35.350143 -13.012326 5.944798  
H -36.758832 -11.255575 7.115909  
H -39.938526 -10.304836 11.395679  
H -41.630369 -15.053360 7.515812  
H -36.216971 -6.443896 7.081091  
H -44.325583 -14.239860 8.337339  
H -38.973282 -13.362614 2.706260  
H -35.487383 -7.203617 3.365623  
H -41.383360 -7.435967 3.269649  
H -41.157440 -8.096898 11.002950  
C -41.374770 -7.492287 8.021797  
H -40.599814 -6.950960 7.468288  
H -42.081685 -7.892754 7.288148  
H -41.897123 -6.779292 8.664292

***trans*-(4-Melm)<sub>2</sub>(5-Melm)<sub>2</sub>, ferric, IEFPCM, PBE0,  
*G*<sup>o</sup> = -2990.250693**

C -37.317941 -12.565666 10.140340  
C -37.186793 -11.866087 8.800462  
O -36.066671 -11.642139 8.318256  
O -38.310992 -11.542146 8.258456  
C -43.933372 -14.037391 6.749867  
C -42.577790 -13.460406 6.942677  
N -41.545208 -14.141597 7.549621  
C -40.456423 -13.352351 7.575413  
N -40.722952 -12.186500 7.009798  
C -42.041237 -12.244670 6.610623  
C -41.130374 -7.828768 9.518399  
N -41.368872 -9.072824 10.047320  
C -40.817617 -9.985675 9.236181  
N -40.231466 -9.395580 8.203099  
C -40.414481 -8.030179 8.366824  
C -35.328512 -6.668623 5.161010  
C -36.166814 -7.637318 5.913913  
N -36.047275 -7.843913 7.272435  
C -36.935895 -8.779370 7.650866  
N -37.636133 -9.192425 6.609803  
C -37.166570 -8.486710 5.521878  
C -41.970534 -8.898678 5.361350  
S -40.383034 -9.641542 4.864764  
C -39.914061 -13.014221 3.817784  
C -38.513318 -12.723810 4.228092  
N -38.155604 -11.889370 5.279498  
C -36.830547 -11.924616 5.362331  
N -36.325173 -12.727432 4.416572  
C -37.367748 -13.243310 3.685689  
Fe -39.249410 -10.623305 6.683292

H -36.337928 -12.813986 10.550338  
H -37.907789 -13.481441 10.030651  
H -43.899662 -14.941532 6.132844  
H -44.575644 -13.309125 6.250891  
H -42.520609 -11.421584 6.104560  
H -39.509197 -13.635714 8.005673  
H -40.851623 -11.049072 9.414125  
H -35.457999 -5.648415 5.537577  
H -34.264713 -6.919186 5.231424  
H -37.583285 -8.625569 4.535478  
H -37.041379 -9.129022 8.665120  
H -42.131507 -8.978218 6.438275  
H -42.787628 -9.400940 4.836003  
H -40.470360 -12.092701 3.626224  
H -40.451186 -13.561526 4.598947  
H -37.215998 -13.924447 2.862611  
H -35.344320 -12.921353 4.277661  
H -36.244130 -11.430988 6.125522  
H -41.876624 -9.273082 10.896777  
H -41.590381 -15.079854 7.921789  
H -35.398028 -7.376461 7.889342  
H -44.396363 -14.301575 7.706496  
H -37.855665 -11.920355 10.842315  
H -39.912217 -13.626269 2.912345  
H -35.611002 -6.679748 4.106467  
H -41.983626 -7.842147 5.081118  
H -41.477979 -6.923606 9.991935  
C -39.878277 -6.995562 7.438930  
H -38.827171 -6.773664 7.652530  
H -39.934568 -7.330412 6.400768  
H -40.445058 -6.067350 7.546261

***trans*-(4-Melm)<sub>2</sub>(5-Melm)<sub>2</sub>, ferrous, IEFPCM,  
PBE0, *G*<sup>o</sup> = -2762.057395**

C -44.176791 -13.962786 7.198439  
C -42.820638 -13.380650 7.019926  
N -41.661641 -14.092909 7.223983  
C -40.608475 -13.285039 6.973226  
N -41.019227 -12.083253 6.614700  
C -42.395745 -12.131354 6.642362  
C -40.717606 -8.693175 10.231090  
N -40.127375 -9.903723 10.495574  
C -39.795783 -10.471112 9.323916  
N -40.136376 -9.686320 8.313244  
C -40.720571 -8.560340 8.865800  
C -35.503217 -6.810295 4.353805  
C -36.518342 -7.477842 5.209888  
N -36.688393 -7.188279 6.544801  
C -37.683924 -7.959404 7.031214  
N -38.175665 -8.734778 6.082895  
C -37.455157 -8.443917 4.945361

C	-40.952792	-7.685390	4.263178	C	-41.097757	-9.987429	9.085521
S	-41.370947	-9.404389	4.723025	N	-40.366017	-9.364336	8.148251
C	-39.264398	-12.691734	3.571425	C	-40.479361	-7.989687	8.399072
C	-38.152521	-12.542430	4.549737	C	-35.201677	-6.727091	5.085283
N	-38.202861	-11.659497	5.613254	C	-36.075193	-7.662595	5.859933
C	-37.057088	-11.781462	6.266180	N	-35.941412	-7.874539	7.230776
N	-36.276307	-12.700968	5.677323	C	-36.873202	-8.782141	7.630003
C	-36.946945	-13.195402	4.585530	N	-37.616100	-9.171355	6.587893
Fe	-39.765998	-10.263445	6.242003	C	-37.127241	-8.478878	5.483610
H	-44.340235	-14.814333	6.529146	C	-41.671001	-8.403556	5.082951
H	-44.933581	-13.207581	6.976539	S	-40.309912	-9.598084	4.760803
H	-42.993396	-11.269230	6.382410	C	-39.934207	-12.859237	3.591236
H	-39.580610	-13.607246	7.054769	C	-38.542902	-12.688064	4.121656
H	-39.322691	-11.438841	9.243725	N	-38.203191	-11.900152	5.232160
H	-35.667975	-5.728601	4.304447	C	-36.878096	-12.032023	5.410481
H	-34.487972	-6.976778	4.729543	N	-36.358038	-12.857239	4.467685
H	-37.647108	-8.947763	4.008442	C	-37.388539	-13.282982	3.642678
H	-38.011428	-7.929484	8.060192	Fe	-39.286527	-10.584689	6.659896
H	-39.895307	-7.587399	4.005715	H	-36.478822	-12.514255	10.817344
H	-41.172310	-6.992505	5.080808	H	-38.119228	-13.107526	10.377738
H	-39.556556	-11.720443	3.160628	H	-39.184242	-13.646821	7.625579
H	-40.152768	-13.122977	4.044536	H	-41.220509	-11.062626	9.180577
H	-36.520507	-13.946999	3.939262	H	-35.278700	-5.691900	5.462019
H	-35.353725	-12.972783	5.984333	H	-34.139482	-7.024585	5.138121
H	-36.766506	-11.222254	7.143549	H	-37.568885	-8.606614	4.497671
H	-39.975222	-10.307212	11.408437	H	-36.977796	-9.123609	8.655084
H	-41.602251	-15.059908	7.509296	H	-41.959557	-8.396678	6.144249
H	-36.158383	-6.512825	7.076849	H	-42.541897	-8.685052	4.469433
H	-44.334195	-14.310075	8.225270	H	-40.358456	-11.901300	3.245988
H	-38.960655	-13.344267	2.749471	H	-40.614021	-13.252571	4.365945
H	-35.558765	-7.208421	3.338625	H	-37.221286	-13.958676	2.807408
H	-41.550089	-7.388640	3.396316	H	-35.377715	-13.125925	4.393476
H	-41.082213	-8.045926	11.013760	H	-36.313241	-11.612222	6.245162
C	-41.248886	-7.439043	8.041776	H	-42.285698	-9.303608	10.700002
H	-40.442937	-6.913260	7.518081	H	-41.053478	-15.395194	7.619689
H	-41.942299	-7.811012	7.280635	H	-35.257963	-7.427288	7.841790
H	-41.770380	-6.716640	8.674054	H	-37.910481	-11.430594	10.918675

**(4-Melm)<sub>3</sub>(5-Melm)<sub>1</sub>, ferric, IEFPCM, BP86,  
G° = -2992.367234**

C	-37.433891	-12.243248	10.343593	H	-39.925010	-13.566381	2.746553
C	-37.222705	-11.798879	8.894783	H	-35.503935	-6.728353	4.027069
O	-36.068112	-11.767201	8.397254	H	-41.348468	-7.393165	4.784014
O	-38.317434	-11.473824	8.261452	H	-43.306977	-14.389861	6.903541
C	-42.377280	-13.829777	6.967223	C	-43.031508	-11.433136	6.254966
N	-41.185528	-14.418134	7.360720	H	-43.031084	-10.567255	6.938693
C	-40.219084	-13.465993	7.351441	H	-42.752527	-11.062169	5.254210
N	-40.724933	-12.284569	6.964669	H	-44.056514	-11.833155	6.206118
C	-42.087478	-12.499128	6.715774	H	-41.640846	-6.915866	10.009607
C	-41.302669	-7.814292	9.499298	C	-39.768152	-6.926752	7.615574
N	-41.675164	-9.082404	9.914040	H	-38.743357	-6.766964	7.994667
				H	-39.682563	-7.199766	6.553612
				H	-40.308409	-5.970021	7.695148

**(4-Melm)<sub>3</sub>(5-Melm)<sub>1</sub>, ferrous, IEFPCM, BP86,  
G° = -2763.916127**

C -42.714837 -13.498740 7.341933  
N -41.541503 -14.213321 7.165011  
C -40.579773 -13.342982 6.748036  
N -41.071200 -12.100705 6.645885  
C -42.417074 -12.182878 7.022880  
C -40.868878 -8.533005 10.091117  
N -40.349561 -9.775514 10.416345  
C -40.026659 -10.415589 9.259256  
N -40.304940 -9.641071 8.200607  
C -40.839112 -8.451112 8.708007  
C -35.393660 -6.820364 4.528731  
C -36.448826 -7.506671 5.338333  
N -36.679581 -7.230744 6.683090  
C -37.706770 -8.015010 7.122082  
N -38.160574 -8.789857 6.131403  
C -37.381777 -8.479883 5.020368  
C -40.817848 -7.683385 4.079023  
S -41.132253 -9.471855 4.447115  
C -39.312745 -12.605737 3.371169  
C -38.204562 -12.477887 4.371321  
N -38.287684 -11.662322 5.506243  
C -37.129480 -11.805737 6.166929  
N -36.312445 -12.671465 5.512206  
C -36.969570 -13.106750 4.371818  
Fe -39.822335 -10.246847 6.183879  
H -39.558025 -13.643724 6.531596  
H -39.609718 -11.419443 9.224328  
H -35.561399 -5.729769 4.481151  
H -34.385410 -6.985475 4.948038  
H -37.537678 -8.976838 4.064304  
H -38.082658 -7.995165 8.142672  
H -39.757470 -7.429512 4.235621  
H -41.437907 -7.036902 4.721396  
H -39.679783 -11.612377 3.061620  
H -40.175893 -13.148954 3.795885  
H -36.514673 -13.806351 3.674884  
H -35.376201 -12.944836 5.808437  
H -36.854146 -11.300741 7.089924  
H -40.234450 -10.151672 11.356601  
H -41.416168 -15.213626 7.313959  
H -36.168818 -6.554396 7.250644  
H -38.964138 -13.157240 2.483703  
H -35.402835 -7.211287 3.499901  
H -41.080731 -7.485219 3.026973  
C -43.336653 -10.999586 7.059693  
H -44.366494 -11.324421 7.278641  
H -43.029106 -10.278139 7.836948  
H -43.325773 -10.460585 6.097102  
H -43.637164 -13.972616 7.669864

H -41.212297 -7.833582 10.849457  
C -41.301070 -7.330641 7.826959  
H -42.063639 -7.680721 7.109687  
H -41.736838 -6.521337 8.433557  
H -40.468672 -6.909400 7.236692

**(4-Melm)<sub>3</sub>(5-Melm)<sub>1</sub>, ferric, IEFPCM, TPSSh,  
G° = -2992.252717**

C -37.234051 -12.101343 10.117481  
C -37.189898 -11.509671 8.712771  
O -36.109733 -11.092144 8.241538  
O -38.330096 -11.485749 8.096266  
C -42.520259 -13.699496 7.401292  
N -41.311026 -14.365227 7.356186  
C -40.344247 -13.462997 7.100458  
N -40.866052 -12.243036 6.972290  
C -42.242450 -12.374941 7.161560  
C -41.497564 -8.260719 9.830567  
N -41.184008 -9.476939 10.403806  
C -40.512498 -10.209992 9.493872  
N -40.378076 -9.532743 8.353261  
C -40.999080 -8.297554 8.549595  
C -35.133741 -7.074882 5.037916  
C -36.236360 -7.762145 5.775101  
N -36.548452 -7.491775 7.098601  
C -37.586727 -8.270557 7.472670  
N -37.977864 -9.034567 6.457974  
C -37.139225 -8.726052 5.397241  
C -40.167163 -8.310957 4.041196  
S -40.907018 -9.681935 5.001860  
C -40.013839 -12.679756 3.465222  
C -38.644076 -12.570268 4.055652  
N -38.337821 -11.859271 5.218752  
C -37.029206 -12.016981 5.431142  
N -36.487012 -12.783703 4.463817  
C -37.489149 -13.148873 3.586316  
Fe -39.468052 -10.583881 6.622031  
H -36.228874 -12.339721 10.469739  
H -37.861955 -12.996480 10.139853  
H -39.296655 -13.704548 7.026326  
H -40.136359 -11.204005 9.670495  
H -35.303444 -5.994144 4.983517  
H -34.166095 -7.239998 5.523709  
H -37.235248 -9.214570 4.440424  
H -38.014067 -8.266458 8.462293  
H -40.974775 -7.773393 3.539702  
H -39.484381 -8.710029 3.286913  
H -40.380054 -11.707532 3.122646  
H -40.733690 -13.054743 4.199010  
H -37.301612 -13.777155 2.730043  
H -35.512625 -13.049667 4.402975

H -36.480273 -11.600011 6.268335  
H -41.408915 -9.770283 11.345941  
H -41.168375 -15.357373 7.496232  
H -36.077716 -6.823349 7.696170  
H -37.679396 -11.368377 10.800298  
H -39.991122 -13.368563 2.616567  
H -35.076982 -7.464247 4.019554  
H -39.622339 -7.627975 4.694952  
H -43.448911 -14.211153 7.597762  
C -43.211097 -11.235938 7.110580  
H -44.207529 -11.591803 7.384101  
H -42.923697 -10.439329 7.803047  
H -43.260832 -10.798149 6.109195  
H -42.029794 -7.492959 10.369334  
C -41.079863 -7.224545 7.511659  
H -40.087884 -6.959398 7.132923  
H -41.681229 -7.549741 6.656957  
H -41.534888 -6.329382 7.943172

**(4-Melm)<sub>3</sub>(5-Melm)<sub>1</sub>, ferrous, IEFPCM, TPSSh,  
*G*<sup>o</sup> = -2763.801979**

C -42.815124 -13.412847 7.230182  
N -41.685233 -14.168382 6.990954  
C -40.692729 -13.326775 6.621832  
N -41.118490 -12.066261 6.610777  
C -42.456466 -12.104767 6.998216  
C -40.747804 -8.585306 10.123024  
N -40.204696 -9.817654 10.424263  
C -39.914191 -10.442506 9.260655  
N -40.235725 -9.674638 8.222996  
C -40.765193 -8.499726 8.749744  
C -35.469464 -6.868559 4.387475  
C -36.515994 -7.528461 5.225373  
N -36.693045 -7.254758 6.572092  
C -37.722564 -8.005880 7.036859  
N -38.227699 -8.757017 6.065875  
C -37.479072 -8.466648 4.936075  
C -40.956531 -7.710066 4.098945  
S -41.115168 -9.537549 4.281692  
C -39.096259 -12.610641 3.383653  
C -38.077781 -12.496750 4.473628  
N -38.248531 -11.679445 5.588794  
C -37.156003 -11.825478 6.335504  
N -36.297239 -12.694187 5.758799  
C -36.860320 -13.129881 4.576383  
Fe -39.850470 -10.260323 6.137765  
H -39.696920 -13.659435 6.376466  
H -39.484197 -11.430689 9.208186  
H -35.606886 -5.782093 4.358463  
H -34.463204 -7.069565 4.770974  
H -37.683067 -8.948931 3.991617

H -38.060224 -7.980198 8.061203  
H -39.947444 -7.379980 4.356158  
H -41.675310 -7.193450 4.740039  
H -39.335622 -11.627716 2.967129  
H -40.032281 -13.039408 3.758096  
H -36.358488 -13.830536 3.928130  
H -35.397930 -12.971717 6.130588  
H -36.956283 -11.324665 7.270030  
H -40.051276 -10.193055 11.351384  
H -41.609488 -15.174190 7.069903  
H -36.147465 -6.603557 7.123049  
H -38.718836 -13.254340 2.585122  
H -35.527732 -7.247701 3.365191  
H -41.162021 -7.443387 3.058808  
C -43.303027 -10.877998 7.129362  
H -42.985808 -10.270239 7.983485  
H -43.220035 -10.256905 6.232164  
H -44.349720 -11.157295 7.277051  
H -43.748210 -13.859576 7.535599  
C -41.276040 -7.390196 7.885837  
H -42.115697 -7.729181 7.269608  
H -41.616926 -6.556488 8.504412  
H -40.498047 -7.024711 7.208257  
H -41.070524 -7.899478 10.890202

**(4-Melm)<sub>3</sub>(5-Melm)<sub>1</sub>, ferric, IEFPCM, PBE0,  
*G*<sup>o</sup> = -2990.246700**

C -37.233036 -12.053630 10.105039  
C -37.203203 -11.487286 8.697926  
O -36.136698 -11.065101 8.220860  
O -38.338371 -11.490228 8.091849  
C -42.509238 -13.677334 7.377357  
N -41.311954 -14.347456 7.320920  
C -40.343859 -13.454025 7.077663  
N -40.853293 -12.234584 6.967118  
C -42.221850 -12.355649 7.156553  
C -41.493026 -8.262996 9.796189  
N -41.189773 -9.473005 10.369351  
C -40.512481 -10.203266 9.472483  
N -40.364695 -9.530247 8.338741  
C -40.980580 -8.300685 8.525063  
C -35.125024 -7.103080 5.071212  
C -36.230168 -7.781343 5.796813  
N -36.549090 -7.512972 7.110123  
C -37.588859 -8.282750 7.472829  
N -37.974833 -9.038797 6.459375  
C -37.131803 -8.736777 5.410442  
C -40.132408 -8.348447 4.049832  
S -40.900655 -9.690578 5.002637  
C -40.011978 -12.690883 3.495511  
C -38.645529 -12.569287 4.072498



N -38.331046 -11.851112 5.218918  
 C -37.026955 -12.004959 5.420859  
 N -36.494522 -12.775492 4.461771  
 C -37.496948 -13.148503 3.600374  
 Fe -39.460935 -10.580551 6.613037  
 H -36.224298 -12.262440 10.465025  
 H -37.840982 -12.961705 10.143609  
 H -39.297161 -13.703154 6.997736  
 H -40.138609 -11.198790 9.653376  
 H -35.286930 -6.021403 5.015383  
 H -34.160597 -7.272901 5.561361  
 H -37.219428 -9.221631 4.449980  
 H -38.024530 -8.278130 8.460265  
 H -40.919851 -7.819378 3.507948  
 H -39.420909 -8.750995 3.324075  
 H -40.393475 -11.722064 3.161231  
 H -40.723831 -13.075678 4.232297  
 H -37.319940 -13.784304 2.746574  
 H -35.522389 -13.039597 4.397128  
 H -36.472114 -11.581487 6.252268  
 H -41.425011 -9.766200 11.306432  
 H -41.176143 -15.340128 7.445823  
 H -36.080349 -6.849846 7.711183  
 H -37.697438 -11.320758 10.774870  
 H -39.990760 -13.376638 2.644650  
 H -35.061557 -7.490074 4.052331  
 H -39.612570 -7.645489 4.703732  
 H -43.444453 -14.180310 7.568956  
 C -43.178586 -11.215317 7.130146  
 H -42.898639 -10.442078 7.851943  
 H -43.212761 -10.742324 6.144521  
 H -44.181242 -11.571712 7.378319  
 H -42.030225 -7.490846 10.325070  
 C -41.044705 -7.229269 7.494870  
 H -40.046735 -6.949365 7.143095  
 H -41.616912 -7.557480 6.621837  
 H -41.520715 -6.340160 7.915574

**(4-Melm)<sub>3</sub>(5-Melm)<sub>1</sub>, ferrous, IEFPCM, PBE0,  
G° = -2762.054185**

C -42.814804 -13.398994 7.221508  
 N -41.691606 -14.153473 6.991397  
 C -40.701398 -13.320620 6.623574  
 N -41.122281 -12.065920 6.604287  
 C -42.452883 -12.096947 6.984361  
 C -40.801488 -8.608854 10.114278  
 N -40.234270 -9.820554 10.419923  
 C -39.917535 -10.435028 9.266081  
 N -40.246040 -9.680371 8.230500  
 C -40.806578 -8.525568 8.744616  
 C -36.475798 -7.557601 5.342261

