Experimental and theoretical investigations on the self-association of Oxaliplatin.

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Electronic Supporting Information

Contents

1. Mass spectrometry

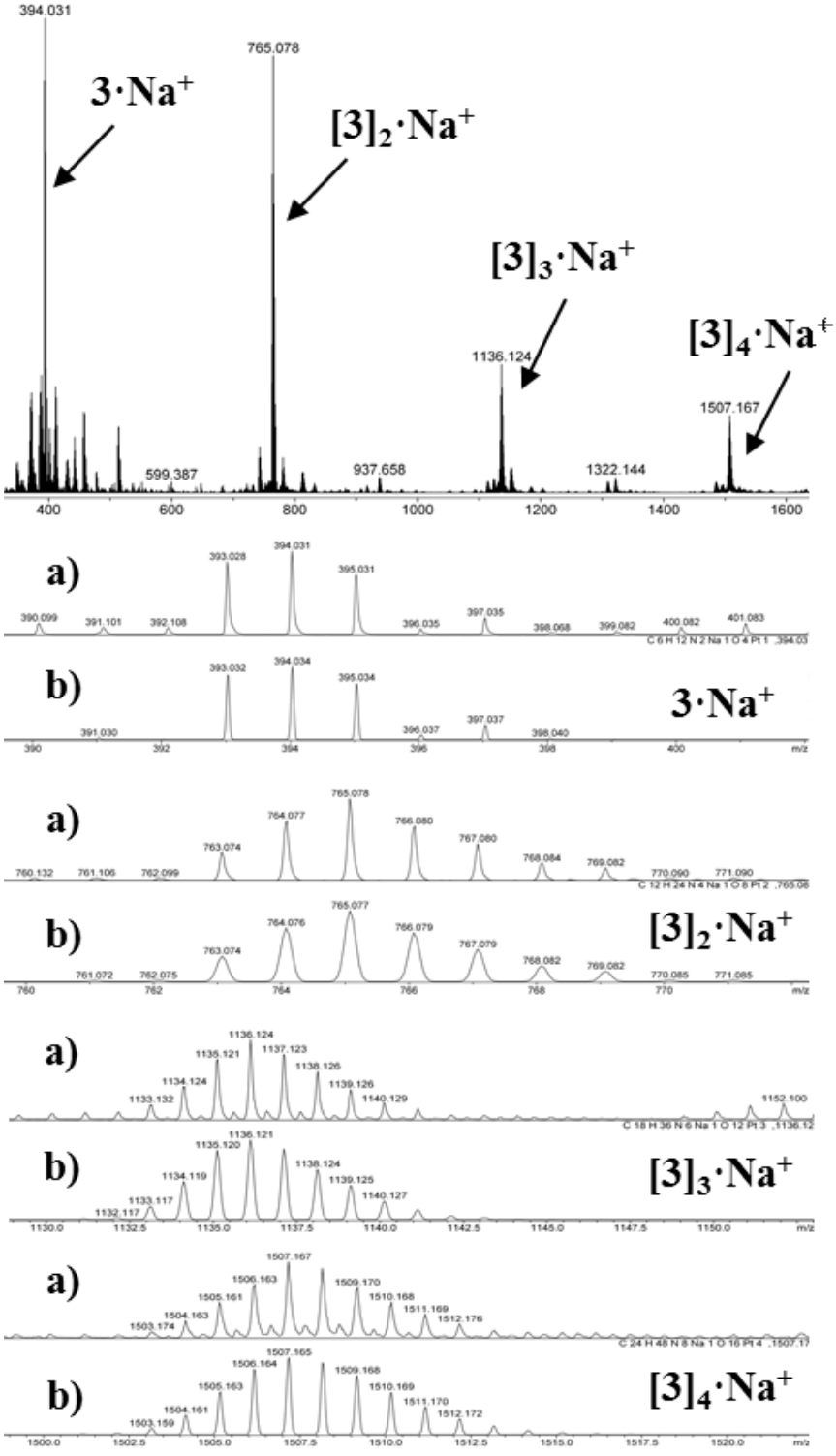


Figure S 1. Selected regions of the ESI^+ mass spectrum of a DMSO solution of **3** containing traces of Na^+ salts: a) experimental spectrum, b) simulated isotopic patterns.

