SUPPORTING INFORMATION

Ni(2,2':6',2''-terpyridine)$_2$: A high-spin octahedral formal Ni(0) complex

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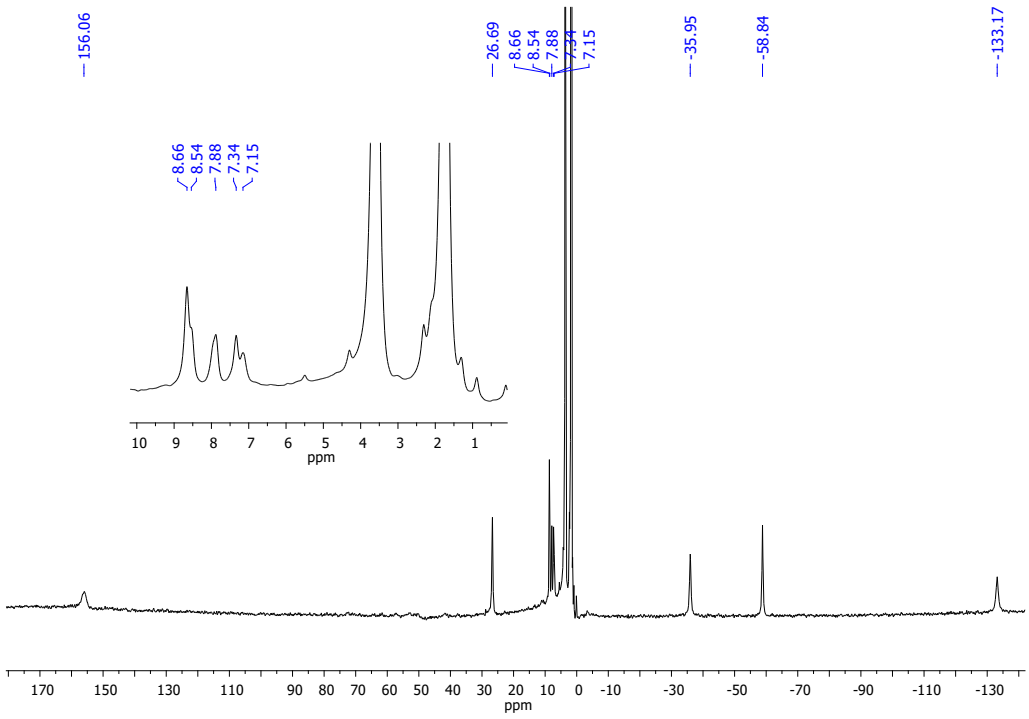
1. Experimental results

Synthesis of complex 1

In a glove-box, a mixture of $Ni(cod)_2$ (74 mg, 0.27 mmol) and terpyridine (125 mg, 0.57 mmol) were dissolved in toluene (3 mL) at room temperature. The resulting dark blue solution is stirred for 10 min, and pentane (5 mL) is added. The resulting precipitate is filtered to give a dark blue solid which is washed with pentane (76 mg, 54%). Crystals suitable for X-ray diffraction were obtained by vapor diffusion toluene/pentane at -25 °C after 24 h. Elemental analysis calculated for $C_{30}H_{22}N_6Ni$: C 68.6 %, H 4.20 %, N 16 %. Found: C 69.04 %, H 3.99 %, N 15.51 %.

Carbon: 69.04 % (expected 68.6 %)
Hydrogen: 3.99 % (expected 4.2 %)
Nitrogen: 15.51 % (expected 16 %)

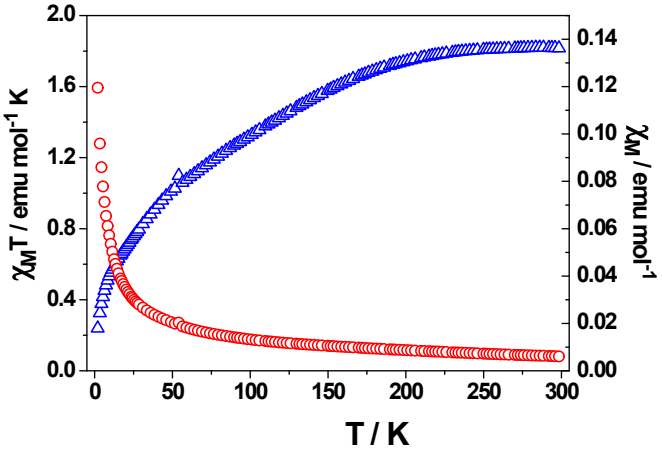


^{1}H-NMR spectrum (d^8-THF, 400 MHz)

Magnetic measurements in the solid state

The variable-temperature magnetic susceptibilities were measured on polycrystalline samples with a Quantum Design MPMSXL SQUID (Superconducting Quantum Interference Device) susceptometer over a temperature range of 2 to 300 K at the constant field of 0.5 T. All data

were corrected for the diamagnetic contribution of both the sample holder and the complex to the susceptibility. The molar diamagnetic corrections were calculated on the basis of Pascal constants.



Temperature dependence of the molar susceptibility χ_M (red circles) and $\chi_M T$ (blue triangles) for solid Ni(tpy)$_2$ at 0.5 T.

Measurement of the effective magnetic moment of 1 in solution

A sealed tube with THF as internal standard was introduced in the NMR tube. Then, a solution of complex **1** in THF (0.5 mL) was added. The experiment was carried out at room temperature with the parameters described in Table S1.

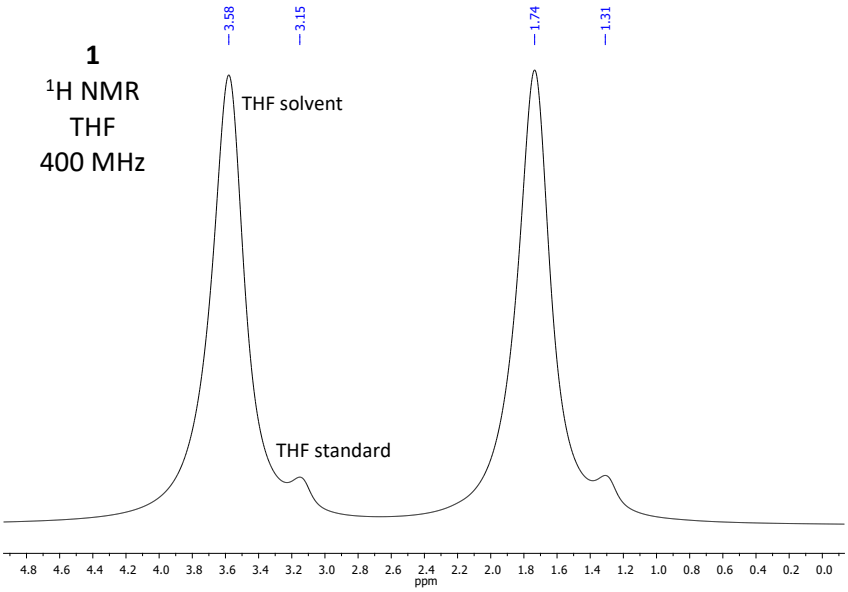
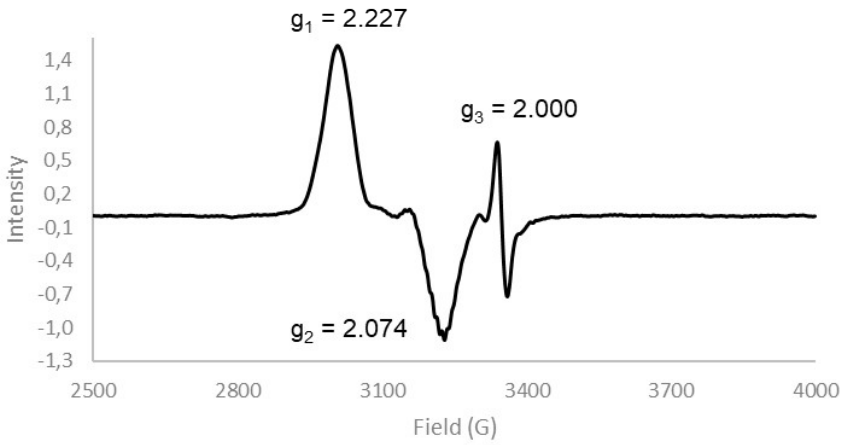


Table S1. *Parameters used for the measurement of μ_{eff}*

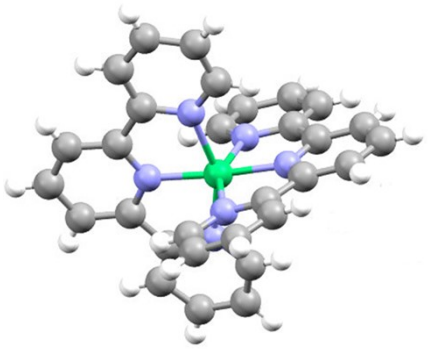
Parameter	Value
temperature	298
frequency shift in Hz	172.0559
spectrometer frequency in Hz	400130000
concentration in moles/L	0.01396
molecular weight in g/mol	525.2414
diamagnetic susceptibility	$- 306 \cdot 10^{-6}$

Magnetic susceptibility:[1] χ(**1**) = 6·(–49·10^{-6} (Py)) + (–12·10^{-6} (Ni)) = –306·10^{-6}
Using a difference of 0.43 ppm of signals shift, we obtained a value of μ_{eff} **= 4.3**. It could correspond to a S = 2 complex.

EPR signal for magnetically active S = ½ minor species (1%)



Crystal data for complex 1



A crystal (0.589 x 0.041 x 0.026 mm^3) was placed onto a thin glass optical fiber or a nylon loop and mounted on a XtaLab Synergy-S Dualflex diffractometer equipped with a HyPix- 6000HE HPC area detector for data collection at 172.99(10) K. A preliminary set of cell constants and an orientation matrix were calculated from a small sampling of reflections. A short pre-experiment was run, from which an optimal data collection strategy was determined. The full data collection was carried out using a PhotonJet (Cu) X-ray Source with frame times of 7.09 and 28.37 seconds and a detector distance of 31.2 mm. Series of frames were collected in 0.50° steps in ω at different 2θ, κ, and ϕ settings. After the intensity data were corrected for absorption, the final cell constants were calculated from the xyz centroids of 23899 strong reflections from the actual data collection after integration. See Table S2 for additional crystal and refinement information. The structure was solved using ShelXT and refined using ShelXL. The space group *Fdd*2 was determined based on systematic absences and intensity statistics. Most or all non-hydrogen atoms were assigned from the solution. Full-matrix least squares / difference Fourier cycles were performed which located any remaining non-hydrogen atoms. All non-hydrogen atoms were refined with anisotropic displacement parameters. All hydrogen atoms were placed in ideal positions and refined as riding atoms with relative isotropic displacement parameters. The

[1] G. A. Bain, J. F. Berry, *J. Chem. Educ.* **2008**, *85*, 532–536.