N -36.734466 -7.239400 6.656664  
 C -37.770650 -7.989183 7.087231  
 N -38.202809 -8.781349 6.123767  
 C -37.400963 -8.521629 5.033564  
 C -40.850374 -7.691594 4.115895  
 S -41.091268 -9.498272 4.266429  
 C -39.123020 -12.631434 3.412111  
 C -38.097155 -12.515947 4.484813  
 N -38.246930 -11.691109 5.585776  
 C -37.153717 -11.836491 6.318230  
 N -36.312381 -12.714343 5.746274  
 C -36.887492 -13.156628 4.581079  
 Fe -39.847845 -10.264587 6.139661  
 H -39.703850 -13.656267 6.383434  
 H -39.461626 -11.413296 9.217924  
 H -38.168764 -7.933213 8.089791  
 H -39.815022 -7.412320 4.327336  
 H -41.506152 -7.147361 4.800856  
 H -39.374777 -11.648278 3.003077  
 H -40.052877 -13.066889 3.794200  
 H -36.400956 -13.868073 3.931700  
 H -35.413271 -12.992681 6.111254  
 H -36.940534 -11.324214 7.245113  
 H -40.082086 -10.191572 11.346391  
 H -41.617592 -15.156529 7.075312  
 H -36.234610 -6.559533 7.211794  
 H -38.754828 -13.268935 2.604614  
 H -41.091375 -7.383741 3.094719  
 C -43.292308 -10.873272 7.105881  
 H -44.341307 -11.145244 7.248677  
 H -42.978301 -10.262617 7.959191  
 H -43.202538 -10.253977 6.207975  
 H -43.752548 -13.838049 7.526140  
 H -41.150599 -7.927222 10.874631  
 C -41.329540 -7.433554 7.878209  
 H -40.548112 -7.035451 7.222863  
 H -42.139207 -7.796129 7.235693  
 H -41.716261 -6.614681 8.489264  
 C -35.397945 -6.914587 4.546011  
 H -35.548587 -5.832591 4.466495  
 H -34.412418 -7.082662 4.993398  
 H -35.387625 -7.330542 3.536517  
 H -37.537085 -9.041931 4.095942

**(4-Melm)<sub>4</sub>(5-Melm)<sub>0</sub>, ferric, IEFPCM, BP86,  
G° = -2992.362166**

C -37.391442 -12.131625 10.274071  
 C -37.222299 -11.737895 8.805353  
 O -36.078736 -11.703683 8.281231  
 O -38.336978 -11.465136 8.183863  
 C -42.359161 -13.875925 7.019811

N -41.132348 -14.446566 7.320377  
 C -40.188322 -13.473333 7.268969  
 N -40.742161 -12.294999 6.944051  
 C -42.113273 -12.534237 6.780715  
 C -41.310062 -7.865136 9.570029  
 N -41.573191 -9.150048 10.016054  
 C -40.985774 -10.025710 9.163343  
 N -40.352868 -9.366646 8.179838  
 C -40.542905 -7.999332 8.424130  
 C -35.981572 -7.650240 6.164238  
 N -36.143788 -7.801377 7.532612  
 C -37.142985 -8.693942 7.742942  
 N -37.642187 -9.126811 6.576611  
 C -36.919012 -8.476456 5.566975  
 C -41.928913 -8.422156 5.258623  
 S -40.517354 -9.520811 4.833274  
 C -40.056172 -12.661443 3.458409  
 C -38.667780 -12.581570 4.016898  
 N -38.305958 -11.844269 5.154482  
 C -36.993825 -12.056601 5.355589  
 N -36.503304 -12.883756 4.398940  
 C -37.539172 -13.228087 3.543440  
 Fe -39.344959 -10.550439 6.610298  
 H -36.419681 -12.351306 10.740395  
 H -38.044934 -13.017488 10.352674  
 H -39.134421 -13.637717 7.471599  
 H -41.028611 -11.105600 9.273601  
 H -37.483618 -8.994488 8.729399  
 H -42.154742 -8.450512 6.334427  
 H -42.814099 -8.747217 4.689048  
 H -40.410627 -11.680259 3.100460  
 H -40.774671 -13.004588 4.222015  
 H -37.394003 -13.891544 2.694352  
 H -35.538213 -13.205335 4.334806  
 H -36.421488 -11.685937 6.210956  
 H -42.121306 -9.400387 10.838458  
 H -40.963266 -15.425794 7.547630  
 H -35.607582 -7.328113 8.258790  
 H -37.887504 -11.315016 10.826600  
 H -40.076878 -13.371736 2.616573  
 H -41.684580 -7.389521 4.962392  
 H -43.279797 -14.454121 7.005008  
 C -43.108467 -11.480510 6.408312  
 H -43.070269 -10.623478 7.101723  
 H -42.916255 -11.093100 5.393512  
 H -44.127086 -11.898718 6.433213  
 H -41.675965 -6.985180 10.093251  
 C -39.947804 -6.904451 7.587401  
 H -38.966307 -6.586339 7.981383  
 H -39.791696 -7.238677 6.551234  
 H -40.606867 -6.021508 7.582577  
 H -35.230404 -6.988680 5.739800

C -37.146861 -8.678559 4.100298  
 H -36.956083 -9.723147 3.800004  
 H -38.189994 -8.448161 3.824010  
 H -36.473149 -8.025207 3.523577

**(4-Melm)<sub>4</sub>(5-Melm)<sub>0</sub>, ferrous, IEFPCM, BP86,  
 G° = -2763.912420**

C -42.738214 -13.464525 7.388322  
 N -41.573218 -14.195916 7.226564  
 C -40.604683 -13.346927 6.781782  
 N -41.083075 -12.102925 6.646250  
 C -42.427882 -12.161136 7.031516  
 C -40.851223 -8.563718 10.053529  
 N -40.311463 -9.799228 10.371699  
 C -39.976367 -10.426596 9.211404  
 N -40.266562 -9.650505 8.156823  
 C -40.821533 -8.472580 8.671027  
 C -36.414692 -7.429695 5.431886  
 N -36.703045 -7.222203 6.771863  
 C -37.714871 -8.061822 7.119916  
 N -38.097597 -8.804106 6.071473  
 C -37.282689 -8.419458 4.999297  
 C -40.855005 -7.682431 4.105848  
 S -41.140523 -9.483817 4.434407  
 C -39.381408 -12.711249 3.419820  
 C -38.258540 -12.585631 4.403307  
 N -38.300108 -11.721583 5.503963  
 C -37.138174 -11.873714 6.156142  
 N -36.358105 -12.791730 5.528093  
 C -37.044480 -13.253573 4.415528  
 Fe -39.791289 -10.256383 6.138352  
 H -39.587325 -13.665625 6.570418  
 H -39.542339 -11.422932 9.171319  
 H -38.140423 -8.103798 8.119582  
 H -39.837497 -7.383232 4.403941  
 H -41.582257 -7.067532 4.660790  
 H -39.703127 -11.718501 3.062020  
 H -40.264977 -13.189591 3.878479  
 H -36.620975 -13.995096 3.742605  
 H -35.427294 -13.083144 5.824440  
 H -36.835298 -11.340231 7.054089  
 H -40.191322 -10.179442 11.309720  
 H -41.457661 -15.193038 7.402269  
 H -36.245255 -6.553080 7.389609  
 H -39.067813 -13.322097 2.558627  
 H -40.983051 -7.487158 3.028525  
 C -43.336183 -10.968610 7.044364  
 H -44.369884 -11.279948 7.265095  
 H -43.025152 -10.237269 7.811065  
 H -43.315613 -10.445555 6.073328  
 H -43.663868 -13.919414 7.733409

H -41.206992 -7.874683 10.815642  
 C -41.297460 -7.351767 7.798056  
 H -42.057460 -7.704775 7.079712  
 H -41.740520 -6.551444 8.411242  
 H -40.470860 -6.917174 7.209197  
 H -35.638693 -6.870112 4.914850  
 C -37.375427 -9.038813 3.637375  
 H -36.937238 -10.052418 3.624481  
 H -38.428313 -9.138383 3.323520  
 H -36.835633 -8.424450 2.899180

**(4-Melm)<sub>4</sub>(5-Melm)<sub>0</sub>, ferric, IEFPCM, TPSSh,  
 G° = -2992.246344**

C -37.202942 -12.037467 10.095804  
 C -37.153056 -11.469831 8.681838  
 O -36.068192 -11.078988 8.199288  
 O -38.294911 -11.436766 8.067791  
 C -42.522031 -13.646524 7.421377  
 N -41.319484 -14.325459 7.413962  
 C -40.343486 -13.447137 7.115130  
 N -40.852167 -12.229515 6.923623  
 C -42.230765 -12.338301 7.116804  
 C -41.527006 -8.335947 9.799075  
 N -41.185309 -9.553568 10.352609  
 C -40.494478 -10.254508 9.432133  
 N -40.373070 -9.556007 8.302517  
 C -41.025688 -8.340976 8.519034  
 C -36.297937 -7.605537 5.778492  
 N -36.619983 -7.433761 7.109367  
 C -37.593742 -8.308480 7.423916  
 N -37.924128 -9.039387 6.359232  
 C -37.109533 -8.611803 5.310202  
 C -40.347019 -8.055055 4.219799  
 S -40.831271 -9.683317 4.905432  
 C -40.039201 -12.784774 3.496989  
 C -38.672244 -12.719386 4.099960  
 N -38.345574 -11.978252 5.237530  
 C -37.047061 -12.182239 5.469782  
 N -36.530358 -13.009573 4.538760  
 C -37.539351 -13.365268 3.665745  
 Fe -39.427090 -10.589454 6.557021  
 H -36.199016 -12.269044 10.455817  
 H -37.829220 -12.933531 10.129287  
 H -39.298689 -13.703775 7.055820  
 H -40.093693 -11.240997 9.594487  
 H -38.031336 -8.393902 8.405085  
 H -41.214395 -7.391778 4.256476  
 H -40.046727 -8.181993 3.176920  
 H -40.350294 -11.808978 3.112249  
 H -40.785242 -13.094274 4.235182  
 H -37.372191 -14.035351 2.837396

H -35.567579 -13.318379 4.497681  
 H -36.483140 -11.746289 6.286746  
 H -41.404668 -9.868234 11.289122  
 H -41.186963 -15.310666 7.604208  
 H -36.204067 -6.763453 7.743448  
 H -37.653236 -11.294830 10.764648  
 H -40.042338 -13.506017 2.675599  
 H -39.525569 -7.614443 4.785675  
 H -43.456487 -14.138762 7.638865  
 C -43.191455 -11.196767 7.008842  
 H -44.193044 -11.537092 7.283738  
 H -42.907406 -10.375431 7.673109  
 H -43.224394 -10.797196 5.991164  
 H -42.079319 -7.590192 10.348417  
 C -41.139766 -7.257901 7.496082  
 H -40.161661 -6.990722 7.085292  
 H -41.775668 -7.571812 6.662807  
 H -41.578327 -6.366096 7.950843  
 H -35.541194 -7.011461 5.291537  
 C -37.137558 -9.206851 3.935611  
 H -36.411514 -10.021540 3.841320  
 H -38.124106 -9.616412 3.710564  
 H -36.888104 -8.447182 3.190110

**(4-Melm)<sub>4</sub>(5-Melm)<sub>0</sub>, ferrous, IEFPCM, TPSSh,  
 G° = -2763.798821**

C -42.713749 -13.459617 7.404234  
 N -41.552045 -14.183322 7.232202  
 C -40.599462 -13.336188 6.778509  
 N -41.080650 -12.102765 6.646165  
 C -42.415147 -12.165250 7.043842  
 C -40.841179 -8.552094 10.045462  
 N -40.309312 -9.784320 10.366583  
 C -39.979104 -10.411189 9.215463  
 N -40.263938 -9.644006 8.165690  
 C -40.811217 -8.467632 8.672532  
 C -36.426886 -7.465778 5.415637  
 N -36.704281 -7.256564 6.751888  
 C -37.717906 -8.078722 7.101526  
 N -38.112642 -8.811124 6.062275  
 C -37.302608 -8.438082 4.990968  
 C -40.851012 -7.674327 4.099058  
 S -41.188924 -9.461141 4.405113  
 C -39.366326 -12.714154 3.434523  
 C -38.248446 -12.590588 4.420165  
 N -38.292867 -11.722479 5.509245  
 C -37.139246 -11.867285 6.158684  
 N -36.361492 -12.783538 5.544489  
 C -37.043131 -13.253309 4.439304  
 Fe -39.806744 -10.262166 6.121434  
 H -39.590885 -13.648364 6.560733

H -39.549302 -11.400045 9.179662  
H -38.135362 -8.114927 8.095167  
H -39.841985 -7.406593 4.421435  
H -41.570714 -7.052290 4.637799  
H -39.638999 -11.733611 3.032782  
H -40.262973 -13.133506 3.903473  
H -36.620262 -13.993602 3.779000  
H -35.438160 -13.069918 5.844038  
H -36.841583 -11.332003 7.046750  
H -40.189741 -10.159286 11.298883  
H -41.429663 -15.172250 7.407304  
H -36.238866 -6.598890 7.364099  
H -39.069110 -13.368822 2.611542  
H -40.946826 -7.470853 3.029045  
C -43.324836 -10.977269 7.064550  
H -43.002707 -10.248305 7.815772  
H -43.325823 -10.468586 6.096199  
H -44.343702 -11.292089 7.305908  
H -43.625470 -13.915058 7.757679  
C -41.283738 -7.354586 7.791891  
H -42.071752 -7.700370 7.114887  
H -41.679184 -6.536515 8.398780  
H -40.469320 -6.964027 7.173019  
H -41.189948 -7.865195 10.800125  
H -35.653380 -6.918786 4.900003  
C -37.415596 -9.058893 3.633904  
H -36.940611 -10.045750 3.608349  
H -38.466633 -9.193534 3.360565  
H -36.927806 -8.427109 2.886820

**(4-Melm)<sub>4</sub>(5-Melm)<sub>0</sub>, ferric, IEFPCM, PBE0,  
*G*<sup>o</sup> = -2990.240566**

C -37.210548 -11.983272 10.093324  
C -37.168794 -11.449115 8.674401  
O -36.094590 -11.058218 8.188359  
O -38.302938 -11.444308 8.065810  
C -42.515577 -13.626147 7.391044  
N -41.326294 -14.311987 7.366421  
C -40.348011 -13.441996 7.084003  
N -40.842319 -12.222070 6.918264  
C -42.212864 -12.318727 7.113264  
C -41.521956 -8.338166 9.765908  
N -41.186844 -9.547835 10.321389  
C -40.490603 -10.246414 9.414144  
N -40.359478 -9.554198 8.289458  
C -41.009505 -8.345754 8.494624  
C -36.286774 -7.640465 5.778475  
N -36.613426 -7.458396 7.098773  
C -37.589814 -8.319120 7.412038  
N -37.918187 -9.051774 6.356418  
C -37.100334 -8.641365 5.314280

C -40.315556 -8.076802 4.239450  
S -40.816506 -9.694093 4.901900  
C -40.023704 -12.788652 3.517619  
C -38.662032 -12.712250 4.113104  
N -38.334865 -11.976142 5.243435  
C -37.041405 -12.175305 5.469819  
N -36.527228 -12.994342 4.540885  
C -37.531353 -13.350668 3.674909  
Fe -39.420501 -10.589473 6.550867  
H -36.205177 -12.191524 10.462741  
H -37.824622 -12.886476 10.148125  
H -39.304961 -13.708286 7.014871  
H -40.090126 -11.233431 9.582159  
H -38.034260 -8.393978 8.392464  
H -41.176272 -7.403795 4.263224  
H -39.996308 -8.190896 3.200406  
H -40.351567 -11.813453 3.146523  
H -40.764455 -13.116088 4.253671  
H -37.368952 -14.019062 2.843367  
H -35.565514 -13.298240 4.497727  
H -36.476106 -11.738351 6.286860  
H -41.413720 -9.861039 11.254019  
H -41.202223 -15.299767 7.534954  
H -36.197711 -6.788776 7.729909  
H -37.673614 -11.233040 10.744508  
H -40.022881 -13.500680 2.688515  
H -39.501799 -7.637131 4.817659  
H -43.457066 -14.109426 7.601713  
C -43.159749 -11.172398 7.041368  
H -42.892048 -10.388155 7.755956  
H -43.162716 -10.716124 6.047643  
H -44.170629 -11.517985 7.271137  
H -42.080048 -7.588067 10.304772  
C -41.114525 -7.267350 7.476590  
H -40.133127 -6.989307 7.080983  
H -41.732700 -7.584356 6.631671  
H -41.567452 -6.379033 7.923541  
H -35.524196 -7.056631 5.286659  
C -37.122548 -9.235591 3.947179  
H -36.417769 -10.069607 3.862896  
H -38.114255 -9.620082 3.702208  
H -36.840848 -8.484817 3.204436

**(4-Melm)<sub>4</sub>(5-Melm)<sub>0</sub>, ferrous, IEFPCM, PBE0,  
*G*<sup>o</sup> = -2762.051367**

C -42.784969 -13.415631 7.303328  
N -41.670574 -14.173464 7.046617  
C -40.694404 -13.345329 6.631905  
N -41.115390 -12.090930 6.605372  
C -42.432436 -12.117243 7.032544  
C -40.803365 -8.590031 10.050155

N -40.256313 -9.810428 10.358483  
 C -39.933462 -10.425506 9.207153  
 N -40.238106 -9.662363 8.169921  
 C -40.790199 -8.501714 8.680993  
 C -36.449924 -7.475649 5.390441  
 N -36.738848 -7.245358 6.712644  
 C -37.753281 -8.054525 7.063113  
 N -38.137983 -8.798687 6.037746  
 C -37.322089 -8.449621 4.974924  
 C -40.880371 -7.707668 4.084809  
 S -41.196992 -9.491084 4.338674  
 C -39.188577 -12.677788 3.409054  
 C -38.152325 -12.581221 4.473102  
 N -38.268629 -11.734988 5.561910  
 C -37.174595 -11.898469 6.289866  
 N -36.364120 -12.808596 5.725444  
 C -36.961067 -13.254323 4.572175  
 Fe -39.818744 -10.269937 6.097558  
 H -39.706148 -13.687244 6.364369  
 H -39.491623 -11.410182 9.160466  
 H -38.180535 -8.074787 8.054481  
 H -39.839881 -7.452483 4.302780  
 H -41.525952 -7.100396 4.725337  
 H -39.412931 -11.691519 2.991519  
 H -40.128087 -13.080933 3.802225  
 H -36.499506 -13.989565 3.931207  
 H -35.470614 -13.107281 6.088485  
 H -36.940592 -11.377726 7.206896  
 H -40.121773 -10.187093 11.285454  
 H -41.592466 -15.175000 7.143426  
 H -36.278763 -6.581850 7.318437  
 H -38.844801 -13.333647 2.605648  
 H -41.090277 -7.447723 3.043545  
 C -43.274653 -10.896726 7.171232  
 H -44.315915 -11.175692 7.352712  
 H -42.936972 -10.275996 8.008008  
 H -43.220734 -10.283214 6.266926  
 H -43.711282 -13.849028 7.648482  
 H -41.153195 -7.906617 10.808536  
 C -41.285893 -7.399319 7.811925  
 H -40.485918 -6.995688 7.182524  
 H -42.077171 -7.754326 7.143281  
 H -41.686569 -6.585771 8.421115  
 H -35.669629 -6.942462 4.869162  
 C -37.420402 -9.087527 3.632925  
 H -36.986240 -10.093207 3.638788  
 H -38.466694 -9.187625 3.327557  
 H -36.886503 -8.491517 2.888391

**(4-Melm)<sub>0</sub>(5-Melm)<sub>4</sub>, ferric, SMD, BP86,**  
**G° = -2992.390799**

C -37.316872 -12.479438 10.193700  
 C -37.051071 -11.882961 8.816378  
 O -35.872532 -11.908278 8.343048  
 O -38.074087 -11.393882 8.188551  
 C -43.527876 -14.473944 6.359388  
 C -42.344979 -13.663348 6.776324  
 N -41.677155 -13.854634 7.983043  
 C -40.649729 -12.966869 8.065136  
 N -40.611523 -12.201098 6.965605  
 C -41.666161 -12.626583 6.160652  
 C -40.905502 -6.462648 10.354060  
 C -40.822927 -7.697801 9.518295  
 N -41.810143 -8.678991 9.506340  
 C -41.436876 -9.670446 8.652842  
 N -40.246493 -9.388371 8.107022  
 C -39.859613 -8.159400 8.638071  
 C -36.188373 -5.673888 5.495646  
 C -36.618146 -7.029451 5.951958  
 N -35.795499 -7.878571 6.687851  
 C -36.469190 -9.030484 6.951491  
 N -37.698348 -8.977674 6.418162  
 C -37.798263 -7.734396 5.795344  
 C -42.044255 -8.958192 5.422130  
 S -40.471583 -9.668743 4.793771  
 C -37.496611 -13.794427 2.020582  
 C -37.574165 -13.061957 3.320160  
 N -36.533230 -13.038703 4.245205  
 C -36.907460 -12.290950 5.317675  
 N -38.151630 -11.823595 5.138086  
 C -38.573901 -12.299906 3.897902  
 Fe -39.200334 -10.570461 6.586426  
 H -37.544435 -13.554481 10.073465  
 H -38.179112 -12.001833 10.684595  
 H -43.278816 -15.547560 6.286312  
 H -43.881967 -14.135442 5.373396  
 H -41.863847 -12.168611 5.193146  
 H -39.969074 -12.906745 8.910589  
 H -40.928712 -6.702519 11.432135  
 H -41.812805 -5.876892 10.123118  
 H -38.917266 -7.688857 8.365489  
 H -42.045032 -10.551209 8.463059  
 H -35.940658 -5.018601 6.349801  
 H -35.294966 -5.728996 4.848431  
 H -38.704749 -7.431557 5.274863  
 H -36.043797 -9.870513 7.501212  
 H -41.843904 -8.143895 6.137263  
 H -42.648898 -9.733333 5.921011  
 H -39.559629 -12.065499 3.500807  
 H -36.284305 -12.127288 6.198693

H -42.679694 -8.661384 10.043478  
H -41.917592 -14.549193 8.693761  
H -34.834549 -7.679428 6.973406  
H -38.441714 -13.672113 1.469264  
H -36.676685 -13.410761 1.387680  
H -35.629799 -13.504765 4.139120  
H -40.027897 -5.825992 10.163008  
H -36.999720 -5.198841 4.922849  
H -37.322758 -14.874443 2.173213  
H -44.360975 -14.373489 7.077702  
H -36.424491 -12.394362 10.833313  
H -42.612189 -8.555272 4.568325