2. NMR spectrometry

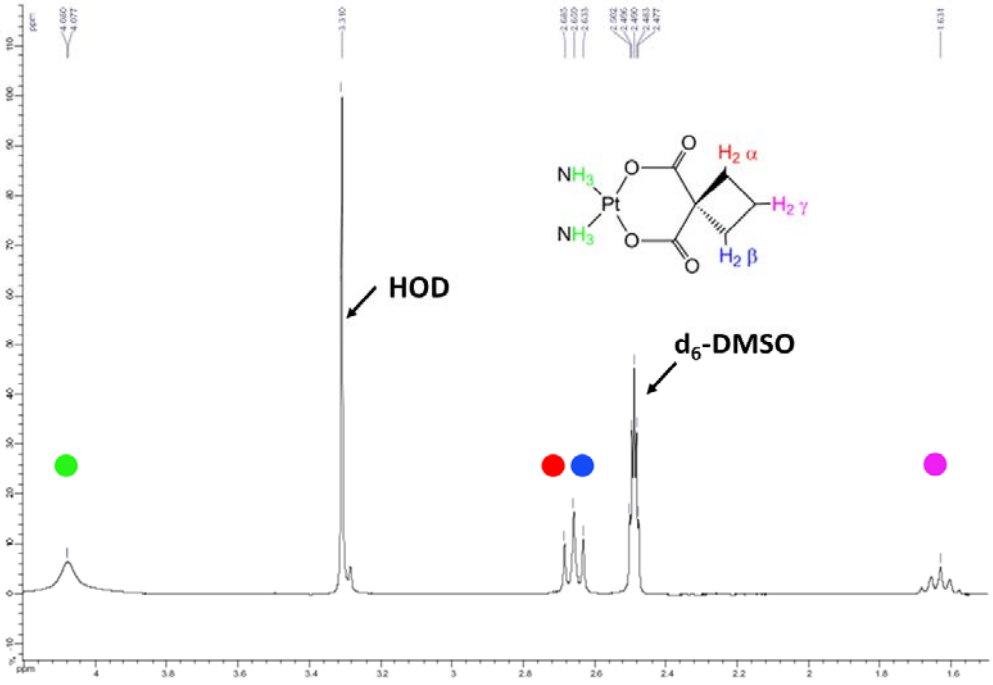


Figure S 2. ^{1}H NMR spectra for **3** in d_6-DMSO

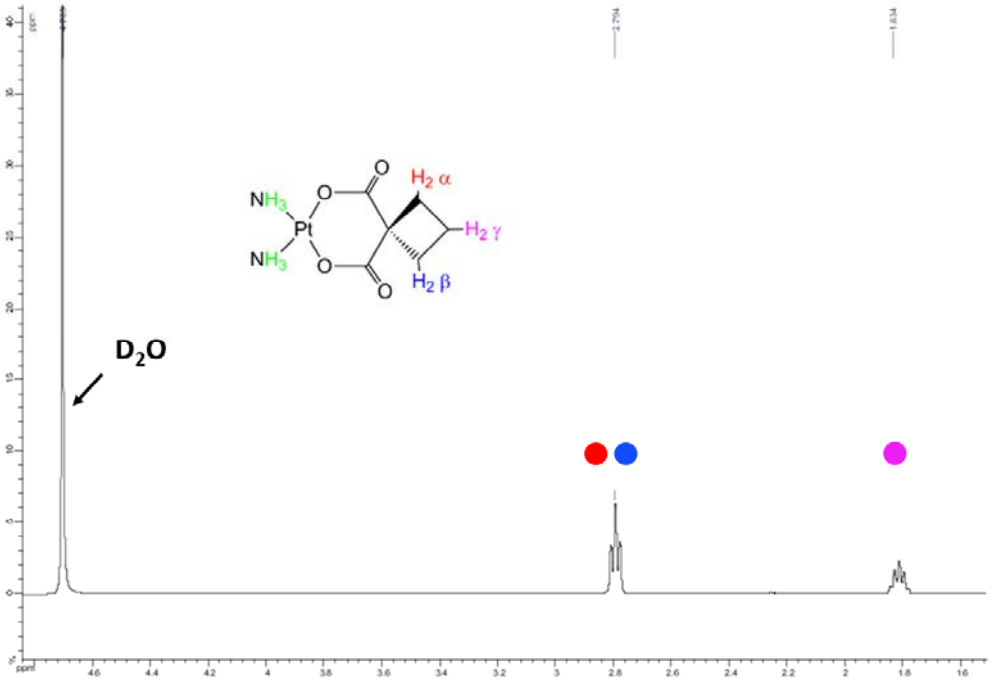


Figure S 3. ^{1}H NMR spectra for **3** in D_2O

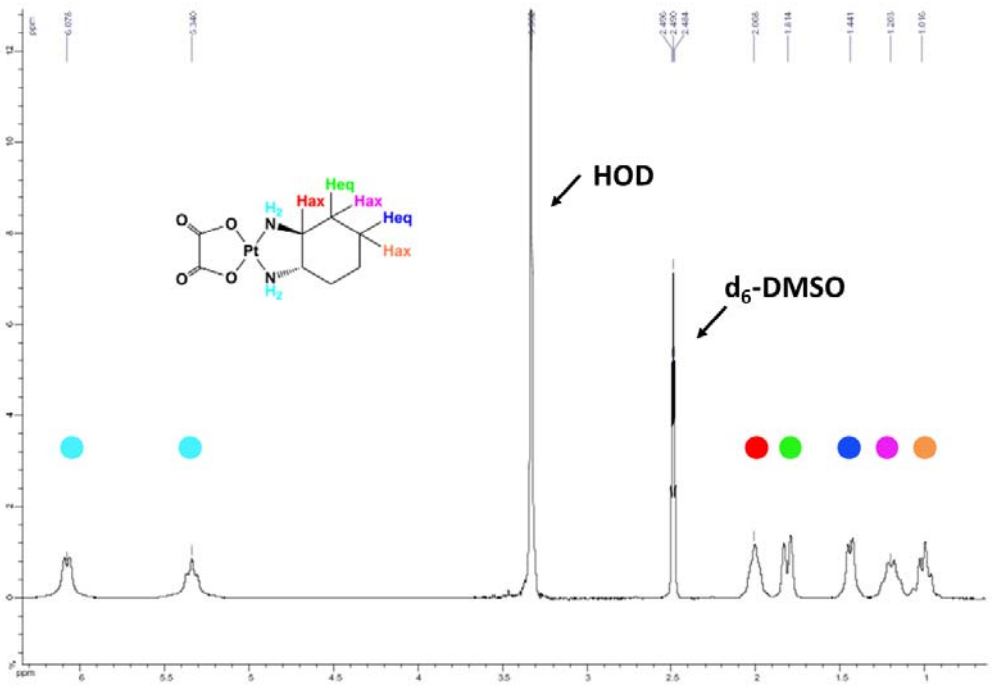


Figure S 4. ^{1}H NMR spectra for **1** in d_6-DMSO

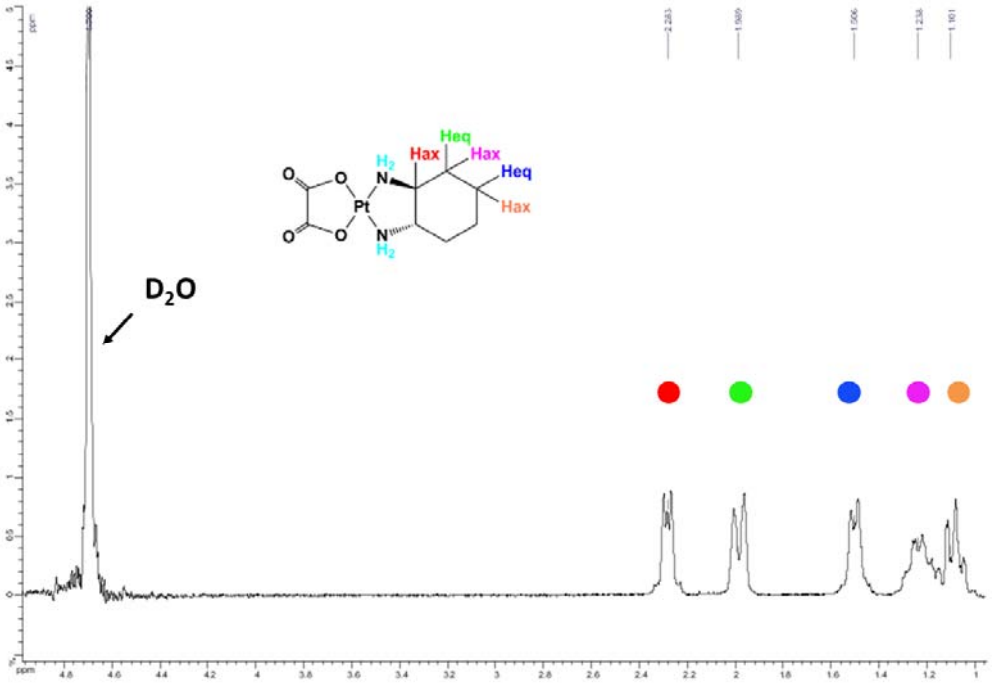


Figure S 5. ^{1}H NMR spectra for **1** in D_2O

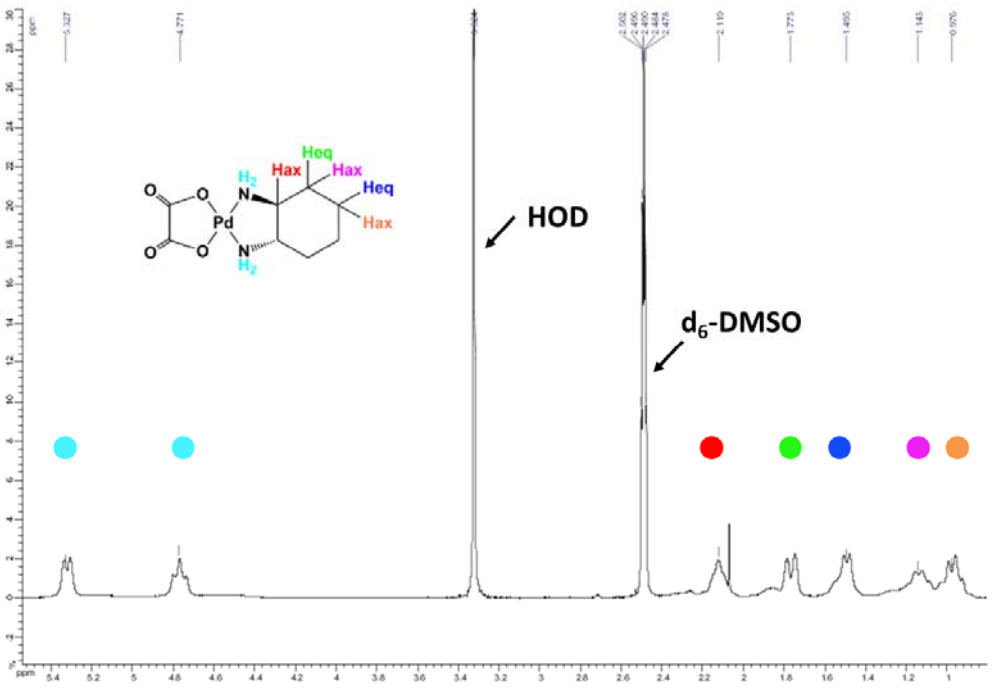


Figure S 6. ^{1}H NMR spectra for **2** in d_6-DMSO

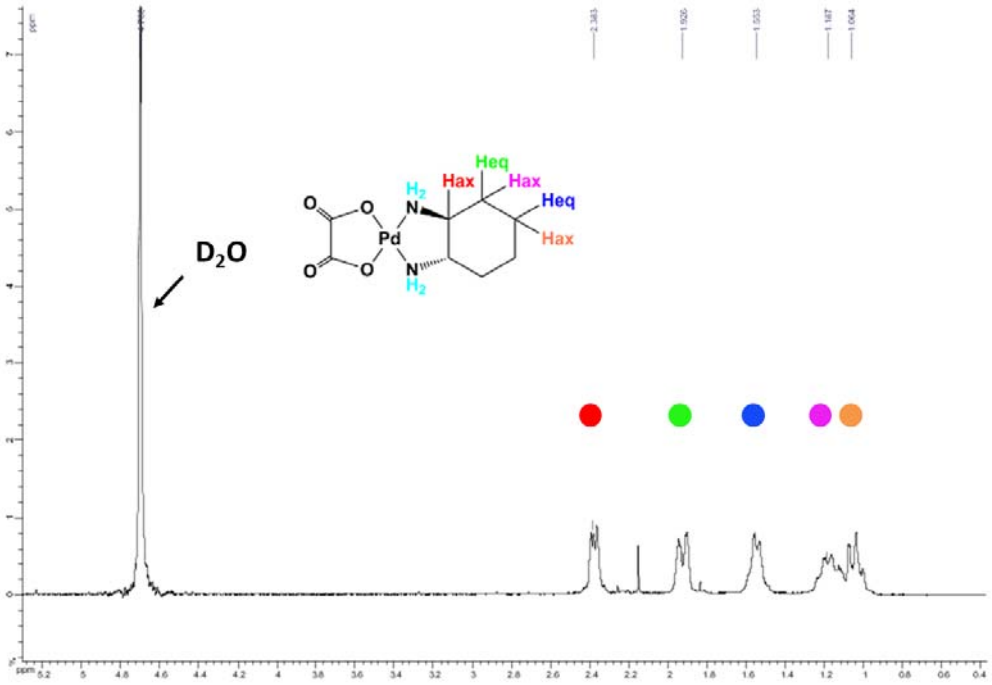


Figure S 7. ^{1}H NMR spectra for **2** in D_2O

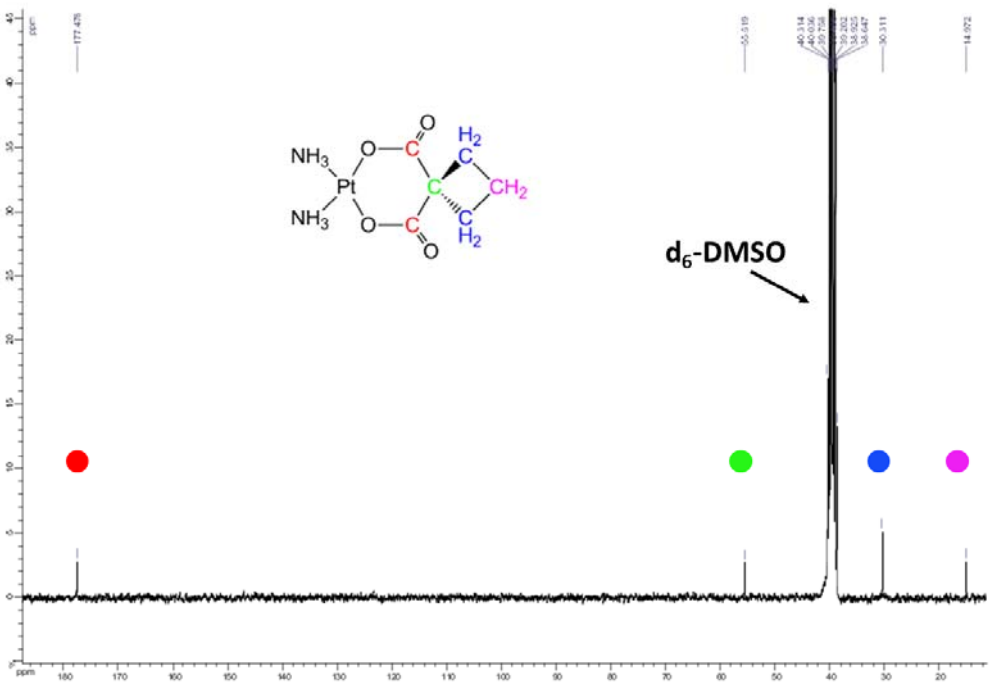


Figure S 8. ^{13}C NMR spectra for **3** in d_6-DMSO

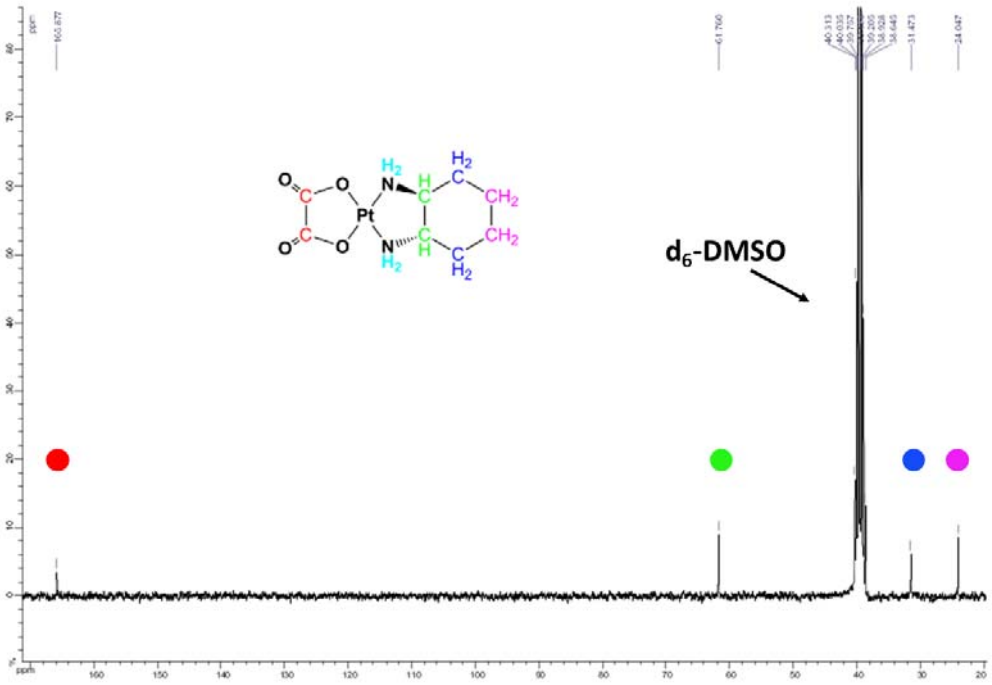


Figure S 9. ^{13}C NMR spectra for **1** in d_6-DMSO

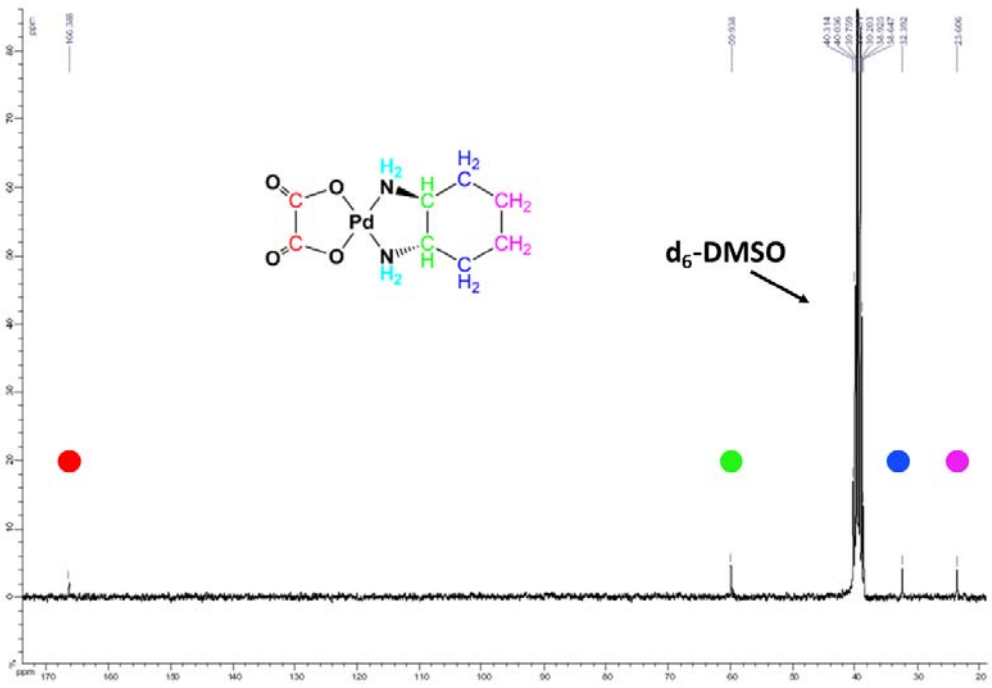


Figure S 10. ^{13}C NMR spectra for **3** in d_6-DMSO

3. ^{1}H DOSY

Table S 1. Hydrodynamic data for compounds **1-3** acquired by two-dimensional ^{1}H DOSY.

entry	cmpd	solvent	c (mM)	D_{exp}^{300K} (10^{-10}m^2/s)	r_h^{exp} (Å)	V_s^{exp} (Å^3)	$D^0_{dimer}[D^0_{monomer}]$ (10^{-10}m^2/s)
1	**1**	D_2O	6.3	5.68	3.55	187.0	6.05[7.63]
2		D_2O	12.6	5.96	3.38	162.2	6.05[7.63]
3		d_6.DMSO	5.0	2.55	4.10	289.0	3.14[3.96]
4		d_6.DMSO	51.8	2.49	4.20	310.4	3.14[3.96]
5	**2**	D_2O	6.8	5.17	3.90	248.2	6.05[7.63]
6		D_2O	67.7	4.98	4.04	276.8	6.05[7.63]
7		d_6.DMSO	9.1	2.20	4.75	448.8	3.14[3.96]
8		d_6.DMSO	63.5	1.99	5.27	611.8	3.14[3.96]
9	**3**	D_2O	6.7	6.24	3.23	141.0	5.08[7.45]
10		D_2O	55.2	6.12	3.29	149.5	5.08[7.45]
11		d_6.DMSO	6.5	2.58	4.06	280.6	2.63[3.87]
		d_6.DMSO	53.9	2.39	4.37	349.7	2.63[3.87]

Practically, if the dynamics of the chemical system are slow with respect to the ^{1}H NMR time-scale the resulting two-dimensional trace should present one set of signals per analyte ordered by the values of respective translational diffusion coefficients. In the contrary, a system consisting of a fast equilibrium between a monomer and a non-covalently bonded dimer within the time frame of ^{1}H NMR spectroscopy, should lead to an averaged ^{1}H NMR response appearing as a single set of averaged signals. This was typically the behaviour observed for **1**-**3**, which all displayed a limited solubility in D_2O and in deuterated dry DMSO. Table S 1 lists the main relevant data of ^{1}H DOSY experiments, that is the millimolar concentration of analyte (c), the measured translational diffusion coefficient (D_{exp}), the experimental hydrodynamic radius (r_h) and the associated spherical volume (V_s).

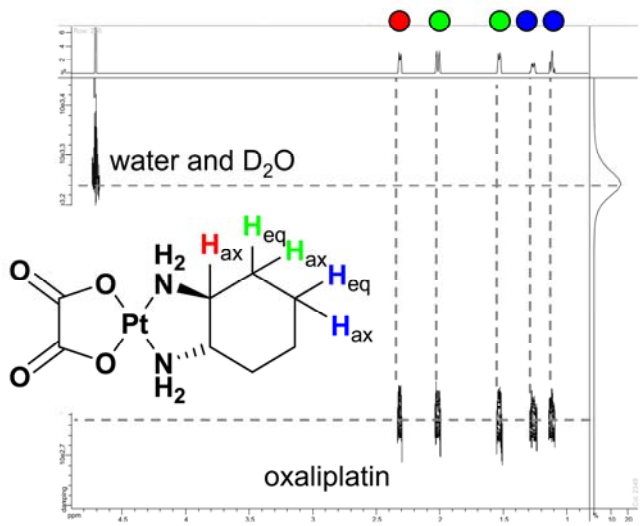


Figure S 11. Two-dimensional plot of a ^{1}H diffusion-ordered NMR experiment carried out with a solution of **1** in D_2O. Ordinates represent the values of the translational diffusion coefficient.

Calculated translational diffusion coefficient (D^0) for monomers and dimers (head-to-tail stacks, vide infra) were obtained by applying the Stoke-Einstein law, roughly approximating the hydrodynamic volume of the analytes with that of the associated solvent-exclusion volume of an ideal triaxial ellipsoid computed from the main dimensions (a, b, c)[1-3] of the structures of either the monomers or the β-stacked dimers produced by COSMO DFT calculations (vide infra).[4]

For each compound a pair of DOSY experiments was carried out by varying the concentration of the analyte: 1) at the highest achievable concentration, which should favour the formation of a dimer, and 2) at a 10 fold lower concentration. Table S 1 indicates that there is no large influence of the concentration on D_{exp}, the values of which surprisingly remain close to the value computed for a dimer in the case of **1** (Figure S 11 and Table S 1 entries 1-4). For d_6.DMSO solutions of **2** the values of D_{exp} also suggested the existence of a dimer. The behaviour of **3** was very similar to that of **1**.

Measures of self-diffusion coefficients were performed on a BRUKER 600 MHz spectrometer - Avance III, developing a pulse field gradient of 50 G/cm.A. The gradient coil was cooled by air flow and the sample was thermo-stated at 298 K. The gradient strength varied linearly between 6 and 305 G/cm in 12 experiments.

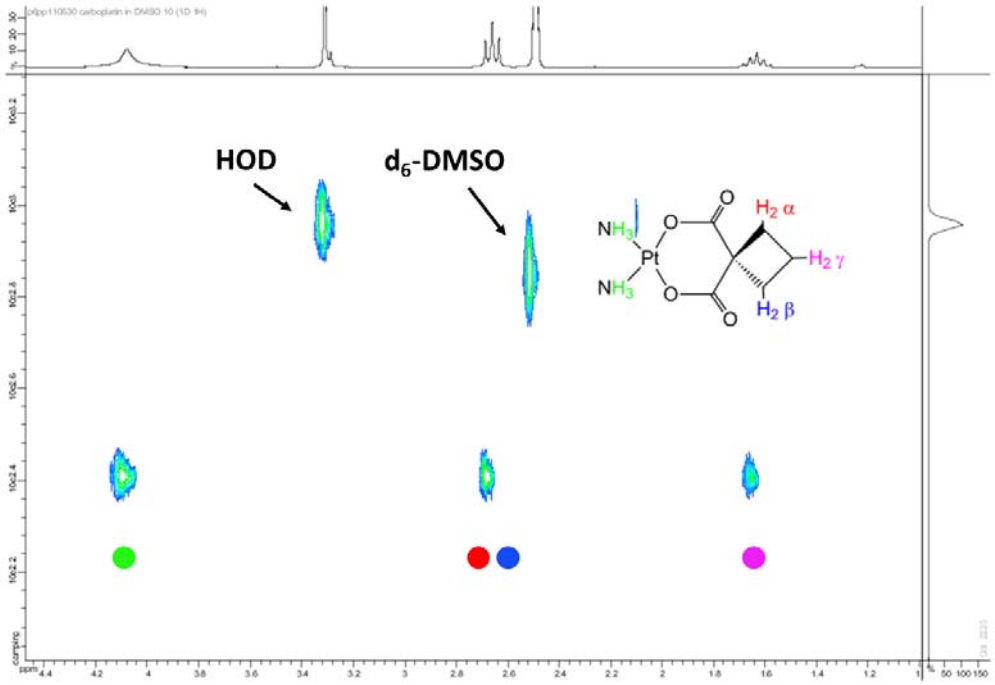


Figure S 12. DOSY spectra for **3** in d_6-DMSO

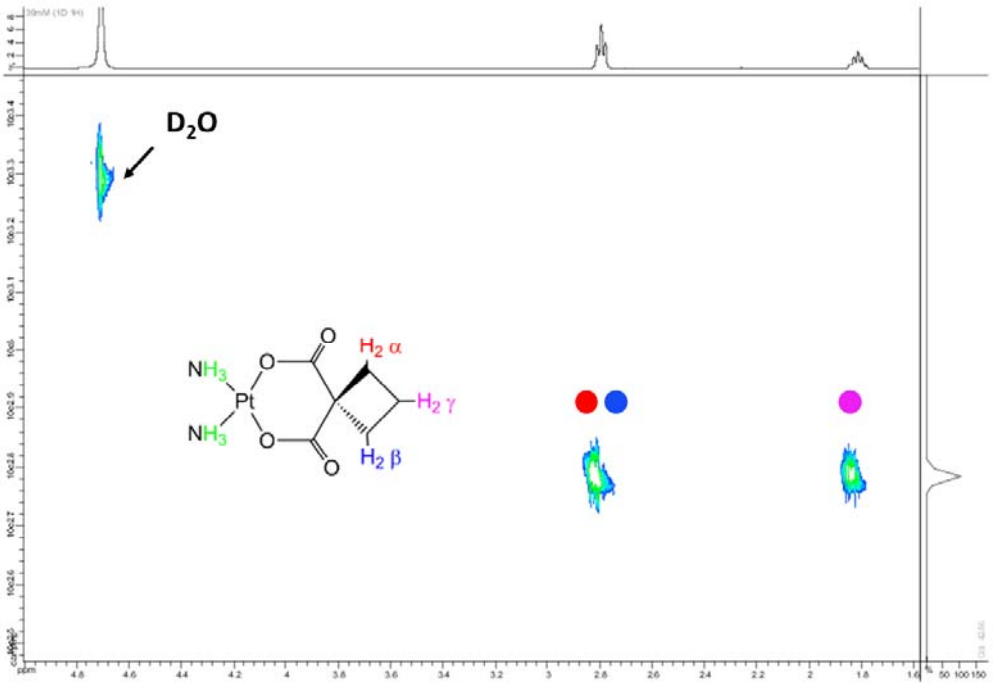


Figure S 13. DOSY spectra for **3** in D_2O

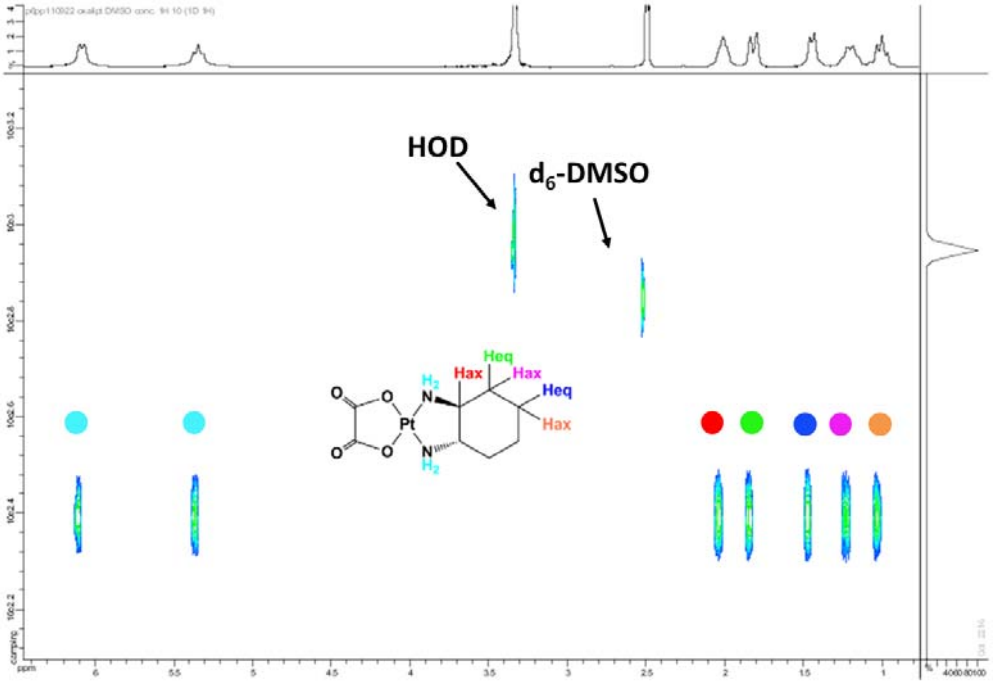


Figure S 14. DOSY spectra for **1** in d_6-DMSO

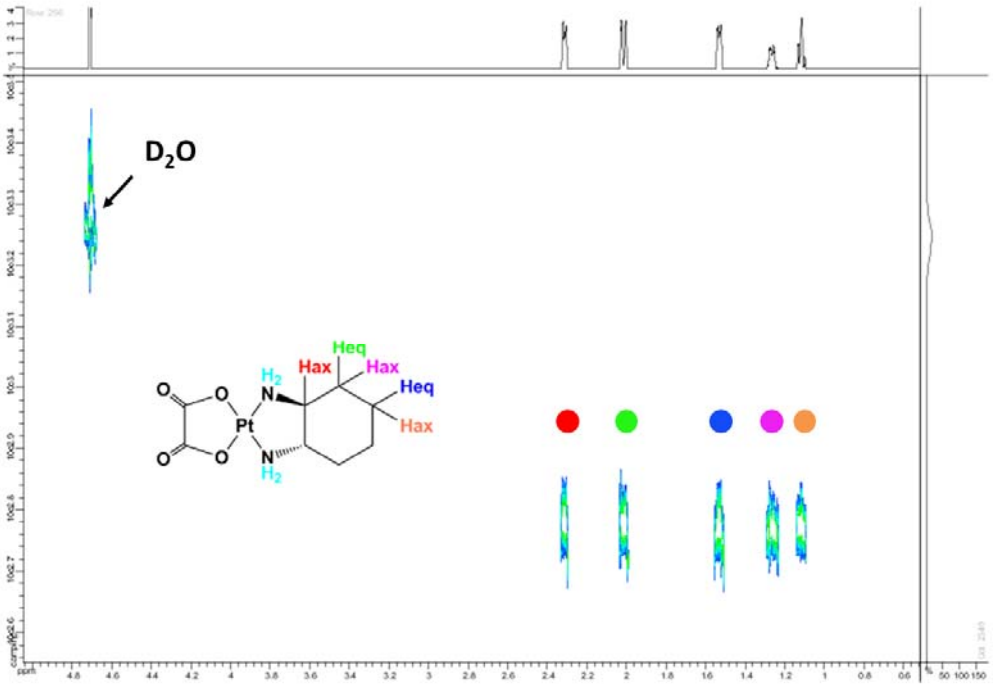


Figure S 15. DOSY spectra for **1** in D_2O

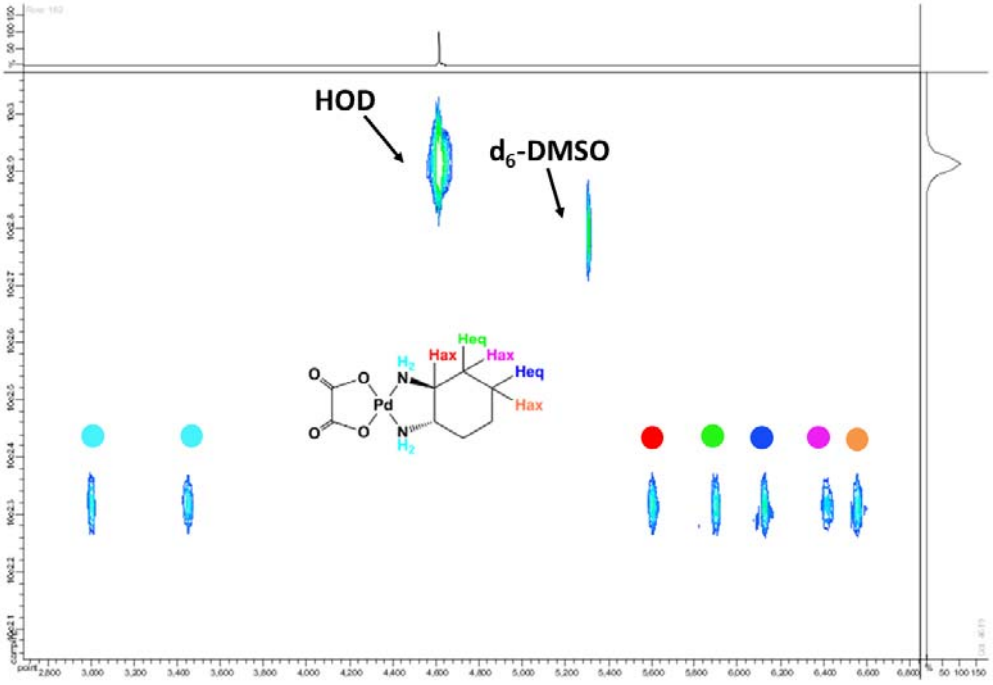


Figure S 16. DOSY spectra for **2** in d_6-DMSO

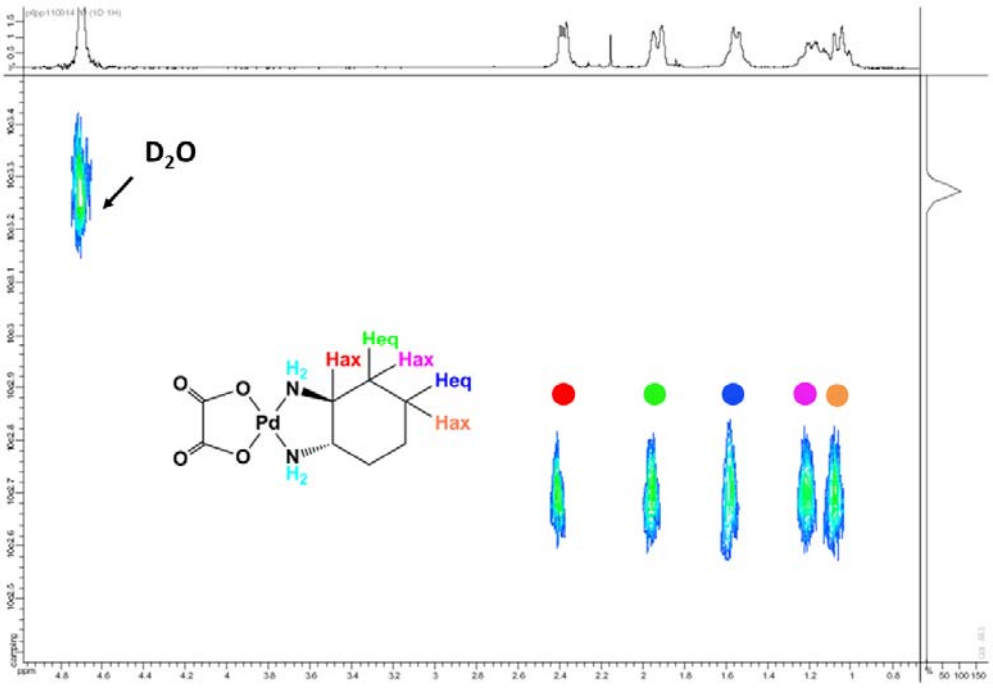


Figure S 17. DOSY spectra for **2** in D_2O

4. UV-visible spectrum of 1 as a function of concentration in pure water

The spectra were recorded between 220 nm and 600 nm on an UVIKON XL spectrometer, using a pair of quartz cells of 1 mm optical path. The large absorption band at 260 nm (ε= 16.4 10^4) and the weaker shoulder at 318 nm (ε= 2.1 10^4) display perfect linearity with respect to concentration, in good accord with Beer Lambert law, which suggest the apparent absence of a second analyte in the concentrated solution.