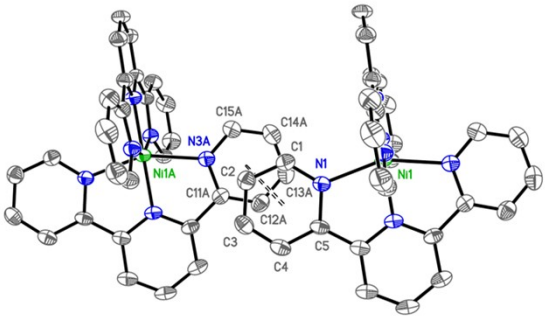
final full matrix least squares refinement converged to $R1 = 0.0327$ ($F2$, $I > 2\sigma$ (I)) and $wR2 = 0.0937$ ($F2$, all data). The structure is similar to the one suggested. The asymmetric unit contains two molecules in general positions. The structure is isomorphous with single crystal X-ray diffraction structures of Ti, Cr, V, Fe, Mo, Ru, and W analogs. Structure manipulation and figure generation were performed using Olex2. Unless noted otherwise all structural diagrams containing thermal displacement ellipsoids are drawn at the 50 % probability level.

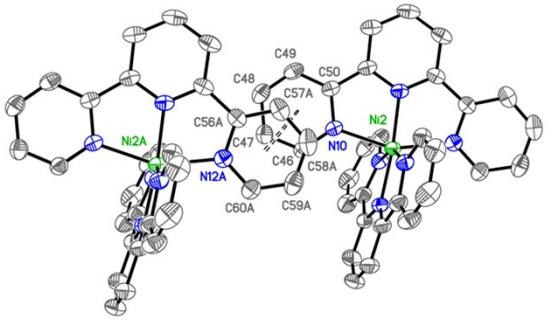
Table S2. *Crystal data and structure refinement***.**

Identification code	CCDC number 1891622
Empirical formula	$C_{30}H_{22}N_6Ni$
Formula weight	525.24
Temperature	172.99(10) K
Wavelength	1.54184 Å
Crystal system	orthorhombic
Space group	*Fdd*2
Unit cell dimensions	a = 56.2329(5) Å, α = 90°b = 39.4759(4) Å, β = 90°, c = 8.49770(10) Å, γ = 90°
Volume	18863.6(3) Å^3
Z	32
Density (calculated)	1.480 mg/m^3
Absorption coefficient	1.444 mm^{-1}
***F*(000)**	8704
Crystal color, morphology	blue-black, needle
Crystal size	0.589 x 0.041 x 0.026 mm^3
Theta range for data collection	2.735 to 77.880°
Index ranges	$-70 \le h \le 64$, $-50 \le k \le 50$, $-10 \le l \le 6$
Reflections collected	31051
Independent reflections	6724 [R(int) = 0.0306]
Observed reflections	6557
Completeness to theta	74.504° 99.9%
Absorption correction	Multi-scan
Max. and min. transmission	1.00000 and 0.71074
Refinement method	Full-matrix least-squares on $F2$
Data / restraints / parameters	6724 / 1 / 668
Goodness-of-fit on *F*2	1.060
Final *R* indices [*I*>2sigma(*I*)]	$R1 = 0.0327$, $wR2 = 0.0930$
***R* indices (all data)**	$R1 = 0.0334$, $wR2 = 0.0937$

Largest diff. peak and hole	0.44(3)

Distances (Å) between pyridine ring centroids for $M(tpy)_2$ complexes (M = Ni, Fe, Ru)





	Ring N1-Ring N3	Ring N4-Ring N6
$Ni(tpy)_2$	3.76	3.72
$Fe(tpy)_2$	3.73	3.69
$Ru(tpy)_2$	3.86	3.81

2. Computational results

2.1. Computational methods

Calculations were performed with Gaussian 09 at DFT level.[2] The geometries of complexes here reported were optimized using the M06-2X hybrid functional[3] that accounts for dispersive interactions. Optimizations were carried out using the standard 6-31G(d) basis set for C, H, and N. The LANL2DZ basis set, which includes the relativistic effective core potential (ECP) of Hay and Wadt and employs a split-valence (double-ζ) basis set, was used for Ni.[4] Harmonic frequencies were calculated at the same level to characterize the stationary points and to determine the zero-point energies (ZPE) for the monomeric complex. Solvent effects were also considered for the monomeric species by performing optimizations in diisopropylether using the polarized continuum model (PCM).

Broken-symmetry calculations were used for the dimers in the singlet state by defining two fragments with opposite spin, either both triplets or both quintets. In theses cases, frequency calculations were not performed and the reported energy values correspond to the energy minima

[2] Gaussian 09, Revision E.01, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, T. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, O. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2013.

[3] Y. Zhao, D.G. Truhlar, *Theor Chem Account.* **2006**, *120*: 215–241.

[4] (a) A. D, Becke, *J. Chem. Phys*. **1993**, *98*, 5648- 5653. (b) A. D. Becke, *Phys. Rev. A* **1988**, *38*, 3098-3100. (c) C. Lee, W. Yang, R. G. Parr, *Phys. Rev. B* **1988**, *37*, 785-789.

[4] *(a)* L. Noodleman, *J. Chem. Phys.*,1981,**74**, 5737; *(b)* L. Noo-dleman, J. G. Norman, J. H. Osborne, A. Aizman and D. Case, *J. Am. Chem. Soc*.,1985, **107**, 3418; *(c)* L. Noodleman and E. R. Davidson, *Chem. Phys.*, 1986, **109**, 131; *(d)* L. Noodleman, D. A.Case and A. J. Aizman, *J. Am. Chem. Soc.*, 1988, **110**, 1001; *(e)* L.Noodleman, C. Y. Peng, D. A. Case and J. M. Monesca, *Coord.Chem. Rev.* 1995, **144**, 199.

I.2. Atomic coordinates and energy values for single-point calculations and the stationary points

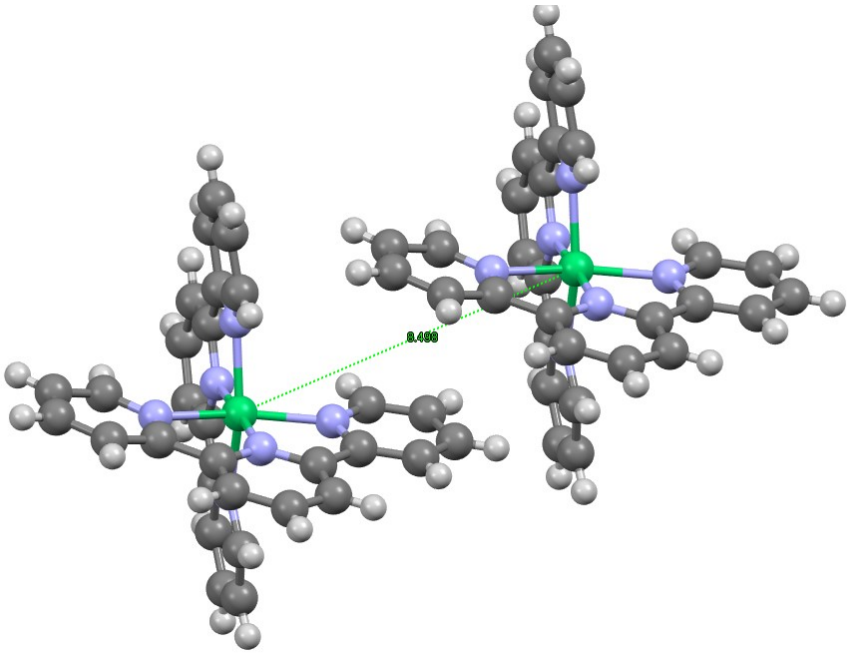
Energy values for different spin states for complex **1** and the dimer

M06-2x

$Ni(tpy)_2$			
Gas phase *E*(au)	S = 0, m = 1 (singlet)	S = 1, m = 3 (triplet)	S = 2, m = 5 (quintuplet)
	-1653.665411	-1653.711479	-1653.735924
Relative *E* ($kcal \cdot mol^{-1}$)	0	-28.9	-44.2
Gas phase *G*(au)	S = 0, m = 1 (singlet)	S = 1, m = 3 (triplet)	S = 2, m = 5 (quintuplet)
	-1653.265043	-1653.315780	-1653.339548
Relative *E* ($kcal \cdot mol^{-1}$)	0	-31.8	-46.8
Di(isopropyl)ether *E*(au)	S = 0, m = 1 (singlet)	S = 1, m = 3 (triplet)	S = 2, m = 5 (quintuplet)
	-1653.678994	-1653.716068	-1653.744597
Relative *E* ($kcal \cdot mol^{-1}$)	0	-23.3	-41.2
Di(isopropyl)ether *G*(au)	S = 0, m = 1 (singlet)	S = 1, m = 3 (triplet)	S = 2, m = 5 (quintuplet)
	-1653.278160	-1653.318266	-1653.347544
Relative *E* ($kcal \cdot mol^{-1}$)	0	-25.2	-43.5
$[Ni(tpy)_2]_2$			
Gas phase *E*(au)	S = 4 (nonaplet)	S = 0 (two triplets)	S = 0, m = 1 (two quintuplets)
	-3307.487585	-3307.478443	-3307.488473*
Relative E ($kcal \cdot mol^{-1}$) SCF=XQC	0	5.7	-0.6* +1,7
Gas phase *G*(au)	S = 4 (nonaplet)	S = 0 (two triplets)	S = 0, m = 1 (two quintuplets)
	-3306.671326	-3306.654013	-3306.667585
Relative G ($kcal \cdot mol^{-1}$) SCF=XQC	0	10.9	2.3
(*) SCF=QC			