**(4-Melm)<sub>0</sub>(5-Melm)<sub>4</sub>, ferrous, SMD, BP86,  
*G*<sup>o</sup> = -2763.927775**

C -43.435726 -14.256678 7.882725  
C -42.231801 -13.548517 7.351374  
N -41.121884 -14.214566 6.841126  
C -40.211168 -13.291040 6.419623  
N -40.664865 -12.050212 6.638035  
C -41.923844 -12.204865 7.220197  
C -41.778868 -6.325728 9.991129  
C -41.291344 -7.575259 9.332527  
N -41.089009 -8.768314 10.020685  
C -40.652419 -9.713359 9.138252  
N -40.559346 -9.198633 7.906832  
C -40.951984 -7.867207 8.021744  
C -34.837604 -6.988577 5.623456  
C -36.037287 -7.708904 6.148149  
N -36.411854 -7.688298 7.488786  
C -37.542821 -8.432955 7.638892  
N -37.929232 -8.944717 6.462967  
C -36.992872 -8.498600 5.531216  
C -42.815618 -9.116411 5.156940  
S -41.085255 -9.133657 4.499208  
C -37.918464 -13.506181 1.673193  
C -37.951280 -12.693715 2.927287  
N -36.870723 -12.587445 3.796255  
C -37.222504 -11.764900 4.830141  
N -38.476699 -11.325883 4.678340  
C -38.938179 -11.906167 3.498728  
Fe -39.739884 -10.156643 6.103687  
H -43.927917 -14.862942 7.101197  
H -44.166153 -13.521797 8.255303  
H -42.530671 -11.348019 7.506879  
H -39.253432 -13.557768 5.978910  
H -41.109281 -6.009620 10.810794  
H -42.788515 -6.458288 10.419851  
H -40.961780 -7.204352 7.157255  
H -40.415447 -10.733631 9.432583  
H -34.912205 -5.898465 5.786164

H -33.910534 -7.334569 6.114595  
H -37.060378 -8.766089 4.478531  
H -38.031527 -8.582306 8.599100  
H -42.861429 -8.651450 6.156070  
H -43.223809 -10.138765 5.222276  
H -39.944422 -11.710381 3.130897  
H -36.548239 -11.525376 5.649646  
H -41.243805 -8.914120 11.020290  
H -41.004683 -15.228229 6.790306  
H -35.922366 -7.199203 8.240824  
H -38.883078 -13.417859 1.149333  
H -37.123433 -13.164562 0.986438  
H -35.963474 -13.042967 3.682495  
H -41.825375 -5.510303 9.252651  
H -34.739012 -7.167592 4.541553  
H -37.738592 -14.575864 1.883326  
H -43.176117 -14.934844 8.715089  
H -43.454005 -8.531610 4.473384

**(4-Melm)<sub>0</sub>(5-Melm)<sub>4</sub>, ferric, SMD, TPSSh,  
*G*<sup>o</sup> = -2992.275180**

C -36.972550 -12.520277 10.116735  
C -37.123847 -12.012476 8.691974  
O -36.210576 -12.219026 7.851312  
O -38.234407 -11.400654 8.439437  
C -43.591454 -14.350758 6.408660  
C -42.333237 -13.644531 6.785540  
N -41.493804 -14.082410 7.797851  
C -40.443207 -13.239124 7.893392  
N -40.548511 -12.265940 6.988951  
C -41.728498 -12.512410 6.297393  
C -41.451290 -6.337567 9.930667  
C -41.136447 -7.665276 9.328954  
N -41.828140 -8.822946 9.645649  
C -41.314482 -9.850056 8.930952  
N -40.313952 -9.421994 8.166617  
C -40.199495 -8.060067 8.404899  
C -35.509261 -6.321746 5.420939  
C -36.267196 -7.402743 6.114241  
N -36.032227 -7.763624 7.432388  
C -36.864856 -8.773486 7.765901  
N -37.640164 -9.091390 6.732435  
C -37.274453 -8.238978 5.698749  
C -41.961150 -8.777118 5.578560  
S -40.454011 -9.609873 4.956379  
C -37.792507 -13.850173 2.123279  
C -37.754629 -12.891079 3.264669  
N -36.600303 -12.229115 3.655109  
C -36.880487 -11.448424 4.720854  
N -38.164507 -11.565725 5.050691  
C -38.716725 -12.462550 4.145497

Fe -39.195548 -10.590605 6.720980  
 H -37.560823 -13.439667 10.223298  
 H -37.362985 -11.793083 10.833830  
 H -43.387873 -15.375842 6.079953  
 H -44.079746 -13.817274 5.590240  
 H -42.052537 -11.868179 5.494450  
 H -39.648456 -13.356860 8.611717  
 H -41.345706 -6.359135 11.020845  
 H -42.476536 -6.028568 9.698791  
 H -39.463567 -7.455133 7.897893  
 H -41.684705 -10.860872 8.998864  
 H -35.646504 -5.356200 5.920257  
 H -34.435712 -6.539529 5.401761  
 H -37.757527 -8.286488 4.734746  
 H -36.887018 -9.224142 8.744828  
 H -41.706173 -7.816185 6.033288  
 H -42.471474 -9.398168 6.319232  
 H -39.759083 -12.738709 4.187969  
 H -36.144601 -10.833735 5.213396  
 H -42.592641 -8.894464 10.308833  
 H -41.639548 -14.903649 8.376037  
 H -35.345301 -7.343635 8.049753  
 H -38.805036 -14.243062 2.008167  
 H -37.500063 -13.365437 1.185327  
 H -35.689917 -12.315415 3.215603  
 H -40.767035 -5.584928 9.532805  
 H -35.861345 -6.230056 4.391222  
 H -37.112307 -14.692508 2.291386  
 H -44.287744 -14.400975 7.253012  
 H -35.929027 -12.747785 10.343201  
 H -42.631649 -8.602135 4.732990

**(4-Melm)<sub>0</sub>(5-Melm)<sub>4</sub>, ferrous, SMD, TPSSh,  
G° = -2763.813697**

C -43.426257 -14.270607 7.885745  
 C -42.228191 -13.558335 7.353330  
 N -41.135158 -14.218032 6.815953  
 C -40.230106 -13.297334 6.405560  
 N -40.668060 -12.066874 6.653473  
 C -41.914947 -12.223781 7.246181  
 C -41.763371 -6.304550 9.952896  
 C -41.284627 -7.562776 9.309809  
 N -41.110854 -8.748520 10.005784  
 C -40.675079 -9.698137 9.141574  
 N -40.556130 -9.197499 7.916948  
 C -40.930676 -7.865604 8.015867  
 C -34.835194 -7.008159 5.634678  
 C -36.037940 -7.720416 6.156774  
 N -36.415908 -7.689695 7.489747  
 C -37.542114 -8.425909 7.638391  
 N -37.923680 -8.941275 6.473143

C -36.986453 -8.505752 5.545455  
 C -42.824508 -9.137100 5.193598  
 S -41.121067 -9.151174 4.491108  
 C -37.917943 -13.484298 1.671651  
 C -37.951258 -12.676235 2.925691  
 N -36.873817 -12.571474 3.789036  
 C -37.223881 -11.760076 4.819790  
 N -38.470333 -11.326900 4.674819  
 C -38.931874 -11.898926 3.498406  
 Fe -39.728718 -10.164734 6.118177  
 H -43.920587 -14.857497 7.103421  
 H -44.143373 -13.543456 8.273307  
 H -42.506063 -11.374443 7.554188  
 H -39.288262 -13.559913 5.949822  
 H -41.101978 -5.996970 10.770469  
 H -42.771156 -6.424928 10.366280  
 H -40.920993 -7.216291 7.152218  
 H -40.458153 -10.711375 9.443246  
 H -34.908786 -5.926855 5.795860  
 H -33.920994 -7.357424 6.127576  
 H -37.051673 -8.779286 4.503255  
 H -38.031885 -8.564519 8.589578  
 H -42.840817 -8.684131 6.189048  
 H -43.228565 -10.151450 5.259596  
 H -39.931893 -11.705062 3.139185  
 H -36.554077 -11.523335 5.632215  
 H -41.282800 -8.886045 10.996172  
 H -41.026716 -15.223621 6.739183  
 H -35.932280 -7.201273 8.235948  
 H -38.876559 -13.395351 1.155329  
 H -37.129262 -13.139171 0.993747  
 H -35.971493 -13.019891 3.673286  
 H -41.789965 -5.502490 9.211846  
 H -34.737981 -7.190013 4.562052  
 H -37.737005 -14.544470 1.882085  
 H -43.157109 -14.955346 8.697610  
 H -43.473645 -8.549629 4.537127

**(4-Melm)<sub>0</sub>(5-Melm)<sub>4</sub>, ferric, SMD, PBE0,  
G° = -2990.270628**

C -36.983555 -12.598868 10.013755  
 C -37.131450 -12.056862 8.610211  
 O -36.234897 -12.255360 7.762803  
 O -38.213148 -11.399095 8.394899  
 C -43.556397 -14.323576 6.372783  
 C -42.311845 -13.614663 6.759109  
 N -41.493770 -14.034304 7.784595  
 C -40.451238 -13.192609 7.885017  
 N -40.542755 -12.237430 6.970423  
 C -41.703741 -12.491760 6.265244  
 C -41.390091 -6.361340 9.959341

C	-41.099588	-7.675335	9.334539
N	-41.866333	-8.798245	9.550534
C	-41.357299	-9.817906	8.835365
N	-40.289522	-9.418345	8.164938
C	-40.122071	-8.081704	8.464952
C	-35.638684	-6.193224	5.500178
C	-36.333163	-7.331686	6.149966
N	-36.002135	-7.797888	7.403478
C	-36.799935	-8.834859	7.708547
N	-37.642176	-9.073042	6.715271
C	-37.361126	-8.137350	5.738772
C	-41.933373	-8.768196	5.601298
S	-40.452376	-9.598660	4.953181
C	-37.740814	-14.025298	2.301854
C	-37.731962	-12.984827	3.359608
N	-36.646650	-12.172283	3.606525
C	-36.945459	-11.340833	4.619348
N	-38.177468	-11.565345	5.046694
C	-38.677695	-12.589494	4.267523
Fe	-39.191614	-10.571903	6.703135
H	-37.821959	-13.266402	10.240104
H	-37.022839	-11.775401	10.734251
H	-43.347682	-15.351555	6.056922
H	-44.036370	-13.801236	5.542269
H	-42.017298	-11.859317	5.447644
H	-39.667658	-13.298292	8.619540
H	-41.373202	-6.424762	11.052713
H	-42.376656	-5.988953	9.662069
H	-39.322237	-7.494764	8.037481
H	-41.781223	-10.811099	8.835926
H	-35.728358	-5.277507	6.094571
H	-34.571434	-6.401241	5.366528
H	-37.917037	-8.101238	4.813370
H	-36.748147	-9.368083	8.645174
H	-41.667475	-7.923821	6.243129
H	-42.555582	-9.463187	6.173087
H	-39.677120	-12.976362	4.404952
H	-36.253929	-10.608526	5.007864
H	-42.680837	-8.855254	10.149175
H	-41.647971	-14.845393	8.371031
H	-35.277560	-7.422500	8.002540
H	-38.695297	-14.556063	2.314012
H	-37.605107	-13.585785	1.307518
H	-35.763273	-12.195579	3.112303
H	-40.640984	-5.630690	9.646613
H	-36.076284	-6.007863	4.516736
H	-36.940138	-14.757085	2.454623
H	-44.265570	-14.367840	7.206507
H	-36.044983	-13.142313	10.134402
H	-42.518030	-8.393561	4.756405

**(4-Melm)<sub>0</sub>(5-Melm)<sub>4</sub>, ferrous, SMD, PBE0,  
G° = -2762.066214**

C	-43.382687	-14.280934	7.935981
C	-42.210771	-13.567862	7.369428
N	-41.166655	-14.214138	6.747757
C	-40.273627	-13.294229	6.332230
N	-40.674673	-12.076190	6.655222
C	-41.884036	-12.238008	7.302692
C	-41.763907	-6.311026	9.938028
C	-41.284587	-7.562174	9.299507
N	-41.062847	-8.726482	10.000909
C	-40.636507	-9.673336	9.140175
N	-40.570247	-9.190789	7.912188
C	-40.968681	-7.873638	8.001922
C	-34.805233	-7.090610	5.656170
C	-36.033886	-7.749542	6.165194
N	-36.482593	-7.607150	7.459187
C	-37.615865	-8.320157	7.604292
N	-37.935138	-8.926553	6.472604
C	-36.950320	-8.576580	5.569636
C	-42.840062	-9.182657	5.227250
S	-41.170704	-9.178379	4.481528
C	-37.872951	-13.394284	1.636693
C	-37.932840	-12.626575	2.905786
N	-36.922560	-12.634383	3.839901
C	-37.283518	-11.839189	4.869911
N	-38.475062	-11.311958	4.657992
C	-38.891211	-11.800699	3.437951
Fe	-39.739440	-10.163644	6.116929
H	-43.921171	-14.840858	7.163300
H	-44.074995	-13.561419	8.379035
H	-42.447212	-11.396683	7.680239
H	-39.362223	-13.552166	5.813165
H	-41.072802	-5.967369	10.715567
H	-42.746115	-6.448753	10.403670
H	-40.999840	-7.232834	7.131235
H	-40.387422	-10.679041	9.447366
H	-34.866552	-6.000906	5.750434
H	-33.915989	-7.422146	6.203771
H	-36.958239	-8.932385	4.549923
H	-38.161971	-8.371269	8.534313
H	-42.869408	-8.615229	6.162562
H	-43.182574	-10.201896	5.430884
H	-39.848481	-11.522628	3.019164
H	-36.656736	-11.678219	5.735438
H	-41.197673	-8.853566	10.996025
H	-41.082196	-15.214173	6.616728
H	-36.038200	-7.060510	8.185857
H	-38.769809	-13.196949	1.044888
H	-36.999730	-13.113909	1.037501
H	-36.048390	-13.139059	3.766025



H -41.850380 -5.522781 9.186659  
H -34.665040 -7.333628 4.600427  
H -37.816785 -14.472886 1.821902  
H -43.083138 -14.991655 8.713952  
H -43.548531 -8.724321 4.530141

**(4-Melm)<sub>1</sub>(5-Melm)<sub>3</sub>, ferric, SMD, BP86,  
G° = -2992.388631**

C -37.121063 -12.716764 10.139201  
C -37.122293 -12.244839 8.688115  
O -36.094615 -12.402363 7.965115  
O -38.232967 -11.698681 8.286205  
C -44.126757 -13.895473 6.930453  
C -42.727640 -13.400436 7.095196  
N -41.781731 -14.041356 7.892069  
C -40.618177 -13.339207 7.846928  
N -40.753179 -12.269886 7.050068  
C -42.063589 -12.301736 6.579376  
C -41.283883 -6.331642 9.845239  
C -41.011120 -7.684172 9.273350  
N -41.655775 -8.839956 9.706424  
C -41.196625 -9.898087 8.985438  
N -40.274024 -9.491191 8.103342  
C -40.155340 -8.113361 8.274458  
C -35.698758 -6.224157 5.598753  
C -36.382609 -7.404087 6.207498  
N -36.072455 -7.889798 7.475312  
C -36.854183 -8.970368 7.738183  
N -37.665410 -9.218601 6.701276  
C -37.379963 -8.245048 5.745482  
C -41.685174 -8.755613 5.233371  
S -40.305375 -9.873145 4.752838  
C -39.713037 -13.659507 4.249396  
C -38.388594 -12.962356 4.257649  
N -38.052850 -11.916695 5.130354  
C -36.792044 -11.562873 4.833644  
N -36.307107 -12.327512 3.824807  
C -37.298786 -13.219372 3.444620  
Fe -39.221108 -10.763017 6.660245  
H -36.133959 -13.103209 10.433877  
H -37.874775 -13.513073 10.271557  
H -44.149933 -14.916961 6.511162  
H -44.678453 -13.230178 6.248490  
H -42.445571 -11.544328 5.898043  
H -39.719564 -13.625700 8.387069  
H -41.086158 -6.302971 10.931470  
H -42.334931 -6.029603 9.689386  
H -39.470288 -7.516818 7.675272  
H -41.538875 -10.918138 9.140015  
H -35.816189 -5.320839 6.223130  
H -34.616292 -6.405175 5.473324

H -37.908737 -8.213639 4.794554  
H -36.815363 -9.520093 8.674757  
H -42.199315 -9.120737 6.136231  
H -42.403472 -8.703555 4.399271  
H -40.543483 -12.945635 4.116200  
H -39.891646 -14.204125 5.192551  
H -37.150233 -13.942946 2.646372  
H -35.372143 -12.251092 3.421174  
H -36.214064 -10.779854 5.316160  
H -42.362814 -8.890253 10.442672  
H -41.932261 -14.899367 8.426665  
H -35.371941 -7.499866 8.109046  
H -40.637420 -5.585435 9.358125  
H -44.662986 -13.919712 7.895919  
H -37.405033 -11.886111 10.807896  
H -39.742299 -14.387035 3.422375  
H -36.128725 -6.015639 4.606988  
H -41.298096 -7.742072 5.430192

**(4-Melm)<sub>1</sub>(5-Melm)<sub>3</sub>, ferrous, SMD, BP86,  
G° = -2763.925277**

C -43.770401 -14.434016 7.285098  
C -42.478158 -13.697973 7.136160  
N -41.237887 -14.286647 7.355450  
C -40.264261 -13.355170 7.122307  
N -40.807930 -12.188323 6.762451  
C -42.185872 -12.392547 6.773731  
C -41.512879 -6.974830 10.725583  
C -41.166589 -8.135037 9.849905  
N -41.279416 -9.459123 10.261298  
C -40.896473 -10.272415 9.235354  
N -40.530056 -9.544871 8.171909  
C -40.695065 -8.212153 8.550208  
C -35.452429 -6.793619 4.614933  
C -36.484676 -7.514486 5.419463  
N -36.480805 -7.544100 6.811466  
C -37.548689 -8.279644 7.235357  
N -38.253331 -8.730767 6.191441  
C -37.593533 -8.261535 5.058410  
C -41.317000 -7.647866 4.752352  
S -41.281100 -9.496189 4.627671  
C -39.567177 -12.790962 3.545603  
C -38.333611 -12.542378 4.357237  
N -38.269547 -11.578246 5.369044  
C -37.026915 -11.632414 5.867466  
N -36.292298 -12.579492 5.224962  
C -37.098951 -13.163185 4.258738  
Fe -39.820387 -10.272323 6.256163  
H -43.830462 -15.295770 6.596348  
H -44.610788 -13.758673 7.060727  
H -42.878483 -11.594030 6.511213

H -39.201807 -13.568700 7.223321  
H -40.914630 -6.972043 11.654177  
H -42.578610 -6.987738 11.016305  
H -40.470846 -7.391467 7.871379  
H -40.892190 -11.357906 9.304309  
H -35.453743 -5.709244 4.826122  
H -34.436274 -7.172411 4.825363  
H -37.951891 -8.490096 4.055600  
H -37.765384 -8.458927 8.286688  
H -40.297430 -7.228460 4.738405  
H -41.823622 -7.322225 5.676269  
H -39.937930 -11.858232 3.085919  
H -40.385167 -13.193377 4.169549  
H -36.732321 -13.947221 3.599781  
H -35.315538 -12.806753 5.417386  
H -36.632295 -11.019782 6.676185  
H -41.597575 -9.774541 11.179771  
H -41.077956 -15.255848 7.635348  
H -35.790346 -7.096253 7.417089  
H -41.316458 -6.033326 10.189232  
H -43.904581 -14.819869 8.311515  
H -39.355995 -13.516176 2.743296  
H -35.654495 -6.934204 3.541683  
H -41.873589 -7.240908 3.891467

**(4-Melm)<sub>1</sub>(5-Melm)<sub>3</sub>, ferric, SMD, TPSSh,  
*G*<sup>o</sup> = -2992.271454**

C -37.195503 -12.715241 10.141387  
C -37.165481 -12.192249 8.714583  
O -36.128522 -12.325903 8.016030  
O -38.263171 -11.641939 8.308295  
C -44.083685 -13.898907 6.945666  
C -42.686764 -13.400937 7.102109  
N -41.727063 -14.061065 7.854559  
C -40.575481 -13.355680 7.811175  
N -40.729028 -12.266745 7.061563  
C -42.043341 -12.289116 6.616070  
C -41.303843 -6.340713 9.812149  
C -41.020629 -7.691057 9.245805  
N -41.646722 -8.845027 9.690374  
C -41.185818 -9.896098 8.976854  
N -40.283119 -9.489393 8.088013  
C -40.176317 -8.114349 8.248429  
C -35.669589 -6.293714 5.545384  
C -36.375458 -7.443153 6.181787  
N -36.102246 -7.877875 7.469692  
C -36.892592 -8.936210 7.752208  
N -37.674694 -9.218505 6.713538  
C -37.359788 -8.288767 5.730934  
C -41.674138 -8.757372 5.239589  
S -40.302321 -9.878621 4.768613

C -39.726185 -13.599764 4.253077  
C -38.392380 -12.927723 4.287492  
N -38.050982 -11.904326 5.175809  
C -36.789725 -11.568945 4.898240  
N -36.308705 -12.321193 3.890976  
C -37.306071 -13.187660 3.488321  
Fe -39.217988 -10.755829 6.668792  
H -36.190259 -12.958055 10.490943  
H -37.808843 -13.623454 10.173233  
H -44.105417 -14.883844 6.466497  
H -44.652926 -13.201884 6.326739  
H -42.437113 -11.514089 5.976980  
H -39.673715 -13.656355 8.319455  
H -41.096326 -6.308032 10.887330  
H -42.352353 -6.059254 9.664231  
H -39.508367 -7.522013 7.641893  
H -41.512635 -10.910541 9.139991  
H -35.824366 -5.368292 6.110947  
H -34.590606 -6.474703 5.487407  
H -37.859591 -8.295619 4.774213  
H -36.877578 -9.447432 8.700911  
H -42.171607 -9.103027 6.148214  
H -42.394972 -8.730846 4.418287  
H -40.535049 -12.868517 4.163349  
H -39.903233 -14.185981 5.160566  
H -37.160842 -13.894852 2.686811  
H -35.374700 -12.253124 3.502379  
H -36.208244 -10.809891 5.394172  
H -42.341817 -8.898413 10.427624  
H -41.860356 -14.931619 8.358507  
H -35.419182 -7.473555 8.101629  
H -40.675375 -5.597492 9.316667  
H -44.584336 -13.987302 7.916154  
H -37.656592 -11.982727 10.809996  
H -39.768965 -14.276239 3.395161  
H -36.049754 -6.146716 4.532160  
H -41.288788 -7.747521 5.404387