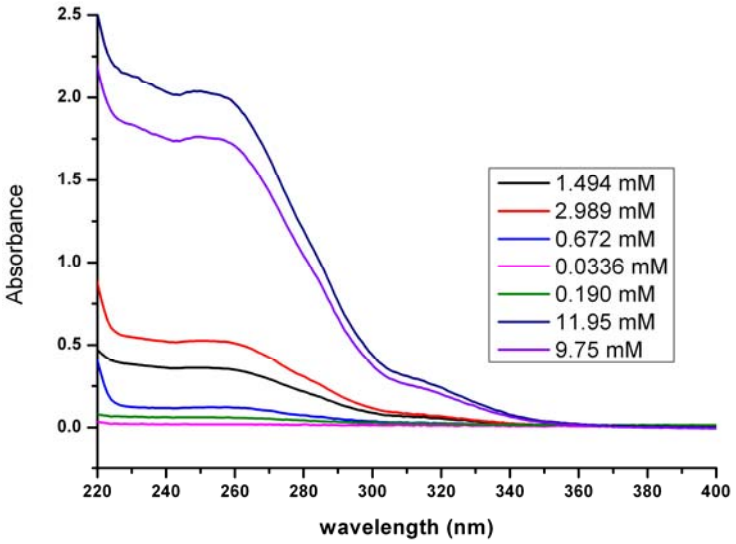


Figure S 18. Stacked UV-visible spectra of aqueous solutions of **1** measured at different concentrations in a 1 mm optical path quartz cell at 25°C.

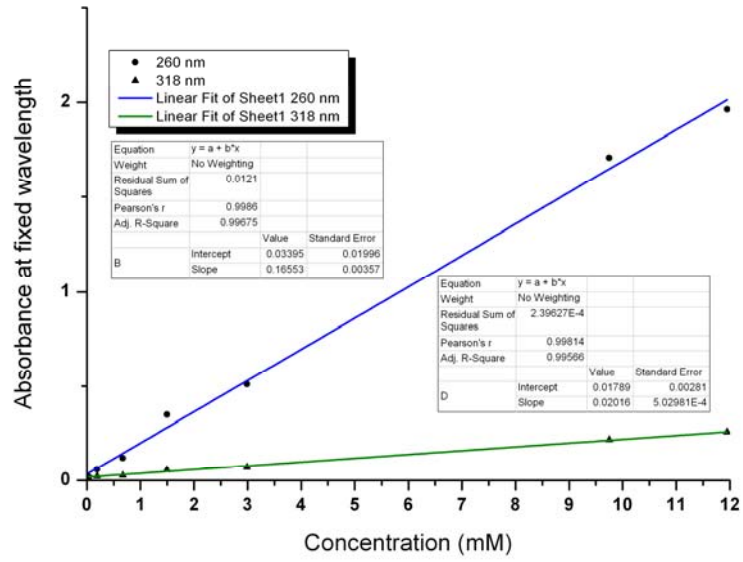


Figure S 19. Linearity of the relationship between absorbance at 216 nm and 318 nm and the concentration of **1** in pure water at 25°C.

5. Calorimetry

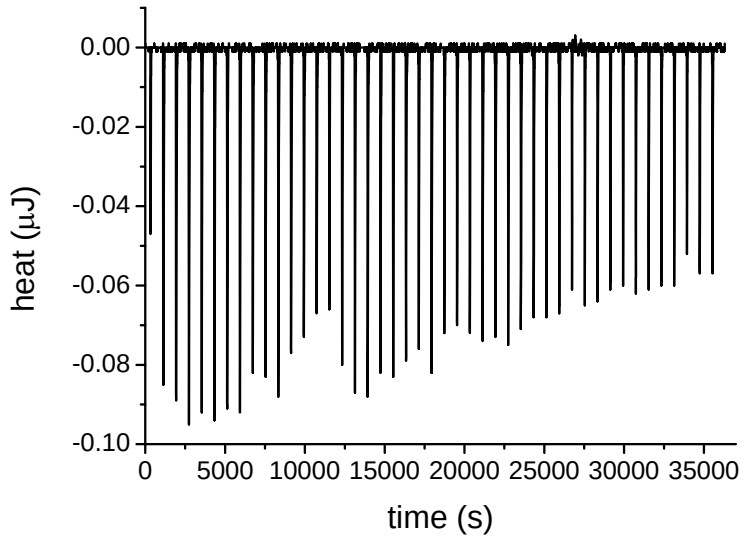


Figure S 20. Thermographic trace of the dilution of a concentrated aqueous solution of **1** (c = 20 mM, v = 2.06 μL) into pure water at 25 °C.

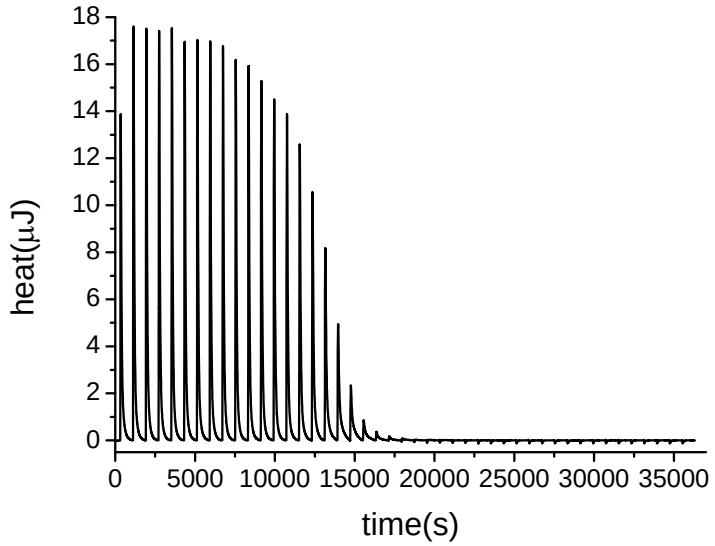


Figure S 21. Heat released in the reaction: titration of **CB**[7] water solution with **1** complex water solution. Reaction was performed on 25^0C. Interval between injections was 800 seconds: **1**: c = 20mM injected into **CB**[7] : c = 2mM. There were 45 injections (of 2.06 μl each).

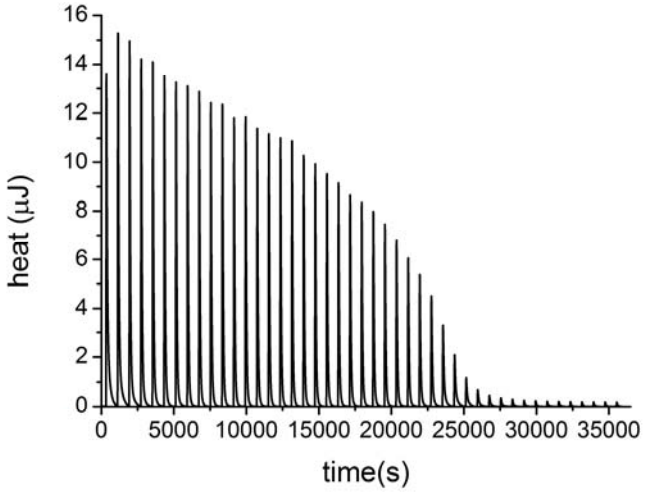


Figure S 22. Heat released in the reaction: titration of **CB**[7] water solution with water solution of complex **2**. Reaction was performed on 25°C. Interval between injections was 800 seconds: **2**: c = 20mM injected into **CB**[7] : c = 2mM. There were 45 injections (of 2.06 μl each).

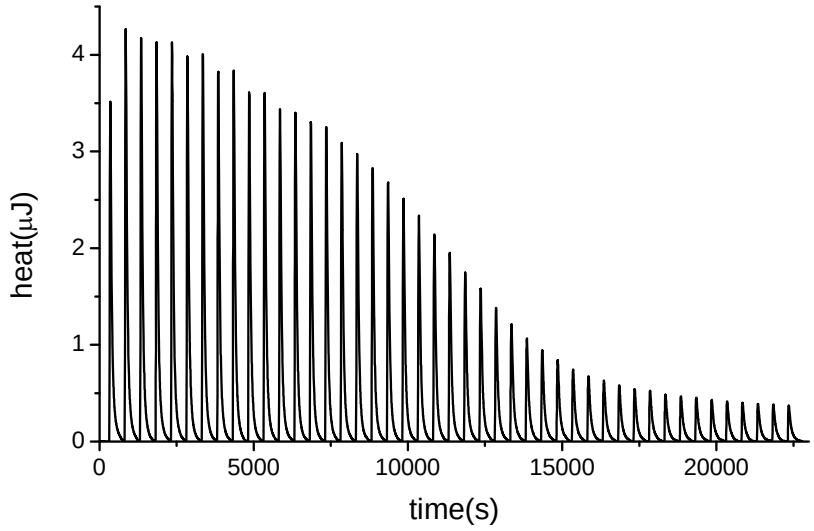


Figure S 23. Heat released in the reaction: titration of **CB**[7] water solution in TRIS buffer (0,1 M) with water solution of complex **2** in TRIS buffer. Reaction was performed on 25°C. Interval between injections was 800 seconds: **2**: c = 20mM injected into **CB**[7] : c = 2mM. There were 45 injections (of 2.06 μl each).

6. Theoretical investigations

Table S 2. Energies obtained by geometry optimization for **1**, **2** and **3**

Molecule	Symmetry	Theory level	Tot. Pauli repulsion	Electrostatic	Orbital interactions	Dispersion	Solvation	Tot. Bonding
			kcal/mol	kcal/mol	kcal/mol	kcal/mol	kcal/mol	kcal/mol
1	C_1	BLYP-D3, TZP	14396.39	-3131.26	-15033.05	-25.23	--	-3793.15
1	C_1	BLYP-D3BJ, TZP	14466.71	-3149.07	-15085.48	-47.01	--	-3814.85
1 water	C_1	BLYP-D3, TZP	14411.85	-3135.14	-15028.45	-25.16	-56.67	-3833.56
1 DMSO	C_1	BLYP-D3, TZP	14409.35	-3134.2	-15027.74	-25.16	-55.09	-3832.84
α[**1**]$_2$	C_2	BLYP, TZP	28901.03	-6286.22	-30178.69	--	--	-7563.87
α[**1**]$_2$	C_1	BLYP, QZ4P	29129.38	-6335.67	-30420.29	--	--	-7626.56
α[**1**]$_2$	C_1	BLYP-D3, TZP	29023.61	-6325.36	-30259.87	-79.69	--	-7641.3
α[**1**]$_2$	C_2	BLYP-D3, TZP	29032.46	-6327.68	-30266.44	-79.63	--	-7641.28
α[**1**]$_2$	C_2	BLYP-D3, QZ4P	29280.76	-6384.39	-30519.67	-79.91	--	-7703.21
α[**1**]$_2$ Na	C_1	BLYP-D3, TZP	29137.58	-6373.6	-30264.9	-80.04	--	-7580.96
α[**1**]$_2$ water	C_2	BLYP-D3, TZP	28998.45	-6312.37	-30234.03	-75.91	-58.87	-7682.73
α[**1**]$_2$ water	C_1	BLYP-D3, TZP	28995.74	-6311.39	-30232.19	-75.88	-58.9	-7682.61
β[**1**]$_2$	C_1	BLYP, TZP	29008.8	-6320.35	-30262.84	--	--	-7574.39
β[**1**]$_2$	C_1	BLYP-D3, TZP	29089.5	-6346.27	-30316.18	-78.86	--	-7651.82
β[**1**]$_2$	C_1	BLYP-D3BJ, TZP	29240.79	-6385.64	-30428.1	-118.87	--	-7691.83
β[**1**]$_2$	C_1	BLYP-D3, TZ2P	29241.79	-6379.61	-30474.76	-78.96	--	-7691.56
β[**1**]$_2$	C_1	BLYP-D3, QZ4P	29335.2	-6393.6h3	-30576.74	-79.21	--	-7714.38
β[**1**]$_2$ Na	C_1	BLYP-D3, TZP	29181.65	-6392.71	-30294.8	-81.22	--	-7587.07
β[**1**]$_2$ DMSO	C_1	BLYP-D3, TZP	29021.55	-6323.71	-30258.64	-77.95	-49.19	-7687.94
β[**1**]$_2$ water	C_1	BLYP-D3, TZP	29020.79	-6324.02	-30256.52	-77.9	-51.46	-7689.1
γ[**1**]$_2$	C_1	BLYP-D3, TZP	28971.08	-6307.49	-30228.52	-62.44	--	-7627.37
γ[**1**]$_2$	C_1	BLYP-D3BJ, TZP	29120.02	-6347	-30337.59	-105.59	--	-7670.15
2	C_1	BLYP-D3, TZP	14054.17	-3029.13	-14750.92	-22.8	--	-3748.68
2	C_1	BLYP-D3BJ, TZP	14116.12	-3043.84	-14798.25	-45.71	--	-3771.69
2 DMSO	C_1	BLYP-D3, TZP	14070.45	-3036.86	-14743.35	-22.75	-54.93	-3787.43
2 water	C_1	BLYP-D3, TZP	14072.04	-3037.63	-14743.07	-22.75	-57.1	-3788.52
α[**2**]$_2$	C_1	BLYP, TZP	28199.45	-6084.78	-29594.27	--	--	-7479.58
α[**2**]$_2$	C_2	BLYP, TZP	28205.25	-6086.35	-29598.45	--	--	-7479.54
α[**2**]$_2$	C_2	BLYP-D3, TZP	28332.76	-6127.11	-29683.55	-72.43	--	-7550.32
α[**2**]$_2$ Na	C_1	BLYP-D3, TZP	28435.5	-6173.86	-29678	-73.16	--	-7489.52
α[**2**]$_2$ water	C_1	BLYP-D3, TZP	28312.39	-6120.19	-29655.89	-69.29	-57.48	-7590.46
β[**2**]$_2$	C_1	BLYP, TZP	28199.45	-6084.78	-29594.27	--	--	-7479.58
β[**2**]$_2$	C_1	BLYP-D3, TZP	28384.37	-6140.49	-29731.91	-69.25	--	-7557.28
β[**2**]$_2$	C_1	BLYP-D3BJ, TZP	28534.22	-6179.72	-29842.16	-115.11	--	-7602.77
β[**2**]$_2$	C_1	BLYP-D3, TZ2P	28544.64	-6176.73	-29894.33	-69.15	--	-7595.57
β[**2**]$_2$ Na	C_1	BLYP-D3, TZP	28475.6	-6187.88	-29709.29	-71.96	--	-7493.52
β[**2**]$_2$ DMSO	C_1	BLYP-D3, TZP	28296.25	-6114.9	-29657.54	-67.34	-49.23	-7592.76
β[**2**]$_2$ water	C_1	BLYP-D3, TZP	28311.26	-6120.01	-29665.56	-68.39	-51.74	-7594.45

Table S 2. (continued)

3	C_1	BLYP-D3, TZP	12036.35	-2609.73	-12633.33	-21.99	--	-3228.7
3	C_1	BLYP-D3BJ, TZP	12097.01	-2626.44	-12677.12	-39.42	--	-3245.97
3 water	C_1	BLYP-D3, TZP	12025.6	-2610.41	-12602.81	-22.43	-57.85	-3267.9
α[**3**]$_2$	C_1	BLYP-D3, TZP	24394.7	-5308.19	-25528.87	-73.54	--	-6515.88
α[**3**]$_2$	C_1	BLYP-D3BJ, TZP	24541.02	-5343.64	-25645.02	-101.19	--	-6548.84
α[3]$_2$ Na	C_1	BLYP-D3, TZP	24404.3	-5324.36	-25456.42	-56.37	--	-6432.84
α[**3**]$_2$ water	C_1	BLYP-D3, TZP	24351.83	-5297.72	-25481.86	-74.29	-49.11	-6551.15
β[**3**]$_2$	C_s	BLYP-D3, TZP	24224.62	-5242.3	-25405.19	-53.56	--	-6479.43
β[**3**]$_2$	C_1	BLYP-D3BJ, TZP	24354.99	-5280.66	-25500.15	-87.87	--	-6513.7
γ[**3**]$_2$	C_1	BLYP-D3, TZP	24228.71	-5262.58	-25410.17	-54.69	--	-6494.38
γ[**3**]$_2$	C_1	BLYP-D3BJ, TZP	24346.01	-5294.55	-25490.92	-88.36	--	-6527.83
β[**1,2**]	C_1	BLYP-D3, TZP	28735.26	-6243.16	-30022.8	-74.23	--	-7604.94
β[**1,2**]	C_1	BLYP-D3BJ, TZP	28887.88	-6283.48	-30134.65	-117.22	--	-7647.46
β[**1,2**] water	C_1	BLYP-D3, TZP	28667.38	-6222.43	-29962.19	-73.23	-51.38	-7641.83
α,α[**1**]$_3$	C_1	BLYP-D3, TZP	43672.01	-9509.08	-45508.12	-132.93	--	-11478.12
α,α[**1**]$_3$ Na	C_1	BLYP-D3, TZP	43836.6	-9586.38	-45551.47	-134.46	--	-11435.71
α,α[**1**]$_3$ Na middle	C_1	BLYP-D3, TZP	43830.46	-9580.48	-45523.71	-136.9	--	-11410.62
α,β[**1**]$_3$	C_1	BLYP-D3, TZP	43666.73	-9518.75	-45502.2	-132.98	--	-11487.19
β,β[**1**]$_3$	C_1	BLYP-D3, TZP	43687.98	-9532.63	-45512.5	-135.88	--	-11493.02
CB[7]	C_1	BLYP-D3, TZP	87740.17	-19339.74	-87016.91	-159.26	--	-18775.61
CB[7] water	C_1	BLYP-D3, TZP	87508.92	-19253.89	-86809.05	-160.14	-201.45	-18915.67
1@CB[7]	C_1	BLYP-D3, TZP,	102540.86	-22550.67	-102382	-226.55	--	-22618.37
2@CB[7]	C_1	BLYP-D3, TZP	102201.19	-22450.9	-102099.7	-223.77	--	-22573.18

Optimized geometries

On the Figures S 24-29 are represented optimized geometries for the dimers with minima energies, with the important distances. Geometries are named as defined in main article (M.a. Figure 7). Blue dashed lines represent hydrogen bonds in these structures.