Single-point calculations on dimers found in the crystal structure

Dimer I



Nonaplet: E(UM062X) = -3306.769226
Singlet (two triplets): E(UM062X) = -3306.723548
Singlet (two quintets): E(UM062X) = -3306.762796

Ni	28.216545	13.858804	4.142374
N	29.065661	14.445811	2.306361
N	28.551130	15.794702	4.453815
N	27.396669	14.185270	6.109846
N	26.221964	13.723007	3.488646
N	27.994987	11.902379	3.903928
N	30.116654	13.083498	4.760666
C	29.283283	13.687874	1.224689
H	28.995370	12.783086	1.251626
C	29.894534	14.131583	0.080473
H	30.034554	13.550497	-0.657807
C	30.309533	15.482448	0.035435
H	30.735216	15.829441	-0.739725
C	30.090225	16.282230	1.120422
H	30.353395	17.194518	1.094164
C	29.477849	15.765095	2.277214
C	29.220302	16.502900	3.483972
C	29.589752	17.837185	3.731170
H	30.054236	18.335766	3.069454
C	29.272036	18.414718	4.941328
H	29.520023	19.315558	5.114681
C	28.585432	17.680861	5.917118
H	28.361625	18.073251	6.752952
C	28.238475	16.364340	5.633550
C	27.507448	15.467052	6.547563

C	26.921501	15.866154	7.738006
H	27.009787	16.765809	8.029987
C	26.215216	14.968472	8.496935
H	25.823835	15.233355	9.321127
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H	26.609971	12.427013	6.537026
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C	23.986706	14.531079	3.185533
H	23.378266	15.260593	3.192076
C	23.546965	13.231137	2.892872
H	22.636554	13.070865	2.673121
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H	24.160465	11.309056	2.722578
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C	26.784855	11.419194	3.470461
C	26.605472	10.048196	3.300677
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H	33.184721	13.733666	5.599474
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N	28.551130	15.794702	-4.043885
N	27.396669	14.185270	-2.387854
N	26.221964	13.723007	-5.009054
N	27.994987	11.902379	-4.593772
N	30.116654	13.083498	-3.737034
C	29.283283	13.687874	-7.273011
H	28.995370	12.783086	-7.246074
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H	30.034554	13.550497	-9.155507
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H	30.735216	15.829441	-9.237425
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C	29.589752	17.837185	-4.766530

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H	29.520023	19.315558	-3.383019
C	28.585432	17.680861	-2.580582
H	28.361625	18.073251	-1.744748
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C	26.921501	15.866154	-0.759694
H	27.009787	16.765809	-0.467713
C	26.215216	14.968472	-0.000765
H	25.823835	15.233355	0.823427
C	26.082506	13.663399	-0.460745
H	25.583720	13.022310	0.031781
C	26.693758	13.321142	-1.650848
H	26.609971	12.427013	-1.960674
C	25.318301	14.723721	-5.035227
H	25.617460	15.606797	-4.853036
C	23.986706	14.531079	-5.312167
H	23.378266	15.260593	-5.305624
C	23.546965	13.231137	-5.604828
H	22.636554	13.070865	-5.824579
C	24.444442	12.192132	-5.570497
H	24.160465	11.309056	-5.775122
C	25.792907	12.442014	-5.229655
C	26.784855	11.419194	-5.027239
C	26.605472	10.048196	-5.197023
H	25.775474	9.710677	-5.513903
C	27.636783	9.185647	-4.903003
H	27.517570	8.249674	-5.013473
C	28.866597	9.686202	-4.439453
H	29.580192	9.098011	-4.222592
C	29.011678	11.052857	-4.306889
C	30.233056	11.733422	-3.865009
C	31.456122	11.086412	-3.624184
H	31.525288	10.143333	-3.716979
C	32.554350	11.829743	-3.252495
H	33.384348	11.403403	-3.074468
C	32.435699	13.202320	-3.141175
H	33.184721	13.733666	-2.898226
C	31.211509	13.787748	-3.388883
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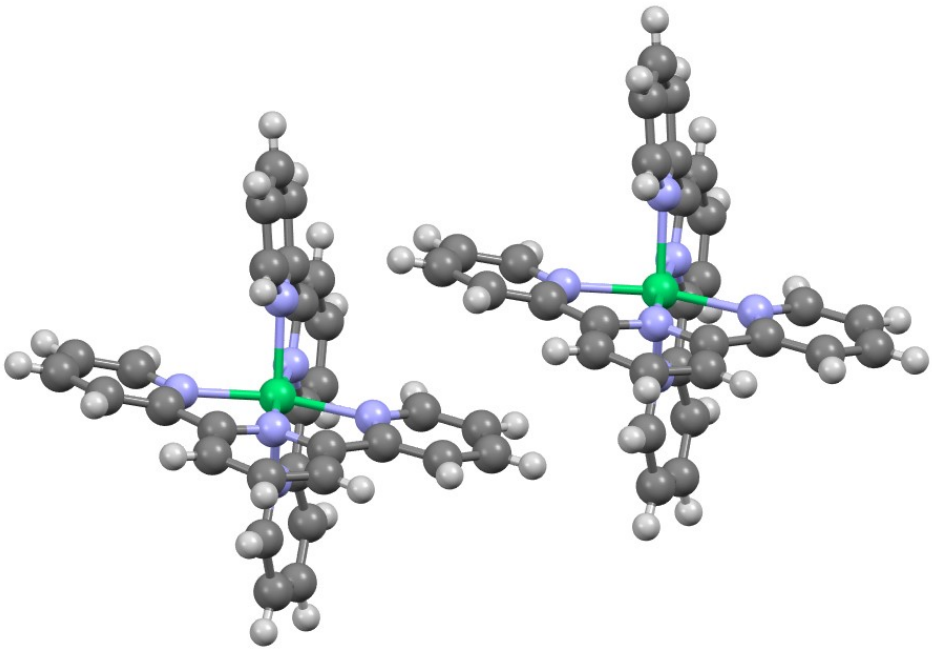
Dimer II



Nonaplet: E(UM062X) = -3306.765759
Singlet (two triplets): E(UM062X) = -3306.700484
Singlet (two quintets): E(UM062X) = -3306.762529

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N	22.039923	9.752126	4.912265
N	20.961376	7.644113	3.878180
N	19.470642	8.698909	6.223546
N	18.199216	9.296969	4.045500
N	19.936250	10.268076	2.398901
C	19.238400	12.489385	4.895355
H	18.380848	12.197658	4.608048
C	19.403724	13.817355	5.177309
H	18.685630	14.431600	5.082984
C	20.663904	14.242115	5.608822
H	20.815170	15.158351	5.810472
C	21.681719	13.331406	5.740111
H	22.536459	13.611290	6.046199
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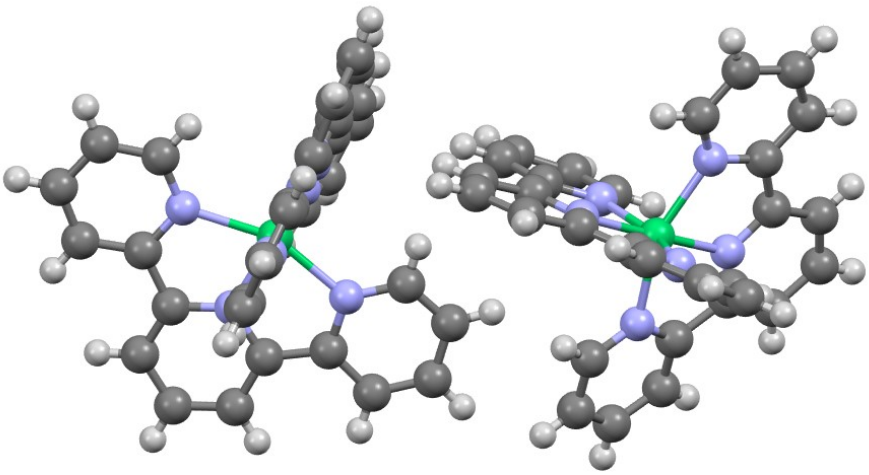
H	22.514529	4.259450	3.850563
C	20.896708	5.328457	3.255384
H	20.443471	4.618680	2.815713
C	20.333254	6.605897	3.325320
H	19.465581	6.740115	2.963148
C	20.212916	8.385865	7.284823
H	21.137947	8.599825	7.263069
C	19.712443	7.767673	8.416377
H	20.277021	7.544239	9.147094
C	18.340923	7.483446	8.443060
H	17.953478	7.071318	9.206238
C	17.566033	7.801227	7.368951
H	16.633129	7.620822	7.389855
C	18.135673	8.392576	6.232978
C	17.427138	8.713515	5.014323
C	16.069114	8.477844	4.772818
H	15.527591	8.062953	5.434109
C	15.521405	8.859181	3.551189
H	14.603122	8.694567	3.373417
C	16.318788	9.485664	2.580412
H	15.947650	9.760022	1.749931
C	17.671751	9.696071	2.865170
C	18.641769	10.317816	1.958295
C	18.324053	10.945878	0.749412
H	17.422077	10.995617	0.455817
C	19.339057	11.493803	-0.012747
H	19.137181	11.922117	-0.836344
C	20.652095	11.416825	0.426245
H	21.363441	11.776450	-0.090925
C	20.894459	10.800606	1.639801
H	21.791373	10.754419	1.949457
Ni	20.135315	9.558300	-4.105239
N	20.214041	11.573544	-3.497653
N	22.039923	9.752126	-3.585435
N	20.961376	7.644113	-4.619520
N	19.470642	8.698909	-2.274154
N	18.199216	9.296969	-4.452200
N	19.936250	10.268076	-6.098799
C	19.238400	12.489385	-3.602345
H	18.380848	12.197658	-3.889652
C	19.403724	13.817355	-3.320391
H	18.685630	14.431600	-3.414716
C	20.663904	14.242115	-2.888878
H	20.815170	15.158351	-2.687228
C	21.681719	13.331406	-2.757589
H	22.536459	13.611290	-2.451501
C	21.453976	11.979357	-3.078632
C	22.456609	10.936798	-3.057303
C	23.761212	11.061147	-2.547525