**(4-Melm)<sub>1</sub>(5-Melm)<sub>3</sub>, ferrous, SMD, TPSSh,  
*G*<sup>o</sup> = -2763.811534**

C -43.805554 -14.414374 7.138899  
C -42.501917 -13.694010 7.048343  
N -41.292340 -14.273093 7.391823  
C -40.306134 -13.358644 7.203700  
N -40.807831 -12.214803 6.755756  
C -42.176172 -12.414768 6.658416  
C -41.417565 -7.007115 10.761852  
C -41.101513 -8.177212 9.891780  
N -41.404237 -9.483637 10.238673  
C -40.996862 -10.305015 9.241292  
N -40.436482 -9.605666 8.258655

C	-40.498996	-8.276969	8.660370	C	-42.666816	-13.393273	7.099584
C	-35.739960	-6.545006	4.433489	N	-41.719868	-14.029327	7.872581
C	-36.608328	-7.385294	5.308211	C	-40.575907	-13.324736	7.827307
N	-36.433387	-7.480974	6.679246	N	-40.723716	-12.258477	7.056825
C	-37.381301	-8.310718	7.180304	C	-42.024558	-12.292999	6.597454
N	-38.167068	-8.763671	6.210178	C	-41.266854	-6.362693	9.817562
C	-37.688346	-8.193274	5.040080	C	-40.998656	-7.704734	9.244489
C	-41.280111	-7.648280	4.903894	N	-41.634311	-8.848876	9.673647
S	-41.239721	-9.481762	4.720219	C	-41.183351	-9.892882	8.956210
C	-39.512294	-12.857745	3.619962	N	-40.277792	-9.490264	8.079173
C	-38.274711	-12.615942	4.422680	C	-40.156530	-8.125641	8.249914
N	-38.195535	-11.646519	5.419771	C	-35.718414	-6.282232	5.559808
C	-36.958852	-11.709957	5.909054	C	-36.405751	-7.438784	6.185292
N	-36.241689	-12.663902	5.277421	N	-36.116988	-7.887995	7.455323
C	-37.056287	-13.246733	4.325672	C	-36.894752	-8.948855	7.730189
Fe	-39.720626	-10.323847	6.325564	N	-37.682852	-9.218906	6.702027
H	-43.800330	-15.331542	6.539495	C	-37.387906	-8.279802	5.733418
H	-44.605593	-13.768320	6.770116	C	-41.653389	-8.766978	5.266252
H	-42.831639	-11.630839	6.308123	S	-40.306175	-9.884498	4.768681
H	-39.264876	-13.567273	7.399136	C	-39.716376	-13.614149	4.291603
H	-40.916250	-7.083932	11.733022	C	-38.395251	-12.932347	4.309298
H	-42.494587	-6.926191	10.946750	N	-38.055428	-11.901934	5.176054
H	-40.112748	-7.480246	8.043069	C	-36.806097	-11.560802	4.884576
H	-41.119359	-11.376399	9.272923	N	-36.329863	-12.316691	3.887417
H	-35.779910	-5.489685	4.725520	C	-37.317040	-13.191931	3.505784
H	-34.693510	-6.866298	4.482078	Fe	-39.219803	-10.750980	6.657473
H	-38.149855	-8.402151	4.085679	H	-36.210507	-13.010721	10.436135
H	-37.454730	-8.550393	8.230138	H	-37.858855	-13.604032	10.130371
H	-40.271426	-7.225456	4.907402	H	-44.068071	-14.901254	6.505938
H	-41.786959	-7.357821	5.829099	H	-44.612752	-13.229069	6.278321
H	-39.868069	-11.931777	3.156560	H	-42.414979	-11.536569	5.932825
H	-40.323599	-13.244113	4.246528	H	-39.677869	-13.611365	8.352743
H	-36.703856	-14.035641	3.679546	H	-41.065827	-6.340009	10.894122
H	-35.272987	-12.895775	5.466285	H	-42.310201	-6.064613	9.666551
H	-36.555756	-11.095715	6.700166	H	-39.480982	-7.530490	7.652795
H	-41.858582	-9.781810	11.095145	H	-41.523336	-10.906091	9.108570
H	-41.161525	-15.222196	7.724182	H	-35.863779	-5.366712	6.143367
H	-35.717835	-7.008039	7.220732	H	-34.640211	-6.457508	5.476980
H	-41.083108	-6.088975	10.273485	H	-37.899815	-8.272077	4.782142
H	-44.037347	-14.692521	8.173338	H	-36.867284	-9.474256	8.672333
H	-39.308702	-13.586095	2.830425	H	-42.212108	-9.167146	6.116059
H	-36.077107	-6.627909	3.397734	H	-42.334708	-8.647102	4.419404
H	-41.831780	-7.218453	4.062221	H	-40.533074	-12.894248	4.184485
<b>(4-Melm)<sub>1</sub>(5-Melm)<sub>3</sub>, ferric, SMD, PBE0,</b>				H	-39.890239	-14.180544	5.212109
<b>G° = -2990.266979</b>				H	-37.176967	-13.909330	2.711349
C	-37.208366	-12.722196	10.100966	H	-35.401885	-12.244225	3.491117
C	-37.178521	-12.180226	8.689613	H	-36.226225	-10.789866	5.366925
O	-36.148631	-12.303989	7.994215	H	-42.331160	-8.901899	10.406203
O	-38.266802	-11.621332	8.299496	H	-41.855953	-14.887427	8.392461
C	-44.053572	-13.895257	6.939041	H	-35.430316	-7.489732	8.083655
				H	-40.626961	-5.621250	9.334015
				H	-44.575230	-13.939711	7.901382

H -37.631876 -11.982896 10.786861  
H -39.754667 -14.311820 3.450774  
H -36.116148 -6.115920 4.556267  
H -41.258927 -7.783799 5.536821

**(4-Melm)<sub>1</sub>(5-Melm)<sub>3</sub>, ferrous, SMD, PBE0,  
G° = -2762.064075**

C -43.689883 -14.491727 7.234177  
C -42.407975 -13.751385 7.123452  
N -41.179854 -14.334650 7.335299  
C -40.221622 -13.401719 7.148150  
N -40.759445 -12.239176 6.830385  
C -42.122379 -12.446014 6.812540  
C -41.462460 -6.848248 10.640795  
C -41.188336 -8.035676 9.793397  
N -41.519236 -9.319525 10.164085  
C -41.135980 -10.164234 9.185820  
N -40.567675 -9.501576 8.192839  
C -40.596505 -8.171970 8.564284  
C -35.480178 -6.808780 4.651667  
C -36.482909 -7.543684 5.462418  
N -36.445685 -7.596563 6.838160  
C -37.489466 -8.334427 7.268439  
N -38.208896 -8.764950 6.247915  
C -37.586024 -8.281653 5.117155  
C -41.348414 -7.706537 4.934324  
S -41.266676 -9.509190 4.637578  
C -39.614407 -12.802660 3.599402  
C -38.349462 -12.546805 4.339771  
N -38.242954 -11.603542 5.346614  
C -36.986635 -11.638560 5.762699  
N -36.281487 -12.554025 5.076595  
C -37.125142 -13.139341 4.163741  
Fe -39.772065 -10.319072 6.303047  
H -43.733832 -15.327180 6.526675  
H -44.522910 -13.818756 7.017928  
H -42.811905 -11.650055 6.567659  
H -39.166075 -13.611022 7.251036  
H -40.955991 -6.921944 11.609512  
H -42.534421 -6.730265 10.834218  
H -40.192832 -7.393240 7.933464  
H -41.283124 -11.232936 9.237994  
H -35.485639 -5.737071 4.879538  
H -34.466631 -7.182652 4.834077  
H -37.965775 -8.490436 4.126392  
H -37.678901 -8.531926 8.314026  
H -40.357167 -7.245679 4.880103  
H -41.783721 -7.480044 5.912347  
H -40.021870 -11.874304 3.185395  
H -40.381565 -13.232177 4.253269  
H -36.790325 -13.903383 3.478200

H -35.301002 -12.763148 5.210086  
H -36.558616 -11.027961 6.545362  
H -41.977100 -9.589667 11.025254  
H -41.017498 -15.302406 7.582288  
H -35.751103 -7.160218 7.430970  
H -41.106129 -5.946621 10.137317  
H -43.832733 -14.900698 8.240510  
H -39.435231 -13.499986 2.776694  
H -35.702999 -6.932862 3.589444  
H -41.978997 -7.242171 4.169704

***cis*-(4-Melm)<sub>2</sub>(5-Melm)<sub>2</sub>, ferric, SMD, BP86,  
G° = -2992.382967**

C -37.201545 -12.328903 10.352658  
C -37.242524 -12.109679 8.842908  
O -36.252443 -12.438844 8.124085  
O -38.341544 -11.581665 8.391410  
C -42.541862 -13.745409 7.093913  
N -41.407242 -14.373979 7.583057  
C -40.379817 -13.491205 7.529022  
N -40.793016 -12.314873 7.029483  
C -42.159189 -12.461361 6.746090  
C -41.350884 -6.322622 9.864124  
C -41.088455 -7.667809 9.270809  
N -41.725162 -8.829251 9.701577  
C -41.280758 -9.877959 8.958878  
N -40.378064 -9.458933 8.061818  
C -40.253139 -8.083917 8.249562  
C -35.498667 -6.450915 5.520978  
C -36.289272 -7.531378 6.182471  
N -36.130378 -7.884445 7.520617  
C -36.983803 -8.901097 7.813118  
N -37.699128 -9.233030 6.729817  
C -37.274437 -8.381096 5.711689  
C -41.295638 -8.349370 5.055210  
S -40.228951 -9.800518 4.699021  
C -39.919102 -13.434515 4.031257  
C -38.537569 -12.875972 4.176900  
N -38.150799 -11.966451 5.173257  
C -36.846589 -11.715803 4.975227  
N -36.382635 -12.417078 3.912017  
C -37.434110 -13.156106 3.390481  
Fe -39.290733 -10.732942 6.665872  
H -36.261062 -12.807833 10.663551  
H -38.053230 -12.957836 10.664588  
H -39.370459 -13.729419 7.852121  
H -41.147262 -6.311260 10.949509  
H -42.401253 -6.012948 9.718407  
H -39.578091 -7.480834 7.645843  
H -41.616170 -10.901404 9.108100  
H -35.661689 -5.472502 6.007033

H -34.415229 -6.663397 5.554308  
H -37.697149 -8.441257 4.710373  
H -37.065753 -9.342628 8.802748  
H -41.935098 -8.526435 5.933464  
H -41.928698 -8.152106 4.174985  
H -40.676460 -12.633723 3.990007  
H -40.182252 -14.099668 4.872074  
H -37.311459 -13.806647 2.527657  
H -35.422446 -12.398204 3.564688  
H -36.223172 -11.050602 5.565509  
H -42.419473 -8.888482 10.449252  
H -41.346782 -15.334590 7.924662  
H -35.478986 -7.454450 8.180548  
H -40.703463 -5.572543 9.384300  
H -37.305666 -11.360758 10.873183  
H -39.982229 -14.022547 3.101483  
H -35.799079 -6.364783 4.465354  
H -40.667106 -7.462898 5.242788  
H -43.504250 -14.249210 7.041323  
C -43.024681 -11.383701 6.173975  
H -43.058246 -10.494312 6.828286  
H -42.654086 -11.050247 5.188626  
H -44.053318 -11.759927 6.053252

***cis*-(4-Melm)<sub>2</sub>(5-Melm)<sub>2</sub>, ferrous, SMD, BP86,  
*G*<sup>°</sup> = -2763.921526**

C -41.897851 -13.914325 7.498704  
N -40.568274 -14.201991 7.764888  
C -39.820607 -13.136824 7.366395  
N -40.602386 -12.172701 6.860330  
C -41.917331 -12.646712 6.939168  
C -41.484315 -6.596263 10.372862  
C -41.235945 -7.831653 9.569473  
N -41.589857 -9.104735 10.003533  
C -41.222876 -10.010269 9.050162  
N -40.643746 -9.393978 8.012721  
C -40.647813 -8.036456 8.332161  
C -35.374459 -6.618236 5.238196  
C -36.370739 -7.525148 5.884605  
N -36.368695 -7.813873 7.245735  
C -37.402565 -8.663344 7.515435  
N -38.077661 -8.948003 6.395690  
C -37.439311 -8.245050 5.376175  
C -41.285942 -7.563760 4.773436  
S -40.955171 -9.343780 4.382186  
C -39.984392 -12.832599 3.459858  
C -38.630215 -12.611008 4.058851  
N -38.372147 -11.614458 5.006215  
C -37.071439 -11.714396 5.311430  
N -36.484455 -12.719407 4.605307  
C -37.455420 -13.298062 3.800490

Fe -39.775414 -10.263855 6.156781  
H -38.736473 -13.103104 7.455939  
H -40.955743 -6.628703 11.342449  
H -42.559508 -6.455906 10.584237  
H -40.231131 -7.288709 7.660223  
H -41.387576 -11.080279 9.157198  
H -35.425742 -5.594637 5.650533  
H -34.341486 -6.983570 5.378598  
H -37.788943 -8.298344 4.346108  
H -37.614724 -9.043360 8.512481  
H -40.344665 -7.010912 4.933579  
H -41.918381 -7.458284 5.670097  
H -40.363837 -11.915720 2.975310  
H -40.720881 -13.124978 4.229113  
H -37.230171 -14.123743 3.128846  
H -35.500708 -12.988481 4.653791  
H -36.530329 -11.097720 6.026112  
H -42.048678 -9.326824 10.888829  
H -40.205251 -15.062853 8.177231  
H -35.706286 -7.448044 7.932283  
H -41.127641 -5.713761 9.819181  
H -39.940151 -13.632333 2.702823  
H -35.573406 -6.561088 4.156647  
H -41.814340 -7.104335 3.921165  
C -43.103936 -11.854345 6.483427  
H -43.998757 -12.496513 6.445569  
H -43.318240 -11.015821 7.171675  
H -42.933922 -11.417520 5.484578  
H -42.696506 -14.618651 7.720384

***cis*-(4-Melm)<sub>2</sub>(5-Melm)<sub>2</sub>, ferric, SMD, TPSSh,  
*G*<sup>°</sup> = -2992.267852**

C -37.350643 -12.538092 10.191022  
C -37.303748 -11.663141 8.949158  
O -36.266929 -10.990327 8.701664  
O -38.370951 -11.661366 8.224365  
C -42.606422 -13.714170 7.211686  
N -41.460639 -14.441589 6.956313  
C -40.446671 -13.575481 6.775187  
N -40.874853 -12.317717 6.900661  
C -42.241611 -12.389857 7.181874  
C -42.207033 -6.865226 10.075899  
C -41.437628 -8.032340 9.556984  
N -40.979057 -9.054958 10.372569  
C -40.319156 -9.957352 9.614071  
N -40.321840 -9.578789 8.338291  
C -41.020567 -8.379823 8.295220  
C -35.311111 -7.069420 4.842981  
C -36.352573 -7.765634 5.651722  
N -36.678402 -7.393055 6.946655  
C -37.651749 -8.209867 7.406431

N	-37.978484	-9.102162	6.475818	C	-41.162919	-7.960922	9.694292
C	-37.174957	-8.830991	5.377329	N	-41.475721	-9.243918	10.112344
C	-40.346291	-7.959905	4.674238	C	-41.114043	-10.117339	9.141289
S	-40.812687	-9.693482	5.037766	N	-40.578422	-9.475456	8.108105
C	-39.779096	-12.672150	3.425345	C	-40.604945	-8.129061	8.448807
C	-38.453929	-12.576287	4.108952	C	-35.443117	-6.671749	4.821941
N	-38.235838	-11.925345	5.326797	C	-36.428811	-7.486784	5.590223
C	-36.942261	-12.084502	5.614357	N	-36.379998	-7.630174	6.967260
N	-36.325726	-12.794436	4.650040	C	-37.412301	-8.418679	7.357595
C	-37.263218	-13.118351	3.689197	N	-38.131549	-8.801314	6.308443
Fe	-39.442420	-10.673917	6.684519	C	-37.521743	-8.226818	5.203401
H	-36.346091	-12.851402	10.484095	C	-41.271237	-7.637744	4.819393
H	-37.987714	-13.411925	10.034613	S	-40.971784	-9.410154	4.413456
H	-39.435622	-13.884127	6.563776	C	-39.711440	-12.812674	3.522637
H	-41.621289	-6.295514	10.805791	C	-38.424891	-12.580798	4.247520
H	-43.131961	-7.187357	10.566942	N	-38.283711	-11.630197	5.256412
H	-41.182678	-7.848871	7.370284	C	-37.016748	-11.697490	5.659558
H	-39.871201	-10.853791	10.010786	N	-36.340127	-12.637308	4.963695
H	-35.555773	-6.010679	4.703577	C	-37.214849	-13.205836	4.057959
H	-34.329592	-7.126440	5.326321	Fe	-39.754808	-10.306637	6.233940
H	-37.243110	-9.409155	4.468431	H	-39.004011	-13.384390	7.242064
H	-38.072976	-8.131945	8.396273	H	-40.882359	-6.793825	11.476569
H	-41.261081	-7.382043	4.518534	H	-42.487831	-6.634625	10.747032
H	-39.750266	-7.926015	3.757984	H	-40.222751	-7.369903	7.783379
H	-40.201816	-11.681415	3.234248	H	-41.248102	-11.184036	9.230842
H	-40.504295	-13.228443	4.029875	H	-35.448500	-5.625872	5.148459
H	-37.010118	-13.696551	2.814306	H	-34.424353	-7.055889	4.946436
H	-35.342776	-13.042928	4.639604	H	-37.912687	-8.378406	4.207631
H	-36.436101	-11.698572	6.486544	H	-37.591730	-8.682443	8.388675
H	-41.121469	-9.124938	11.374723	H	-40.328582	-7.106391	4.981844
H	-41.385919	-15.451519	6.905469	H	-41.895679	-7.534518	5.711254
H	-36.258382	-6.631484	7.469489	H	-40.092486	-11.882017	3.089243
H	-42.468419	-6.200441	9.249806	H	-40.482453	-13.204512	4.195178
H	-37.777997	-11.951215	11.013112	H	-36.904562	-13.980234	3.373764
H	-39.657855	-13.194808	2.472640	H	-35.360767	-12.870515	5.082022
H	-35.237643	-7.538846	3.859583	H	-36.564058	-11.096831	6.433732
H	-39.770911	-7.521923	5.491672	H	-41.904352	-9.493308	10.997139
H	-43.557729	-14.189835	7.391776	H	-40.632124	-15.241022	7.808120
C	-43.112855	-11.203418	7.440379	H	-35.690670	-7.213941	7.584005
H	-44.157863	-11.522395	7.479143	H	-41.087992	-5.858077	9.984081
H	-42.864511	-10.731032	8.396656	H	-39.559985	-13.534481	2.715331
H	-43.002373	-10.448412	6.656669	H	-35.692873	-6.701469	3.758924
<b><i>cis</i>-(4-Melm)<sub>2</sub>(5-Melm)<sub>2</sub>, ferrous, SMD, TPSSh, G° = -2763.808290</b>				H	-41.790735	-7.166408	3.979627
C	-42.208192	-13.867714	7.333154	C	-43.218799	-11.606451	6.599813
N	-40.913576	-14.314035	7.509404	H	-43.362895	-10.881973	7.410796
C	-40.078834	-13.298648	7.193482	H	-42.997274	-11.039281	5.690377
N	-40.762875	-12.217190	6.827565	H	-44.157610	-12.151392	6.466759
C	-42.111057	-12.560814	6.913786	H	-43.061191	-14.503779	7.512117
C	-41.421094	-6.747698	10.523487				

***cis*-(4-Melm)<sub>2</sub>(5-Melm)<sub>2</sub>, ferric, SMD, PBE0,  
G° = -2990.262027**

C -37.346003 -12.520210 10.163567  
C -37.309686 -11.647959 8.928943  
O -36.282778 -10.981069 8.669819  
O -38.377613 -11.654434 8.221010  
C -42.595862 -13.685137 7.220956  
N -41.460190 -14.412248 6.961934  
C -40.449101 -13.554451 6.778819  
N -40.868997 -12.301326 6.905750  
C -42.226330 -12.366170 7.190818  
C -42.209643 -6.877005 10.046110  
C -41.435030 -8.034546 9.535656  
N -40.961454 -9.038331 10.351469  
C -40.301131 -9.935550 9.599377  
N -40.318331 -9.570585 8.327222  
C -41.026409 -8.386486 8.276901  
C -35.286627 -7.106885 4.875752  
C -36.339037 -7.786406 5.670347  
N -36.692378 -7.394561 6.942968  
C -37.670324 -8.200537 7.391799  
N -37.974869 -9.103026 6.473860  
C -37.151385 -8.853949 5.395213  
C -40.254782 -7.999900 4.643712  
S -40.805107 -9.685561 5.046475  
C -39.790096 -12.668284 3.454947  
C -38.467578 -12.570054 4.127288  
N -38.239191 -11.919699 5.333671  
C -36.950766 -12.081488 5.611904  
N -36.345945 -12.792407 4.651272  
C -37.284686 -13.115275 3.702511  
Fe -39.437987 -10.663936 6.681283  
H -36.347044 -12.660344 10.580671  
H -37.795647 -13.490889 9.936664  
H -39.438990 -13.867968 6.563359  
H -41.627185 -6.293421 10.767432  
H -43.128685 -7.202562 10.545623  
H -41.207493 -7.866173 7.348266  
H -39.839140 -10.824603 10.000064  
H -35.531666 -6.052924 4.704888  
H -34.316721 -7.146060 5.383327  
H -37.191984 -9.447575 4.493393  
H -38.114378 -8.106483 8.371753  
H -41.115502 -7.436314 4.273613  
H -39.492260 -8.024613 3.860448  
H -40.216585 -11.679271 3.264925  
H -40.512643 -13.222965 4.064010  
H -37.043384 -13.697534 2.825998  
H -35.365893 -13.042908 4.637128  
H -36.436692 -11.694230 6.480448  
H -41.093483 -9.100045 11.353357