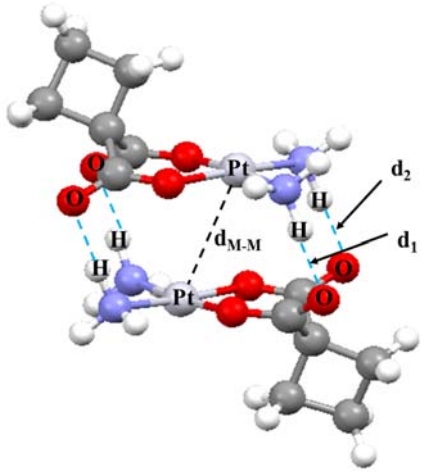


Figure S 24. $\alpha[\mathbf{3}]_2$; d_1 = 1.798 Å; d_2 = 1.805 Å; d_{MM} = 3.5 Å

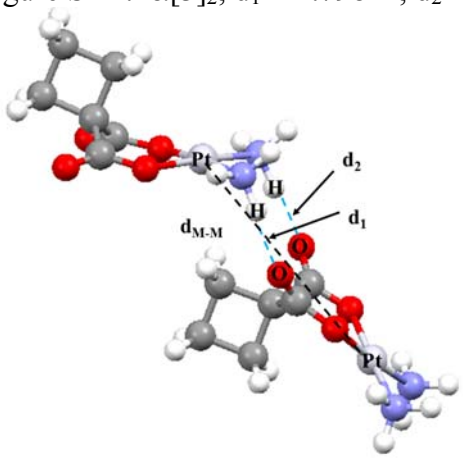


Figure S 25. $\beta[\mathbf{3}]_2$; $d_1 = d_2$ = 1.877 Å; d_{MM} = 7.238 Å

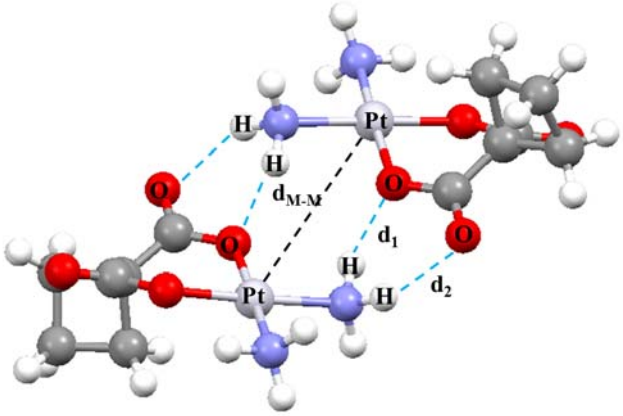


Figure S 26. $\gamma[\mathbf{3}]_2$; d_1 = 1.944 Å; d_2 = 2.134 Å; d_{MM} = 5.429 Å

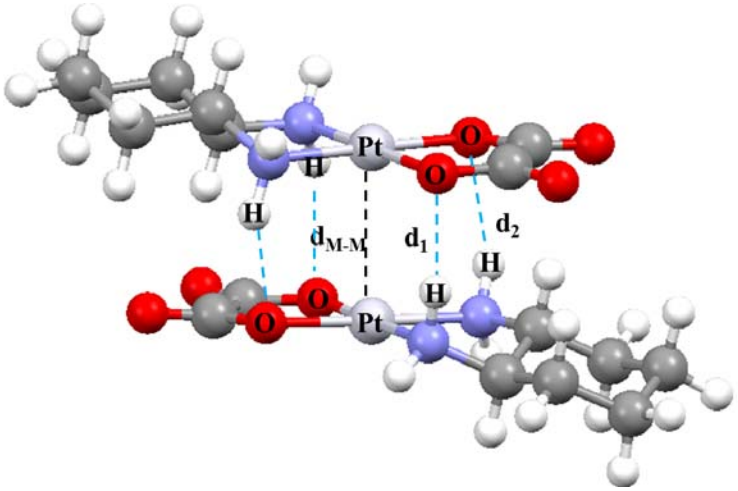


Figure S 27. $\alpha[\mathbf{1}]_2$; d_1 = 2.143Å; d_2 = 2.487 Å; d_{MM} = 3.202 Å

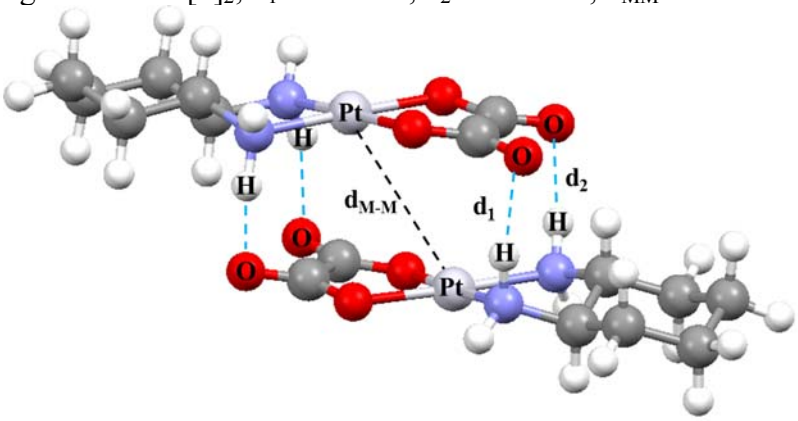


Figure S 28. $\beta[\mathbf{1}]_2$; d_1 = 1.951 Å ;d_2 = 2.016 Å; d_{MM} = 3.945 Å

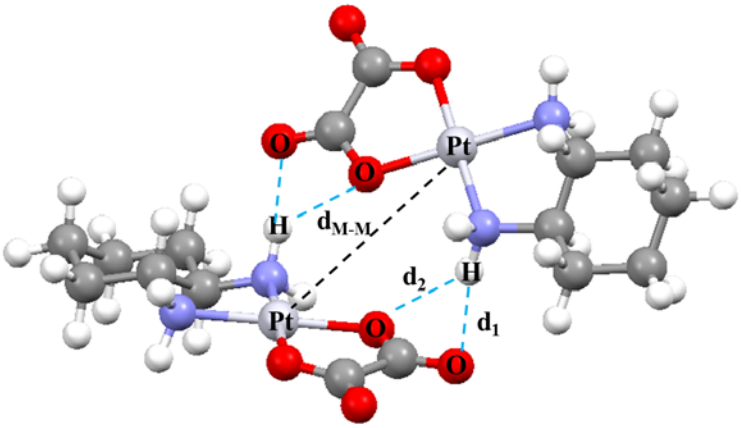


Figure S 29. $\gamma[\mathbf{1}]_2$; d_1 = 2.255 Å; d_2 = 2.298 Å; d_{MM} = 5.182 Å

BSSE

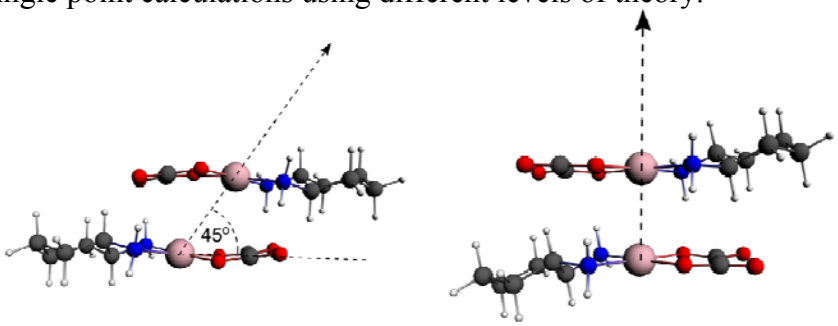
The basis set superposition error (BSSE) was calculated by re-performing all the calculations using a mixed basis sets, and the error is then subtracted a posteriori from the uncorrected energy. The mixed basis sets are realized by introducing "ghost orbitals", basis set functions which have no electrons or protons.
Calculations showed that when larger basis sets (TZ2P and QZ4P) were used changes to BSSE were very small, so we opted for more optimal TZP, for which BSSE is less than 4% of the total interaction energy for the selected cases - Table S 3. , so we decided not to calculate it for all the systems that were studied.

Table S 3. BSSE for selected systems

Molecule	BSSE	TBE(ΔE_{int})	% BSSE in TBE
	kcal/mol	kcal/mol	
α[**1**]$_2$	-2.22	-60.13	3.7
β[**1**]$_2$	-2.02	-73.41	2.7
α[**2**]$_2$	-1.72	-57.48	3.0
β[**2**]$_2$	-1.52	-67.63	2.2
1@CB[7]	-1.57	-51.71	3.0
2@CB[7]	-1.48	-50.64	3.0

6.1 Potential energy curves (PEC)

The M-M distances have been varied between 2.65 and 9 Å following the axes as defined below. Positions of the rest of the atoms in the fragments were frozen (rigid model) relative to their respective metals. For every M-M distance total bonding energies were calculated by performing single point calculations using different levels of theory.



a) b)

Figure S 30. a) M-M distance was increased following the direction of the line that goes through two metals and builds the angle of 45° with the mean plane of the oxalate ring; b) M-M distance was increased following the direction of the line that goes through two metals and is perpendicular to the mean plane of the oxalate ring.

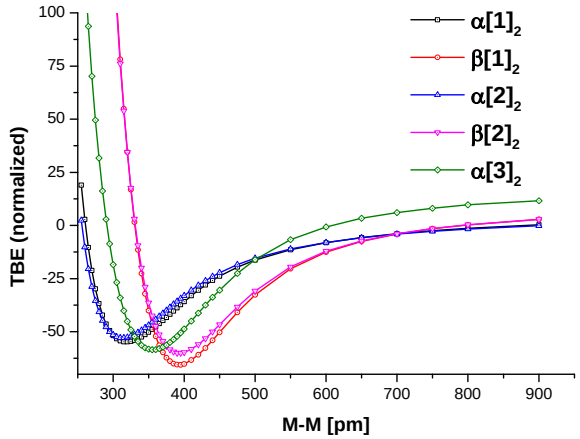


Figure S 31. PEC based on single point calculations: BLYP-D3(0) with ZORA/AE-TZP level of theory

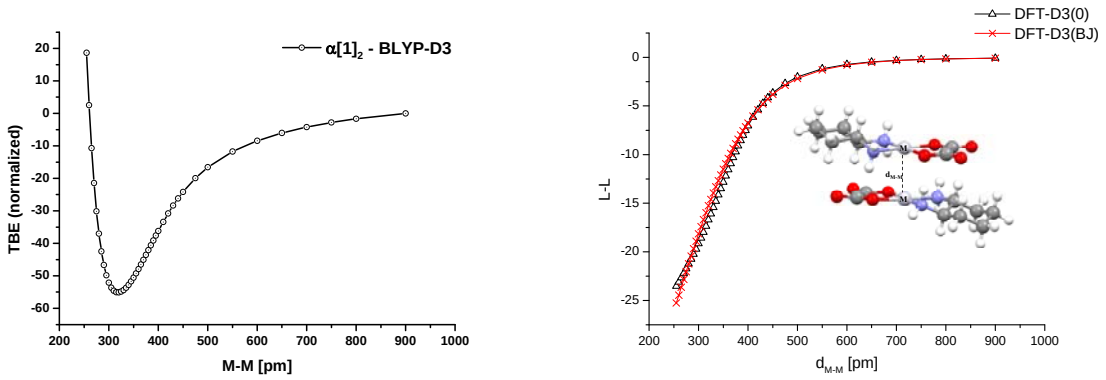


Figure S 32. PEC for $\alpha[1]_2$ without (left) and with BJ-damping (right)

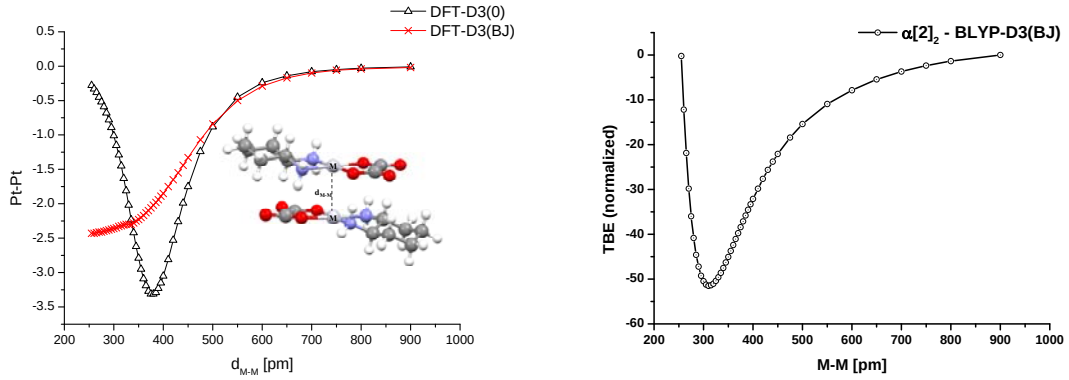


Figure S 33. PEC for $\alpha[2]_2$ without (left) and with BJ-damping (right)

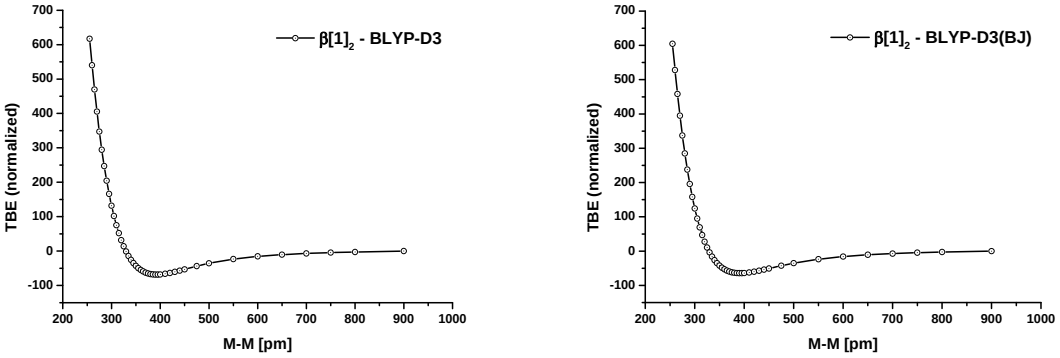


Figure S 34. PEC for $\beta[1]_2$ without (left) and with BJ-damping (right)

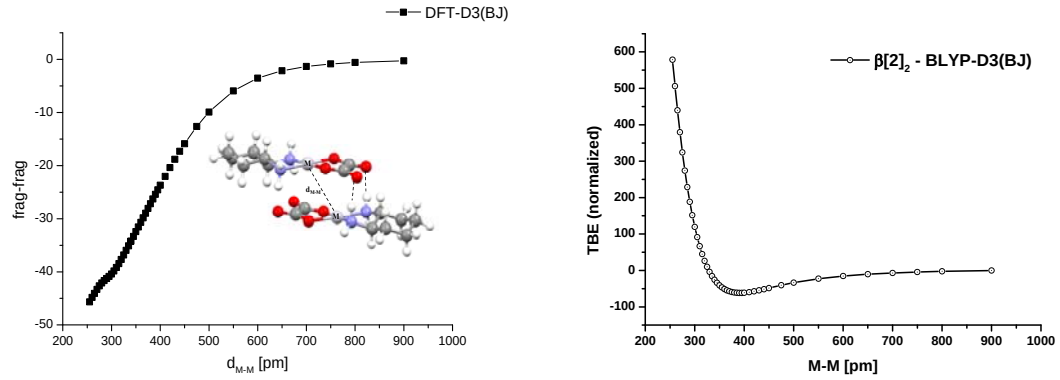


Figure S 35. PEC for $\beta[2]_2$ without (left) and with BJ-damping (right)

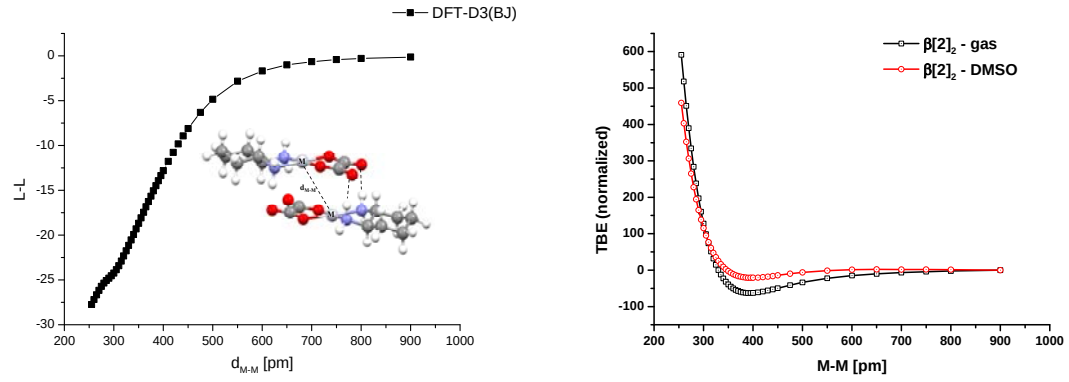
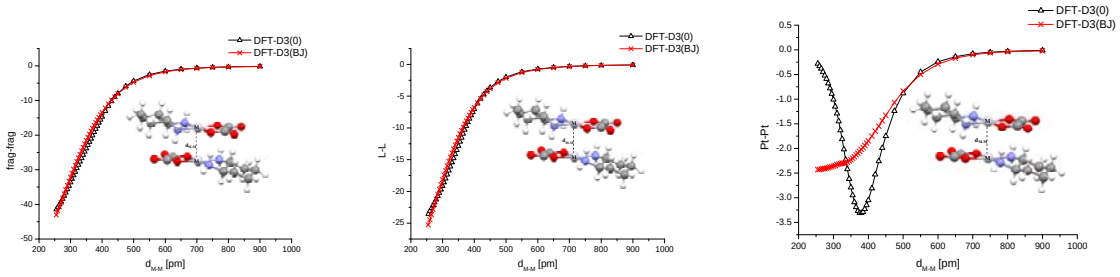


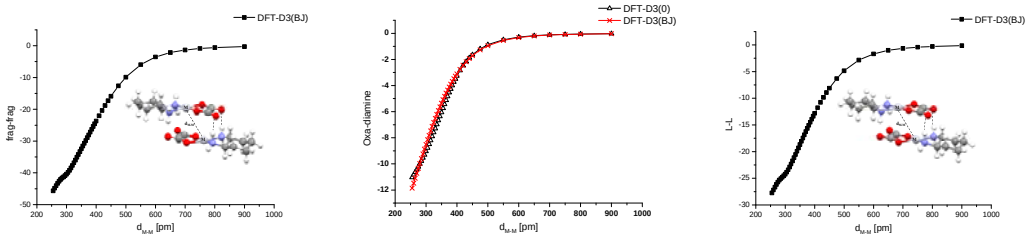
Figure S 36. PEC for $\alpha[2]_2$ (left) and for $\beta[2]_2$ (right) in gas phase and DMSO(COSMO)

6.2 Dispersion energy curves

Interfragment dispersion interaction were analyzed as such: frag-frag (contribution for the interaction between monomers), L-L (contribution between monomers without the metals) and M-M (contribution between the metals). L-L contribution to the total dispersion is ca 55%, and M-M only ca 5% in the case of α–[**1**]$_2$ and 55% (L-L); 8% (M-M) in the case of β–[**1**]$_2$. Similar results were obtained for the other complexes. On the Figure S 37.a and Figure S 38, for the sake of comparison, schematically is represented the dispersion contribution with "zero-damping" and "BJ-damping".



a)



b)

Figure S 37. DFT-D3 calculated for geometries optimized using BLYP-D3 with (ZORA)/AE-TZP level of theory. a. α[1]$_2$; b. β[1]$_2$

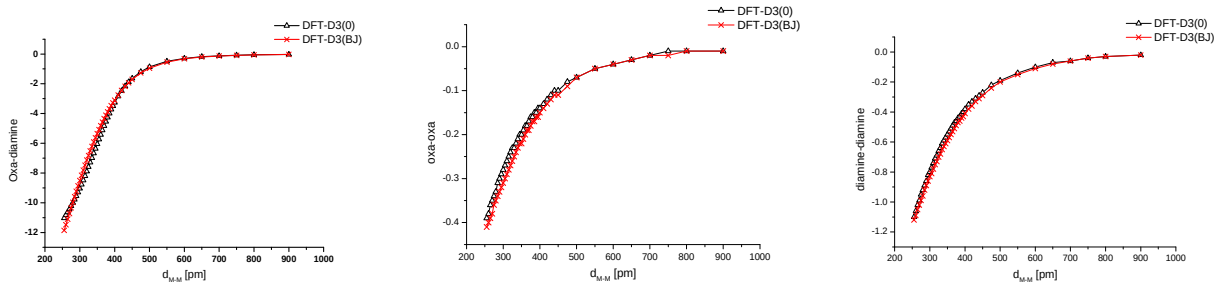


Figure S 38. Dispersion energy contribution for interactions of predefined $\alpha[1]_2$ fragments: between oxalate and diamine ligand of different fragments, between two oxalates, between two diamine ligands.