H	24.066557	11.890141	-2.197420
C	24.590085	9.957796	-2.564861
H	25.481376	10.033195	-2.244243
C	24.128413	8.725358	-3.052204
H	24.685681	7.955973	-3.036143
C	22.840117	8.657854	-3.557137
C	22.204685	7.449102	-4.099885
C	22.792881	6.181531	-4.084504
H	23.644247	6.051655	-3.682818
C	22.127646	5.127130	-4.655720
H	22.514529	4.259450	-4.647137
C	20.896708	5.328457	-5.242316
H	20.443471	4.618680	-5.681987
C	20.333254	6.605897	-5.172380
H	19.465581	6.740115	-5.534552
C	20.212916	8.385865	-1.212877
H	21.137947	8.599825	-1.234631
C	19.712443	7.767673	-0.081323
H	20.277021	7.544239	0.649394
C	18.340923	7.483446	-0.054640
H	17.953478	7.071318	0.708538
C	17.566033	7.801227	-1.128749
H	16.633129	7.620822	-1.107845
C	18.135673	8.392576	-2.264722
C	17.427138	8.713515	-3.483377
C	16.069114	8.477844	-3.724882
H	15.527591	8.062953	-3.063591
C	15.521405	8.859181	-4.946511
H	14.603122	8.694567	-5.124283
C	16.318788	9.485664	-5.917288
H	15.947650	9.760022	-6.747769
C	17.671751	9.696071	-5.632530
C	18.641769	10.317816	-6.539405
C	18.324053	10.945878	-7.748288
H	17.422077	10.995617	-8.041883
C	19.339057	11.493803	-8.510447
H	19.137181	11.922117	-9.334044
C	20.652095	11.416825	-8.071455
H	21.363441	11.776450	-8.588625
C	20.894459	10.800606	-6.857899
H	21.791373	10.754419	-6.548243

Dimer **III**



Nonaplet: E(UM062X) = -3306.766108
Singlet (two triplets): E(UM062X) = -3306.720573
Singlet (two quintets): E(UM062X) = -3306.706463

Ni	28.216545	13.858804	4.142374
N	29.065661	14.445811	2.306361
N	28.551130	15.794702	4.453815
N	27.396669	14.185270	6.109846
N	26.221964	13.723007	3.488646
N	27.994987	11.902379	3.903928
N	30.116654	13.083498	4.760666
C	29.283283	13.687874	1.224689
H	28.995370	12.783086	1.251626
C	29.894534	14.131583	0.080473
H	30.034554	13.550497	-0.657807
C	30.309533	15.482448	0.035435
H	30.735216	15.829441	-0.739725
C	30.090225	16.282230	1.120422
H	30.353395	17.194518	1.094164
C	29.477849	15.765095	2.277214
C	29.220302	16.502900	3.483972
C	29.589752	17.837185	3.731170
H	30.054236	18.335766	3.069454
C	29.272036	18.414718	4.941328
H	29.520023	19.315558	5.114681
C	28.585432	17.680861	5.917118
H	28.361625	18.073251	6.752952
C	28.238475	16.364340	5.633550
C	27.507448	15.467052	6.547563
C	26.921501	15.866154	7.738006
H	27.009787	16.765809	8.029987
C	26.215216	14.968472	8.496935
H	25.823835	15.233355	9.321127
C	26.082506	13.663399	8.036955

H	25.583720	13.022310	8.529481
C	26.693758	13.321142	6.846852
H	26.609971	12.427013	6.537026
C	25.318301	14.723721	3.462473
H	25.617460	15.606797	3.644664
C	23.986706	14.531079	3.185533
H	23.378266	15.260593	3.192076
C	23.546965	13.231137	2.892872
H	22.636554	13.070865	2.673121
C	24.444442	12.192132	2.927203
H	24.160465	11.309056	2.722578
C	25.792907	12.442014	3.268045
C	26.784855	11.419194	3.470461
C	26.605472	10.048196	3.300677
H	25.775474	9.710677	2.983797
C	27.636783	9.185647	3.594697
H	27.517570	8.249674	3.484227
C	28.866597	9.686202	4.058247
H	29.580192	9.098011	4.275108
C	29.011678	11.052857	4.190811
C	30.233056	11.733422	4.632691
C	31.456122	11.086412	4.873516
H	31.525288	10.143333	4.780721
C	32.554350	11.829743	5.245205
H	33.384348	11.403403	5.423232
C	32.435699	13.202320	5.356525
H	33.184721	13.733666	5.599474
C	31.211509	13.787748	5.108817
H	31.136719	14.731616	5.187421
Ni	22.039360	19.427275	2.268036
N	21.960634	21.442519	2.875622
N	20.134752	19.621101	2.787840
N	21.213299	17.513088	1.753755
N	22.704033	18.567884	4.099121
N	23.975459	19.165944	1.921075
N	22.238425	20.137051	0.274476
C	22.936275	22.358360	2.770930
H	23.793827	22.066633	2.483623
C	22.770951	23.686330	3.052884
H	23.489045	24.300575	2.958559
C	21.510771	24.111090	3.484397
H	21.359505	25.027326	3.686047
C	20.492956	23.200381	3.615686
H	19.638216	23.480265	3.921774
C	20.720699	21.848332	3.294643
C	19.718066	20.805773	3.315972
C	18.413463	20.930122	3.825750
H	18.108118	21.759116	4.175855
C	17.584590	19.826771	3.808414
H	16.693299	19.902170	4.129032
C	18.046262	18.594333	3.321071
H	17.488994	17.824948	3.337132

C	19.334558	18.526829	2.816138
C	19.969990	17.318077	2.273390
C	19.381794	16.050506	2.288771
H	18.530428	15.920630	2.690457
C	20.047029	14.996105	1.717555
H	19.660146	14.128425	1.726138
C	21.277967	15.197432	1.130959
H	21.731204	14.487655	0.691288
C	21.841421	16.474872	1.200895
H	22.709094	16.609090	0.838723
C	21.961759	18.254840	5.160398
H	21.036728	18.468800	5.138644
C	22.462232	17.636648	6.291952
H	21.897654	17.413214	7.022669
C	23.833752	17.352421	6.318635
H	24.221197	16.940293	7.081813
C	24.608642	17.670202	5.244526
H	25.541546	17.489797	5.265430
C	24.039002	18.261551	4.108553
C	24.747537	18.582490	2.889898
C	26.105561	18.346819	2.648393
H	26.647084	17.931928	3.309684
C	26.653270	18.728156	1.426764
H	27.571553	18.563542	1.248992
C	25.855887	19.354639	0.455987
H	26.227025	19.628997	-0.374494
C	24.502924	19.565046	0.740745
C	23.532906	20.186791	-0.166130
C	23.850622	20.814853	-1.375013
H	24.752598	20.864592	-1.668608
C	22.835618	21.362778	-2.137172
H	23.037494	21.791092	-2.960769
C	21.522580	21.285800	-1.698180
H	20.811234	21.645425	-2.215350
C	21.280216	20.669581	-0.484624
H	20.383302	20.623394	-0.174968

COORDINATES – M062X / Diisopropylether (PCM)

1 – Singlet

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	4.555835	2.066345	2.909289
2	6	0	3.662945	1.670355	2.434459
3	7	0	1.361030	0.680090	1.200370
4	6	0	3.587835	0.344104	2.110079
5	6	0	2.554504	2.523955	2.170972
6	6	0	1.447211	1.971065	1.574352
7	6	0	2.421477	-0.176598	1.479649
8	1	0	4.409236	-0.328938	2.336079

9	1	0	2.571802	3.575649	2.430244
10	1	0	0.571772	2.579788	1.355393
11	6	0	2.170521	-1.517531	1.135950
12	6	0	1.465864	-3.931059	-0.056067
13	6	0	3.089058	-2.568945	1.099142
14	7	0	0.813534	-1.770318	0.809059
15	6	0	0.570649	-2.891093	0.008845
16	6	0	2.732226	-3.804193	0.573366
17	1	0	4.110190	-2.395349	1.430791
18	1	0	3.453415	-4.611523	0.518704
19	1	0	1.232620	-4.814445	-0.643650
20	6	0	-0.667226	-2.805234	-0.717331
21	6	0	-3.050426	-2.336447	-2.043997
22	6	0	-1.351679	-3.878834	-1.324401
23	7	0	-1.197038	-1.540980	-0.748524
24	6	0	-2.351541	-1.334917	-1.403538
25	6	0	-2.531769	-3.646785	-1.992768
26	1	0	-0.940041	-4.879800	-1.250682
27	1	0	-2.714056	-0.310577	-1.412432
28	1	0	-3.060351	-4.465350	-2.471076
29	1	0	-3.971017	-2.110311	-2.568369
30	28	0	-0.100479	-0.240062	0.276570
31	1	0	-6.077477	0.497405	1.628131
32	6	0	-4.992402	0.485616	1.624887
33	7	0	-2.211214	0.442714	1.593026
34	6	0	-4.285545	1.287147	0.734995
35	6	0	-4.287923	-0.339427	2.494936
36	6	0	-2.895686	-0.327445	2.436060
37	6	0	-2.890217	1.232639	0.756324
38	1	0	-4.806889	1.915477	0.020865
39	1	0	-4.799693	-0.984368	3.200205
40	1	0	-2.299643	-0.961129	3.087066
41	6	0	-2.064257	2.036214	-0.188432
42	6	0	-0.461693	3.449390	-1.898835
43	6	0	-2.505540	3.269858	-0.667762
44	7	0	-0.874292	1.521601	-0.541308
45	6	0	-0.075362	2.215537	-1.373386
46	6	0	-1.693509	3.980470	-1.541508
47	1	0	-3.455729	3.673193	-0.337588
48	1	0	-2.014614	4.940509	-1.931893
49	1	0	0.197927	3.969629	-2.584303
50	6	0	1.272320	1.646515	-1.668057
51	6	0	3.730888	0.503584	-1.927009
52	6	0	2.395081	2.470443	-1.636505
53	7	0	1.338201	0.323705	-1.862333
54	6	0	2.543543	-0.231636	-1.974981
55	6	0	3.651746	1.879403	-1.770631
56	1	0	2.294326	3.536346	-1.460975
57	1	0	2.560540	-1.311078	-2.105714
58	1	0	4.549990	2.487001	-1.730610
59	1	0	4.687164	-0.001341	-2.008313