H -41.388372 -15.420077 6.910183  
H -36.284399 -6.626655 7.461748  
H -42.484152 -6.220548 9.217500  
H -37.976044 -12.036708 10.919554  
H -39.676473 -13.193934 2.503070  
H -35.184340 -7.596421 3.904735  
H -39.842437 -7.488539 5.516699  
H -43.551120 -14.153142 7.405090  
C -43.091088 -11.184450 7.451019  
H -42.833795 -10.704968 8.401299  
H -42.990521 -10.432239 6.663484  
H -44.135877 -11.501817 7.503416

***cis*-(4-Melm)<sub>2</sub>(5-Melm)<sub>2</sub>, ferrous, SMD, PBE0,  
G° = -2762.061010**

C -42.206896 -13.874063 7.282757  
N -40.920540 -14.326619 7.444150  
C -40.087242 -13.311212 7.157001  
N -40.764086 -12.223304 6.824194  
C -42.104955 -12.560109 6.901071  
C -41.459747 -6.760756 10.507103  
C -41.191396 -7.967017 9.684877  
N -41.504484 -9.243490 10.094722  
C -41.130272 -10.110057 9.132075  
N -40.585881 -9.468971 8.112561  
C -40.619143 -8.130545 8.449752  
C -35.417531 -6.714185 4.849334  
C -36.419271 -7.500204 5.611952  
N -36.389010 -7.629349 6.982224  
C -37.432927 -8.393883 7.365813  
N -38.142479 -8.772918 6.318231  
C -37.516587 -8.223402 5.219820  
C -41.257376 -7.650878 4.833111  
S -40.982815 -9.406820 4.403569  
C -39.707602 -12.798873 3.549849  
C -38.423008 -12.564295 4.262528  
N -38.276047 -11.617798 5.261528  
C -37.013273 -11.680883 5.654645  
N -36.342665 -12.616522 4.960970  
C -37.216720 -13.186504 4.067332  
Fe -39.754853 -10.304363 6.240429  
H -39.011193 -13.401819 7.200585  
H -40.930985 -6.804014 11.465735  
H -42.528404 -6.648571 10.721010  
H -40.231154 -7.366498 7.791598  
H -41.263081 -11.178742 9.217038  
H -35.414689 -5.662191 5.155216  
H -34.404841 -7.106087 4.995786  
H -37.895810 -8.376908 4.218754  
H -37.629173 -8.645050 8.398395  
H -40.310364 -7.126521 4.996582

H -41.873706 -7.545163 5.730958  
H -40.096747 -11.868929 3.121833  
H -40.473768 -13.194818 4.225653  
H -36.913610 -13.963241 3.381325  
H -35.364236 -12.846141 5.074027  
H -36.556532 -11.075273 6.424635  
H -41.943230 -9.494519 10.971477  
H -40.642389 -15.259783 7.717872  
H -35.702148 -7.218271 7.601414  
H -41.124205 -5.868579 9.973365  
H -39.562118 -13.517399 2.738709  
H -35.648678 -6.758663 3.782531  
H -41.777624 -7.155561 4.007379  
C -43.204437 -11.599064 6.613796  
H -44.146773 -12.134091 6.467227  
H -43.345974 -10.893521 7.441560  
H -42.981874 -11.008830 5.719079  
H -43.065404 -14.508798 7.443933

***trans*-(4-Melm)<sub>2</sub>(5-Melm)<sub>2</sub>, ferric, SMD, BP86,  
*G*<sup>o</sup> = -2992.384673**

C -36.786462 -12.233822 10.123574  
C -37.421593 -12.422060 8.748485  
O -37.184713 -13.477145 8.083546  
O -38.207288 -11.463965 8.361771  
C -44.022402 -13.994590 6.929790  
C -42.631082 -13.458457 7.012114  
N -41.560900 -14.193960 7.514870  
C -40.437248 -13.429629 7.466733  
N -40.721474 -12.224493 6.952568  
C -42.083799 -12.236049 6.664367  
C -41.368738 -7.863072 9.445204  
N -41.673826 -9.125971 9.928867  
C -41.044830 -10.040090 9.149287  
N -40.340338 -9.429027 8.182690  
C -40.534281 -8.050983 8.357172  
C -35.286759 -6.581756 5.355817  
C -36.119876 -7.605431 6.054949  
N -35.924838 -7.967939 7.385980  
C -36.840150 -8.915789 7.723107  
N -37.626971 -9.192592 6.675142  
C -37.185608 -8.380860 5.633565  
C -41.992126 -8.893478 5.265643  
S -40.371177 -9.641087 4.825932  
C -39.829378 -13.092795 3.830819  
C -38.425744 -12.717509 4.189721  
N -38.083818 -11.820383 5.213279  
C -36.741839 -11.770575 5.246158  
N -36.213110 -12.578927 4.296063  
C -37.257333 -13.184477 3.613345  
Fe -39.264925 -10.637108 6.668078

H -36.002220 -12.983184 10.309212  
H -37.566307 -12.336995 10.899452  
H -44.069292 -14.905712 6.307212  
H -44.687281 -13.238272 6.484828  
H -42.591438 -11.376237 6.233431  
H -39.453512 -13.775187 7.783080  
H -41.114489 -11.112478 9.313821  
H -35.373484 -5.591735 5.838055  
H -34.217941 -6.860018 5.355084  
H -37.661556 -8.398451 4.654987  
H -36.903363 -9.370120 8.708853  
H -42.192415 -8.963621 6.345453  
H -42.791541 -9.410887 4.709548  
H -40.456737 -12.198460 3.676900  
H -40.303976 -13.693904 4.625654  
H -37.086322 -13.881376 2.796105  
H -35.215878 -12.707987 4.116616  
H -36.136992 -11.179362 5.928732  
H -42.269914 -9.339428 10.730275  
H -41.604410 -15.155893 7.857555  
H -35.217415 -7.580143 8.013242  
H -44.415649 -14.253853 7.928974  
H -36.363417 -11.219686 10.220645  
H -39.829768 -13.690467 2.905056  
H -35.618372 -6.483739 4.310622  
H -41.995766 -7.832816 4.964707  
H -41.758290 -6.958537 9.906534  
C -39.905086 -6.993648 7.504328  
H -38.826562 -6.889082 7.715432  
H -40.007364 -7.223267 6.431259  
H -40.385333 -6.022039 7.703711

***trans*-(4-Melm)<sub>2</sub>(5-Melm)<sub>2</sub>, ferrous, SMD, BP86,  
*G*<sup>o</sup> = -2763.922356**

C -44.121900 -13.956471 7.562503  
C -42.785798 -13.393599 7.198790  
N -41.606455 -14.125230 7.279861  
C -40.571360 -13.330778 6.869827  
N -41.016204 -12.118490 6.524311  
C -42.393008 -12.148713 6.732094  
C -40.745361 -8.588544 10.073996  
N -40.311790 -9.876198 10.349565  
C -40.089871 -10.507514 9.164151  
N -40.349505 -9.686614 8.135946  
C -40.766017 -8.472599 8.694004  
C -35.453745 -6.659994 4.647459  
C -36.493226 -7.425107 5.400271  
N -36.637840 -7.350461 6.782879  
C -37.676613 -8.151351 7.158485  
N -38.220770 -8.744356 6.090120  
C -37.485524 -8.301798 4.993546



C -41.013581 -7.714789 4.130381  
 S -41.194213 -9.535254 4.417699  
 C -39.351492 -12.907709 3.526484  
 C -38.195836 -12.622561 4.435250  
 N -38.232540 -11.656532 5.448886  
 C -37.031342 -11.684615 6.046034  
 N -36.232587 -12.619986 5.469321  
 C -36.946918 -13.220705 4.443685  
 Fe -39.796336 -10.276744 6.109519  
 H -44.397551 -14.806900 6.913092  
 H -44.895513 -13.180261 7.454447  
 H -43.016994 -11.279602 6.528075  
 H -39.537752 -13.670370 6.846059  
 H -39.744484 -11.537008 9.091006  
 H -35.569909 -5.570620 4.789405  
 H -34.433194 -6.930634 4.972540  
 H -37.711287 -8.638137 3.982473  
 H -37.991212 -8.271803 8.193529  
 H -39.955368 -7.406178 4.152283  
 H -41.567760 -7.136370 4.888087  
 H -39.825717 -11.971824 3.184198  
 H -40.131559 -13.501769 4.036604  
 H -36.513741 -13.998422 3.818643  
 H -35.268353 -12.826740 5.734892  
 H -36.713285 -11.057290 6.876572  
 H -40.194265 -10.289196 11.275705  
 H -41.527700 -15.098345 7.580525  
 H -36.064738 -6.785815 7.413063  
 H -44.140625 -14.317086 8.606490  
 H -39.011411 -13.476843 2.646198  
 H -35.538732 -6.875942 3.571108  
 H -41.427957 -7.467725 3.138303  
 C -41.173294 -7.293326 7.866597  
 H -42.024617 -7.538619 7.207652  
 H -41.474311 -6.458740 8.520262  
 H -40.346636 -6.945194 7.222596  
 H -41.003238 -7.886033 10.863352

***trans*-(4-Melm)<sub>2</sub>(5-Melm)<sub>2</sub>, ferric, SMD, TPSSh,  
G° = -2992.266329**

C -37.230920 -12.395937 10.263342  
 C -37.213537 -12.114461 8.769967  
 O -36.203616 -12.411030 8.081937  
 O -38.292880 -11.580265 8.300966  
 C -44.023027 -13.935185 6.915213  
 C -42.629052 -13.421279 7.044787  
 N -41.618192 -14.122458 7.683898  
 C -40.483823 -13.388931 7.643529  
 N -40.698779 -12.241207 7.004822  
 C -42.033837 -12.256022 6.627546  
 C -41.312709 -7.863307 9.356077

N -41.618366 -9.109443 9.865820  
 C -40.997698 -10.034909 9.109380  
 N -40.298825 -9.451950 8.133478  
 C -40.486798 -8.075594 8.278743  
 C -35.319798 -6.586865 5.386650  
 C -36.143743 -7.620592 6.077081  
 N -35.968657 -7.963102 7.409527  
 C -36.863044 -8.921575 7.735362  
 N -37.616329 -9.227719 6.682811  
 C -37.175388 -8.417790 5.645383  
 C -41.906029 -8.925667 5.227243  
 S -40.330465 -9.755213 4.790671  
 C -39.845025 -13.317220 4.022159  
 C -38.460701 -12.775319 4.170905  
 N -38.075797 -11.841594 5.138863  
 C -36.769166 -11.634649 4.962314  
 N -36.302356 -12.378927 3.942757  
 C -37.355974 -13.107221 3.425820  
 Fe -39.222981 -10.682057 6.655445  
 H -36.248644 -12.717206 10.614649  
 H -37.960951 -13.186365 10.471282  
 H -44.050715 -14.878207 6.358271  
 H -44.633046 -13.202020 6.382850  
 H -42.480930 -11.439443 6.083309  
 H -39.551003 -13.713079 8.075337  
 H -41.068129 -11.094400 9.296262  
 H -35.433262 -5.606049 5.861612  
 H -34.255937 -6.847715 5.405525  
 H -37.629112 -8.459450 4.666992  
 H -36.938318 -9.345013 8.723847  
 H -42.117903 -9.005042 6.294879  
 H -42.716979 -9.390602 4.659500  
 H -40.582352 -12.510470 3.981047  
 H -40.109878 -13.972563 4.858482  
 H -37.231244 -13.783839 2.595017  
 H -35.342089 -12.391364 3.617679  
 H -36.144608 -10.974370 5.540041  
 H -42.207643 -9.303912 10.667771  
 H -41.709267 -15.035575 8.116823  
 H -35.286552 -7.559389 8.042952  
 H -44.473975 -14.111689 7.897997  
 H -37.548106 -11.503931 10.812089  
 H -39.907120 -13.900920 3.099546  
 H -35.636199 -6.503267 4.344718  
 H -41.848699 -7.870250 4.946928  
 C -39.857464 -7.040734 7.402377  
 H -40.391122 -6.093090 7.515962  
 H -38.809157 -6.872313 7.671506  
 H -39.883811 -7.338676 6.351357  
 H -41.697924 -6.956128 9.794513

***trans*-(4-Melm)<sub>2</sub>(5-Melm)<sub>2</sub>, ferrous, SMD, TPSSh,  
*G*<sup>o</sup> = -2763.807564**

C -44.121256 -14.047105 7.302523  
C -42.776121 -13.441332 7.079621  
N -41.593966 -14.142169 7.244542  
C -40.556753 -13.314093 6.955503  
N -40.998775 -12.112521 6.606663  
C -42.381182 -12.182326 6.688282  
C -40.717222 -8.512391 10.140704  
N -40.326454 -9.803790 10.435337  
C -40.104772 -10.448188 9.268100  
N -40.325088 -9.639017 8.233973  
C -40.712594 -8.412894 8.769073  
C -35.497366 -6.710149 4.528565  
C -36.504854 -7.458345 5.335080  
N -36.570422 -7.387763 6.717677  
C -37.594481 -8.167334 7.143771  
N -38.203987 -8.741994 6.113292  
C -37.527104 -8.308348 4.983489  
C -41.036823 -7.701228 4.213490  
S -41.265915 -9.502282 4.529287  
C -39.398044 -12.898980 3.627567  
C -38.217814 -12.617616 4.501529  
N -38.226258 -11.654631 5.509585  
C -37.016439 -11.680025 6.067004  
N -36.237533 -12.609011 5.473914  
C -36.977302 -13.209968 4.474333  
Fe -39.783936 -10.268178 6.193660  
H -44.301035 -14.883693 6.617726  
H -44.894060 -13.293753 7.133270  
H -43.000484 -11.329027 6.452972  
H -39.524477 -13.624801 7.010924  
H -39.789535 -11.479083 9.212743  
H -35.589380 -5.628761 4.679747  
H -34.474846 -6.999037 4.796244  
H -37.817105 -8.632076 3.994267  
H -37.848855 -8.288686 8.185919  
H -40.030121 -7.371827 4.483348  
H -41.763689 -7.113351 4.781740  
H -39.885806 -11.968303 3.321275  
H -40.145995 -13.507971 4.148356  
H -36.563420 -13.981626 3.844046  
H -35.273104 -12.812137 5.711954  
H -36.677062 -11.054850 6.878943  
H -40.230929 -10.206958 11.360364  
H -41.512951 -15.112939 7.526693  
H -35.955557 -6.845094 7.314883  
H -44.226057 -14.424948 8.325753  
H -39.079825 -13.443012 2.733977  
H -35.648145 -6.922825 3.467737  
H -41.193980 -7.501846 3.148919

H -40.963147 -7.800337 10.912962  
C -41.070958 -7.237278 7.918512  
H -40.234852 -6.940728 7.276292  
H -41.923575 -7.464842 7.270070  
H -41.337262 -6.386469 8.551503

***trans*-(4-Melm)<sub>2</sub>(5-Melm)<sub>2</sub>, ferric, SMD, PBE0,  
*G*<sup>o</sup> = -2990.261918**

C -37.353481 -12.584780 10.191422  
C -37.254569 -12.131582 8.752152  
O -36.212195 -12.345187 8.097609  
O -38.295541 -11.532974 8.301728  
C -43.983299 -13.895615 6.981650  
C -42.592952 -13.385878 7.071654  
N -41.562392 -14.102902 7.638459  
C -40.438333 -13.367376 7.582399  
N -40.679890 -12.203121 7.001559  
C -42.020396 -12.206342 6.676283  
C -41.275196 -7.844040 9.353794  
N -41.577367 -9.083613 9.860794  
C -40.964988 -10.003976 9.104317  
N -40.274830 -9.424291 8.129493  
C -40.457938 -8.056128 8.274846  
C -35.330616 -6.577271 5.365506  
C -36.144024 -7.608555 6.055640  
N -35.952796 -7.962734 7.373870  
C -36.843044 -8.914808 7.701693  
N -37.609361 -9.204101 6.662975  
C -37.182939 -8.393047 5.631203  
C -41.885650 -8.920296 5.252923  
S -40.324936 -9.735104 4.792559  
C -39.834812 -13.315353 4.077835  
C -38.455431 -12.780227 4.227770  
N -38.071778 -11.828861 5.166271  
C -36.770190 -11.632040 4.990774  
N -36.304051 -12.401578 3.999782  
C -37.351478 -13.135721 3.499893  
Fe -39.214337 -10.647729 6.646251  
H -36.452546 -13.113634 10.506856  
H -38.223950 -13.237774 10.313621  
H -44.032079 -14.825758 6.405132  
H -44.615695 -13.153138 6.489788  
H -42.495379 -11.371917 6.183011  
H -39.486174 -13.707989 7.958984  
H -41.036194 -11.064950 9.290252  
H -35.434167 -5.599096 5.847850  
H -34.267041 -6.839313 5.367196  
H -37.651214 -8.419244 4.658151  
H -36.905061 -9.352669 8.686325  
H -42.089377 -9.003983 6.322291  
H -42.708152 -9.379408 4.696665

H -40.568222 -12.506259 4.020141  
H -40.111503 -13.958649 4.919681  
H -37.230185 -13.834799 2.686253  
H -35.344437 -12.424624 3.680487  
H -36.145419 -10.957521 5.554293  
H -42.160804 -9.278716 10.663981  
H -41.633573 -15.030623 8.037586  
H -35.261582 -7.569100 8.000142  
H -44.399234 -14.095884 7.975163  
H -37.508904 -11.714523 10.837903  
H -39.894656 -13.911466 3.163171  
H -35.658869 -6.482631 4.328090  
H -41.842875 -7.860782 4.984382  
H -41.654530 -6.933602 9.792620  
C -39.837669 -7.023481 7.401713  
H -38.780914 -6.871778 7.646148  
H -39.891775 -7.303498 6.346822  
H -40.353745 -6.069485 7.539812

***trans*-(4-Melm)<sub>2</sub>(5-Melm)<sub>2</sub>, ferrous, SMD, PBE0,  
*G*<sup>o</sup> = -2762.061873**

C -44.084287 -13.907087 7.639025  
C -42.761677 -13.365901 7.237167  
N -41.609232 -14.117205 7.241010  
C -40.588059 -13.340143 6.817904  
N -41.013177 -12.123351 6.536047  
C -42.365914 -12.126813 6.799834  
C -40.809190 -8.599466 10.073698  
N -40.401160 -9.880571 10.353865  
C -40.139296 -10.496498 9.188179  
N -40.348977 -9.677987 8.168369  
C -40.773440 -8.477040 8.708354  
C -35.417583 -6.739869 4.694558  
C -36.479806 -7.465365 5.434929  
N -36.619176 -7.401774 6.803598  
C -37.670578 -8.165097 7.166001  
N -38.229693 -8.720280 6.105562  
C -37.490840 -8.294678 5.022369  
C -40.912960 -7.771828 4.054861  
S -41.305455 -9.506633 4.474493  
C -39.335540 -12.865724 3.539266  
C -38.180188 -12.588335 4.435050  
N -38.210764 -11.639353 5.443496  
C -37.018726 -11.663774 6.022515  
N -36.228708 -12.580871 5.442386  
C -36.941169 -13.175289 4.429711  
Fe -39.787371 -10.282528 6.125339  
H -44.390416 -14.739713 6.995883  
H -44.841944 -13.123490 7.565214  
H -42.974300 -11.245101 6.653245  
H -39.571124 -13.697803 6.739293

H -39.803700 -11.521935 9.122243  
H -35.490529 -5.657240 4.846036  
H -34.418625 -7.053711 5.017379  
H -37.725232 -8.607493 4.014271  
H -37.985709 -8.287284 8.192863  
H -39.953630 -7.688774 3.536037  
H -40.879312 -7.136271 4.944661  
H -39.812169 -11.934588 3.216962  
H -40.101458 -13.465878 4.043929  
H -36.515416 -13.942181 3.800143  
H -35.270475 -12.780589 5.697948  
H -36.699750 -11.041187 6.846653  
H -40.320348 -10.297309 11.271843  
H -41.537643 -15.091633 7.504394  
H -36.032366 -6.871107 7.434865  
H -44.071304 -14.273087 8.671654  
H -39.002724 -13.416282 2.655299  
H -35.509304 -6.942004 3.624929  
H -41.689134 -7.377623 3.391079  
H -41.092470 -7.903246 10.848723  
C -41.131660 -7.298099 7.875228  
H -40.253049 -6.876246 7.374618  
H -41.854042 -7.571828 7.099252  
H -41.572933 -6.517177 8.500264

**(4-Melm)<sub>3</sub>(5-Melm)<sub>1</sub>, ferric, SMD, BP86,  
*G*<sup>o</sup> = -2992.377489**

C -37.258625 -12.100729 10.450186  
C -37.520351 -12.125805 8.945339  
O -36.899113 -12.963108 8.219663  
O -38.415517 -11.292038 8.514745  
C -42.315404 -13.824743 7.014750  
N -41.112113 -14.394724 7.400985  
C -40.153617 -13.438157 7.343407  
N -40.677905 -12.268317 6.941145  
C -42.044612 -12.499125 6.723973  
C -41.415969 -7.738960 9.352112  
N -41.861241 -8.991680 9.743200  
C -41.261960 -9.918277 8.956186  
N -40.445798 -9.325413 8.069662  
C -40.529974 -7.946043 8.309057  
C -35.143027 -6.742255 5.252394  
C -36.020817 -7.708618 5.977665  
N -35.806789 -8.086094 7.301335  
C -36.768440 -8.974502 7.668014  
N -37.604095 -9.201106 6.644495  
C -37.145264 -8.414868 5.589733  
C -41.716308 -8.437570 5.071198  
S -40.320961 -9.585897 4.745197  
C -39.963102 -13.054155 3.794613  
C -38.550465 -12.691716 4.133894