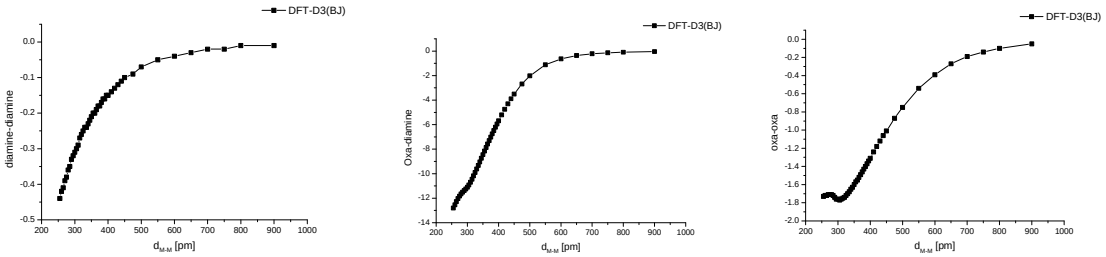


Figure S 39. Dispersion energy contribution for interactions of predefined $\beta[1]_2$ fragments: between diamine ligands, between oxalate and diamine ligand of two different fragments, between two different oxalates.

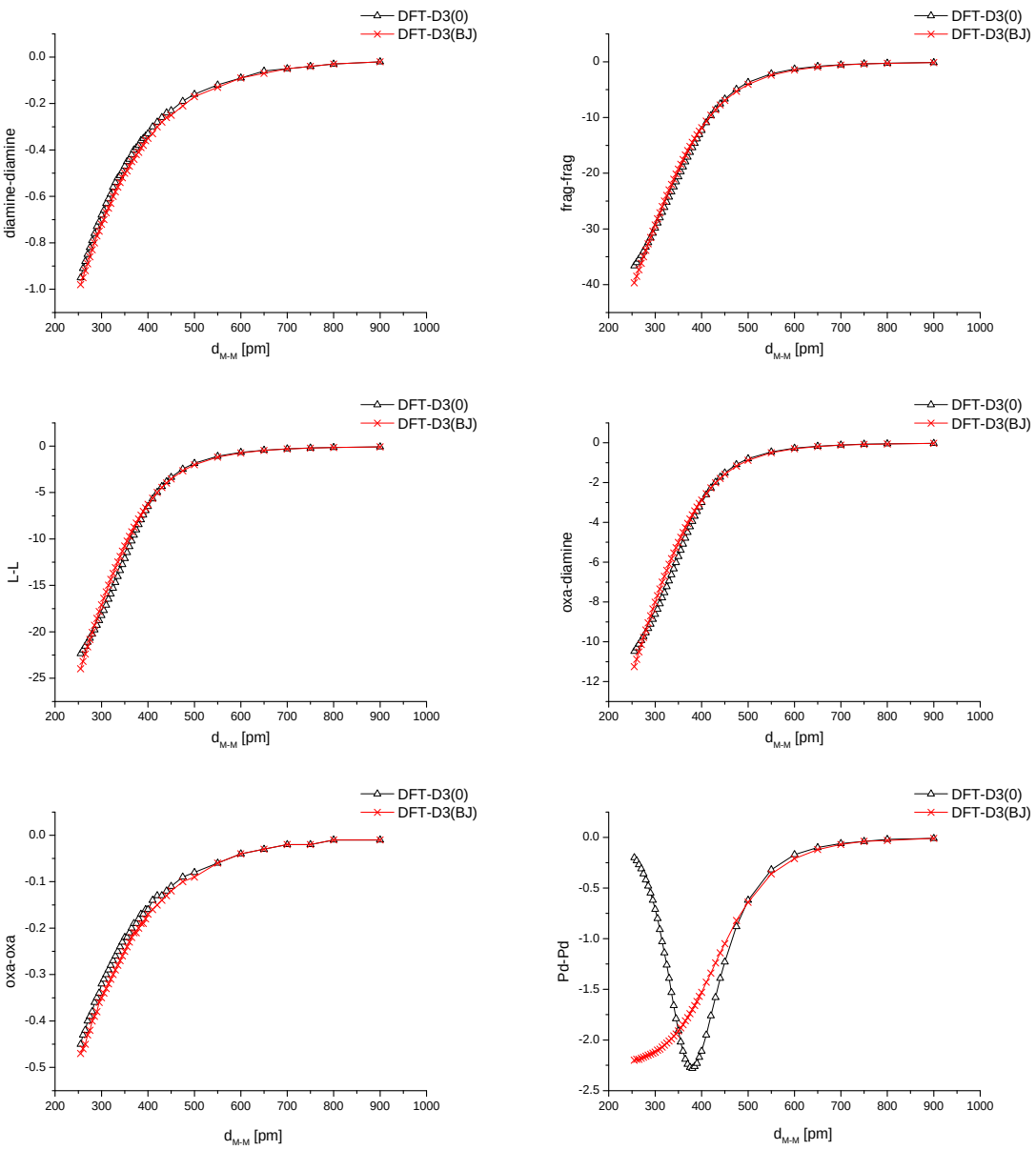


Figure S 40. Dispersion energy contribution for interactions of predefined $\alpha[2]_2$ fragments

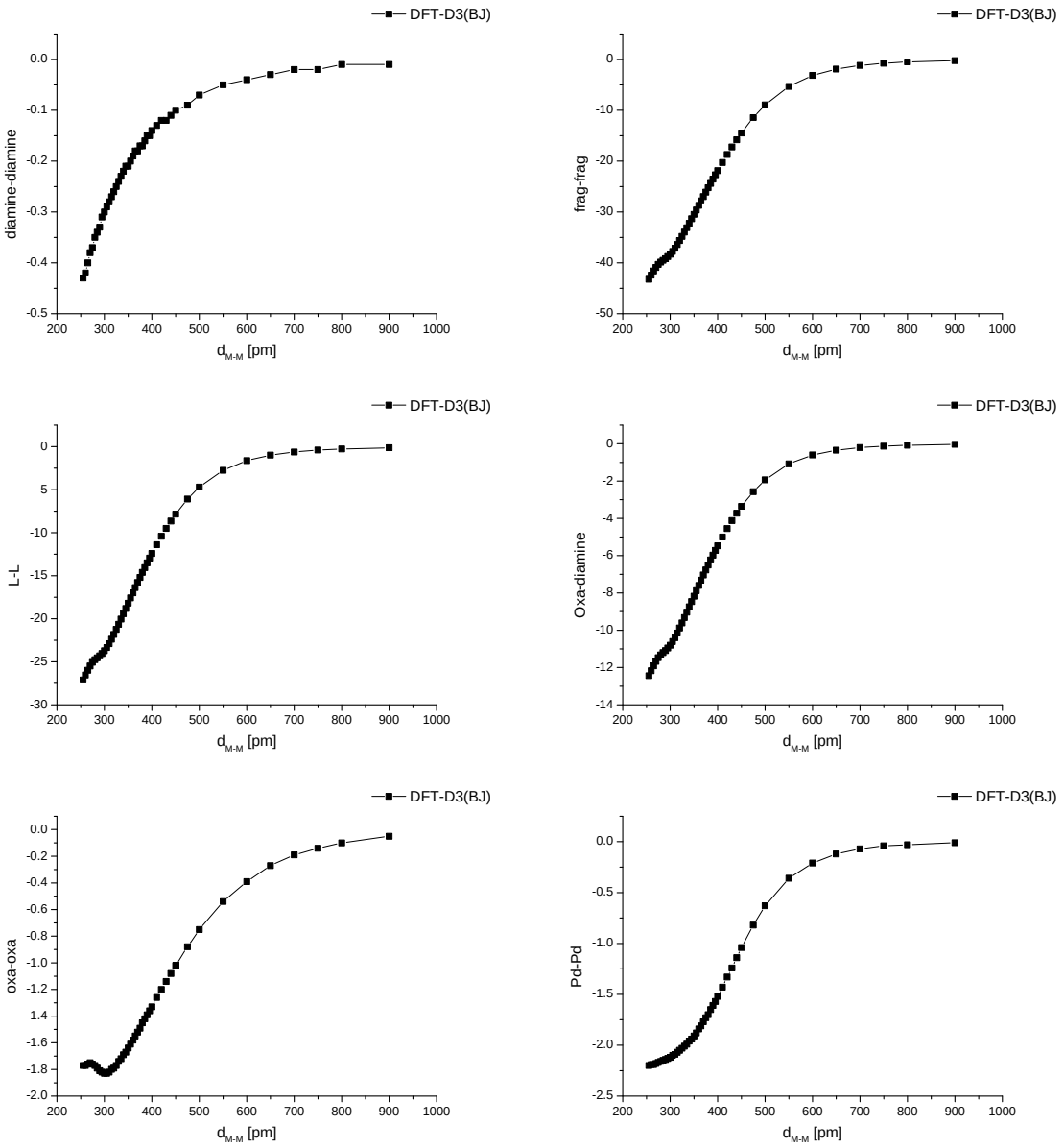


Figure S 41. Dispersion energy contribution for interactions of predefined $\beta[2]_2$ fragments

6.3 Analysis of the bonding interaction

Wiberg bond indices

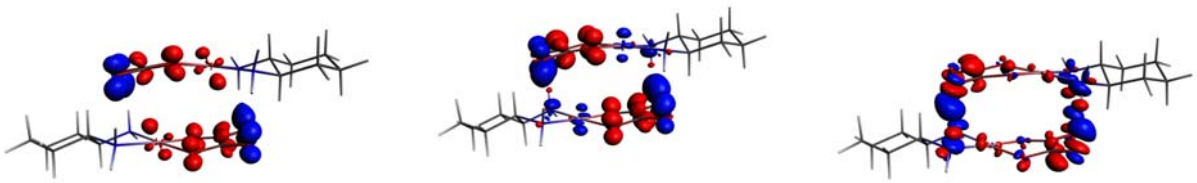
Molecules	Interacting atoms	Wiberg bond indices
α[**1**]$_2$	Pt-Pt	0.0225
β[**1**]$_2$	Pt-Pt	0.0050
α[**2**]$_2$	Pd-Pd	0.0202
β[**2**]$_2$	Pd-Pd	0.0045
α[**3**]$_2$	Pt-Pt	0.0099
β[**3**]$_2$	Pt-Pt	0.0009
β [**1,2**]	Pt-Pd	0.0055

Wiberg bond indices in all the aggregates have the low values which support the non-bonding situation within these complexes. Indices were computed from the Natural Atomic Orbital basis for the M-M segment.

NOCV analysis

The NOCV are defined as eigenvectors that diagonalize the deformation density matrix, ΔP: $\Delta P = P - P^0$, where P and P^0 correspond to the density matrices of the combined molecule and the fragments considered.
The deformation density, $\Delta\rho$ = ρ**(molecule) -** ρ^0**(fragments),** can be expressed in the NOCV representation as a sum of pairs of complementary eigenfunctions (ψ_{-k}, ψ_k) corresponding to the eigenvalues $-\nu_k$ and $+\nu_k$ with the same absolute value but opposite signs. The orbitals with negative eigenvalues exhibit "anti-bonding" character and those corresponding to positive eigenvalues are mostly "bonding".

Apart from interaction that can be related directly to H-bonding, the NOCV-ETS analysis did not reveal any significant bonding between fragments where metal orbitals would be involved (example for one of the cases is shown below).



NOCV deformation density $\Delta\rho_1$ (left up; ΔE_{orb} = -5.84 kcal/mol; ω = 15%), $\Delta\rho_2$ (right up; ΔE_{orb} = -4.07 kcal/mol; ω = 11%) and $\Delta\rho_5$(down; ΔE_{orb} = -3.58 kcal/mol; ω = 9%) for $\beta[1]_2$

ΔE_{orb} – orbital stabilization energy for corresponding deformation density
ΔE_{torb} – energy of total orbital interactions in the corresponding dimer
ω - % of ΔE_{orb} in the ΔE_{torb}

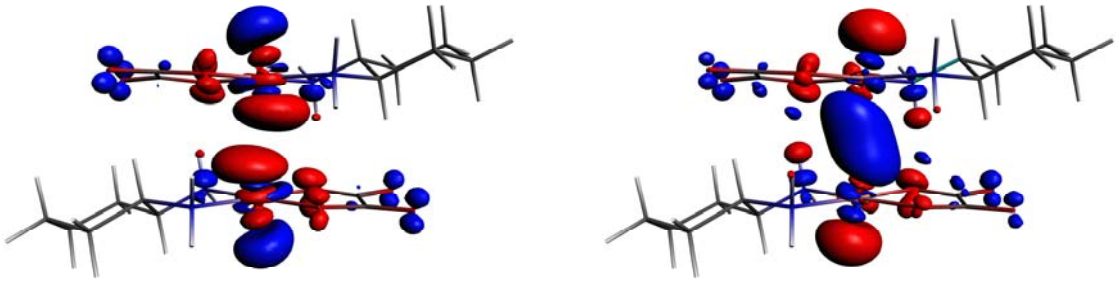


Figure S 42. NOCV deformation density $\Delta\rho_1$ (left; ΔE_{orb} = -3.76 kcal/mol; ω = 14%) and $\Delta\rho_2$(right; ΔE_{orb} = -2.94 kcal/mol; ω = 11%) for $\alpha[\mathbf{1}]_2$

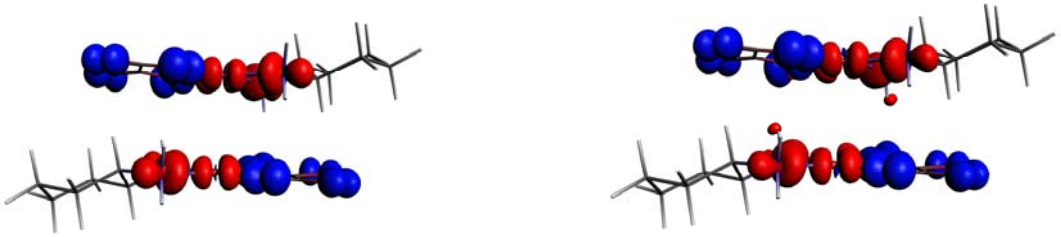


Figure S 43. NOCV deformation density $\Delta\rho_1$ (left; ΔE_{orb} = -2.45 kcal/mol; ω = 10%) and $\Delta\rho_2$ (right; ΔE_{orb} = -2.47 kcal/mol; ω = 10%) for $\alpha[\mathbf{2}]_2$

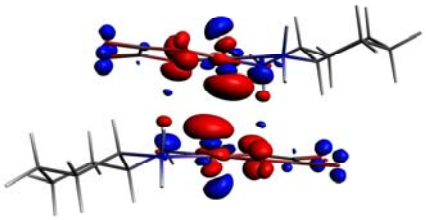


Figure S 44. NOCV deformation density $\Delta\rho_3$ (ΔE_{orb} = -2.71 kcal/mol; ω = 11%) for $\alpha[2]_2$

Figure S 45. NOCV deformation density $\Delta\rho_1$ (left; ΔE_{orb} = -4.87 kcal/mol; ω = 13%) and $\Delta\rho_3$ (right; ΔE_{orb} = -3.89 kcal/mol; ω = 10%) for $\beta[\mathbf{2}]_2$

Figure S 46. NOCV deformation density $\Delta\rho_4$ (left; ΔE_{orb} = -4.13 kcal/mol; ω = 11%) and $\Delta\rho_5$ (right; ΔE_{orb} = -3.76 kcal/mol; ω = 10%) for $\beta[\mathbf{2}]_2$

Figure S 47. NOCV deformation density $\Delta\rho_1$ (left; ΔE_{orb} = -7.63 kcal/mol; ω = 19%) and $\Delta\rho_2$(right; ΔE_{orb} = -6.18 kcal/mol; ω = 15%) for $\alpha[3]_2$

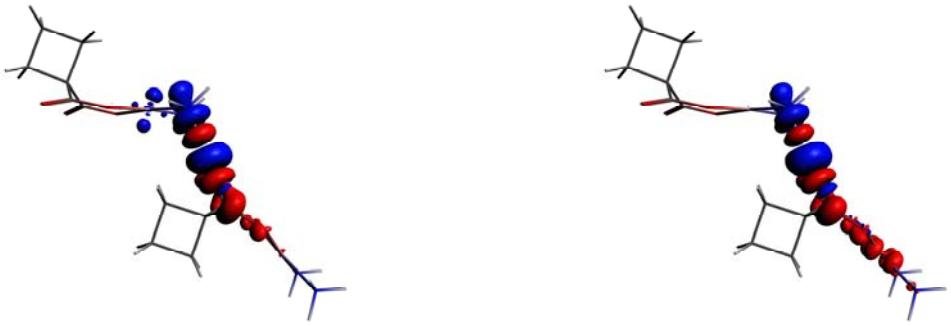


Figure S 48. NOCV deformation density $\Delta\rho_1$ (left; ΔE_{orb} = -4.50 kcal/mol; ω = 30%) and $\Delta\rho_2$(right; ΔE_{orb} = -4.19 kcal/mol; ω = 28%) for $\beta[\mathbf{3}]_2$

ELF

The electron localization function was introduced by Becke and Edgecombe[5] as a measure of the probability of finding an electron in the neighborhood of another electron with the same spin, thus being the measure of Pauli repulsion. ELF is formulated as[6]:

$ELF = [1 + [K(r)/K_h(\rho(r)]^2]^{-1}$,

Parameter K is the curvature of the electron pair density for electrons of identical spin, $\rho(r)$ the density at (r), and K_h the value of K in a homogeneous electron gas with density ρ. ELF is defined in such way to conveniently take the values between 0 and 1. Values are close to 1 when in the vicinity of one electron, no others with the same spin could be found, e.g. in bonding pairs or lone pairs. Small values of ELF are typical for the region between two electron shells. In a homogeneous electron gas ELF has everywhere the value 0.5.

Figure S 49 displays two-dimensional (2D) cross section in the plane that contains metals, and split the rest of the molecules nearly through the middle. In this 2D representation ELF values are coded in a color scale. Savin et al.[7] have shown that in the case of existence of the M-M bond, localization should be found in between metal centers. Because of the selection of the ELF cross section plane, Pauli repulsion between the metals can clearly be seen, but the hydrogen bond can't be observed (Figure S49).

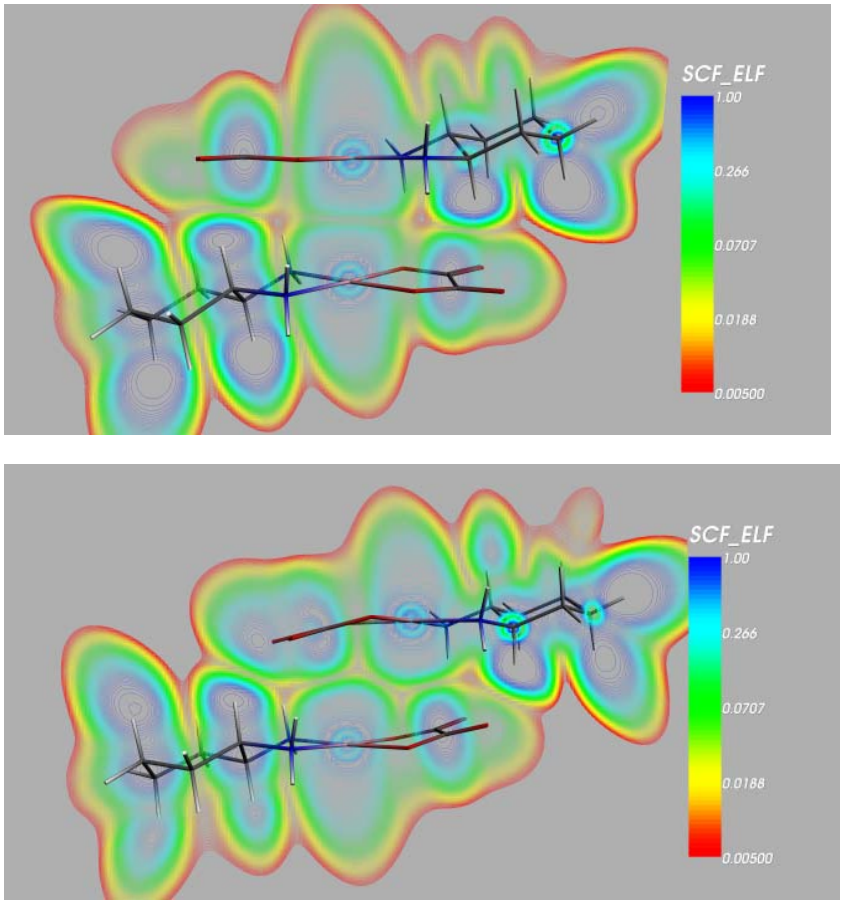


Figure S 49. ELF for $\alpha[\mathbf{1}]_2$ left and $\beta[\mathbf{1}]_2$ right

Model system used for calculations at the CCSD(T)/CBS level

The model system used for the estimation of the CCSD(T)/CBS limit was constructed in such a way as to conserve as much as possible the „original“ β[**1**]$_2$ system without the contribution of H-bonding though. The resulting model system shown on Figure S 50 retained the core of the β[**1**]$_2$ dimer, where two metals and respective chelates are interacting. CCSD(T)/CBS calculations on this model system were done on a supercomputer at Texas A&M at Qatar - the most demanding job lasted for 27 days. In the reduced model system there are no hydrogen bonds; however, interactions of metals with chelate rings are preserved; our intention was to gauge the BLYP-D3 and TPSS-D3 functionals in their ability to describe non-covalent interactions between metals and chelates without the interference of H- bonding, which are known to be rather well described otherwise by DFT functionals.