Zero-point correction=	0.460270
(Hartree/Particle)	
Thermal correction to Energy=	0.489007
Thermal correction to Enthalpy=	0.489951
Thermal correction to Gibbs Free Energy=	0.400834
Sum of electronic and zero-point Energies=	-1653.218724
Sum of electronic and thermal Energies=	-1653.189987
Sum of electronic and thermal Enthalpies=	-1653.189043
Sum of electronic and thermal Free Energies=	-1653.278160

1 – Triplet

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	5.501843	-1.732421	2.043594
2	6	0	4.497616	-1.394788	1.806171
3	7	0	1.929304	-0.530885	1.171432
4	6	0	3.574493	-2.280842	1.287627
5	6	0	4.126451	-0.058195	2.015343
6	6	0	2.831626	0.310574	1.675368
7	6	0	2.274996	-1.830697	0.973653
8	1	0	3.859206	-3.310856	1.105403
9	1	0	4.817979	0.669082	2.424199
10	1	0	2.491772	1.336979	1.802897
11	6	0	1.246455	-2.694399	0.399755
12	6	0	-0.757695	-4.176674	-0.802265
13	6	0	1.404478	-4.086792	0.243584
14	7	0	0.098468	-2.084191	-0.001747
15	6	0	-0.857955	-2.803341	-0.602320
16	6	0	0.402905	-4.825182	-0.352615
17	1	0	2.302667	-4.580878	0.595563
18	1	0	0.517575	-5.896766	-0.481791
19	1	0	-1.544163	-4.717468	-1.315845
20	6	0	-2.056125	-2.042292	-1.058526
21	6	0	-4.203813	-0.519687	-1.792786
22	6	0	-3.337921	-2.591649	-0.962439
23	7	0	-1.834811	-0.805083	-1.519382
24	6	0	-2.888101	-0.068288	-1.870843
25	6	0	-4.427983	-1.814474	-1.336235
26	1	0	-3.474480	-3.592730	-0.566903
27	1	0	-2.666132	0.936845	-2.223506
28	1	0	-5.436365	-2.208370	-1.255449
29	1	0	-5.024070	0.127967	-2.081971
30	28	0	-0.000127	-0.000067	0.334101
31	1	0	-5.501845	1.733328	2.043275
32	6	0	-4.497654	1.395556	1.805892
33	7	0	-1.929445	0.531311	1.171260
34	6	0	-3.574416	2.281473	1.287324
35	6	0	-4.126665	0.058918	2.015134
36	6	0	-2.831875	-0.310021	1.675213
37	6	0	-2.274962	1.831153	0.973399
38	1	0	-3.858994	3.311514	1.105044
39	1	0	-4.818296	-0.668248	2.424014
40	1	0	-2.492142	-1.336461	1.802790
41	6	0	-1.246291	2.694659	0.399470
42	6	0	0.758095	4.176535	-0.802662
43	6	0	-1.404078	4.087080	0.243239
44	7	0	-0.098415	2.084242	-0.002027
45	6	0	0.858107	2.803188	-0.602659
46	6	0	-0.402388	4.825263	-0.353014
47	1	0	-2.302172	4.581339	0.595223
48	1	0	-0.516868	5.896862	-0.482227
49	1	0	1.544646	4.717172	-1.316280
50	6	0	2.056148	2.041896	-1.058821
51	6	0	4.203573	0.518858	-1.792954
52	6	0	3.338035	2.591051	-0.962823
53	7	0	1.834620	0.804688	-1.519573
54	6	0	2.887781	0.067682	-1.870968

55	6	0	4.427965	1.813652	-1.336541
56	1	0	3.474769	3.592150	-0.567392
57	1	0	2.665640	-0.937449	-2.223530
58	1	0	5.436414	2.207389	-1.255804
59	1	0	5.023715	-0.128971	-2.082073

Zero-point correction= 0.461028
(Hartree/Particle)
Thermal correction to Energy= 0.490639
Thermal correction to Enthalpy= 0.491583
Thermal correction to Gibbs Free Energy= 0.397801
Sum of electronic and zero-point Energies= -1653.255040
Sum of electronic and thermal Energies= -1653.225429
Sum of electronic and thermal Enthalpies= -1653.224485
Sum of electronic and thermal Free Energies= -1653.318266

1 – Quintet

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	2.858435	3.583800	3.957327
2	6	0	2.307434	2.949964	3.268641
3	7	0	0.887240	1.327665	1.509348
4	6	0	2.976179	2.024146	2.506675
5	6	0	0.903754	3.073057	3.155130
6	6	0	0.259987	2.235803	2.262247
7	6	0	2.255202	1.192724	1.607118
8	1	0	4.053115	1.922722	2.591488
9	1	0	0.344229	3.790704	3.742507
10	1	0	-0.820067	2.278562	2.127864
11	6	0	2.847605	0.195803	0.771704
12	6	0	3.719048	-1.793193	-0.996552
13	6	0	4.231106	-0.113434	0.677943
14	7	0	1.963548	-0.511264	-0.011688
15	6	0	2.387012	-1.459990	-0.864133
16	6	0	4.656887	-1.089490	-0.187568
17	1	0	4.951408	0.423374	1.286614
18	1	0	5.713351	-1.325966	-0.262227
19	1	0	4.054285	-2.553436	-1.690816
20	6	0	1.283841	-2.093966	-1.642922
21	6	0	-0.888932	-3.130456	-2.978433
22	6	0	1.471716	-3.153804	-2.531932
23	7	0	0.058876	-1.577045	-1.433280
24	6	0	-0.995112	-2.079031	-2.075864
25	6	0	0.373457	-3.673011	-3.205861
26	1	0	2.459157	-3.571366	-2.689032
27	1	0	-1.950787	-1.612531	-1.846308
28	1	0	0.501726	-4.496575	-3.900922
29	1	0	-1.769718	-3.511455	-3.481950
30	28	0	-0.000075	-0.000198	0.088567
31	1	0	-2.862820	-3.581559	3.956311
32	6	0	-2.311128	-2.948248	3.267701
33	7	0	-0.889096	-1.327264	1.508689
34	6	0	-2.978993	-2.022491	2.504905
35	6	0	-0.907412	-3.071978	3.155159
36	6	0	-0.262707	-2.235345	2.262379
37	6	0	-2.257095	-1.191768	1.605423
38	1	0	-4.055939	-1.920553	2.589001
39	1	0	-0.348554	-3.789599	3.743204

40	1	0	0.817430	-2.278543	2.128790
41	6	0	-2.848467	-0.195069	0.769010
42	6	0	-3.717655	1.794248	-0.999971
43	6	0	-4.231688	0.115146	0.674580
44	7	0	-1.963587	0.510888	-0.014454
45	6	0	-2.385919	1.459918	-0.867084
46	6	0	-4.656351	1.091347	-0.191315
47	1	0	-4.952651	-0.421006	1.283039
48	1	0	-5.712604	1.328597	-0.266478
49	1	0	-4.052035	2.554953	-1.694146
50	6	0	-1.281928	2.092977	-1.645469
51	6	0	0.892165	3.128020	-2.979911
52	6	0	-1.468941	3.151731	-2.535950
53	7	0	-0.057187	1.576322	-1.433984
54	6	0	0.997449	2.077615	-2.076030
55	6	0	-0.370002	3.670227	-3.209333
56	1	0	-2.456268	3.568926	-2.694709
57	1	0	1.952896	1.611334	-1.845065
58	1	0	-0.497611	4.492873	-3.905589
59	1	0	1.773483	3.508448	-3.482931

Zero-point correction=	0.459189
(Hartree/Particle)	
Thermal correction to Energy=	0.488206
Thermal correction to Enthalpy=	0.489150
Thermal correction to Gibbs Free Energy=	0.397052
Sum of electronic and zero-point Energies=	-1653.285408
Sum of electronic and thermal Energies=	-1653.256391
Sum of electronic and thermal Enthalpies=	-1653.255447
Sum of electronic and thermal Free Energies=	-1653.347544

COORDINATES – M062X Gas phase

1 – Singlet

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	-4.466969	-2.448176	2.619951
2	6	0	-3.572295	-1.972600	2.229307
3	7	0	-1.271347	-0.777583	1.197469
4	6	0	-3.563819	-0.627931	1.974778
5	6	0	-2.393005	-2.736609	2.010395
6	6	0	-1.289952	-2.085868	1.513547
7	6	0	-2.398043	-0.003930	1.455143
8	1	0	-4.443120	-0.021902	2.170572
9	1	0	-2.353395	-3.796833	2.229082
10	1	0	-0.362432	-2.624383	1.326620
11	6	0	-2.225185	1.363283	1.158984
12	6	0	-1.646051	3.852905	0.060118
13	6	0	-3.213707	2.349642	1.110273
14	7	0	-0.890817	1.705587	0.859005
15	6	0	-0.687065	2.870565	0.126820
16	6	0	-2.924968	3.617200	0.625346
17	1	0	-4.229593	2.099488	1.405696
18	1	0	-3.696547	4.376052	0.567032
19	1	0	-1.447404	4.772059	-0.483089
20	6	0	0.571766	2.881482	-0.571141
21	6	0	2.981041	2.579954	-1.895139