N -38.175820 -11.822240 5.170819  
 C -36.833194 -11.774804 5.161200  
 N -36.334997 -12.563040 4.178148  
 C -37.401369 -13.148482 3.512361  
 Fe -39.311402 -10.562296 6.649601  
 H -36.265190 -12.512299 10.686280  
 H -38.017495 -12.731249 10.948864  
 H -39.109410 -13.623724 7.586589  
 H -41.431731 -10.986658 9.060113  
 H -35.093224 -5.770720 5.775085  
 H -34.110635 -7.124493 5.160289  
 H -37.653134 -8.402378 4.627363  
 H -36.832523 -9.413262 8.660032  
 H -42.048472 -8.487426 6.118621  
 H -42.555859 -8.703418 4.408181  
 H -40.597146 -12.156806 3.697581  
 H -40.417589 -13.699828 4.565939  
 H -37.257624 -13.825280 2.673258  
 H -35.343839 -12.690013 3.966838  
 H -36.205104 -11.201414 5.837243  
 H -42.524422 -9.192129 10.493822  
 H -40.960693 -15.367602 7.672211  
 H -35.060812 -7.740361 7.908292  
 H -37.352153 -11.082154 10.859572  
 H -39.983456 -13.604926 2.840278  
 H -35.537642 -6.569425 4.239318  
 H -41.405350 -7.406436 4.834817  
 H -43.241872 -14.393538 6.984028  
 C -43.012127 -11.460484 6.252768  
 H -43.027961 -10.580732 6.919374  
 H -42.755523 -11.103905 5.240383  
 H -44.027828 -11.886604 6.221744  
 H -41.754424 -6.827216 9.838845  
 C -39.740103 -6.908667 7.572657  
 H -38.694430 -6.874045 7.925355  
 H -39.714142 -7.104904 6.489602  
 H -40.185297 -5.914557 7.739442

**(4-Melm)<sub>3</sub>(5-Melm)<sub>1</sub>, ferrous, SMD, BP86,  
G° = -2763.918648**

C -42.674558 -13.471489 7.407349  
 N -41.481322 -14.169898 7.309481  
 C -40.535872 -13.314736 6.827800  
 N -41.056008 -12.099865 6.608998  
 C -42.403458 -12.181340 6.979600  
 C -40.813317 -8.515202 10.034309  
 N -40.409182 -9.806579 10.335588  
 C -40.152365 -10.450594 9.163613  
 N -40.360835 -9.634761 8.120285  
 C -40.780909 -8.411001 8.653233  
 C -35.398318 -6.702213 4.656124

C -36.455431 -7.445403 5.406377  
 N -36.592095 -7.379466 6.790133  
 C -37.649086 -8.157598 7.163186  
 N -38.211413 -8.728945 6.092478  
 C -37.470240 -8.294500 4.996696  
 C -40.961749 -7.670827 4.100320  
 S -41.064646 -9.510269 4.286018  
 C -39.395577 -12.838966 3.476641  
 C -38.238646 -12.582744 4.392295  
 N -38.271147 -11.642094 5.430588  
 C -37.071132 -11.694354 6.028281  
 N -36.276988 -12.619996 5.428742  
 C -36.993605 -13.189025 4.386848  
 Fe -39.810538 -10.241671 6.095867  
 H -39.503033 -13.611434 6.659132  
 H -39.816222 -11.484355 9.112925  
 H -35.480846 -5.611491 4.810643  
 H -34.384551 -7.006515 4.972875  
 H -37.711735 -8.614199 3.983757  
 H -37.964076 -8.276349 8.198237  
 H -39.958628 -7.296271 4.362431  
 H -41.708463 -7.168617 4.737271  
 H -39.826755 -11.891906 3.108664  
 H -40.205246 -13.390226 3.989059  
 H -36.565000 -13.953839 3.742949  
 H -35.314877 -12.840545 5.690933  
 H -36.749590 -11.091368 6.875489  
 H -40.322972 -10.211841 11.268555  
 H -41.332714 -15.151979 7.544637  
 H -36.001349 -6.836506 7.422969  
 H -39.069267 -13.440198 2.612576  
 H -35.495075 -6.904235 3.578060  
 H -41.170369 -7.407086 3.049889  
 C -43.346639 -11.020397 6.902239  
 H -44.375415 -11.348394 7.122986  
 H -43.072956 -10.232520 7.627246  
 H -43.323486 -10.557044 5.900818  
 H -43.590254 -13.939943 7.761872  
 H -41.089876 -7.802277 10.807821  
 C -41.138686 -7.234074 7.799754  
 H -41.982971 -7.466613 7.126897  
 H -41.430741 -6.380739 8.432932  
 H -40.289223 -6.919491 7.168554

**(4-Melm)<sub>3</sub>(5-Melm)<sub>1</sub>, ferric, SMD, TPSSh,  
G° = -2992.261324**

C -37.263870 -12.033681 10.187822  
 C -37.194803 -11.483355 8.772040  
 O -36.103104 -11.029931 8.332682  
 O -38.298298 -11.517499 8.106298  
 C -42.517405 -13.681740 7.371407

N -41.319318 -14.363758 7.288725  
 C -40.348163 -13.471798 7.018490  
 N -40.854719 -12.241854 6.917764  
 C -42.229017 -12.358682 7.139115  
 C -41.476223 -8.304289 9.832097  
 N -41.211030 -9.542992 10.381202  
 C -40.550789 -10.274788 9.462690  
 N -40.372325 -9.574577 8.341173  
 C -40.958931 -8.325134 8.558919  
 C -35.163396 -7.069876 4.967598  
 C -36.252872 -7.757261 5.718472  
 N -36.571895 -7.454317 7.033080  
 C -37.600183 -8.236325 7.426051  
 N -37.976568 -9.035665 6.430944  
 C -37.137711 -8.745427 5.363250  
 C -40.164392 -8.193685 4.133516  
 S -40.874141 -9.660192 4.965850  
 C -40.008978 -12.735426 3.477548  
 C -38.643267 -12.624458 4.073209  
 N -38.336581 -11.891043 5.223240  
 C -37.032647 -12.064938 5.446774  
 N -36.490869 -12.857972 4.502020  
 C -37.492349 -13.226816 3.624953  
 Fe -39.464807 -10.580530 6.594717  
 H -36.264718 -12.211518 10.590395  
 H -37.848188 -12.957741 10.216318  
 H -39.309930 -13.741360 6.911856  
 H -40.222556 -11.286671 9.633405  
 H -35.349633 -5.992557 4.895894  
 H -34.192828 -7.211172 5.455701  
 H -37.224804 -9.253862 4.415754  
 H -38.021991 -8.206967 8.418102  
 H -40.979658 -7.652664 3.646733  
 H -39.444825 -8.507762 3.373016  
 H -40.391404 -11.759177 3.164832  
 H -40.725268 -13.151779 4.193852  
 H -37.306538 -13.875694 2.783380  
 H -35.516323 -13.133655 4.456821  
 H -36.473764 -11.643988 6.271486  
 H -41.461137 -9.855721 11.312910  
 H -41.182393 -15.360369 7.415590  
 H -36.111406 -6.758803 7.610713  
 H -37.773391 -11.300213 10.824074  
 H -39.970827 -13.395087 2.606165  
 H -35.102825 -7.477106 3.955952  
 H -39.667858 -7.537362 4.849969  
 H -43.448709 -14.183731 7.582079  
 C -43.192984 -11.216461 7.106059  
 H -44.180089 -11.569577 7.416589  
 H -42.886144 -10.409280 7.777652  
 H -43.279716 -10.793920 6.100113  
 H -41.993072 -7.532703 10.380999

C -41.002388 -7.226124 7.547714  
 H -40.001989 -6.969469 7.184697  
 H -41.607024 -7.509325 6.679820  
 H -41.442386 -6.333346 8.000576

**(4-Melm)<sub>3</sub>(5-Melm)<sub>1</sub>, ferrous, SMD, TPSSh,  
 G° = -2763.804616**

C -42.669794 -13.419875 7.409263  
 N -41.493434 -14.132844 7.290696  
 C -40.543119 -13.288784 6.826453  
 N -41.039461 -12.068804 6.639688  
 C -42.379950 -12.134012 7.014141  
 C -40.941343 -8.626702 10.085798  
 N -40.414953 -9.871054 10.371309  
 C -40.053495 -10.446414 9.202117  
 N -40.309583 -9.636674 8.177836  
 C -40.873084 -8.484971 8.719089  
 C -35.331022 -6.819772 4.544470  
 C -36.416378 -7.487559 5.320159  
 N -36.696058 -7.181791 6.642304  
 C -37.734286 -7.950222 7.054368  
 N -38.148528 -8.743667 6.073069  
 C -37.329986 -8.460657 4.989187  
 C -40.774200 -7.620571 4.127327  
 S -41.054240 -9.431458 4.312483  
 C -39.423065 -12.814034 3.494221  
 C -38.246594 -12.591142 4.389835  
 N -38.251165 -11.675074 5.441735  
 C -37.050233 -11.752166 6.012476  
 N -36.280301 -12.668112 5.386923  
 C -37.017590 -13.206636 4.350672  
 Fe -39.769259 -10.245537 6.120765  
 H -39.525055 -13.596740 6.646130  
 H -39.621448 -11.433833 9.138315  
 H -35.495234 -5.738282 4.479502  
 H -34.351062 -6.981875 5.007311  
 H -37.450325 -8.969434 4.043887  
 H -38.135132 -7.906618 8.055342  
 H -39.734485 -7.357988 4.339368  
 H -41.427503 -7.051692 4.794857  
 H -39.850991 -11.860358 3.168993  
 H -40.215281 -13.374265 4.005034  
 H -36.610715 -13.957150 3.690901  
 H -35.323525 -12.901166 5.628369  
 H -36.710418 -11.175150 6.858899  
 H -40.318386 -10.287527 11.290336  
 H -41.360162 -15.115306 7.500566  
 H -36.209387 -6.496012 7.209554  
 H -39.118393 -13.384789 2.612683  
 H -35.303243 -7.224587 3.530293  
 H -41.002321 -7.333271 3.096635

C	-43.294234	-10.950675	6.980704
H	-43.079625	-10.262529	7.806744
H	-43.172769	-10.392621	6.047188
H	-44.334250	-11.276695	7.071934
H	-43.583480	-13.878165	7.755040
C	-41.336497	-7.339103	7.878503
H	-42.077355	-7.669389	7.142459
H	-41.795270	-6.574856	8.511642
H	-40.506415	-6.878698	7.331904
H	-41.316415	-7.973874	10.858597

**(4-Melm)<sub>3</sub>(5-Melm)<sub>1</sub>, ferric, SMD, PBE0,  
G° = -2990.256780**

C	-37.361463	-12.352087	10.168549
C	-37.297625	-11.551780	8.887040
O	-36.262115	-10.902479	8.614040
O	-38.348239	-11.594452	8.157011
C	-42.622365	-13.591789	7.260267
N	-41.484730	-14.325361	7.029418
C	-40.469439	-13.472096	6.845443
N	-40.888429	-12.216763	6.946631
C	-42.250061	-12.274014	7.212429
C	-41.423433	-8.211908	9.800048
N	-41.085685	-9.390328	10.416750
C	-40.427358	-10.149997	9.531124
N	-40.316596	-9.524387	8.365086
C	-40.945948	-8.295817	8.518326
C	-35.234162	-7.121106	4.826864
C	-36.305906	-7.773847	5.618152
N	-36.635729	-7.390616	6.900208
C	-37.640457	-8.165231	7.341923
N	-37.989187	-9.038213	6.410313
C	-37.160113	-8.804384	5.331199
C	-40.181309	-8.323607	4.131059
S	-40.864613	-9.772787	4.985004
C	-39.795189	-12.721497	3.459166
C	-38.474444	-12.579624	4.127552
N	-38.246658	-11.876003	5.304043
C	-36.954604	-12.012416	5.579139
N	-36.346764	-12.755300	4.644730
C	-37.288166	-13.129253	3.717818
Fe	-39.448127	-10.595223	6.646245
H	-36.366691	-12.504120	10.591748
H	-37.848859	-13.316454	10.001267
H	-39.457074	-13.790216	6.647294
H	-40.051727	-11.135365	9.756611
H	-35.446974	-6.058763	4.664724
H	-34.264905	-7.194694	5.331794
H	-37.227251	-9.381867	4.420891
H	-38.067729	-8.076098	8.329626
H	-40.998985	-7.808600	3.619509

H	-39.445602	-8.633627	3.383780
H	-40.189542	-11.754860	3.133243
H	-40.541177	-13.166009	4.126279
H	-37.046690	-13.747502	2.866337
H	-35.364779	-12.998125	4.636094
H	-36.440394	-11.589415	6.430926
H	-41.291134	-9.648430	11.373275
H	-41.413784	-15.333990	6.996018
H	-36.195553	-6.648284	7.429858
H	-37.968237	-11.799173	10.895617
H	-39.689466	-13.371184	2.586019
H	-35.149227	-7.605817	3.851754
H	-39.705833	-7.632209	4.829456
H	-43.580967	-14.054863	7.439548
C	-43.119287	-11.087285	7.437414
H	-42.890707	-10.596731	8.389494
H	-43.001233	-10.343796	6.644176
H	-44.165404	-11.403454	7.465365
H	-41.956073	-7.423897	10.310829
C	-41.060897	-7.263971	7.454234
H	-40.079930	-6.959750	7.074722
H	-41.642518	-7.633401	6.603755
H	-41.559108	-6.378360	7.857714

**(4-Melm)<sub>3</sub>(5-Melm)<sub>1</sub>, ferrous, SMD, PBE0,  
G° = -2762.058400**

C	-42.686256	-13.442476	7.364083
N	-41.563195	-14.181626	7.085261
C	-40.613586	-13.337813	6.642791
N	-41.057768	-12.090885	6.621684
C	-42.363739	-12.139528	7.080345
C	-41.071764	-8.674241	10.089360
N	-40.571271	-9.917095	10.390352
C	-40.127493	-10.470762	9.248228
N	-40.304878	-9.648367	8.226583
C	-40.904778	-8.511833	8.737493
C	-35.374468	-6.928267	4.385881
C	-36.441673	-7.539098	5.217412
N	-36.805724	-7.050309	6.452158
C	-37.798445	-7.820578	6.944043
N	-38.101744	-8.788483	6.098557
C	-37.260523	-8.620923	5.018365
C	-40.685465	-7.592027	4.237386
S	-41.065741	-9.373362	4.389057
C	-39.195902	-12.556453	3.356929
C	-38.131995	-12.487303	4.393971
N	-38.234789	-11.700467	5.527791
C	-37.125078	-11.895031	6.223272
N	-36.317456	-12.767583	5.597656
C	-36.933386	-13.153296	4.432585
Fe	-39.762603	-10.265646	6.172684

H -39.626878 -13.669644 6.355867  
H -39.690173 -11.458165 9.199662  
H -35.599704 -5.882220 4.150508  
H -34.405386 -6.952809 4.896508  
H -37.292867 -9.282756 4.163874  
H -38.249955 -7.648762 7.910468  
H -39.639791 -7.382525 4.480681  
H -41.323055 -6.991067 4.892761  
H -39.497893 -11.554869 3.034763  
H -40.092769 -13.057858 3.739646  
H -36.479161 -13.850521 3.744654  
H -35.412290 -13.074361 5.929472  
H -36.874395 -11.431899 7.166914  
H -40.538541 -10.346710 11.305371  
H -41.460337 -15.182635 7.184056  
H -36.396381 -6.250673 6.918694  
H -38.840010 -13.116736 2.488269  
H -35.279275 -7.477182 3.446300  
H -40.865678 -7.271850 3.206516  
C -43.221763 -10.932630 7.230167  
H -44.271584 -11.225205 7.321400  
H -42.952286 -10.357495 8.123307  
H -43.112029 -10.269522 6.366213  
H -43.597459 -13.893244 7.728164  
H -41.503479 -8.029381 10.840115  
C -41.324370 -7.364690 7.888411  
H -40.475822 -6.912749 7.364634  
H -42.046102 -7.684100 7.128543  
H -41.793822 -6.594048 8.505671

**(4-Melm)<sub>4</sub>(5-Melm)<sub>0</sub>, ferric, SMD, BP86,  
*G*<sup>o</sup> = -2992.370626**

C -37.168794 -12.082418 10.295687  
C -37.531657 -12.254452 8.823340  
O -37.036289 -13.217904 8.158625  
O -38.376103 -11.392491 8.351733  
C -42.379758 -13.840150 7.043915  
N -41.158797 -14.420386 7.350544  
C -40.202630 -13.462612 7.269304  
N -40.745431 -12.281686 6.927633  
C -42.121707 -12.506940 6.776031  
C -41.404587 -7.767869 9.390737  
N -41.775433 -9.029621 9.828252  
C -41.175169 -9.947334 9.031787  
N -40.427398 -9.339345 8.095881  
C -40.560176 -7.959459 8.310927  
C -35.981884 -7.648721 6.322354  
N -36.040384 -7.991626 7.663788  
C -37.041223 -8.891569 7.825835  
N -37.636487 -9.155211 6.650509  
C -36.976122 -8.374141 5.688759

C -41.895569 -8.471174 5.158004  
S -40.510755 -9.612174 4.769379  
C -40.009403 -13.003362 3.728428  
C -38.602217 -12.662192 4.109828  
N -38.245192 -11.795629 5.155522  
C -36.902251 -11.771294 5.190062  
N -36.387042 -12.570588 4.225628  
C -37.441399 -13.140158 3.527553  
Fe -39.374067 -10.557457 6.605644  
H -36.312859 -12.714874 10.575890  
H -38.037798 -12.368327 10.915548  
H -39.146471 -13.653247 7.455398  
H -41.296292 -11.019954 9.159191  
H -37.302584 -9.331087 8.784311  
H -42.170993 -8.510325 6.222031  
H -42.765965 -8.748764 4.541631  
H -40.621970 -12.096688 3.589229  
H -40.504310 -13.618962 4.499428  
H -37.282319 -13.823561 2.696639  
H -35.391963 -12.717026 4.047484  
H -36.288905 -11.204421 5.885327  
H -42.394458 -9.240539 10.612898  
H -40.994342 -15.399674 7.588838  
H -35.442007 -7.630487 8.408319  
H -36.941672 -11.026564 10.519724  
H -40.008073 -13.576289 2.787122  
H -41.602536 -7.441522 4.893833  
H -43.307927 -14.407066 7.047555  
C -43.114762 -11.457088 6.390337  
H -43.063847 -10.580517 7.058672  
H -42.944505 -11.099563 5.360331  
H -44.133749 -11.873101 6.445774  
H -41.759389 -6.861205 9.875281  
C -39.854238 -6.903779 7.516099  
H -38.811048 -6.773916 7.854207  
H -39.823685 -7.150002 6.443700  
H -40.369155 -5.937489 7.640925  
H -35.249458 -6.943329 5.936315  
C -37.294633 -8.367582 4.226634  
H -37.160042 -9.366152 3.774606  
H -38.339287 -8.066709 4.037609  
H -36.624565 -7.662849 3.708066

**(4-Melm)<sub>4</sub>(5-Melm)<sub>0</sub>, ferrous, SMD, BP86,  
*G*<sup>o</sup> = -2763.916583**

C -42.688002 -13.475649 7.501361  
N -41.501957 -14.181256 7.375136  
C -40.565054 -13.333648 6.863938  
N -41.083808 -12.116897 6.651045  
C -42.421898 -12.189931 7.057146  
C -40.880806 -8.548216 10.031547

N -40.424080 -9.820896 10.337547  
 C -40.111137 -10.447105 9.170175  
 N -40.333687 -9.637068 8.125183  
 C -40.823197 -8.436159 8.652058  
 C -36.374026 -7.476101 5.483225  
 N -36.659291 -7.317241 6.831318  
 C -37.710265 -8.125233 7.135373  
 N -38.121221 -8.799573 6.051969  
 C -37.281831 -8.405672 5.002400  
 C -40.856516 -7.677784 4.107487  
 S -41.144183 -9.484060 4.395904  
 C -39.416144 -12.762546 3.415132  
 C -38.275312 -12.588064 4.369123  
 N -38.317346 -11.715944 5.463463  
 C -37.137914 -11.832622 6.091051  
 N -36.346407 -12.736367 5.456417  
 C -37.043954 -13.221834 4.360274  
 Fe -39.801704 -10.265766 6.111162  
 H -39.538992 -13.637608 6.670225  
 H -39.734946 -11.467206 9.121869  
 H -38.129691 -8.199888 8.136521  
 H -39.836948 -7.379151 4.400918  
 H -41.580007 -7.070227 4.676477  
 H -39.810087 -11.784748 3.087653  
 H -40.253947 -13.311678 3.882390  
 H -36.614037 -13.956790 3.683394  
 H -35.398098 -12.996324 5.733024  
 H -36.829048 -11.289936 6.982384  
 H -40.342362 -10.226876 11.270681  
 H -41.351918 -15.162478 7.612860  
 H -36.176442 -6.697618 7.483582  
 H -39.088259 -13.331142 2.529976  
 H -40.991117 -7.457334 3.035074  
 C -43.368285 -11.030437 6.993494  
 H -44.384417 -11.354611 7.271703  
 H -43.063555 -10.223010 7.683471  
 H -43.396993 -10.592906 5.980817  
 H -43.596600 -13.936567 7.883049  
 H -41.209186 -7.852288 10.800266  
 C -41.210207 -7.268958 7.798079  
 H -41.942535 -7.564364 7.026896  
 H -41.660025 -6.478441 8.420177  
 H -40.337165 -6.837634 7.275703  
 H -35.569664 -6.929102 4.996127  
 C -37.379164 -8.968400 3.617205  
 H -36.988571 -10.001553 3.573930  
 H -38.427071 -9.003344 3.273081  
 H -36.791581 -8.354514 2.915297