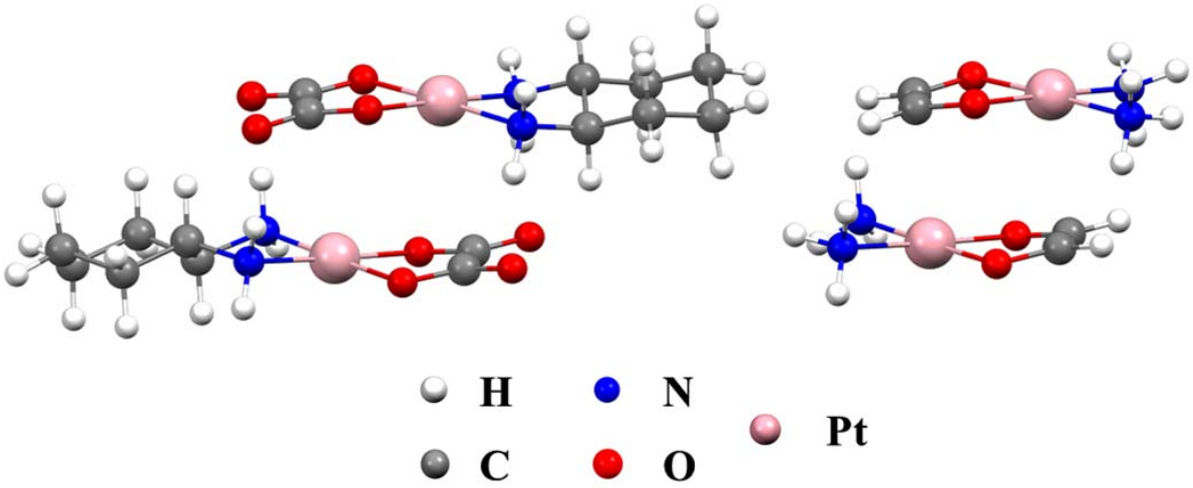


Figure S 50. β[1]$_2$ (left); model system used for calculations at the CCSD(T)/CBS level (right)

Table S 4. Interaction energies calculated for model system shown on Figure S 50.

Method	ΔE_{int} (kcal/mol)
CCSD(T)/CBS	-1
BLYP-D3(0)/TZP	-3
BLYP-D3(BJ)/TZP	-1
TPSS-D3(0)/TZP	-3
TPSS-D3(BJ)/TZP	-1

6.4 Geometry optimizations

NOTE: legend for the designations of the geometry optimization calculations

E.g. α[**1**]$_2$-DMSO-tzp-blyp-d3;C_1 Na,α[**1**]$_2$-tzp-blyp-d3;C_1

α (interaction type) **[1]$_2$** (molecule) - **DMSO** (solvent) - **tzp** (basis set) - **blyp-d3** (level of theory); **C_1** (symmetry group)
Na - sodium molecule present in the geometry

1-tzp-blyp-d3;C_1

Coordinates in Geometry Cycle 10

Atom	X	Y	Z (Angstrom)
1.Pt	-0.903170	2.475596	0.493891
2.O	-1.643211	3.836552	-0.803719
3.O	-2.720893	3.923185	-2.781027
4.N	-0.161757	3.864401	1.912838
5.H	0.683901	4.309755	1.536761
6.H	-0.839347	4.617132	2.073112
7.H	-0.907024	0.632508	2.384172
8.O	-2.657935	1.047765	-2.823773
9.C	-2.213153	3.271458	-1.882412
10.H	2.972646	1.903831	4.637103
11.H	2.143282	1.189971	6.020832
12.C	0.156100	3.151600	3.206263
13.H	-0.814297	2.971412	3.691350
14.C	1.065083	3.956853	4.151865
15.H	0.122625	0.731826	4.634849
16.C	1.983843	1.767648	5.101470
17.H	0.583154	4.912492	4.402007
18.H	2.004893	4.195088	3.626686
19.C	1.076531	0.968929	4.135153
20.H	1.545388	0.012862	3.862727
21.H	1.720549	1.962869	2.315324
22.C	1.378091	3.149856	5.434758
23.H	2.063198	3.722132	6.073105
24.H	0.449221	3.012819	6.009470
25.C	-2.179098	1.694251	-1.905688
26.O	-1.586093	1.122817	-0.842922
27.C	0.783451	1.782166	2.861820
28.N	-0.127627	1.077393	1.884620
29.H	0.374751	0.325128	1.401816

current energy		-6.04476726 Hartree	
energy change	-0.00000229	0.00100000	T
constrained gradient max	0.00088527	0.00100000	T
constrained gradient rms	0.00021721	0.00066667	T
gradient max		0.00088527	
gradient rms		0.00021721	
cart. step max	0.00117277	0.01000000	T
cart. step rms	0.00039265	0.00666667	T
GEOMETRY CONVERGED			

	hartree	eV	kcal/mol	kJ/mol
Total Pauli Repulsion:	22.942105887605482	624.2865	14396.39	60234.49
Electrostatic Energy:	-4.989986077015767	-135.7844	-3131.26	-13101.21
Total Orbital Interactions:	-23.956685280478258	-651.8946	-15033.05	-62898.27
Dispersion Energy:	-0.040200382800140	-1.0939	-25.23	-105.55
Total Bonding Energy:	-6.044770457205533	-164.4866	-3793.15	-15870.54

Frequency cm-1	Dipole Strength 1e-40 esu2 cm2	Absorption Intensity (degeneracy not counted) km/mole
21.462711	474.255674	2.551380
58.762365	3.555133	0.052364
67.869424	22.886319	0.389339
87.392104	295.177398	6.465965
124.025548	0.653378	0.020312
176.768014	4.530093	0.200719
180.006938	55.766909	2.516193
197.366383	0.028915	0.001430
225.165380	118.624092	6.695031
246.464509	20.065082	1.239577
296.368883	190.195017	14.128947
328.479125	31.876325	2.624545
332.484634	16.156027	1.346431
345.300686	14.584087	1.262277
371.588149	37.109029	3.456364
418.856179	12.843017	1.348373
429.361858	45.519767	4.898934
436.512383	202.381427	22.143450
484.638662	94.977743	11.537666
528.940266	238.374466	31.604173
533.297476	8.479892	1.133543
541.462643	1.406363	0.190873
556.865473	3.413934	0.476523
570.754887	14.542081	2.080436
650.342533	1.142125	0.186180

684.406669		44.953054	7.711724
760.666424		164.695459	31.401757
764.546052		0.058838	0.011276
782.669677		0.009039	0.001773
824.486266		52.331724	10.815000
827.107455		6.140788	1.273105
846.331605		4.263866	0.904528
854.432244		0.509624	0.109145
905.071722		6.319546	1.433663
922.849330		2.330271	0.539033
970.401650		350.416709	85.234301
1010.730854		136.349204	34.543489
1018.568735		6.126614	1.564188
1023.535896		5.637431	1.446313
1036.648437		36.488158	9.481161
1047.277622		26.473668	6.949507
1076.227812		44.298566	11.950111
1095.670857		8.554087	2.349264
1104.999423		154.203601	42.710498
1116.787788		0.741290	0.207509
1150.396900		4.579670	1.320566
1182.863057		14.238382	4.221562
1212.127943		1491.997102	453.309179
1224.700247		10.395805	3.191288
1258.428145		8.262492	2.606259
1289.433129		2.157688	0.697374
1304.719402		2.707318	0.885390
1332.850983		10.218151	3.413752
1334.778816		6.778683	2.267946
1338.898782		7.228514	2.425911
1350.468935		9.461154	3.202630
1351.847876		4.884697	1.655173
1369.066419		0.415463	0.142572
1390.522810		24.443913	8.519751
1460.535741		2.502494	0.916143
1462.385257		8.710948	3.193047
1467.271428		24.273894	8.927461
1477.087521		8.267652	3.061022
1610.449124		121.918773	49.214793
1613.080687		4.030189	1.629520
1672.455153		287.099231	120.355123
1682.438871		1699.155352	716.556519
2920.859530		28.445446	20.825790
2922.449587		0.582091	0.426399
2933.924486		16.743766	12.313461
2940.607946		32.008577	23.592913
2949.809193		0.745431	0.551162
2962.943760		17.566084	13.045972
2979.710529		0.693077	0.517647
2982.534837		50.687908	37.893783
2992.478878		54.629505	40.976648
2994.657667		36.744690	27.581625
3325.092594		6.976248	5.814384
3326.590709		9.385832	7.826187
3392.951685		22.068209	18.768209
3393.835457	31.821918	27.070433	

Zero-Point Energy :	0.228817	a.u.
========== 6.226437 eV		

Statistical Thermal Analysis *** ideal gas assumed ***				
Temp	Transl	Rotat	Vibrat	Total
----	------	-----	------	-----
298.15 Entropy (cal/mole-K):	43.828	32.839	48.398	125.066
Internal Energy (Kcal/mole):	0.889	0.889	151.161	152.938
Constant Volume Heat Capacity (cal/mole-K):	2.981	2.981	51.443	57.405

1-tzp-blyp-d3bj;C_1

```
 Coordinates       in       Geometry       Cycle       27
   Atom          X           Y           Z   (Angstrom)
   1.Pt          -0.022457     -0.047279     -0.002725
   2.O           -1.572504      0.351393     -1.237868
   3.O           -3.753279      0.907601     -1.136985
   4.N            1.421805     -0.391565     -1.505254
   5.H            1.241955     -1.303264     -1.940730
   6.H            1.342266      0.310208     -2.247320
   7.H            1.922407      0.429989      1.699184
   8.O           -3.550376      0.783751      1.721529
   9.C           -2.706745      0.628227     -0.573684
  10.H            5.001484     -2.713373      0.181592
  11.H            6.166598     -1.549323      0.812442
  12.C            2.798252     -0.366343     -0.894132
  13.H            3.027650      0.695158     -0.725011
  14.C            3.881776     -0.993655     -1.784693
  15.H            4.339133      0.029545      1.413666
  16.C            5.197750     -1.637762      0.305748
  17.H            3.926824     -0.460183     -2.744099
  18.H            3.601953     -2.036706     -2.005372
  19.C            4.091232     -1.020871      1.189847
  20.H            4.023810     -1.549758      2.150460
  21.H            2.435635     -2.114215      0.312639
  22.C            5.256549     -0.963611     -1.080710
  23.H            6.005429     -1.457548     -1.711990
  24.H            5.578971      0.082222     -0.965454
  25.C           -2.594191      0.567167      0.993923
  26.O           -1.374039      0.261325      1.465206
  27.C            2.731211     -1.068384      0.476689
  28.N            1.611209     -0.448570      1.269142
  29.H          1.323591   -1.065521    2.034967
```

```
E-test:          old,new=          -6.07935,          -6.07936     hartree
max    gradient:                         0.00066758    au/angstrom,radian
max      cart.      step:                        0.00147163      angstrom
Geometry Converged
```

	hartree	eV	kcal/mol	kJ/mol
Total Pauli Repulsion:	23.054168318443239	627.3358	14466.71	60528.71
Electrostatic Energy:	-5.018365838747616	-136.5567	-3149.07	-13175.72
Total Orbital Interactions:	-24.040242627996580	-654.1683	-15085.48	-63117.65
Dispersion Energy:	-0.074913750620457	-2.0385	-47.01	-196.69
Total Bonding Energy:	-6.079357739331448	-165.4277	-3814.85	-15961.35

1-water-tzp-blyp-d3;C_1

Coordinates	in	Geometry	Cycle	7
Atom	X	Y	Z	(Angstrom)
1.Pt	-0.894659	2.474102	0.523351	
2.O	-1.646114	3.837500	-0.837141	
3.O	-2.742409	3.907165	-2.806023	
4.N	-0.153139	3.839561	1.914079	
5.H	0.702480	4.268291	1.540139	
6.H	-0.810281	4.608723	2.080711	
7.H	-0.918143	0.669940	2.409368	
8.O	-2.654335	1.067093	-2.864652	
9.C	-2.212299	3.271082	-1.885852	
10.H	2.972033	1.900874	4.635387	
11.H	2.138629	1.189789	6.021902	
12.C	0.160268	3.142153	3.222417	
13.H	-0.809752	2.966890	3.706566	
14.C	1.066982	3.962290	4.151779	
15.H	0.121377	0.727387	4.633896	
16.C	1.983806	1.766690	5.101187	
17.H	0.577973	4.913354	4.401501	
18.H	2.003348	4.198216	3.621398	
19.C	1.076271	0.962388	4.137243	
20.H	1.548618	0.010932	3.858719	
21.H	1.726304	1.964397	2.324662	
22.C	1.380664	3.151081	5.433360	
23.H	2.070412	3.723012	6.067182	
24.H	0.452051	3.016220	6.008818	
25.C	-2.178476	1.695630	-1.910338	
26.O	-1.619223	1.120855	-0.862488	
27.C	0.792095	1.789115	2.874704	
28.N	-0.137748	1.099460	1.896919	
29.H	0.356621	0.330835	1.432144	

```
E-test:          old,new=          -6.10931,          -6.10916     hartree
max    gradient:                          0.00098084    au/angstrom,radian
max      cart.      step:                        0.00079543      angstrom
Geometry Converged
```

	hartree	eV	kcal/mol	kJ/mol
Total Pauli Repulsion:	22.966745467875434	624.9569	14411.85	60299.18
Electrostatic Energy:	-4.996156296927075	-135.9523	-3135.14	-13117.41
Total Orbital Interactions:	-23.949354198945777	-651.6951	-15028.45	-62879.02
Solvation:	-0.090304150948753	-2.4573	-56.67	-237.09
Dispersion Energy:	-0.040091150768103	-1.0909	-25.16	-105.26
Total Bonding Energy:	-6.109161180067348	-166.2387	-3833.56	-16039.60

Frequency	Dipole Strength	Absorption Intensity (degeneracy not counted)	
cm-1	1e-40 esu2 cm2		km/mole
-19.284967	2750.367692		-13.294981
48.316816	0.756397		0.009161
65.514849	85.792927		1.408865
76.139264	1106.411057		21.115591
120.859872	0.692783		0.020987
176.734708	2.927407		0.129683
185.468917	105.030537		4.882753
190.494381	419.187950		20.015619
214.718242	419.376277		22.571004
249.965675	108.948781		6.826229
280.225597	802.565059		56.372348
323.574758	42.653584		3.459459
334.423594	67.282222		5.639951
336.858446	69.218227		5.844481
343.298051	120.038451		10.329274
425.907667	45.225012		4.828055
432.173263	46.998493		5.091197
435.868149	529.691508		57.870364
486.685713	87.630848		10.690147
509.795766	362.160264		46.278055
549.436096	9.047688		1.246043
559.928081	34.268784		4.809601
560.932518	135.247425		19.015935
578.467151	47.591437		6.900580
674.221668	4.439570		0.750277
716.027504	219.193774		39.340148
754.948668	518.129622		98.046911
770.929309	1.535342		0.296686
795.206210	0.002332		0.000465

821.014851		25.564760	5.261030
839.973799		59.956040	12.623412
842.357570		20.795728	4.390851
858.451731		1.575507	0.339011
897.418283		39.759868	8.943714
919.136323		6.806226	1.568066
964.597874		349.008579	84.384071
1012.561315		5.900189	1.497495
1025.093773		139.883833	35.942575
1027.062654		4.999924	1.287177
1035.676500		21.387110	5.552062
1058.958415		33.391687	8.863298
1109.005879		25.271936	7.025066
1126.427964		0.810176	0.228750
1136.430811		262.514646	74.778131
1161.815615		202.803869	59.059738
1180.029787		20.199361	5.974598
1184.504842		5.543324	1.645831
1222.522131		3.017643	0.924704
1242.900066		5.427323	1.690830
1260.288488		2826.946592	893.029166
1282.313580		8.001228	2.571751
1299.745992		2.220485	0.723410
1324.089728		0.657263	0.218140
1324.809777		1.219296	0.404893
1332.670636		11.784712	3.936587
1342.304961		10.948740	3.683778
1350.770013		0.648175	0.219458
1365.516882		0.213618	0.073116
1385.993084		49.966320	17.358672
1443.578144		3.491898	1.263514
1444.273008		25.340852	9.173785
1444.897705		61.730329	22.357012
1455.298029		6.747325	2.461284
1563.155643		358.325100	140.396902
1565.225214		44.777256	17.567598
1584.724385		587.762479	233.471390
1592.573120		4638.852452	1851.774122
2929.856066		43.741713	32.123299
2930.971809		2.433398	1.787734
2934.511440		30.938514	22.756912
2938.140438		81.646024	60.129232
2966.690208		0.701810	0.521879
2978.173503		36.507544	27.252772
2987.617555		65.361224	48.946681
2988.948570		47.149316	35.324165
2990.043964		17.981029	13.476285
2993.813768		102.462546	76.889670
3330.080056		33.390821	27.871468
3332.118657		133.178656	111.232873
3399.033352		109.793326	93.542600
3400.347888	130.962881	111.621959	

Zero-Point Energy :	0.228559	a.u.
==========	6.219397	eV
(imaginary frequencies were excluded from the summation)		

Statistical Thermal Analysis *** ideal gas assumed ***

Temp		Transl	Rotat	Vibrat	Total
298.15	Entropy (cal/mole-K):	43.828	32.837	42.826	119.492
	Internal Energy (Kcal/mole):	0.889	0.889	150.478	152.256
	Constant Volume Heat Capacity (cal/mole-K):	2.981	2.981	49.309	55.271

1-DMSO-tzp-blyp-d3;C_1

Coordinates in Geometry Cycle 16				
Atom	X	Y	Z	(Angstrom)
1.Pt	0.006210	0.025175	0.000485	
2.O	1.412671	-0.343552	1.467540	
3.O	3.580786	-0.914672	1.700947	
4.N	-1.619136	0.407011	1.253630	
5.H	-1.941724	-0.476095	1.667685	
6.H	-1.358984	1.014279	2.038056	
7.H	-1.247141	1.333686	-1.880738	
8.O	3.794538	-0.930204	-1.136723	
9.C	2.604319	-0.649611	0.988781	
10.H	-5.566575	-0.140733	-0.987348	
11.H	-6.012709	1.401482	-1.725237	
12.C	-2.753151	1.040045	0.471713	
13.H	-2.464417	2.089462	0.324055	
14.C	-4.107384	0.967275	1.193119	
15.H	-3.611771	2.014855	-2.005948	
16.C	-5.260592	0.911205	-1.094037	
17.H	-4.044493	1.496588	2.153310	
18.H	-4.340671	-0.087345	1.409095	
19.C	-3.882093	0.967357	-1.798187	
20.H	-3.912061	0.435276	-2.758464	
21.H	-3.023322	-0.722012	-0.740516	
22.C	-5.217028	1.577144	0.300538	
23.H	-6.187289	1.470156	0.802190	
24.H	-5.032550	2.656029	0.184282	
25.C	2.722507	-0.658843	-0.581977	
26.O	1.615323	-0.360598	-1.237056	
27.C	-2.808573	0.344068	-0.893927	
28.N	-1.413312	0.401237	-1.482504	
29.H	-1.338534	-0.260960	-2.261972	