22	6	0	1.211597	4.010722	-1.118033
23	7	0	1.158636	1.645572	-0.653770
24	6	0	2.323330	1.519669	-1.307891
25	6	0	2.406039	3.862549	-1.785478
26	1	0	0.754584	4.987646	-1.000849
27	1	0	2.728063	0.511926	-1.356799
28	1	0	2.902348	4.725360	-2.218626
29	1	0	3.914224	2.419516	-2.421669
30	28	0	0.137484	0.249563	0.317974
31	1	0	6.143509	-0.594688	1.538838
32	6	0	5.059524	-0.543593	1.514290
33	7	0	2.287157	-0.397642	1.429482
34	6	0	4.340767	-1.345467	0.636293
35	6	0	4.371754	0.337004	2.344849
36	6	0	2.982357	0.376535	2.258673
37	6	0	2.946803	-1.240076	0.628639
38	1	0	4.850211	-2.012865	-0.050871
39	1	0	4.896449	0.983806	3.038971
40	1	0	2.393969	1.054109	2.872127
41	6	0	2.094180	-2.032792	-0.295898
42	6	0	0.406886	-3.423200	-1.939068
43	6	0	2.480635	-3.293076	-0.750531
44	7	0	0.920393	-1.476212	-0.645315
45	6	0	0.077530	-2.161857	-1.441378
46	6	0	1.625475	-3.993214	-1.592453
47	1	0	3.419756	-3.724797	-0.422904
48	1	0	1.900437	-4.975864	-1.962059
49	1	0	-0.287672	-3.934145	-2.596745
50	6	0	-1.256666	-1.551693	-1.699174
51	6	0	-3.678967	-0.314112	-1.754597
52	6	0	-2.404190	-2.335778	-1.614552
53	7	0	-1.283206	-0.221716	-1.855721
54	6	0	-2.472504	0.378134	-1.876221
55	6	0	-3.644353	-1.695805	-1.635888
56	1	0	-2.332056	-3.406723	-1.456547
57	1	0	-2.457154	1.462266	-1.969158
58	1	0	-4.559581	-2.269446	-1.531711
59	1	0	-4.616374	0.231535	-1.739241

Zero-point correction=	0.459362 (Hartree/Particle)
Thermal correction to Energy=	0.488096
Thermal correction to Enthalpy=	0.489040
Thermal correction to Gibbs Free Energy=	0.400368
Sum of electronic and zero-point Energies=	-1653.206049
Sum of electronic and thermal Energies=	-1653.177314
Sum of electronic and thermal Enthalpies=	-1653.176370
Sum of electronic and thermal Free Energies=	-1653.265043

1 – Triplet

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	5.407845	-1.337023	2.363212
2	6	0	4.412486	-1.048611	2.036329
3	7	0	1.866019	-0.307128	1.176700
4	6	0	3.572767	-1.989063	1.495337
5	6	0	3.974363	0.287355	2.175099

6	6	0	2.698267	0.578468	1.722762
7	6	0	2.264874	-1.621424	1.063075
8	1	0	3.910124	-3.014908	1.398446
9	1	0	4.603254	1.057864	2.604797
10	1	0	2.312928	1.597669	1.782164
11	6	0	1.325071	-2.536718	0.496354
12	6	0	-0.589085	-4.209452	-0.654679
13	6	0	1.598572	-3.923398	0.303528
14	7	0	0.090273	-2.033530	0.127417
15	6	0	-0.800602	-2.856257	-0.442860
16	6	0	0.660625	-4.746223	-0.258132
17	1	0	2.557958	-4.329987	0.603075
18	1	0	0.875983	-5.799878	-0.408677
19	1	0	-1.339025	-4.816243	-1.148316
20	6	0	-2.092146	-2.238849	-0.861056
21	6	0	-4.438159	-1.027290	-1.591981
22	6	0	-3.305459	-2.896706	-0.617916
23	7	0	-2.037803	-1.037895	-1.449429
24	6	0	-3.184467	-0.459330	-1.803410
25	6	0	-4.493399	-2.279216	-0.985832
26	1	0	-3.300267	-3.862617	-0.123463
27	1	0	-3.093327	0.516501	-2.277302
28	1	0	-5.447474	-2.762725	-0.796866
29	1	0	-5.338061	-0.503358	-1.895970
30	28	0	-0.040037	0.045074	0.296922
31	1	0	-5.294315	2.285911	2.232699
32	6	0	-4.364871	1.852557	1.877109
33	7	0	-1.987191	0.758371	0.962927
34	6	0	-3.400367	2.658218	1.284393
35	6	0	-4.121100	0.489582	2.008409
36	6	0	-2.911254	-0.009749	1.538235
37	6	0	-2.215076	2.073362	0.833022
38	1	0	-3.574673	3.722448	1.177588
39	1	0	-4.847134	-0.176318	2.460933
40	1	0	-2.665153	-1.066688	1.605907
41	6	0	-1.128553	2.845156	0.162884
42	6	0	0.954973	4.080711	-1.125027
43	6	0	-1.207951	4.215170	-0.095015
44	7	0	-0.055097	2.127096	-0.192939
45	6	0	0.957148	2.713845	-0.844174
46	6	0	-0.144344	4.836947	-0.738416
47	1	0	-2.078934	4.790859	0.193695
48	1	0	-0.182660	5.900355	-0.952125
49	1	0	1.787120	4.526562	-1.659188
50	6	0	2.075255	1.814991	-1.241571
51	6	0	4.024579	-0.013977	-1.744527
52	6	0	3.404557	2.200710	-1.080726
53	7	0	1.709223	0.604994	-1.677809
54	6	0	2.666494	-0.284366	-1.923041
55	6	0	4.397395	1.257308	-1.329715
56	1	0	3.651133	3.190952	-0.709874
57	1	0	2.328810	-1.263955	-2.252494
58	1	0	5.442300	1.504969	-1.171495
59	1	0	4.763072	-0.788307	-1.919389

Zero-point correction= 0.459764 (Hartree/Particle)
Thermal correction to Energy= 0.489414
Thermal correction to Enthalpy= 0.490358
Thermal correction to Gibbs Free Energy= 0.395699
Sum of electronic and zero-point Energies= -1653.251715

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 Sum of electronic and thermal Energies=            -1653.222065
 Sum of electronic and thermal Enthalpies=          -1653.221121
 Sum of electronic and thermal Free Energies=       -1653.315780
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1 – Quintet

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	-2.952379	-3.498090	3.956927
2	6	0	-2.385541	-2.877993	3.268593
3	7	0	-0.928424	-1.293648	1.511384
4	6	0	-3.033142	-1.944788	2.496892
5	6	0	-0.985550	-3.025608	3.166742
6	6	0	-0.320323	-2.205685	2.273585
7	6	0	-2.291245	-1.132609	1.599499
8	1	0	-4.108372	-1.822302	2.573899
9	1	0	-0.443053	-3.748689	3.763203
10	1	0	0.759686	-2.265290	2.146883
11	6	0	-2.855903	-0.125066	0.754616
12	6	0	-3.666479	1.878475	-1.023065
13	6	0	-4.228642	0.210252	0.644437
14	7	0	-1.946509	0.562917	-0.019343
15	6	0	-2.343690	1.520861	-0.876130
16	6	0	-4.628498	1.193821	-0.226124
17	1	0	-4.965296	-0.313354	1.245234
18	1	0	-5.679216	1.449808	-0.313121
19	1	0	-3.978441	2.644885	-1.721732
20	6	0	-1.220994	2.133108	-1.640885
21	6	0	0.989946	3.128721	-2.946186
22	6	0	-1.373177	3.206525	-2.521552
23	7	0	-0.010645	1.584795	-1.426344
24	6	0	1.061536	2.066903	-2.053180
25	6	0	-0.256998	3.704545	-3.179704
26	1	0	-2.349039	3.649983	-2.680688
27	1	0	2.002532	1.574735	-1.815931
28	1	0	-0.357915	4.538936	-3.866801
29	1	0	1.884836	3.493881	-3.436672
30	28	0	0.000042	0.000044	0.093867
31	1	0	2.954094	3.496585	3.957046
32	6	0	2.386977	2.876770	3.268687
33	7	0	0.929151	1.293162	1.511410
34	6	0	3.034242	1.943746	2.496486
35	6	0	0.986970	3.024572	3.167316
36	6	0	0.321380	2.205012	2.274096
37	6	0	2.291981	1.131946	1.599046
38	1	0	4.109484	1.821122	2.573111
39	1	0	0.444736	3.747521	3.764177
40	1	0	-0.758662	2.264770	2.147747
41	6	0	2.856245	0.124640	0.753615
42	6	0	3.665957	-1.878538	-1.024866
43	6	0	4.228887	-0.210920	0.642984
44	7	0	1.946525	-0.562865	-0.020386
45	6	0	2.343282	-1.520661	-0.877527
46	6	0	4.628318	-1.194310	-0.227972
47	1	0	4.965801	0.312332	1.243772
48	1	0	5.678960	-1.450499	-0.315302
49	1	0	3.977582	-2.644862	-1.723778
50	6	0	1.220249	-2.132459	-1.642152
51	6	0	-0.991243	-3.127258	-2.947139

52	6	0	1.372000	-3.205557	-2.523283
53	7	0	0.010050	-1.584042	-1.427032
54	6	0	-1.062396	-2.065757	-2.053720
55	6	0	0.255543	-3.703172	-3.181269
56	1	0	2.347751	-3.649082	-2.682914
57	1	0	-2.003244	-1.573531	-1.816007
58	1	0	0.356129	-4.537315	-3.868716
59	1	0	-1.886341	-3.492101	-3.437481

Zero-point correction= 0.458808 (Hartree/Particle)
Thermal correction to Energy= 0.487879
Thermal correction to Enthalpy= 0.488823
Thermal correction to Gibbs Free Energy= 0.396375
Sum of electronic and zero-point Energies= -1653.277116
Sum of electronic and thermal Energies= -1653.248044
Sum of electronic and thermal Enthalpies= -1653.247100
Sum of electronic and thermal Free Energies= -1653.339548

Dimer nonaplet

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	28	0	4.647516	-0.014478	0.081398
2	7	0	5.953183	-0.319516	1.731961
3	7	0	5.729626	-1.622282	-0.520717
4	7	0	3.819710	-0.508170	-1.894840
5	7	0	2.832632	-0.742279	0.930920
6	7	0	3.632042	1.704490	0.458911
7	7	0	5.975535	1.565937	-0.668966
8	6	0	5.973973	0.377810	2.870356
9	1	0	5.196674	1.135114	2.960384
10	6	0	6.900485	0.175998	3.876902
11	1	0	6.872147	0.769093	4.782608
12	6	0	7.874433	-0.826157	3.674839
13	1	0	8.624380	-1.020008	4.436151
14	6	0	7.871505	-1.559278	2.513874
15	1	0	8.613367	-2.334764	2.354822
16	6	0	6.888852	-1.306286	1.520461
17	6	0	6.777992	-2.014234	0.282609
18	6	0	7.631032	-3.049828	-0.179122
19	1	0	8.463799	-3.380083	0.433477
20	6	0	7.407717	-3.629855	-1.402656
21	1	0	8.062961	-4.418340	-1.757928
22	6	0	6.320297	-3.196572	-2.215260
23	1	0	6.151709	-3.633242	-3.192054
24	6	0	5.518341	-2.190432	-1.720311
25	6	0	4.344804	-1.620127	-2.440644
26	6	0	3.778170	-2.195242	-3.579754
27	1	0	4.197772	-3.102395	-3.999075
28	6	0	2.652148	-1.610028	-4.143934
29	1	0	2.190683	-2.052226	-5.021276
30	6	0	2.112168	-0.463759	-3.564486
31	1	0	1.221960	0.013046	-3.959630
32	6	0	2.738838	0.051696	-2.436145
33	1	0	2.366044	0.937446	-1.924149
34	6	0	2.481545	-2.022088	1.092474
35	1	0	3.249761	-2.746614	0.825624
36	6	0	1.242893	-2.426018	1.554434
37	1	0	1.000980	-3.477552	1.649570