**(4-Melm)<sub>4</sub>(5-Melm)<sub>0</sub>, ferric, SMD, TPSSh,  
 G° = -2992.255570**

C -37.314901 -12.118025 10.174084  
 C -37.209057 -11.479082 8.798917  
 O -36.114020 -10.978427 8.423165  
 O -38.288022 -11.494660 8.094739  
 C -42.517383 -13.649151 7.398421  
 N -41.325829 -14.342650 7.319576  
 C -40.351320 -13.465395 7.015405  
 N -40.848548 -12.233993 6.888687  
 C -42.221442 -12.334548 7.130053  
 C -41.443517 -8.320287 9.817808  
 N -41.175674 -9.564879 10.352009  
 C -40.521011 -10.286766 9.421884  
 N -40.349681 -9.575531 8.305773  
 C -40.935087 -8.329093 8.541107  
 C -36.383507 -7.559629 5.649995  
 N -36.672046 -7.367608 6.986901  
 C -37.602737 -8.269144 7.348825  
 N -37.935437 -9.039832 6.311641  
 C -37.167004 -8.606801 5.228635  
 C -40.394187 -8.059559 4.240465  
 S -40.863701 -9.690742 4.925041  
 C -39.971232 -12.781719 3.485407  
 C -38.617607 -12.706794 4.113626  
 N -38.316493 -11.963602 5.257094  
 C -37.023856 -12.170164 5.515155  
 N -36.485550 -13.001041 4.601383  
 C -37.475175 -13.351903 3.703939  
 Fe -39.432198 -10.585217 6.552875  
 H -36.328836 -12.261941 10.619896  
 H -37.839231 -13.076029 10.111751  
 H -39.316900 -13.747190 6.904843  
 H -40.190223 -11.299481 9.580754  
 H -38.003178 -8.338797 8.347366  
 H -41.280739 -7.420104 4.234085  
 H -40.051829 -8.186639 3.210044  
 H -40.303780 -11.801107 3.131439  
 H -40.721830 -13.145223 4.195047  
 H -37.289646 -14.023177 2.880022  
 H -35.517813 -13.302649 4.581419  
 H -36.467369 -11.741525 6.336447  
 H -41.418849 -9.887465 11.282126  
 H -41.194795 -15.336732 7.470186  
 H -36.265878 -6.666364 7.596295  
 H -37.905637 -11.460976 10.823379  
 H -39.938484 -13.469913 2.636240  
 H -39.608330 -7.587322 4.830954  
 H -43.450180 -14.137818 7.632590  
 C -43.180552 -11.188679 7.085529  
 H -44.166124 -11.533375 7.410482



H -42.864792 -10.372028 7.741218  
H -43.272494 -10.781154 6.074135  
H -41.956272 -7.553934 10.377766  
C -40.992345 -7.222705 7.539375  
H -40.006027 -7.005865 7.118138  
H -41.660983 -7.473761 6.709842  
H -41.368054 -6.315616 8.020725  
H -35.662410 -6.950422 5.127983  
C -37.205484 -9.230631 3.868857  
H -36.503423 -10.068566 3.795123  
H -38.201333 -9.613810 3.637246  
H -36.925407 -8.491395 3.113450

**(4-Melm)<sub>4</sub>(5-Melm)<sub>0</sub>, ferrous, SMD, TPSSh,  
*G*<sup>o</sup> = -2763.802671**

C -42.664582 -13.475925 7.497625  
N -41.510958 -14.200650 7.274639  
C -40.576072 -13.350798 6.789765  
N -41.060943 -12.116212 6.685175  
C -42.377554 -12.178820 7.138552  
C -40.998057 -8.533363 10.001986  
N -40.558915 -9.797729 10.342244  
C -40.161701 -10.419159 9.209360  
N -40.313639 -9.620399 8.155718  
C -40.842728 -8.426679 8.639535  
C -36.372311 -7.515374 5.432325  
N -36.637764 -7.343682 6.777136  
C -37.689171 -8.130268 7.096502  
N -38.118966 -8.802606 6.030679  
C -37.291606 -8.429658 4.973193  
C -40.857090 -7.707454 4.095503  
S -41.201166 -9.490691 4.410526  
C -39.382489 -12.745669 3.422687  
C -38.244459 -12.584289 4.378309  
N -38.289486 -11.723963 5.473856  
C -37.116445 -11.838310 6.093451  
N -36.325657 -12.728638 5.457684  
C -37.019654 -13.208934 4.364113  
Fe -39.786408 -10.276369 6.123206  
H -39.575217 -13.665889 6.539950  
H -39.781345 -11.429386 9.191008  
H -38.097044 -8.191128 8.093739  
H -39.878807 -7.416907 4.486726  
H -41.622988 -7.081078 4.562009  
H -39.747407 -11.770355 3.084846  
H -40.225720 -13.268152 3.889720  
H -36.589881 -13.931801 3.688281  
H -35.383357 -12.984629 5.731345  
H -36.811730 -11.303730 6.980579  
H -40.537023 -10.195479 11.274284  
H -41.380710 -15.192250 7.438535

H -36.141671 -6.731436 7.414808  
H -39.060880 -13.326353 2.553879  
H -40.870762 -7.521189 3.017364  
C -43.274167 -10.984298 7.221260  
H -43.013884 -10.349643 8.076463  
H -43.189327 -10.372275 6.317958  
H -44.313243 -11.304632 7.340944  
H -43.563171 -13.934776 7.880324  
C -41.187714 -7.277689 7.748101  
H -41.942488 -7.569824 7.010125  
H -41.584464 -6.449654 8.341479  
H -40.309739 -6.919101 7.199809  
H -41.378950 -7.842950 10.738398  
H -35.573182 -6.986284 4.936591  
C -37.421539 -9.002024 3.597490  
H -37.010327 -10.017253 3.550206  
H -38.472054 -9.058317 3.295598  
H -36.876638 -8.382543 2.879567

**(4-Melm)<sub>4</sub>(5-Melm)<sub>0</sub>, ferric, SMD, PBE0,  
*G*<sup>o</sup> = -2990.251251**

C -37.331399 -12.051244 10.191236  
C -37.226011 -11.464765 8.800949  
O -36.139978 -10.968551 8.421170  
O -38.292586 -11.515370 8.096390  
C -42.532519 -13.635204 7.313648  
N -41.360601 -14.341058 7.196884  
C -40.373229 -13.470629 6.952723  
N -40.842699 -12.230239 6.901172  
C -42.209765 -12.315935 7.132934  
C -41.411393 -8.303285 9.789961  
N -41.128941 -9.528467 10.340941  
C -40.481652 -10.258379 9.422778  
N -40.327517 -9.570534 8.297423  
C -40.916050 -8.331783 8.512671  
C -36.380551 -7.589863 5.649944  
N -36.680964 -7.382189 6.973742  
C -37.613412 -8.271462 7.334483  
N -37.936749 -9.049907 6.309066  
C -37.160841 -8.636543 5.234656  
C -40.379235 -8.112958 4.244067  
S -40.852961 -9.729205 4.924322  
C -39.938429 -12.774772 3.486935  
C -38.596244 -12.696957 4.122158  
N -38.302432 -11.966435 5.265198  
C -37.017082 -12.171867 5.525930  
N -36.475399 -12.990064 4.613539  
C -37.453954 -13.334618 3.713737  
Fe -39.424499 -10.593556 6.554691  
H -36.345021 -12.222184 10.626596  
H -37.901506 -12.984225 10.178849

H -39.343785 -13.767133 6.822327  
H -40.142596 -11.267360 9.595535  
H -38.023658 -8.328529 8.331301  
H -41.261563 -7.467178 4.227831  
H -40.028358 -8.234785 3.215495  
H -40.266342 -11.799133 3.116320  
H -40.698539 -13.124015 4.193536  
H -37.267942 -14.000268 2.884324  
H -35.508957 -13.288420 4.597292  
H -36.464195 -11.747654 6.353359  
H -41.360737 -9.836599 11.276369  
H -41.247996 -15.342789 7.281877  
H -36.279721 -6.677581 7.578768  
H -37.876185 -11.343499 10.827543  
H -39.903127 -13.475791 2.648529  
H -39.597687 -7.633328 4.835081  
H -43.478591 -14.114985 7.514283  
C -43.139866 -11.155949 7.189690  
H -42.896157 -10.480942 8.016462  
H -43.109151 -10.568167 6.267979  
H -44.160082 -11.520139 7.337578  
H -41.924963 -7.527167 10.337160  
C -40.989376 -7.245344 7.501052  
H -40.006066 -7.010673 7.082024  
H -41.645840 -7.519916 6.669579  
H -41.387172 -6.339389 7.966293  
H -35.653435 -6.990437 5.123259  
C -37.184244 -9.265506 3.884920  
H -36.512347 -10.129268 3.832780  
H -38.184953 -9.613589 3.621390  
H -36.854696 -8.542215 3.134106

**(4-Melm)<sub>4</sub>(5-Melm)<sub>0</sub>, ferrous, SMD, PBE0,  
*G*<sup>o</sup> = -2762.057627**

C -42.682568 -13.456730 7.456665  
N -41.548817 -14.193496 7.218693  
C -40.605658 -13.357146 6.747589  
N -41.065563 -12.118767 6.666506  
C -42.373657 -12.163103 7.119013  
C -41.042322 -8.550980 9.986936  
N -40.608882 -9.805977 10.337966  
C -40.179300 -10.422595 9.223189  
N -40.304236 -9.629779 8.170735  
C -40.849226 -8.445294 8.633082  
C -36.379557 -7.511192 5.460855  
N -36.664526 -7.321843 6.791257  
C -37.702879 -8.114472 7.108129  
N -38.106528 -8.807758 6.054441  
C -37.277217 -8.443835 5.007226  
C -40.799149 -7.719268 4.108677  
S -41.179663 -9.483145 4.403461

C -39.355597 -12.740785 3.440373  
C -38.220452 -12.583096 4.388781  
N -38.265805 -11.745339 5.490168  
C -37.094196 -11.856536 6.097840  
N -36.302383 -12.725347 5.448724  
C -36.993356 -13.194170 4.358049  
Fe -39.770520 -10.293611 6.135587  
H -39.610635 -13.686603 6.487440  
H -39.794693 -11.432836 9.215505  
H -38.122779 -8.166030 8.102369  
H -39.818561 -7.446246 4.507933  
H -41.551369 -7.074804 4.573927  
H -39.733477 -11.764817 3.118428  
H -40.192830 -13.277450 3.901989  
H -36.564335 -13.904030 3.666808  
H -35.358357 -12.974862 5.713677  
H -36.788889 -11.330248 6.991318  
H -40.612427 -10.203151 11.268014  
H -41.434738 -15.187554 7.364100  
H -36.188285 -6.693789 7.424881  
H -39.035271 -13.305171 2.560580  
H -40.799440 -7.515102 3.033435  
C -43.245739 -10.961082 7.222181  
H -44.290075 -11.263006 7.342166  
H -42.972425 -10.340976 8.083789  
H -43.154935 -10.336832 6.327726  
H -43.590828 -13.901851 7.834851  
H -41.447654 -7.858211 10.709168  
C -41.175301 -7.303920 7.736486  
H -40.282703 -6.922559 7.228519  
H -41.888990 -7.606384 6.962532  
H -41.615441 -6.486157 8.313130  
H -35.582234 -6.980661 4.962053  
C -37.381857 -9.031503 3.643646  
H -36.989818 -10.054969 3.619826  
H -38.424543 -9.074030 3.312924  
H -36.807794 -8.433603 2.930431

**(4-Melm)<sub>1</sub>(5-Melm)<sub>2</sub>(5-Me-1,3-Th)<sub>1</sub>, ferric, in  
*vacuo*, TPSSh, *G*<sup>o</sup> = -3335.026486**

C -37.460768 -12.652647 10.323977  
C -37.343848 -11.827375 9.048995  
O -36.235834 -11.427060 8.660425  
O -38.474832 -11.615266 8.424429  
C -43.879681 -14.310821 6.370106  
C -42.606575 -13.638770 6.770158  
N -41.728848 -14.170201 7.705639  
C -40.673387 -13.331606 7.845670  
N -40.817235 -12.278046 7.049685  
C -42.015475 -12.463068 6.377229  
C -41.401205 -6.245471 9.945393

C -41.013103 -7.601544 9.452425  
 N -41.213327 -8.762183 10.188494  
 C -40.754218 -9.819304 9.473528  
 N -40.270865 -9.408131 8.310086  
 C -40.426451 -8.032074 8.287542  
 C -35.671302 -6.658756 4.743312  
 C -36.319674 -7.536541 5.771889  
 C -37.045638 -8.711576 7.799804  
 N -37.710706 -9.134779 6.747545  
 C -37.302654 -8.472225 5.601250  
 C -42.068375 -8.951975 5.542714  
 S -40.449339 -9.647266 5.040550  
 C -39.602355 -12.716230 3.572839  
 C -38.280073 -12.558412 4.252800  
 N -38.076961 -11.835624 5.431712  
 C -36.781210 -11.942610 5.735460  
 N -36.149471 -12.692200 4.810140  
 C -37.076367 -13.092116 3.864733  
 Fe -39.319887 -10.694858 6.810114  
 H -36.565096 -12.531496 10.934370  
 H -37.550764 -13.712649 10.057195  
 H -43.694234 -15.298771 5.934175  
 H -44.394190 -13.704958 5.621829  
 H -42.360560 -11.749204 5.646351  
 H -39.836195 -13.494218 8.505051  
 H -40.880533 -5.989666 10.874818  
 H -42.479092 -6.176484 10.129369  
 H -40.102910 -7.448893 7.439046  
 H -40.769887 -10.840058 9.820398  
 H -35.822298 -5.597989 4.967599  
 H -34.593333 -6.839654 4.683231  
 H -37.779714 -8.711882 4.660148  
 H -37.179611 -9.109065 8.794174  
 H -42.372390 -9.317480 6.525107  
 H -42.812283 -9.234598 4.793379  
 H -39.999074 -11.753345 3.239090  
 H -40.340591 -13.161586 4.246501  
 H -36.808785 -13.705817 3.019235  
 H -35.166425 -12.928342 4.824290  
 H -36.313249 -11.536470 6.626893  
 H -41.628544 -8.812720 11.109840  
 H -41.847212 -15.047704 8.195601  
 H -41.139681 -5.495342 9.196668  
 H -44.554979 -14.437623 7.223565  
 H -38.350125 -12.374820 10.897016  
 H -39.490680 -13.369652 2.703841  
 H -36.107725 -6.865195 3.762954  
 H -42.002404 -7.861494 5.567009  
 S -35.888422 -7.486367 7.463178

**(4-Melm)<sub>1</sub>(5-Melm)<sub>2</sub>(5-Me-1,3-Th)<sub>1</sub>, ferrous, in vacuo, TPSSh, G° = -3106.569711**

C -44.033960 -14.199994 6.875560  
 C -42.672145 -13.585312 6.909544  
 N -41.523323 -14.303252 7.208295  
 C -40.454675 -13.464023 7.129718  
 N -40.848416 -12.240779 6.803065  
 C -42.226046 -12.307374 6.665805  
 C -41.368677 -7.040237 10.750284  
 C -40.991735 -8.220136 9.914439  
 N -41.187861 -9.531587 10.321156  
 C -40.762701 -10.363599 9.336860  
 N -40.290347 -9.666132 8.311416  
 C -40.430221 -8.331328 8.665181  
 C -35.988110 -6.664858 4.009182  
 C -36.638087 -7.397341 5.145028  
 C -37.351489 -8.319652 7.302269  
 N -38.093583 -8.792315 6.324805  
 C -37.690993 -8.273502 5.107380  
 C -41.348131 -7.806872 4.999158  
 S -41.024244 -9.583302 4.642893  
 C -39.261150 -12.605643 3.662579  
 C -38.098495 -12.526347 4.599601  
 N -38.093751 -11.709179 5.729405  
 C -36.904743 -11.861450 6.303553  
 N -36.146045 -12.739316 5.605253  
 C -36.885130 -13.168565 4.519166  
 Fe -39.707183 -10.373237 6.351384  
 H -44.098606 -14.994996 6.124269  
 H -44.771423 -13.437034 6.619332  
 H -42.789710 -11.437034 6.364457  
 H -39.436369 -13.780097 7.297978  
 H -40.836091 -7.035752 11.707793  
 H -42.443998 -7.022546 10.959394  
 H -40.135244 -7.540902 7.992555  
 H -40.825925 -11.438842 9.391847  
 H -36.072809 -5.580379 4.131089  
 H -34.925113 -6.912457 3.926185  
 H -38.231579 -8.577105 4.218170  
 H -37.495148 -8.576031 8.344239  
 H -40.416516 -7.248935 5.132139  
 H -41.968681 -7.695958 5.891862  
 H -39.480668 -11.625767 3.226973  
 H -40.165078 -12.937190 4.182263  
 H -36.490443 -13.866738 3.797974  
 H -35.201141 -13.018419 5.832318  
 H -36.560871 -11.358611 7.194530  
 H -41.591081 -9.822344 11.202407  
 H -41.482895 -15.290152 7.427485  
 H -41.115418 -6.120147 10.220186  
 H -44.311801 -14.626884 7.845845

H -39.045570 -13.308344 2.854040  
H -36.478345 -6.942205 3.072924  
H -41.886081 -7.388069 4.145785  
S -36.120330 -7.218559 6.801094

**(4-Melm)<sub>1</sub>(5-Melm)<sub>2</sub>(5-Me-1,3-Ox)<sub>1</sub>, ferric, in vacuo, TPSSh,  $G^\circ = -3012.051523$**

C -37.574406 -12.656210 10.339647  
C -37.367383 -11.894565 9.037955  
O -36.217931 -11.588538 8.674432  
O -38.449430 -11.640260 8.355897  
C -43.894965 -14.344081 6.409017  
C -42.624131 -13.660990 6.797365  
N -41.751764 -14.165231 7.752143  
C -40.697460 -13.322537 7.874118  
N -40.836755 -12.290889 7.048990  
C -42.031365 -12.496268 6.375364  
C -41.025616 -6.164319 9.932932  
C -40.745535 -7.543461 9.430868  
N -40.995205 -8.687297 10.177210  
C -40.627878 -9.772662 9.451679  
N -40.158050 -9.395561 8.271587  
C -40.226892 -8.012739 8.248819  
C -35.862292 -6.259910 5.141055  
C -36.502406 -7.433595 5.789125  
C -36.652560 -8.991542 7.308364  
N -37.686676 -9.190450 6.531336  
C -37.601218 -8.195755 5.550046  
C -42.140450 -9.018003 5.696703  
S -40.555566 -9.676625 5.055178  
C -39.693105 -12.636411 3.441024  
C -38.388951 -12.633481 4.172183  
N -38.158241 -11.970239 5.380119  
C -36.891018 -12.214614 5.720590  
N -36.303053 -12.995387 4.791767  
C -37.230895 -13.273037 3.805271  
Fe -39.318152 -10.727927 6.747812  
H -36.753470 -12.450306 11.028001  
H -37.567029 -13.731789 10.125098  
H -43.707047 -15.344052 6.002583  
H -44.404888 -13.759769 5.640731  
H -42.373916 -11.803046 5.623675  
H -39.862453 -13.471033 8.539122  
H -40.450668 -5.940509 10.838298  
H -42.088147 -6.026113 10.161704  
H -39.893858 -7.451832 7.389088  
H -40.699073 -10.789148 9.803635  
H -35.807532 -5.410714 5.829855  
H -34.843962 -6.497975 4.817298  
H -38.337090 -8.119104 4.765023  
H -36.330120 -9.591367 8.148204

H -42.395245 -9.465765 6.658782  
H -42.923494 -9.233299 4.965405  
H -39.970678 -11.632760 3.107447  
H -40.500981 -13.007108 4.078691  
H -36.995779 -13.884862 2.948864  
H -35.347729 -13.324817 4.827267  
H -36.405932 -11.874415 6.629811  
H -41.381075 -8.709643 11.112287  
H -41.872485 -15.028576 8.266114  
H -40.748641 -5.433906 9.170375  
H -44.575365 -14.446358 7.261692  
H -38.531652 -12.407280 10.805478  
H -39.618845 -13.286499 2.565545  
H -36.444642 -5.962922 4.266606  
H -42.062934 -7.934354 5.812634  
O -35.896572 -7.950375 6.922655

**(4-Melm)<sub>1</sub>(5-Melm)<sub>2</sub>(5-Me-1,3-Ox)<sub>1</sub>, ferrous, in vacuo, TPSSh,  $G^\circ = -2783.593531$**

C -44.073988 -14.197559 6.952972  
C -42.707715 -13.591934 6.949658  
N -41.556393 -14.316394 7.221668  
C -40.484674 -13.484532 7.112168  
N -40.878579 -12.259915 6.790744  
C -42.259603 -12.318014 6.689355  
C -41.291220 -7.047832 10.731580  
C -40.926309 -8.229147 9.892362  
N -41.077110 -9.539537 10.320647  
C -40.679417 -10.373816 9.326599  
N -40.267098 -9.678508 8.274338  
C -40.418305 -8.343043 8.620497  
C -35.891431 -6.522711 4.296269  
C -36.727027 -7.392818 5.163318  
C -37.382288 -8.205195 7.073448  
N -38.148591 -8.793675 6.196751  
C -37.737348 -8.281685 4.963554  
C -41.396679 -7.852823 4.926306  
S -41.087102 -9.639083 4.608584  
C -39.263598 -12.643637 3.642119  
C -38.110979 -12.561067 4.591173  
N -38.119664 -11.739996 5.717992  
C -36.939341 -11.893179 6.309346  
N -36.172864 -12.774880 5.624296  
C -36.897955 -13.206143 4.529618  
Fe -39.737589 -10.397875 6.305652  
H -44.163143 -14.994925 6.206704  
H -44.812653 -13.430601 6.712629  
H -42.825275 -11.445454 6.398550  
H -39.464477 -13.806720 7.255544  
H -40.716921 -7.020963 11.664267  
H -42.356325 -7.050708 10.988187

H -40.174588 -7.554199 7.925763  
H -40.718962 -11.449488 9.394967  
H -36.022766 -5.467315 4.555777  
H -34.829202 -6.766895 4.398941  
H -38.220948 -8.592169 4.049272  
H -37.380573 -8.313987 8.146856  
H -40.460863 -7.297275 5.037275  
H -42.008657 -7.717297 5.821651  
H -39.485555 -11.663512 3.208415  
H -40.170469 -12.982612 4.152076  
H -36.495129 -13.908131 3.816683  
H -35.232170 -13.056279 5.865675  
H -36.607926 -11.391231 7.205622  
H -41.434945 -9.828472 11.221882  
H -41.516831 -15.302811 7.443118  
H -41.081956 -6.128693 10.181026  
H -44.329804 -14.618841 7.931733  
H -39.036162 -13.342223 2.833302  
H -36.182128 -6.662913 3.253380  
H -41.940428 -7.450656 4.068610  
O -36.496460 -7.347460 6.529193