E-test:	old,new=	-6.10801,	-6.10801 hartree
max gradient:		0.00098278	au/angstrom,radian
max cart. step:		0.00334202	angstrom
Geometry Converged			

	hartree	eV	kcal/mol	kJ/mol
Total Pauli Repulsion:	22.962758842260719	624.8485	14409.35	60288.71
Electrostatic Energy:	-4.994662688561360	-135.9117	-3134.20	-13113.49
Total Orbital Interactions:	-23.948228978431921	-651.6645	-15027.74	-62876.07
Solvation:	-0.087798697918370	-2.3891	-55.09	-230.52
Dispersion Energy:	-0.040094353008416	-1.0910	-25.16	-105.27
Total Bonding Energy:	-6.108026252214991	-166.2079	-3832.84	-16036.62

Frequency	Dipole Strength	Absorption Intensity (degeneracy not counted)
cm-1	1e-40 esu2 cm2	km/mole
15.001960	0.000000	0.000000
51.273569	0.818192	0.010515
66.239449	93.715225	1.555983
79.773687	1138.866491	22.772491
121.251619	1.853685	0.056338
176.215984	6.325300	0.279386
187.021084	128.273619	6.013205
189.887785	367.556967	17.494428
216.219246	436.954416	23.681464
249.508463	112.188375	7.016349
280.725944	785.389445	55.264428
322.989939	41.056541	3.323911
335.141082	62.744401	5.270851
336.238625	61.469143	5.180633
344.125710	115.745185	9.983852
425.322598	42.686755	4.550820
432.068517	51.145834	5.539122
436.064180	526.630149	57.561778
486.116045	92.645676	11.288680
511.399226	363.286574	46.567989
548.894292	11.798325	1.623256
559.201671	122.948012	17.233284
560.055440	31.219775	4.382671
577.812052	45.633827	6.609240
674.862293	5.598123	0.946969
716.580630	209.928890	37.706424
755.566853	507.210129	96.059182
771.376225	1.346548	0.260355
794.920642	0.045216	0.009009

821.294820		22.521223	4.636274
840.489727		61.407227	12.936892
842.506287		18.304811	3.865596
858.410147		2.910395	0.626217
897.795449		38.550725	8.675370
919.122326		5.402417	1.244628
963.833143		351.304403	84.871821
1012.442258		5.956883	1.511706
1025.416412		133.754732	34.378545
1027.117607		6.508424	1.675615
1035.268434		25.194671	6.537922
1060.166630		29.766117	7.909962
1109.237500		27.227044	7.570126
1128.620829		0.508071	0.143731
1137.249284		260.791407	74.340764
1159.494033		195.899908	56.935196
1180.701085		8.384217	2.481307
1185.918467		3.866481	1.149341
1223.209577		2.978267	0.913151
1243.558849		7.678154	2.393322
1258.768445		2811.200175	886.983802
1282.819548		6.085404	1.956740
1299.983931		2.634989	0.858608
1324.447701		0.408600	0.135647
1324.816326		0.967193	0.321179
1332.904710		14.080582	4.704330
1342.439547		10.302082	3.466553
1351.013093		0.596239	0.201910
1366.436123		0.317658	0.108800
1386.296656		52.154391	18.122793
1444.627858		3.591413	1.300467
1445.600850		19.290525	6.989893
1446.155944		65.282137	23.663967
1456.659675		7.253011	2.648223
1565.290708		358.889481	140.810100
1567.479807		47.273408	18.573636
1587.712361		593.002609	235.997010
1596.597178		4523.985152	1810.483614
2931.052832		29.721040	21.835630
2931.834108		19.282681	14.170491
2934.616034		28.598199	21.036236
2938.377005		78.886732	58.101796
2966.090281		0.701223	0.521337
2977.843609		34.663483	25.873319
2988.146555		58.706528	43.971002
2988.884545		51.598160	38.656402
2989.892091		20.240408	15.168856
2994.319637		101.030804	75.828076
3331.232189		16.368539	13.667620
3332.273216		150.320921	125.556182
3397.855517		215.390138	183.446230
3399.303833		20.628940	17.577008
1340.327733		34.237397	11.502436
1345.257980		24.695221	8.327153
1350.227076		12.440001	4.210225
1350.647494		4.525937	1.532246
1354.666996		6.085571	2.066388
1370.110170		4.137779	1.421022
1373.355445		3.914513	1.347531
1387.396232		14.924150	5.190010
1388.154781		34.942621	12.158260
1408.827696		16.144028	5.700958
1459.259469		7.348281	2.687796
1462.442104		2.637050	0.966663
1464.147659		7.994453	2.933943
1464.156800		11.267068	4.135010
1467.960590		27.169580	9.997131
1468.685600		23.213653	8.545754
1477.967881		20.910913	7.746688
1478.783521		11.813446	4.378842
1534.313790		363.071306	139.631751
1550.701716		444.101560	172.619016
1558.979099		2113.296203	825.807334
1577.756739		1035.654093	409.574434
1603.148708		165.876595	66.655654
1613.452547		236.024540	95.453405
1616.143079		47.891999	19.400854
1624.677906		1270.328562	517.322547
2898.508991		43.935900	31.920688
2914.765754		24.623165	17.989770
2917.551918		19.520641	14.275481
2928.968094		14.375943	10.554291
2933.362058		23.074439	16.965821
2941.481257	10.183107	7.508004	
2945.266326		24.535020	18.112945
2947.441926		24.802816	18.324170
2949.720431		18.128015	13.403221
2959.402538		4.880107	3.620024
2972.505030		15.189496	11.317332
2985.436650		44.661991	33.421352
2985.778911		2.562945	1.918117

2988.717804		5.566434	4.170038
2990.719314		29.728731	22.285896
2996.092693		46.709247	35.078109
2996.820185		35.187756	26.432018
2998.683979		27.274462	20.500524
2999.395528		31.318115	23.545473
3009.976155		6.373524	4.808623
3126.521773		258.264669	202.397212
3242.122825		123.372678	100.259729
3269.372646		68.730014	56.323408
3312.596538		15.578615	12.935269
3361.266148		60.324317	50.824532
3380.687597		43.336708	36.723074
3381.536855		47.605073	40.350176
3390.386737	45.307622	38.503356	

Zero-Point Energy : 0.228672 a.u.
========== 6.222486 eV

Statistical Thermal Analysis *** ideal gas assumed ***

Temp		Transl	Rotat	Vibrat	Total
298.15	Entropy (cal/mole-K):	43.828	32.838	42.572	119.238
	Internal Energy (Kcal/mole):	0.889	0.889	150.516	152.294
	Constant Volume Heat Capacity (cal/mole-K):	2.981	2.981	49.293	55.255

α[**1**]$_2$-tzp-blyp;C_2

```
   Coordinates      in      Geometry      Cycle      47
   Atom          X           Y           Z   (Angstrom)
   1.Pt          -0.628196    -1.638476      0.144872
   2.O            0.696173    -2.220897      1.590060
   3.O            2.843758    -2.874220      1.816797
   4.N           -2.281565    -1.340199      1.412448
   5.H           -2.515912    -2.229779      1.866768
   6.H           -2.027845    -0.681238      2.156561
   7.H           -1.895543    -0.037461     -1.498115
   8.O            3.128687    -2.608762     -1.008347
   9.C            1.893311    -2.548912      1.111930
  10.H           -6.088300    -2.184363     -1.028795
  11.H           -6.727026    -0.642527     -1.599992
  12.C           -3.481443    -0.805618      0.647876
  13.H           -3.363777     0.283725      0.623365
  14.C           -4.828806    -1.137433      1.312242
  15.H           -4.430650     0.320951     -1.748163
  16.C           -5.923196    -1.095008     -1.005154
  17.H           -4.859737    -0.699744      2.319929
  18.H           -4.922642    -2.231365      1.423611
  19.C           -4.554808    -0.768465     -1.655741
  20.H           -4.503983    -1.196427     -2.668072
  21.H           -3.486535    -2.437213     -0.767915
  22.C           -5.999026    -0.593260      0.455292
  23.H           -6.952981    -0.891391      0.909992
  24.H           -5.967880     0.505661      0.467294
  25.C            2.056627    -2.397692     -0.448446
  26.O            0.983356    -1.928173     -1.092026
  27.C           -3.412105    -1.339812     -0.795223
  28.N           -2.022478    -1.047662     -1.317239
  29.H           -1.867208    -1.537738     -2.203349
  30.Pt           0.628196     1.638476      0.144872
  31.O           -0.983356     1.928173     -1.092026
  32.O           -3.128687     2.608762     -1.008347
  33.N            2.022478     1.047662     -1.317239
  34.H            1.895543     0.037461     -1.498115
  35.H            1.867208     1.537738     -2.203349
  36.H            2.515912     2.229779      1.866768
  37.O           -2.843758     2.874220      1.816797
  38.C           -2.056627     2.397692     -0.448446
  39.H            5.967880    -0.505661      0.467294
  40.H            6.952981     0.891391      0.909992
  41.C            3.412105     1.339812     -0.795223
  42.H            3.486535     2.437213     -0.767915
  43.C            4.554808     0.768465     -1.655741
  44.H            4.922642     2.231365      1.423611
  45.C            5.999026     0.593260      0.455292
  46.H            4.503983     1.196427     -2.668072
  47.H            4.430650    -0.320951     -1.748163
  48.C            4.828806     1.137433      1.312242
  49.H            4.859737     0.699744      2.319929
  50.H            3.363777    -0.283725      0.623365
  51.C            5.923196     1.095008     -1.005154
  52.H            6.727026     0.642527     -1.599992
  53.H            6.088300     2.184363     -1.028795
  54.C           -1.893311     2.548912      1.111930
  55.O           -0.696173     2.220897      1.590060
  56.C            3.481443     0.805618      0.647876
  57.N            2.281565     1.340199      1.412448
  58.H         2.027845    0.681238    2.156561
```

```
E-test:            old,new=      -12.05373,      -12.05375      hartree
max    gradient:                        0.00096109    au/angstrom,radian
max      cart.      step:                        0.00784647      angstrom
Geometry Converged
```

	hartree	eV	kcal/mol	kJ/mol
Total Pauli Repulsion:	46.056719339993933	1253.2671	28901.03	120921.90
Electrostatic Energy:	-10.017733888820132	-272.5964	-6286.22	-26301.56
Total Orbital Interactions:	-48.092801919315171	-1308.6717	-30178.69	-126267.63
Total Bonding Energy:	-12.053787142282193	-328.0002	-7563.87	-31647.21

α[**1**]$_2$-tzp-blyp;C_1

```
 Coordinates       in       Geometry       Cycle      93
   Atom          X            Y            Z    (Angstrom)
   1.Pt          -0.688589     -1.722114      0.145531
   2.O            0.601008     -2.346963      1.601033
   3.O            2.793128     -2.796925      1.895898
   4.N           -2.378506     -1.522443      1.380902
   5.H           -2.640811     -2.448290      1.738061
   6.H           -2.145426     -0.944902      2.195833
   7.H           -1.902963     -0.048959     -1.463772
   8.O            3.149606     -2.445095     -0.910188
   9.C            1.842275     -2.533698      1.165537
  10.H           -6.151249     -2.112426     -1.175740
  11.H           -6.729992     -0.524944     -1.682916
  12.C           -3.542903     -0.900429      0.626948
  13.H           -3.387201      0.184060      0.670358
  14.C           -4.916152     -1.226495      1.239827
  15.H           -4.406731      0.374363     -1.735475
  16.C           -5.953934     -1.031273     -1.094504
  17.H           -4.960160     -0.844973      2.269790
  18.H           -5.046412     -2.321438      1.287730
  19.C           -4.562671     -0.713434     -1.698235
  20.H           -4.499396     -1.095517     -2.728133
  21.H           -3.550346     -2.450079     -0.876038
  22.C           -6.047768     -0.599872      0.387104
  23.H           -7.021328     -0.887331      0.805730
  24.H           -5.980046      0.495357      0.454669
  25.C            2.047782     -2.319333     -0.381026
  26.O            0.970374     -1.902503     -1.050818
  27.C           -3.453358     -1.354217     -0.842847
  28.N           -2.046589     -1.063249     -1.320307
  29.H           -1.878393     -1.522998     -2.220230
  30.Pt           0.687707      1.717285      0.145760
  31.O           -0.972441      1.897411     -1.048926
  32.O           -3.148417      2.453646     -0.910086
  33.N            2.047207      1.060609     -1.320417
  34.H            1.907049      0.045989     -1.464257
  35.H            1.877845      1.519877     -2.220283
  36.H            2.636268      2.442111      1.743579
  37.O           -2.788633      2.813968      1.894641
  38.C           -2.047401      2.323104     -0.380435
  39.H            5.988328     -0.482369      0.452954
  40.H            7.022794      0.905038      0.805728
  41.C            3.452693      1.356518     -0.842296
  42.H            3.545008      2.452786     -0.873933
  43.C            4.565057      0.721959     -1.698427
  44.H            5.040848      2.328858      1.289127
  45.C            6.050642      0.613302      0.386718
  46.H            4.499847      1.104992     -2.727901
  47.H            4.414362     -0.366535     -1.736996
  48.C            4.915954      1.233301      1.240191
  49.H            4.961928      0.850990      2.269726
  50.H            3.393704     -0.184049      0.669328
  51.C            5.954625      1.046116     -1.094251
  52.H            6.733431      0.544858     -1.683388
  53.H            6.146178      2.128454     -1.173985
  54.C           -1.840146      2.540814      1.165102
  55.O           -0.600473      2.344160      1.601226
  56.C            3.544099      0.901229      0.627117
  57.N            2.377071      1.517108      1.382116
  58.H          2.144324    0.935379    2.194152
```

```
E-test:            old,new=      -12.05498,      -12.05500      hartree
max    gradient:                       0.00089072    au/angstrom,radian
max      cart.      step:                        0.00776654      angstrom
Geometry Converged
```

	hartree	eV	kcal/mol	kJ/mol
Total Pauli Repulsion:	46.060746364157865	1253.3767	28903.56	120932.47
Electrostatic Interaction:	-10.015817672842791	-272.5443	-6285.02	-26296.53
Total Orbital Interactions:	-48.099972164370982	-1308.8668	-30183.19	-126286.46
Total Bonding Energy:	-12.055016188153258	-328.0337	-7564.64	-31650.44

α[**1**]$_2$-tzp-blyp-d3;C$_1$

Coordinates	in	Geometry	Cycle	7
Atom	X	Y	Z	(Angstrom)
1.Pt	-0.518867	-1.514435	0.137891	
2.O	0.861859	-1.960592	1.588343	
3.O	2.994646	-2.664093	1.795604	
4.N	-2.119620	-1.055090	1.421812	
5.H	-2.337920	-1.863253	2.014624	
6.H	-1.829959	-0.284996	2.039167	
7.H	-1.813266	-0.030415	-1.565567	
8.O	3.193914	-2.620626	-1.051044	
9.C	2.025231	-2.385212	1.097492	
10.H	-6.019849	-2.034046	-0.872809	
11.H	-6.628616	-0.511650	-1.527796	
12.C	-3.350394	-0.621119	0.642950	
13.H	-3.258464	0.458121	0.515630	
14.C	-4.676564	-0.889613	1.365961	
15.H	-4.304208	0.369390	-1.773300	
16.C	-5.824536	-0.950728	-0.923410	
17.H	-4.664973	-0.392215	2.345321	
18.H	-4.792856	-1.973394	1.537942	
19.C	-4.463383	-0.709086	-1.623122	
20.H	-4.446186	-1.192996	-2.610794	
21.H	-3.419134	-2.354785	-0.651391	
22.C	-5.847768	-0.355592	0.503632	
23.H	-6.802253	-0.584185	0.995351	
24.H	-5.766709	0.739362	0.444639	
25.C	2.137984	-2.364077	-0.482298	
26.O	1.052560	-1.923776	-1.124466	
27.C	-3.321659	-1.263940	-0.753414	
28.N	-1.940648	-1.028327	-1.325610	
29.H	-1.814911	-1.570534	-2.185978	
30.Pt	0.518867	1.514435	0.137891	
31.O	-1.052560	1.923776	-1.124466	
32.O	-3.193914	2.620626	-1.051044	
33.N	1.940648	1.028327	-1.325610	
34.H	1.813266	0.030415	-1.565567	
35.H	1.814911	1.570534	-2.185978	
36.H	2.337920	1.863253	2.014624	
37.O	-2.994646	2.664093	1.795604	
38.C	-2.137984	2.364077	-0.482298	
39.H	5.766709	-0.739362	0.444639	
40.H	6.802253	0.584185	0.995351	
41.C	3.321659	1.263940	-0.753414	
42.H	3.419134	2.354785	-0.651391	
43.C	4.463383	0.709086	-1.623122	
44.H	4.792856	1.973394	1.537942	
45.C	5.847768	0.355592	0.503632	
46.H	4.446186	1.192996	-2.610794	
47.H	4.304208	-0.369390	-1.773300	
48.C	4.676564	0.889613	1.365961	
49.H	4.664973	0.392215	2.345321	
50.H	3.258464	-0.458121	0.515630	
51.C	5.824536	0.950728	-0.923410	
52.H	6.628616	0.511650	-1.527796	
53.H	6.019849	2.034046	-0.872809	
54.C	-2.025231	2.385212	1.097492	
55.O	-0.861859	1.960592	1.588343	
56.C	3.350394	0.621119	0.642950	
57.N	2.119620	1.055090	1.421812	
58.H	1.829959	0.284996	2.039167	

```
E-test:            old,new=      -12.17713,      -12.17715      hartree
max    gradient:                        0.00083134    au/angstrom,radian
max      cart.      step:                         0.00588312      angstrom
Geometry Converged
```

	hartree	eV	kcal/mol	kJ/mol
Total Pauli Repulsion:	46.266171084374179	1258.9666	29032.46	121471.81
Electrostatic Energy:	-10.083802075960831	-274.3942	-6327.68	-26475.02
Total Orbital Interactions:	-48.232631764867598	-1312.4767	-30266.44	-126634.76
Dispersion Energy:	-0.126893385203091	-3.4529	-79.63	-333.16
Total Bonding Energy:	-12.177159486897814	-331.3574	-7641.28	-31971.13

α[**1**]$_2$-tzp-blyp-d3bj;C_1

```
 Coordinates       in       Geometry       Cycle      12
   Atom          X            Y            Z    (Angstrom)
   1.Pt          -0.523385     -1.484172      0.137777
   2.O            0.850868     -1.941380      1.588605
   3.O            2.967364     -2.690239      1.792076
   4.N           -2.120942     -1.043410      1.419568
   5.H           -2.329737     -1.856710      2.007435
   6.H           -1.835314     -0.273001      2.037279
   7.H           -1.812415      0.002306     -1.549429
   8.O            3.177284     -2.618259     -1.043900
   9.C            2.005238     -2.384019      1.095520
  10.H           -5.993775     -2.068147     -0.886755
  11.H           -6.623320     -0.549444     -1.529587
  12.C           -3.351968     -0.621523      0.642111
  13.H           -3.279486      0.460315      0.523515
  14.C           -4.672211     -0.919962      1.359608
  15.H           -4.315823      0.366357     -1.765483
  16.C           -5.814479     -0.982212     -0.927861
  17.H           -4.672662     -0.431016      2.342787
  18.H           -4.768779     -2.006740      1.521636
  19.C           -4.457691     -0.714648     -1.621684
  20.H           -4.432821     -1.192889     -2.611455
  21.H           -3.391789     -2.347278     -0.657683
  22.C           -5.849900     -0.400703      0.501983
  23.H           -6.800489     -0.650658      0.989895
  24.H           -5.788316      0.695447      0.452426
  25.C            2.122125     -2.352881     -0.477782
  26.O            1.045597     -1.897160     -1.121986
  27.C           -3.310642     -1.255420     -0.754826
  28.N           -1.936607     -0.999367     -1.321805
  29.H           -1.800423     -1.535286     -2.183382
  30.Pt           0.523370      1.483821      0.138124
  31.O           -1.045796      1.896124     -1.121719
  32.O           -3.177103      2.618366     -1.043957
  33.N            1.936402      0.998984     -1.321531
  34.H            1.812446     -0.002680     -1.549233
  35.H            1.799960      1.534924     -2.183060
  36.H            2.329702      1.857429      2.007509
  37.O           -2.967062      2.691577      1.791976
  38.C           -2.122054      2.352783     -0.477735
  39.H            5.788279     -0.694430      0.452898
  40.H            6.800649      0.651832      0.989590
  41.C            3.310437      1.255450     -0.754748
  42.H            3.391325      2.347366     -0.657903
  43.C            4.457437      0.714770     -1.621672
  44.H            4.768763      2.008376      1.520671
  45.C            5.849968      0.401741      0.501942
  46.H            4.432320      1.192895     -2.611486
  47.H            4.315703     -0.366276     -1.765320
  48.C            4.672423      0.921459      1.359479
  49.H            4.673202      0.433236      2.343024
  50.H            3.280053     -0.459858      0.524412
  51.C            5.814332      0.982619     -0.928152
  52.H            6.623082      0.549608     -1.529820
  53.H            5.993636      2.068571     -0.887505
  54.C           -2.005092      2.384619      1.095551
  55.O           -0.850909      1.941578      1.588800
  56.C            3.352119      0.622061      0.642438
  57.N            2.121063      1.043878      1.419932
  58.H          1.835713    0.273596    2.037921
```

```
E-test:            old,new=      -12.24369,      -12.24370      hartree
max    gradient:                        0.00065030    au/angstrom,radian
max      cart.      step:                        0.00580382      angstrom
Geometry Converged
```

	hartree	eV	kcal/mol	kJ/mol
Total Pauli Repulsion:	46.510268854434827	1265.6088	29185.64	122112.69
Electrostatic Interaction:	-10.150561537802254	-276.2108	-6369.57	-26650.30
Total Orbital Interactions:	-48.409293565191618	-1317.2839	-30377.29	-127098.58
Dispersion Energy:	-0.194104826464562	-5.2819	-121.80	-509.62
Total Bonding Energy:	-12.243696314773567	-333.1679	-7683.04	-32145.82