38	6	0	0.305196	-1.420629	1.881151
39	1	0	-0.688921	-1.693775	2.225852
40	6	0	0.648620	-0.099319	1.735556
41	1	0	-0.061498	0.687875	1.967906
42	6	0	1.931526	0.250866	1.235404
43	6	0	2.363237	1.589982	0.982229
44	6	0	1.607903	2.774469	1.189817
45	1	0	0.604006	2.714676	1.597950
46	6	0	2.137975	3.993279	0.848160
47	1	0	1.560174	4.899208	1.000895
48	6	0	3.443036	4.076537	0.283026
49	1	0	3.855396	5.033851	-0.010268
50	6	0	4.140823	2.898674	0.113681
51	6	0	5.508972	2.812433	-0.472620
52	6	0	6.285044	3.926718	-0.798412
53	1	0	5.905679	4.927122	-0.626626
54	6	0	7.552595	3.734827	-1.332218
55	1	0	8.169369	4.590292	-1.589336
56	6	0	8.024278	2.439239	-1.527352
57	1	0	9.009771	2.250115	-1.936990
58	6	0	7.194020	1.381764	-1.175457
59	1	0	7.501609	0.344553	-1.292824
60	28	0	-4.692402	-0.073816	-0.122998
61	7	0	-3.459564	-1.781162	-0.446681
62	7	0	-2.958614	0.768387	-0.769712
63	7	0	-5.103032	2.087043	-0.101419
64	7	0	-6.044860	-0.326436	-1.746357
65	7	0	-6.358449	-0.770321	0.810598
66	7	0	-4.136587	-0.133205	2.001042
67	6	0	-3.804812	-3.060746	-0.280732
68	1	0	-4.852198	-3.227255	-0.033356
69	6	0	-2.919294	-4.115822	-0.404976
70	1	0	-3.252868	-5.136247	-0.261243
71	6	0	-1.578198	-3.808952	-0.722714
72	1	0	-0.843555	-4.602448	-0.825927
73	6	0	-1.199382	-2.501101	-0.902780
74	1	0	-0.167979	-2.257360	-1.136577
75	6	0	-2.159315	-1.464464	-0.762004
76	6	0	-1.876275	-0.071294	-0.920801
77	6	0	-0.601870	0.499136	-1.168463
78	1	0	0.266943	-0.143841	-1.271101
79	6	0	-0.460456	1.864047	-1.230713
80	1	0	0.515576	2.310542	-1.395168
81	6	0	-1.588896	2.708871	-1.018941
82	1	0	-1.472551	3.785930	-1.009665
83	6	0	-2.806713	2.104768	-0.788886
84	6	0	-4.066876	2.845732	-0.503997
85	6	0	-4.202660	4.229004	-0.641504
86	1	0	-3.367358	4.828013	-0.985097
87	6	0	-5.423894	4.820296	-0.348394
88	1	0	-5.547391	5.894072	-0.450805
89	6	0	-6.488580	4.023302	0.066483
90	1	0	-7.459076	4.447822	0.296209
91	6	0	-6.277884	2.653900	0.170155
92	1	0	-7.067850	1.970852	0.475934
93	6	0	-5.799457	-0.079490	-3.035764
94	1	0	-4.785944	0.253071	-3.254739
95	6	0	-6.739295	-0.226408	-4.039321
96	1	0	-6.485888	-0.012665	-5.070413
97	6	0	-8.028770	-0.664798	-3.665711
98	1	0	-8.800609	-0.796816	-4.418221

99	6	0	-8.306020	-0.926524	-2.347105
100	1	0	-9.293670	-1.264690	-2.051989
101	6	0	-7.295824	-0.755402	-1.363425
102	6	0	-7.473078	-0.998017	0.034578
103	6	0	-8.662368	-1.437241	0.672930
104	1	0	-9.554633	-1.631964	0.086723
105	6	0	-8.684184	-1.617282	2.033106
106	1	0	-9.593148	-1.951501	2.522595
107	6	0	-7.517016	-1.365077	2.809840
108	1	0	-7.533386	-1.492801	3.885060
109	6	0	-6.385466	-0.946237	2.142619
110	6	0	-5.084150	-0.646000	2.805566
111	6	0	-4.819981	-0.887079	4.155997
112	1	0	-5.584019	-1.311188	4.796959
113	6	0	-3.558874	-0.596874	4.660655
114	1	0	-3.334940	-0.787418	5.705622
115	6	0	-2.584098	-0.073906	3.813526
116	1	0	-1.581611	0.148376	4.163700
117	6	0	-2.926541	0.141655	2.483868
118	1	0	-2.215369	0.534336	1.759830

SCF=QC

Zero-point correction= 0.919502
(Hartree/Particle)
Thermal correction to Energy= 0.979680
Thermal correction to Enthalpy= 0.980624
Thermal correction to Gibbs Free Energy= 0.816258
Sum of electronic and zero-point Energies= -3306.568083
Sum of electronic and thermal Energies= -3306.507905
Sum of electronic and thermal Enthalpies= -3306.506960
Sum of electronic and thermal Free Energies= -3306.671326

SCF=XQC

Zero-point correction= 0.919497
(Hartree/Particle)
Thermal correction to Energy= 0.979676
Thermal correction to Enthalpy= 0.980620
Thermal correction to Gibbs Free Energy= 0.816246
Sum of electronic and zero-point Energies= -3306.568088
Sum of electronic and thermal Energies= -3306.507909
Sum of electronic and thermal Enthalpies= -3306.506964
Sum of electronic and thermal Free Energies= -3306.671339

Dimer singlet with two triplet subunits

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	28	0	4.106412	0.004233	0.064282
2	7	0	5.995642	-0.808270	0.624906
3	7	0	3.938988	-1.926369	-0.548368
4	7	0	2.139045	-0.063012	-0.921810
5	7	0	3.288600	-0.109775	2.011934
6	7	0	3.919842	1.975180	0.561113
7	7	0	4.979877	1.086691	-1.652271
8	6	0	7.016526	-0.160336	1.190481
9	1	0	6.869022	0.911479	1.315209
10	6	0	8.185572	-0.773545	1.603154
11	1	0	8.982609	-0.197877	2.057215

12	6	0	8.288728	-2.170000	1.416021
13	1	0	9.186696	-2.698107	1.723394
14	6	0	7.250764	-2.861936	0.843961
15	1	0	7.324679	-3.933914	0.694152
16	6	0	6.077374	-2.171266	0.437003
17	6	0	4.941465	-2.789959	-0.170608
18	6	0	4.750955	-4.182049	-0.390901
19	1	0	5.526525	-4.888506	-0.113773
20	6	0	3.575123	-4.631272	-0.934712
21	1	0	3.423581	-5.694256	-1.093920
22	6	0	2.542215	-3.714310	-1.282482
23	1	0	1.603000	-4.067706	-1.689154
24	6	0	2.786879	-2.370969	-1.070436
25	6	0	1.808570	-1.286528	-1.375531
26	6	0	0.619389	-1.499820	-2.072372
27	1	0	0.372549	-2.488019	-2.442816
28	6	0	-0.244901	-0.432478	-2.290313
29	1	0	-1.179781	-0.580009	-2.824870
30	6	0	0.105055	0.825808	-1.808217
31	1	0	-0.545370	1.682537	-1.942302
32	6	0	1.309453	0.960719	-1.126959
33	1	0	1.625465	1.920082	-0.721684
34	6	0	3.100382	-1.215680	2.734577
35	1	0	3.495273	-2.129805	2.290328
36	6	0	2.442796	-1.232080	3.952297
37	1	0	2.310700	-2.158247	4.497923
38	6	0	1.954275	-0.000346	4.445896
39	1	0	1.418777	0.035655	5.389842
40	6	0	2.162670	1.155528	3.733933
41	1	0	1.797555	2.104394	4.113290
42	6	0	2.862272	1.107255	2.495965
43	6	0	3.169291	2.241644	1.682710
44	6	0	2.747507	3.580045	1.913719
45	1	0	2.170656	3.822669	2.800962
46	6	0	3.054204	4.559515	1.003468
47	1	0	2.722677	5.579290	1.171188
48	6	0	3.790394	4.242805	-0.173365
49	1	0	3.991287	5.000546	-0.920327
50	6	0	4.192469	2.932073	-0.337489
51	6	0	4.921191	2.425523	-1.536378
52	6	0	5.519605	3.256765	-2.484238
53	1	0	5.486923	4.333521	-2.364740
54	6	0	6.173929	2.682510	-3.566768
55	1	0	6.646932	3.312695	-4.313533
56	6	0	6.225169	1.295682	-3.677418
57	1	0	6.730736	0.810771	-4.504388
58	6	0	5.614257	0.536655	-2.685774
59	1	0	5.627217	-0.550667	-2.702036
60	28	0	-4.051957	0.076975	-0.030701
61	7	0	-2.215600	-1.071115	0.398425
62	7	0	-2.818952	1.452417	0.756919
63	7	0	-5.303353	1.817007	0.024307
64	7	0	-3.664415	0.281935	-2.125279
65	7	0	-5.020698	-1.524159	-0.805058
66	7	0	-5.058175	-0.828431	1.712207
67	6	0	-2.021613	-2.378953	0.224629
68	1	0	-2.835244	-2.917308	-0.257725
69	6	0	-0.858854	-3.022762	0.630974
70	1	0	-0.734610	-4.087564	0.467114
71	6	0	0.128810	-2.264255	1.254796
72	1	0	1.051911	-2.724199	1.595160