**(4-Melm)<sub>1</sub>(5-Melm)<sub>2</sub>(4-MePy)<sub>1</sub>, ferric, in vacuo,  
TPSSH,  $G^\circ = -2992.184891$**

C -37.705307 -12.348463 10.370936  
C -37.696660 -11.260751 9.311135  
O -37.155454 -10.159685 9.563263  
O -38.252542 -11.559894 8.179175  
C -43.784371 -14.535760 6.771720  
C -42.491342 -13.815705 6.978006  
N -41.408097 -14.376130 7.643324  
C -40.389611 -13.481742 7.659563  
N -40.753439 -12.365731 7.039499  
C -42.057894 -12.564735 6.609828  
C -40.878526 -6.654185 10.614511  
C -40.814186 -7.887257 9.773603  
N -41.650288 -8.977832 9.959981  
C -41.334060 -9.934103 9.051398  
N -40.335176 -9.521357 8.281966  
C -40.006752 -8.249971 8.723592  
C -35.826740 -6.660351 4.539902  
C -36.476053 -7.621646 5.495360  
N -37.906394 -9.144409 6.388637  
C -37.611532 -8.422114 5.286809  
C -41.218203 -8.064656 5.463380  
S -40.786553 -9.788637 5.030996  
C -39.828670 -12.746149 3.503239  
C -38.482840 -12.671365 4.150060  
N -38.225744 -11.971315 5.328132  
C -36.931274 -12.124655 5.592088  
N -36.343806 -12.885543 4.644268

C -37.309876 -13.244401 3.722309  
Fe -39.393093 -10.680078 6.675039  
H -37.138675 -12.032993 11.247028  
H -37.275637 -13.270141 9.965582  
H -43.645419 -15.453238 6.189163  
H -44.477528 -13.893250 6.225549  
H -42.579179 -11.799802 6.053845  
H -39.424820 -13.646985 8.112225  
H -40.669715 -6.874813 11.667135  
H -41.861658 -6.174378 10.554324  
H -39.209713 -7.685346 8.267198  
H -41.839106 -10.883833 8.975809  
H -36.351184 -5.698484 4.522339  
H -34.788962 -6.467022 4.823853  
H -38.226572 -8.528920 4.403796  
H -37.005142 -9.296425 8.259363  
H -41.833064 -8.048095 6.365765  
H -41.780392 -7.638235 4.630509  
H -40.153076 -11.763815 3.146906  
H -40.585364 -13.110087 4.204691  
H -37.085590 -13.858287 2.864460  
H -35.366878 -13.144681 4.618193  
H -36.416438 -11.711919 6.444636  
H -42.377722 -9.051626 10.659261  
H -41.377906 -15.304208 8.045976  
H -35.287156 -7.539119 7.414255  
H -40.132151 -5.936816 10.268396  
H -44.253345 -14.806704 7.724173  
H -38.737736 -12.566311 10.665714  
H -39.792681 -13.428210 2.650305  
H -35.828579 -7.056476 3.520354  
H -40.313876 -7.475727 5.633606  
N -36.969027 -8.817783 7.307730  
C -36.102470 -7.913116 6.810479

**(4-Melm)<sub>1</sub>(5-Melm)<sub>2</sub>(4-MePy)<sub>1</sub>, ferrous, in vacuo,  
TPSSH,  $G^\circ = -2763.712678$**

C -44.117426 -13.764033 7.562695  
C -42.727843 -13.278778 7.304584  
N -41.621397 -14.115517 7.298264  
C -40.518009 -13.373984 7.011879  
N -40.846735 -12.102050 6.838206  
C -42.218201 -12.034106 7.020845  
C -42.254020 -7.872447 10.773981  
C -41.274828 -8.666632 9.971492  
N -40.329371 -9.504792 10.542213  
C -39.604099 -10.084928 9.548583  
N -40.025524 -9.667768 8.362219  
C -41.067698 -8.784398 8.616475  
C -35.466054 -6.605068 4.732712  
C -36.509541 -7.307143 5.554554

N -37.989261 -8.885913 6.284161  
 C -37.075547 -8.583278 5.345640  
 C -40.476615 -7.878630 4.154918  
 S -41.218724 -9.351987 4.970742  
 C -39.660426 -12.566667 3.505394  
 C -38.375927 -12.545204 4.272086  
 N -38.186168 -11.751292 5.403032  
 C -36.942892 -11.973322 5.819715  
 N -36.324064 -12.872582 5.017253  
 C -37.215158 -13.241955 4.027409  
 Fe -39.623947 -10.354083 6.283723  
 H -44.430996 -14.504015 6.817904  
 H -44.812225 -12.923584 7.511438  
 H -42.747383 -11.099235 6.910812  
 H -39.525292 -13.789627 6.930709  
 H -41.750535 -7.177998 11.455622  
 H -42.904993 -8.521257 11.370360  
 H -41.603248 -8.324597 7.797563  
 H -38.805072 -10.787403 9.732069  
 H -35.804805 -6.463089 3.701430  
 H -35.240325 -5.620334 5.149004  
 H -36.875789 -9.291667 4.553940  
 H -38.672513 -7.805884 7.866439  
 H -39.803864 -8.181621 3.349147  
 H -39.928068 -7.258646 4.867696  
 H -40.038099 -11.551936 3.348792  
 H -40.437363 -13.113725 4.049812  
 H -36.950045 -13.942850 3.251546  
 H -35.372350 -13.199705 5.115768  
 H -36.463652 -11.497877 6.662060  
 H -40.200345 -9.661983 11.533547  
 H -41.633628 -15.112751 7.467572  
 H -37.054087 -5.913542 7.241503  
 H -42.885918 -7.287492 10.103167  
 H -44.210741 -14.220125 8.554775  
 H -39.514275 -13.051185 2.536874  
 H -34.532830 -7.176722 4.700425  
 H -41.291237 -7.290148 3.727017  
 C -37.151081 -6.842610 6.698048  
 N -38.015615 -7.806331 7.096388

**(4-Melm)<sub>1</sub>(5-Melm)<sub>2</sub>(5-Me-1,2,3-Tr)<sub>1</sub>, ferric, in vacuo, TPSSh,  $G^\circ = -3008.207169$**

C -37.231401 -11.689019 10.289234  
 C -37.186275 -11.554438 8.775211  
 O -36.106200 -11.416023 8.184171  
 O -38.357271 -11.600142 8.182588  
 C -43.886198 -14.393789 6.634132  
 C -42.582453 -13.710747 6.891496  
 N -41.546772 -14.297398 7.607147  
 C -40.505452 -13.431431 7.665595

N -40.809934 -12.309788 7.024482  
 C -42.096878 -12.475138 6.538863  
 C -41.445038 -6.421823 10.095528  
 C -41.036168 -7.743629 9.531440  
 N -41.110560 -8.929980 10.250180  
 C -40.666296 -9.944174 9.467471  
 N -40.313381 -9.481347 8.277420  
 C -40.536702 -8.115767 8.307885  
 C -35.077083 -6.978037 5.349808  
 C -36.119930 -7.798194 6.037150  
 N -36.303931 -7.829264 7.388822  
 N -37.772771 -9.154086 6.656849  
 C -37.092486 -8.664241 5.579276  
 C -42.169468 -8.892521 5.534617  
 S -40.548257 -9.564769 5.009266  
 C -39.988537 -12.510548 3.366782  
 C -38.628230 -12.497087 3.988517  
 N -38.301628 -11.844188 5.181336  
 C -37.009933 -12.086902 5.416165  
 N -36.496102 -12.851766 4.430608  
 C -37.501003 -13.125707 3.520537  
 Fe -39.391430 -10.691688 6.710334  
 H -36.233440 -11.884801 10.683146  
 H -37.918046 -12.485381 10.592076  
 H -43.750199 -15.321397 6.067061  
 H -44.535293 -13.736798 6.052070  
 H -42.580436 -11.703086 5.961515  
 H -39.565007 -13.622987 8.157897  
 H -40.850251 -6.157291 10.976981  
 H -42.501911 -6.415173 10.384713  
 H -40.316843 -7.496569 7.451940  
 H -40.596796 -10.971868 9.786081  
 H -35.195941 -5.912822 5.572970  
 H -34.069923 -7.281726 5.653518  
 H -37.346195 -8.950583 4.570896  
 H -42.417755 -9.189197 6.555119  
 H -42.933912 -9.259628 4.844283  
 H -40.286047 -11.514817 3.026792  
 H -40.743691 -12.851690 4.080874  
 H -37.335211 -13.729931 2.642613  
 H -35.542139 -13.183946 4.389456  
 H -36.464635 -11.760512 6.300764  
 H -41.438095 -9.024360 11.202687  
 H -41.558965 -15.225042 8.011166  
 H -35.778321 -7.346494 8.107567  
 H -41.298319 -5.642580 9.345089  
 H -44.404868 -14.639423 7.567509  
 H -37.602762 -10.749200 10.713752  
 H -39.990110 -13.189435 2.509833  
 H -35.159981 -7.108558 4.269609  
 H -42.147482 -7.801669 5.470152  
 N -37.294530 -8.644526 7.764477

**(4-Melm)<sub>1</sub>(5-Melm)<sub>2</sub>(5-Me-1,2,3-Tr)<sub>1</sub>, ferrous, in vacuo, TPSSh, G° = -2779.756057**

C -43.975471 -14.450769 6.370162  
C -42.715423 -13.687785 6.623391  
N -41.682084 -14.170483 7.412472  
C -40.681432 -13.247375 7.427034  
N -41.009367 -12.193147 6.694818  
C -42.273973 -12.458294 6.191027  
C -40.243198 -7.448641 11.245130  
C -40.434398 -8.377652 10.090399  
N -41.569322 -9.160095 9.929214  
C -41.440052 -9.890191 8.793739  
N -40.281541 -9.622410 8.202298  
C -39.651094 -8.680537 9.003523  
C -36.334125 -6.272882 3.859619  
C -36.975199 -7.220616 4.821073  
N -36.507114 -7.473183 6.075412  
N -38.237756 -8.692665 5.925256  
C -38.097299 -8.024524 4.743438  
C -41.721158 -7.925895 5.077470  
S -41.174032 -9.599807 4.534802  
C -38.976849 -12.732270 3.860512  
C -37.964991 -12.577556 4.950786  
N -38.130772 -11.672421 5.996145  
C -37.052317 -11.770640 6.765732  
N -36.201519 -12.700740 6.269893  
C -36.761704 -13.220627 5.117317  
Fe -39.800644 -10.327753 6.244853  
H -43.776246 -15.404657 5.868874  
H -44.632482 -13.864336 5.725061  
H -42.757464 -11.747822 5.535683  
H -39.756575 -13.384546 7.966515  
H -40.253270 -7.983570 12.201410  
H -41.023384 -6.679956 11.277902  
H -38.682027 -8.286357 8.738441  
H -42.186002 -10.580040 8.431003  
H -36.322080 -5.251846 4.254919  
H -35.302953 -6.566028 3.637029  
H -38.803177 -8.177509 3.939674  
H -40.868188 -7.265630 5.258918  
H -42.322070 -7.987814 5.988148  
H -39.156472 -11.777950 3.354620  
H -39.935788 -13.074933 4.261043  
H -36.265320 -13.977120 4.530357  
H -35.310278 -12.961215 6.669653  
H -36.851780 -11.186967 7.651332  
H -42.368839 -9.176959 10.548814  
H -41.668140 -15.063171 7.888398  
H -35.696016 -7.078757 6.536437  
H -39.279418 -6.944163 11.152878  
H -44.516044 -14.663067 7.299525

H -38.629514 -13.456572 3.119944  
H -36.894689 -6.266959 2.923564  
H -42.334516 -7.497910 4.281241  
N -37.266080 -8.360434 6.744183

**(4-Melm)<sub>1</sub>(5-Melm)<sub>2</sub>(5-Me-1,2,4-Tr)<sub>1</sub>, ferric, in vacuo, TPSSh, G° = -3008.231154**

C -37.588721 -12.129518 10.460239  
C -37.310785 -11.563808 9.074964  
O -36.131288 -11.351244 8.719080  
O -38.350271 -11.366786 8.323542  
C -43.756358 -14.551555 6.792590  
C -42.505700 -13.778606 7.059610  
N -41.581577 -14.141221 8.029879  
C -40.561021 -13.248484 8.020883  
N -40.770966 -12.322420 7.095157  
C -41.978542 -12.643716 6.492161  
C -40.687605 -7.078897 11.034204  
C -40.756523 -8.032629 9.885910  
N -41.948672 -8.558790 9.408214  
C -41.675366 -9.382051 8.364280  
N -40.370351 -9.418880 8.140529  
C -39.790902 -8.586508 9.080574  
C -36.518257 -6.192835 4.682668  
C -36.823654 -7.409968 5.488313  
N -35.941573 -8.026957 6.347597  
C -36.597718 -9.090586 6.878782  
N -37.817487 -9.125131 6.372800  
C -41.161339 -8.129509 5.117924  
S -40.735676 -9.897257 4.944593  
C -39.629539 -12.692817 3.413215  
C -38.382417 -12.770934 4.233272  
N -38.181016 -12.082787 5.431338  
C -36.961386 -12.407984 5.860867  
N -36.373781 -13.263461 4.996989  
C -37.256595 -13.509133 3.962633  
Fe -39.366923 -10.685869 6.655603  
H -36.780217 -11.865853 11.143869  
H -37.623938 -13.224130 10.395879  
H -43.536139 -15.577212 6.476123  
H -44.321580 -14.068238 5.993376  
H -42.376802 -12.037064 5.692285  
H -39.709099 -13.279743 8.679983  
H -41.097224 -7.519026 11.950203  
H -41.238141 -6.154793 10.825560  
H -38.722591 -8.443796 9.119879  
H -42.425065 -9.923253 7.807619  
H -36.268319 -5.342708 5.325735  
H -35.677223 -6.368312 4.004102  
H -36.189720 -9.812365 7.586890  
H -41.640731 -7.942624 6.081929

H -41.848523 -7.870490 4.310212  
H -39.781004 -11.687691 3.010022  
H -40.511528 -12.946614 4.008895  
H -37.016457 -14.169006 3.144070  
H -35.450934 -13.661597 5.105967  
H -36.496365 -12.058504 6.775650  
H -42.871184 -8.359674 9.772534  
H -41.654088 -14.940072 8.646678  
H -34.987293 -7.755227 6.547710  
H -39.646424 -6.812994 11.226847  
H -44.399047 -14.600894 7.678717  
H -38.548700 -11.777320 10.845502  
H -39.565398 -13.396839 2.579683  
H -37.396713 -5.937234 4.089363  
H -40.244481 -7.543237 5.045356  
N -37.962465 -8.067375 5.496133

**(4-Melm)<sub>1</sub>(5-Melm)<sub>2</sub>(5-Me-1,2,4-Tr)<sub>1</sub>, ferrous, in vacuo, TPSSh, G° = -2779.776317**

C -44.484990 -13.520068 6.816364  
C -43.110405 -12.944770 6.931890  
N -42.105896 -13.526074 7.691740  
C -40.984140 -12.762447 7.582354  
N -41.205990 -11.721687 6.794232  
C -42.525605 -11.826027 6.385387  
C -41.387580 -9.063203 11.678233  
C -40.581453 -9.253978 10.434557  
N -39.215845 -9.014731 10.371964  
C -38.785003 -9.262264 9.108625  
N -39.797635 -9.655560 8.346236  
C -40.917032 -9.655178 9.164359  
C -35.076582 -6.681628 6.572414  
C -36.458628 -7.166331 6.288530  
N -37.455072 -6.407064 5.725870  
C -38.547835 -7.215755 5.632504  
N -38.245117 -8.405117 6.106219  
C -40.291258 -8.995511 3.098258  
S -41.220350 -9.040539 4.688902  
C -40.070386 -12.906400 4.001854  
C -38.694116 -12.528843 4.452747  
N -38.442866 -11.480315 5.337386  
C -37.122366 -11.422001 5.496628  
N -36.516035 -12.385940 4.766603  
C -37.494053 -13.093026 4.092268  
Fe -39.807546 -10.074434 6.213022  
H -44.467579 -14.526366 6.382737  
H -45.091349 -12.885626 6.167082  
H -42.949283 -11.096111 5.710756  
H -40.056775 -12.996054 8.083232  
H -41.354013 -8.024519 12.025502  
H -41.034087 -9.705191 12.492901

H -41.886409 -9.936381 8.782779  
H -37.763188 -9.135967 8.782542  
H -34.567224 -6.377276 5.652281  
H -35.087029 -5.825878 7.255199  
H -39.517725 -6.939999 5.239718  
H -40.137054 -10.002085 2.702080  
H -39.315113 -8.513768 3.214063  
H -40.696133 -12.016785 3.889127  
H -40.563145 -13.562066 4.727200  
H -37.255867 -13.908119 3.427306  
H -35.519417 -12.544565 4.708965  
H -36.595377 -10.687725 6.089334  
H -38.633945 -8.709680 11.141145  
H -42.190153 -14.376071 8.233719  
H -37.393752 -5.441675 5.428036  
H -42.430949 -9.315624 11.479581  
H -44.983409 -13.579448 7.790563  
H -40.023241 -13.433181 3.045189  
H -34.507836 -7.490062 7.033397  
H -40.882225 -8.424521 2.378477  
N -36.924825 -8.377694 6.526646

**(4-Melm)<sub>1</sub>(5-Melm)<sub>2</sub>(5-MeTe<sup>-</sup>)<sub>1</sub>, ferric, in vacuo, TPSSh, G° = -3023.832180**

C -36.864917 -11.415196 10.027172  
C -37.803502 -12.222570 9.148930  
O -37.752909 -13.469844 9.112440  
O -38.676025 -11.533689 8.472099  
C -43.470464 -14.974797 5.997609  
C -42.409739 -14.090361 6.568416  
N -41.634450 -14.443476 7.665190  
C -40.766682 -13.432081 7.932659  
N -40.944500 -12.438687 7.071928  
C -41.957542 -12.841755 6.218877  
C -41.003609 -5.960490 9.876935  
C -40.772107 -7.380547 9.475342  
N -40.729844 -8.429381 10.386039  
C -40.466473 -9.578326 9.710639  
N -40.352889 -9.332440 8.417338  
C -40.537835 -7.971397 8.259063  
C -35.906051 -6.938221 4.957358  
C -36.628431 -7.859371 5.887376  
N -36.347230 -7.980546 7.207673  
N -37.956075 -9.300306 6.656431  
C -42.637815 -9.553677 6.183444  
S -41.016358 -9.675658 5.333713  
C -38.622640 -10.881340 3.193904  
C -38.141891 -11.957502 4.112373  
N -38.451875 -12.008868 5.469969  
C -37.858905 -13.090949 5.966651  
N -37.182571 -13.740272 4.991761



C -37.346969 -13.036965 3.810770  
 Fe -39.524440 -10.678539 6.868587  
 H -36.001434 -12.018096 10.314339  
 H -37.400725 -11.120794 10.938449  
 H -43.062914 -15.936458 5.663380  
 H -43.925280 -14.486244 5.133119  
 H -42.271664 -12.211815 5.400387  
 H -39.989691 -13.481132 8.683850  
 H -40.218004 -5.598222 10.550485  
 H -41.970050 -5.828749 10.378285  
 H -40.460552 -7.517005 7.282320  
 H -40.339638 -10.541086 10.178525  
 H -35.898625 -5.917101 5.351557  
 H -34.863439 -7.249438 4.829205  
 H -42.720271 -10.285382 6.990400  
 H -43.433394 -9.725660 5.452645  
 H -38.370686 -9.897296 3.602345  
 H -39.709296 -10.925887 3.069457  
 H -36.894221 -13.353496 2.884463  
 H -36.627704 -14.573529 5.124741  
 H -37.887868 -13.417245 7.000487  
 H -40.842196 -8.350020 11.387275  
 H -41.680707 -15.317048 8.171930  
 H -40.997423 -5.327061 8.987455  
 H -44.265786 -15.179704 6.724385  
 H -36.568681 -10.499524 9.508689  
 H -38.152858 -10.996223 2.212527  
 H -36.393608 -6.937843 3.979744  
 H -42.760290 -8.551617 6.603776  
 N -37.192207 -8.892792 7.670330  
 N -37.628466 -8.666988 5.517341

**(4-Melm)<sub>1</sub>(5-Melm)<sub>2</sub>(5-MeTe<sup>-</sup>)<sub>1</sub>, ferrous, in vacuo, TPSSh, G° = -2795.387527**

C -42.451968 -14.738889 8.435835  
 C -41.489625 -13.658008 8.063112  
 N -40.275626 -13.466943 8.709267  
 C -39.637061 -12.409243 8.136915  
 N -40.374942 -11.910488 7.156606  
 C -41.527698 -12.675501 7.103525  
 C -41.565557 -7.181842 10.819061  
 C -41.509398 -7.758901 9.441504  
 N -42.423949 -7.440070 8.446926  
 C -42.085803 -8.118756 7.314928  
 N -41.009766 -8.858501 7.524904  
 C -40.642785 -8.641214 8.841976  
 C -35.239558 -7.474218 7.285728  
 C -36.386595 -8.430969 7.365662  
 N -36.592588 -9.284946 8.389392  
 N -38.152595 -9.496309 6.902924  
 C -41.150710 -9.488399 2.834134

S -41.795817 -9.850682 4.517055  
 C -40.074885 -13.169769 3.791904  
 C -38.894143 -12.267452 3.627349  
 N -38.686206 -11.162520 4.444547  
 C -37.567178 -10.585016 4.027587  
 N -37.040106 -11.267881 2.980305  
 C -37.871078 -12.342551 2.711480  
 Fe -39.978460 -10.153586 5.992521  
 H -42.011374 -15.736343 8.318554  
 H -43.330120 -14.683116 7.788771  
 H -42.298955 -12.462329 6.377618  
 H -38.686927 -12.002005 8.459164  
 H -42.498632 -7.440312 11.334857  
 H -41.478729 -6.088485 10.807195  
 H -39.766191 -9.116634 9.258050  
 H -42.619464 -8.062056 6.376662  
 H -35.246979 -6.785442 8.136836  
 H -34.282562 -8.006471 7.301724  
 H -40.444301 -10.256793 2.507546  
 H -40.652594 -8.515316 2.810993  
 H -40.996300 -12.577774 3.824677  
 H -40.010436 -13.732819 4.729120  
 H -37.665337 -13.042081 1.916269  
 H -36.192147 -11.028062 2.486939  
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 H -41.993959 -9.466421 2.138376  
 N -37.709537 -9.942973 8.073475  
 N -37.338687 -8.539739 6.423930

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