73	6	0	-0.068062	-0.900667	1.432894
74	1	0	0.687831	-0.296285	1.922140
75	6	0	-1.256630	-0.325517	0.978489
76	6	0	-1.559069	1.128568	1.096947
77	6	0	-0.631089	2.073796	1.485300
78	1	0	0.391345	1.805061	1.723949
79	6	0	-1.051819	3.433484	1.513699
80	1	0	-0.339784	4.206045	1.787887
81	6	0	-2.340570	3.768971	1.183233
82	1	0	-2.654825	4.807496	1.203512
83	6	0	-3.259645	2.757518	0.796587
84	6	0	-4.622943	2.949231	0.413197
85	6	0	-5.294517	4.201186	0.415500
86	1	0	-4.765856	5.096604	0.725029
87	6	0	-6.610436	4.272188	0.031446
88	1	0	-7.124910	5.228778	0.034664
89	6	0	-7.291210	3.100491	-0.367038
90	1	0	-8.327514	3.120691	-0.681119
91	6	0	-6.580362	1.913759	-0.350116
92	1	0	-7.042795	0.975876	-0.655097
93	6	0	-3.104476	1.320046	-2.745458
94	1	0	-2.896247	2.179668	-2.107971
95	6	0	-2.785959	1.328532	-4.093220
96	1	0	-2.327251	2.196554	-4.550479
97	6	0	-3.080261	0.162791	-4.836418
98	1	0	-2.832843	0.112811	-5.892789
99	6	0	-3.694526	-0.904561	-4.226673
100	1	0	-3.943778	-1.791799	-4.799214
101	6	0	-4.024668	-0.833721	-2.844901
102	6	0	-4.744298	-1.832214	-2.119869
103	6	0	-5.182115	-3.085655	-2.626531
104	1	0	-4.995427	-3.345460	-3.663430
105	6	0	-5.828030	-3.971401	-1.802706
106	1	0	-6.157501	-4.931019	-2.187578
107	6	0	-6.056973	-3.644026	-0.435963
108	1	0	-6.524073	-4.356002	0.232890
109	6	0	-5.629357	-2.407294	0.002387
110	6	0	-5.755839	-1.937467	1.411578
111	6	0	-6.544357	-2.573801	2.371557
112	1	0	-7.121965	-3.452600	2.109670
113	6	0	-6.594059	-2.049467	3.656732
114	1	0	-7.203500	-2.528218	4.416941
115	6	0	-5.865950	-0.900850	3.955997
116	1	0	-5.885671	-0.459187	4.945639
117	6	0	-5.112266	-0.321030	2.942001
118	1	0	-4.529993	0.583764	3.101734

SCF=XQC

Zero-point correction= 0.920712
(Hartree/Particle)
Thermal correction to Energy= 0.980321
Thermal correction to Enthalpy= 0.981265
Thermal correction to Gibbs Free Energy= 0.824430
Sum of electronic and zero-point Energies= -3306.557731
Sum of electronic and thermal Energies= -3306.498122
Sum of electronic and thermal Enthalpies= -3306.497178
Sum of electronic and thermal Free Energies= -3306.654013

Dimer singlet with two quintet subunits

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	28	0	4.553982	0.006590	0.068851
2	7	0	5.886606	-0.186782	1.717490
3	7	0	5.562453	-1.696617	-0.390120
4	7	0	3.708053	-0.621132	-1.859383
5	7	0	2.758635	-0.608730	1.039322
6	7	0	3.580622	1.771049	0.337879
7	7	0	5.875978	1.495668	-0.857824
8	6	0	5.976575	0.632013	2.768758
9	1	0	5.255346	1.448104	2.779695
10	6	0	6.904322	0.480022	3.782959
11	1	0	6.932544	1.172045	4.615537
12	6	0	7.800609	-0.606599	3.689214
13	1	0	8.547114	-0.767396	4.461435
14	6	0	7.726314	-1.463908	2.619423
15	1	0	8.409541	-2.303150	2.542188
16	6	0	6.749733	-1.252851	1.610736
17	6	0	6.579802	-2.080409	0.456293
18	6	0	7.346894	-3.223921	0.115735
19	1	0	8.151455	-3.550946	0.766538
20	6	0	7.074244	-3.916330	-1.037745
21	1	0	7.662407	-4.789354	-1.300366
22	6	0	6.021022	-3.490539	-1.897166
23	1	0	5.811588	-4.020733	-2.818031
24	6	0	5.301615	-2.377053	-1.520308
25	6	0	4.173674	-1.802479	-2.305871
26	6	0	3.594445	-2.427465	-3.412303
27	1	0	3.965422	-3.386468	-3.754780
28	6	0	2.519153	-1.819094	-4.047319
29	1	0	2.047294	-2.299510	-4.898585
30	6	0	2.045287	-0.597630	-3.574077
31	1	0	1.196519	-0.097416	-4.026515
32	6	0	2.681695	-0.036333	-2.474071
33	1	0	2.360005	0.911500	-2.047582
34	6	0	2.397620	-1.863342	1.327188
35	1	0	3.130696	-2.624353	1.062579
36	6	0	1.191563	-2.200012	1.912687
37	1	0	0.938438	-3.234521	2.109564
38	6	0	0.301281	-1.149044	2.228869
39	1	0	-0.665707	-1.369469	2.673575
40	6	0	0.658091	0.148629	1.956999
41	1	0	-0.014079	0.969506	2.187767
42	6	0	1.905384	0.427478	1.336395
43	6	0	2.348566	1.731454	0.952047
44	6	0	1.637673	2.948394	1.122801
45	1	0	0.660054	2.945134	1.594630
46	6	0	2.173766	4.125241	0.664287
47	1	0	1.629559	5.055903	0.787836
48	6	0	3.443605	4.132005	0.017425
49	1	0	3.863626	5.056967	-0.357497
50	6	0	4.099476	2.926263	-0.114099
51	6	0	5.432322	2.762389	-0.761833
52	6	0	6.200564	3.827003	-1.238166
53	1	0	5.840176	4.845055	-1.149565
54	6	0	7.435175	3.564060	-1.816198
55	1	0	8.045717	4.380492	-2.189327
56	6	0	7.883861	2.248534	-1.905031

57	1	0	8.844469	2.005226	-2.344184
58	6	0	7.063762	1.243966	-1.406341
59	1	0	7.353966	0.195704	-1.434212
60	28	0	-4.574496	-0.127294	-0.116212
61	7	0	-3.313325	-1.843324	-0.190978
62	7	0	-2.822686	0.658188	-0.782535
63	7	0	-5.007654	2.018192	-0.360222
64	7	0	-5.837176	-0.608304	-1.758832
65	7	0	-6.299132	-0.673775	0.812476
66	7	0	-4.127834	0.092852	2.022442
67	6	0	-3.655993	-3.102283	0.095103
68	1	0	-4.707651	-3.250308	0.335984
69	6	0	-2.763210	-4.158549	0.093892
70	1	0	-3.094203	-5.161687	0.333412
71	6	0	-1.418981	-3.877359	-0.233659
72	1	0	-0.680575	-4.674171	-0.249300
73	6	0	-1.042756	-2.591466	-0.536349
74	1	0	-0.010898	-2.366114	-0.785039
75	6	0	-2.007948	-1.551309	-0.508925
76	6	0	-1.728282	-0.178471	-0.800901
77	6	0	-0.450095	0.375892	-1.061743
78	1	0	0.427965	-0.262948	-1.054277
79	6	0	-0.318043	1.728192	-1.264241
80	1	0	0.659738	2.170038	-1.429684
81	6	0	-1.460435	2.576728	-1.189855
82	1	0	-1.352955	3.649753	-1.293730
83	6	0	-2.681698	1.986311	-0.942705
84	6	0	-3.958097	2.739341	-0.795568
85	6	0	-4.095064	4.098191	-1.088252
86	1	0	-3.248373	4.665591	-1.456744
87	6	0	-5.331922	4.704990	-0.916991
88	1	0	-5.456527	5.759953	-1.140966
89	6	0	-6.409906	3.946908	-0.465359
90	1	0	-7.391935	4.383881	-0.326144
91	6	0	-6.196712	2.599068	-0.203568
92	1	0	-6.995210	1.944606	0.140411
93	6	0	-5.510290	-0.570412	-3.053034
94	1	0	-4.476862	-0.295026	-3.257376
95	6	0	-6.394502	-0.854809	-4.077472
96	1	0	-6.075787	-0.811209	-5.111662
97	6	0	-7.715599	-1.203337	-3.720159
98	1	0	-8.446904	-1.434409	-4.489292
99	6	0	-8.075627	-1.252141	-2.396512
100	1	0	-9.087482	-1.523708	-2.114857
101	6	0	-7.118862	-0.950828	-1.391261
102	6	0	-7.380327	-0.974914	0.014457
103	6	0	-8.622543	-1.259917	0.639109
104	1	0	-9.489804	-1.509712	0.036531
105	6	0	-8.729534	-1.213364	2.006362
106	1	0	-9.679947	-1.425469	2.485019
107	6	0	-7.597548	-0.879124	2.804133
108	1	0	-7.681933	-0.820477	3.882225
109	6	0	-6.411064	-0.621614	2.150771
110	6	0	-5.139006	-0.255776	2.837068
111	6	0	-4.963618	-0.280906	4.222621
112	1	0	-5.779248	-0.575421	4.872506
113	6	0	-3.724861	0.055281	4.753243
114	1	0	-3.569603	0.034228	5.827416
115	6	0	-2.683816	0.406236	3.896273
116	1	0	-1.697270	0.659022	4.270562
117	6	0	-2.938006	0.409501	2.529632

118	1	0	-2.170570	0.656937	1.797989

SCF=QC
Energy= -3307.488473

SCF=XQC

Zero-point correction= (Hartree/Particle)	0.919186
Thermal correction to Energy=	0.979574
Thermal correction to Enthalpy=	0.980518
Thermal correction to Gibbs Free Energy=	0.817366
Sum of electronic and zero-point Energies=	-3306.565765
Sum of electronic and thermal Energies=	-3306.505377
Sum of electronic and thermal Enthalpies=	-3306.504433
Sum of electronic and thermal Free Energies=	-3306.667585