α[**1**]$_2$-qz4p-blyp;C_1

Coordinates in Geometry Cycle 63

Atom	X	Y	Z (Angstrom)
1.Pt	-0.654563	-1.682386	0.143824
2.O	0.669375	-2.276022	1.568939
3.O	2.838741	-2.828559	1.803006
4.N	-2.304466	-1.435074	1.412231
5.H	-2.553853	-2.342729	1.816778
6.H	-2.053438	-0.823575	2.194171
7.H	-1.902137	-0.076284	-1.505146
8.O	3.123813	-2.488610	-1.016504
9.C	1.883810	-2.534395	1.099803
10.H	-6.130236	-2.118048	-1.038047
11.H	-6.721927	-0.550635	-1.579429
12.C	-3.487650	-0.847975	0.662542
13.H	-3.338390	0.236465	0.664553
14.C	-4.843349	-1.155993	1.316480
15.H	-4.404853	0.347352	-1.711953
16.C	-5.932854	-1.036380	-0.994011
17.H	-4.864199	-0.742731	2.332870
18.H	-4.969011	-2.247003	1.403499
19.C	-4.558237	-0.737180	-1.637456
20.H	-4.518312	-1.147173	-2.655625
21.H	-3.529944	-2.446843	-0.784904
22.C	-5.994279	-0.560114	0.472303
23.H	-6.955660	-0.836788	0.920526
24.H	-5.931104	0.535434	0.505539
25.C	2.046891	-2.342146	-0.454866
26.O	0.956641	-1.909562	-1.087750
27.C	-3.431524	-1.351975	-0.790259
28.N	-2.037893	-1.079972	-1.311001
29.H	-1.886559	-1.578645	-2.191141
30.Pt	0.654563	1.682386	0.143824
31.O	-0.956641	1.909562	-1.087750
32.O	-3.123813	2.488610	-1.016504
33.N	2.037893	1.079972	-1.311001
34.H	1.902137	0.076284	-1.505146
35.H	1.886559	1.578645	-2.191141
36.H	2.553853	2.342729	1.816778
37.O	-2.838741	2.828559	1.803006
38.C	-2.046891	2.342146	-0.454866
39.H	5.931104	-0.535434	0.505539
40.H	6.955660	0.836788	0.920526
41.C	3.431524	1.351975	-0.790259
42.H	3.529944	2.446843	-0.784904
43.C	4.558237	0.737180	-1.637456
44.H	4.969011	2.247003	1.403499
45.C	5.994279	0.560114	0.472303
46.H	4.518312	1.147173	-2.655625
47.H	4.404853	-0.347352	-1.711953
48.C	4.843349	1.155993	1.316480
49.H	4.864199	0.742731	2.332870
50.H	3.338390	-0.236465	0.664553
51.C	5.932854	1.036380	-0.994011
52.H	6.721927	0.550635	-1.579429
53.H	6.130236	2.118048	-1.038047
54.C	-1.883810	2.534395	1.099803
55.O	-0.669375	2.276022	1.568939
56.C	3.487650	0.847975	0.662542
57.N	2.304466	1.435074	1.412231
58.H	2.053438	0.823575	2.194171

```
E-test:            old,new=      -12.11282,      -12.11344      hartree
max    gradient:                        0.00099644    au/angstrom,radian
max      cart.      step:                        0.00360737      angstrom
Geometry Converged
```

	hartree	eV	kcal/mol	kJ/mol
Total Pauli Repulsion:	46.420616378069880	1263.1692	29129.38	121877.31
Electrostatic Energy:	-10.096535154119872	-274.7407	-6335.67	-26508.45
Total Orbital Interactions:	-48.477805002962405	-1319.1482	-30420.29	-127278.46
Total Bonding Energy:	-12.153689628768248	-330.7187	-7626.56	-31909.51

$\alpha[\mathbf{1}]_2$-qz4p-blyp-d3;C_2

Coordinates in Geometry Cycle 11

Atom	X	Y	Z (Angstrom)
1.Pt	-0.536431	-1.503873	0.137695
2.O	0.838316	-1.944024	1.578971
3.O	2.965178	-2.641090	1.796556
4.N	-2.130543	-1.067215	1.422909
5.H	-2.344982	-1.884624	2.001240
6.H	-1.847592	-0.309406	2.054522
7.H	-1.825243	-0.045726	-1.586105
8.O	3.174932	-2.554379	-1.052561
9.C	2.003358	-2.364200	1.096447
10.H	-6.021511	-2.041542	-0.880493
11.H	-6.629772	-0.519080	-1.526690
12.C	-3.358655	-0.630578	0.644313
13.H	-3.267707	0.448044	0.523018
14.C	-4.683531	-0.906682	1.361993
15.H	-4.309299	0.363885	-1.765991
16.C	-5.827088	-0.959497	-0.924406
17.H	-4.675532	-0.418002	2.343744
18.H	-4.796149	-1.989754	1.527336
19.C	-4.467141	-0.713001	-1.619266
20.H	-4.447443	-1.191117	-2.607615
21.H	-3.426410	-2.359172	-0.651336
22.C	-5.854108	-0.373128	0.503324
23.H	-6.806467	-0.608847	0.991608
24.H	-5.780194	0.721007	0.451475
25.C	2.119199	-2.327861	-0.481051
26.O	1.028934	-1.896711	-1.113611
27.C	-3.328076	-1.269364	-0.751805
28.N	-1.948943	-1.036306	-1.326148
29.H	-1.819938	-1.592212	-2.175222
30.Pt	0.536431	1.503873	0.137695
31.O	-1.028934	1.896711	-1.113611
32.O	-3.174932	2.554379	-1.052561
33.N	1.948943	1.036306	-1.326148
34.H	1.825243	0.045726	-1.586105
35.H	1.819938	1.592212	-2.175222
36.H	2.344982	1.884624	2.001240
37.O	-2.965178	2.641090	1.796556
38.C	-2.119199	2.327861	-0.481051
39.H	5.780194	-0.721007	0.451475
40.H	6.806467	0.608847	0.991608
41.C	3.328076	1.269364	-0.751805
42.H	3.426410	2.359172	-0.651336
43.C	4.467141	0.713001	-1.619266
44.H	4.796149	1.989754	1.527336
45.C	5.854108	0.373128	0.503324
46.H	4.447443	1.191117	-2.607615
47.H	4.309299	-0.363885	-1.765991
48.C	4.683531	0.906682	1.361993
49.H	4.675532	0.418002	2.343744
50.H	3.267707	-0.448044	0.523018
51.C	5.827088	0.959497	-0.924406
52.H	6.629772	0.519080	-1.526690
53.H	6.021511	2.041542	-0.880493
54.C	-2.003358	2.364200	1.096447
55.O	-0.838316	1.944024	1.578971
56.C	3.358655	0.630578	0.644313
57.N	2.130543	1.067215	1.422909
58.H	1.847592	0.309406	2.054522

```
E-test:            old,new=      -12.23498,      -12.23473      hartree
max    gradient:                        0.00095761    au/angstrom,radian
max      cart.      step:                       0.00163027      angstrom
Geometry Converged
```

	hartree	eV	kcal/mol	kJ/mol
Total Pauli Repulsion:	46.661862168382783	1269.7339	29280.76	122510.70
Electrostatic Energy:	-10.174170154476958	-276.8533	-6384.39	-26712.28
Total Orbital Interactions:	-48.636190702391232	-1323.4581	-30519.67	-127694.30
Dispersion Energy:	-0.127347500266592	-3.4653	-79.91	-334.35
Total Bonding Energy:	-12.275850580169845	-334.0429	-7703.21	-32230.24

Na,α[**1**]$_2$-tzp-blyp-d3;C$_1$

Coordinates in Geometry Cycle 100

Atom	X	Y	Z	(Angstrom)
1.Pt	-0.730406	-1.435683	0.150095	
2.O	0.682796	-1.890456	1.612989	
3.O	2.773644	-2.725741	1.793927	
4.N	-2.362637	-1.110368	1.407029	
5.H	-2.521761	-1.954596	1.969455	
6.H	-2.168310	-0.341099	2.063816	
7.H	-2.110620	-0.061096	-1.589827	
8.O	3.005969	-2.619807	-0.990950	
9.C	1.793064	-2.337695	1.117005	
10.H	-6.164506	-2.340563	-0.951702	
11.H	-6.854774	-0.848434	-1.592809	
12.C	-3.623812	-0.759399	0.617368	
13.H	-3.607147	0.325466	0.500724	
14.C	-4.926224	-1.137921	1.329484	
15.H	-4.586391	0.176096	-1.800129	
16.C	-6.036034	-1.247372	-0.981746	
17.H	-4.960999	-0.649402	2.312494	
18.H	-4.967060	-2.228466	1.489658	
19.C	-4.683215	-0.910800	-1.662315	
20.H	-4.620724	-1.385260	-2.652114	
21.H	-3.547638	-2.491956	-0.683049	
22.C	-6.120845	-0.677563	0.453893	
23.H	-7.061679	-0.982852	0.927692	
24.H	-6.121036	0.421002	0.413445	
25.C	1.922427	-2.290254	-0.454956	
26.O	0.898806	-1.820891	-1.101945	
27.C	-3.527777	-1.396124	-0.772704	
28.N	-2.148432	-1.057215	-1.320160	
29.H	-1.963734	-1.601636	-2.169454	
30.Pt	0.727360	1.608798	0.128767	
31.O	-0.867481	1.928885	-1.109141	
32.O	-3.104337	2.101229	-0.985722	
33.N	2.143170	1.162442	-1.358600	
34.H	2.011619	0.182407	-1.648211	
35.H	2.013770	1.740374	-2.195595	
36.H	2.591481	2.116367	1.905691	
37.O	-2.867249	2.080238	1.855646	
38.C	-2.004658	2.085169	-0.436861	
39.H	6.007107	-0.624891	0.406387	
40.H	7.018737	0.714714	0.946427	
41.C	3.526207	1.373288	-0.783803	
42.H	3.639660	2.462238	-0.685696	
43.C	4.660290	0.807612	-1.654202	
44.H	5.016640	2.083452	1.492144	
45.C	6.064873	0.475665	0.461012	
46.H	4.634847	1.277197	-2.647196	
47.H	4.495139	-0.272437	-1.798016	
48.C	4.894585	1.000667	1.327588	
49.H	4.891541	0.519624	2.315738	
50.H	3.403015	-0.332605	0.517360	
51.C	6.026903	1.057460	-0.970570	
52.H	6.831159	0.626791	-1.579485	
53.H	6.213378	2.140901	-0.923703	
54.C	-1.871020	2.086283	1.136904	
55.O	-0.633699	1.971583	1.602662	
56.C	3.551845	0.747494	0.625113	
57.N	2.355470	1.249522	1.408330	
58.H	2.086721	0.560426	2.120920	
59.Na	4.436175	-3.549400	0.505485	

```
E-test:            old,new=      -12.08090,      -12.08095      hartree
max    gradient:                        0.00090188    au/angstrom,radian
max      cart.      step:                       0.01000000      angstrom
Geometry Converged
```

	hartree	eV	kcal/mol	kJ/mol
Total Pauli Repulsion:	46.433687345637942	1263.5249	29137.58	121911.63
Electrostatic Energy:	-10.156982635781103	-276.3856	-6373.60	-26667.15
Total Orbital Interactions:	-48.230182911364778	-1312.4101	-30264.90	-126628.33
Dispersion Energy:	-0.127557987593029	-3.4710	-80.04	-334.90
Total Bonding Energy:	-12.081032602863843	-328.7416	-7580.96	-31718.75

Frequency	Dipole Strength	Absorption Intensity (degeneracy not counted)
cm-1	1e-40 esu2 cm2	km/mole
-26.596603	153.335464	-1.022226
13.389601	0.000000	0.000000
18.938635	0.000000	0.000000
36.600967	536.184918	4.919095
46.153723	4.364312	0.050489
52.787893	119.409399	1.579978
58.799586	52.613747	0.775446
61.644445	123.045307	1.901241
65.240638	24.446704	0.399776
79.382427	148.835257	2.961476
86.051618	75.066309	1.619132
93.381298	55.973330	1.310144
108.962530	1655.712429	45.221000
109.221537	57.491891	1.573957
132.890845	22.352826	0.744570
146.970987	540.946660	19.928019
154.142024	153.546313	5.932511
176.699787	103.118251	4.567196
182.354923	20.314692	0.928551
190.648314	44.419019	2.122658
193.101005	426.799456	20.657914
197.065899	42.467790	2.097728
205.362113	11.504320	0.592188
223.155398	12.231499	0.684172
228.408571	486.216274	27.836842
236.862354	105.328742	6.253469
250.405743	82.062084	5.150684
251.457378	180.990302	11.407691
259.062690	20.568659	1.335638
298.318180	199.803456	14.940351
302.871065	818.241695	62.117999
328.437481	17.430809	1.434988
328.856377	20.999662	1.730998
335.594108	42.652859	3.587902
345.059018	11.697134	1.011698
355.386299	32.907883	2.931424
359.003293	41.883556	3.768947
365.363486	46.203245	4.231318
395.230699	315.400145	31.245727
422.138690	20.668027	2.186917
425.048599	16.563252	1.764665
432.918475	39.254980	4.259699
436.181004	39.725207	4.343212
441.149973	258.976528	28.636816
449.405536	264.065865	29.746012
492.456742	27.874982	3.440810
498.037995	2.595218	0.323977
506.069285	143.053789	18.146272
518.893366	214.234412	27.864126
543.656320	7.633473	1.040219
550.814965	63.490985	8.765887
557.941644	19.244483	2.691368
559.169659	2.195106	0.307664
562.025675	9.999069	1.408620
567.375783	34.065575	4.844674
575.494217	14.374157	2.073487
586.753514	15.568190	2.289665
686.724876	8.350472	1.437381
715.713990	11.580113	2.077449
729.942667	97.358388	17.813128
759.082261	38.672545	7.358167
759.688286	252.609939	48.102089
769.871580	136.522660	26.345176
774.025849	0.691377	0.134137
786.724149	3.422547	0.674916
799.054902	8.881837	1.778924
801.224434	0.032273	0.006481
823.428274	15.879504	3.277485
825.097454	8.667623	1.792600
834.520561	26.967000	5.640891
837.547597	3.395066	0.712748
842.745955	2.839383	0.599789
845.158802	0.736965	0.156122
858.933438	0.065095	0.014015
864.955151	2.142736	0.464558
905.076053	1.701909	0.386100
905.302763	8.584604	1.948015
919.629481	9.280737	2.139309
922.387648	4.809240	1.111906
955.013803	204.576197	48.971434
970.906459	225.114101	54.784558
1009.122851	8.036418	2.032753
1019.554699	24.849819	6.350557
1024.298130	23.249912	5.969333
1027.359782	7.502278	1.931941
1030.369077	41.227047	10.647634
1031.359067	37.521812	9.700001
1035.025521	34.069766	8.838901

1046.016033		27.875614	7.308712
1056.979569		17.885958	4.738674
1062.481540		21.552312	5.739755
1097.962696		28.114126	7.737314
1114.655381		15.537413	4.341076
1124.127596		41.310230	11.639955
1126.386496		159.836912	45.127636
1127.402948		4.276710	1.208557
1140.019914		34.330764	9.810112
1147.906900		53.328539	15.344206
1161.298420		8.824111	2.568579
1181.256987		10.348242	3.064002
1186.633603		4.795659	1.426405
1193.252077		4.546541	1.359851
1228.269190		2.335483	0.719032
1234.254086		129.555268	40.080924
1237.210646		95.184205	29.517978
1247.516528		909.334929	284.346739
1255.516424		12.710710	4.000095
1257.463801		32.456639	10.230035
1290.855169		10.107447	3.270371
1291.496569		0.304032	0.098422
1306.586636		1.750089	0.573161
1309.285289		0.290549	0.095352
1318.840105		338.605373	111.934525
1329.940387		4.821541	1.607297
1332.091191		7.975903	2.663127
1334.554271		5.153376	1.723877
1334.995715		5.845822	1.956156
1340.995051		21.049795	7.075434
1348.162867		15.391186	5.201068
1350.477375		3.007509	1.018057
1354.717444		5.561589	1.888538
1358.357837		4.948453	1.684852
1363.701231		3.332006	1.138946
1374.195537		15.389527	5.300928
1386.638685		10.134921	3.522587
1392.301034		20.258573	7.070011
1416.600686		22.623735	8.033223
1456.218656		10.326963	3.769444
1462.009182		3.093964	1.133818
1462.370433		7.971897	2.922114
1465.151194		15.616405	5.735108
1469.607552		18.411113	6.782027
1469.624141		23.963470	8.827425
1477.155822		34.486298	12.768826
1480.744001		29.570588	10.975341
1570.497877		230.066264	90.566663
1593.200356		2826.560075	1128.773189
1600.402547		226.245324	90.758418
1610.912957		132.046654	53.318454
1614.305231		223.578689	90.467821
1624.385038		47.260756	19.242776
1646.399955		111.380918	45.964677
1653.974888		1536.824115	637.134538
2900.157849		57.222926	41.597743
2917.497322		27.201745	19.892314
2929.782532		13.698739	10.059909
2931.661408		9.555854	7.022009
2933.693331		30.203976	22.210427
2945.139411	24.901053	18.382376	
2946.740989		19.971157	14.751061
2955.017137		12.083398	8.950085
2955.674490		12.127163	8.984499
2961.609180		4.038492	2.997955
2981.187401		20.138727	15.048713
2986.993763		17.523945	13.120315
2987.299355		20.406399	15.279994
2992.399274		15.702493	11.777855
2999.247530		20.838584	15.666017
3000.591984		50.121467	37.697174
3000.771086		23.886140	17.966228
3004.854876		28.386676	21.380414
3016.715899		4.029363	3.046835
3060.943050		39.332083	30.177292
3269.698990		87.712056	71.886135
3293.131759		39.954591	32.980244
3300.118309		50.118914	41.458084
3322.396982		13.231229	11.018685
3372.034426		57.429547	48.540636
3383.876217		44.680828	37.897778
3385.760827		41.265273	35.020236
3388.556830	53.113213	45.112347	

Zero-Point Energy :	0.462492	a.u.
==========	12.585050	eV
(imaginary frequencies were excluded from the summation)		

```
Statistical      Thermal      Analysis             ***             ideal       gas       assumed             ***
     Temp                                                                Transl      Rotat     Vibrat      Total
     ----                                                                ------      -----     ------      -----

     298.15    Entropy (cal/mole-K):                                     45.980     37.181    109.226    192.386
               Internal Energy (Kcal/mole):                              0.889       0.889    307.395    309.173
               Constant Volume Heat Capacity (cal/mole-K):       2.981    2.981   112.633   118.595
```

α[**1**]$_2$-water-tzp-blyp-d3;C_2

Coordinates in Geometry Cycle 4

Atom	X	Y	Z	(Angstrom)
1.Pt	-0.489464	-1.580461	0.143556	
2.O	0.911906	-2.085218	1.589808	
3.O	2.974861	-2.978491	1.772721	
4.N	-2.101410	-1.196766	1.415017	
5.H	-2.355924	-2.060403	1.908072	
6.H	-1.837441	-0.515588	2.134946	
7.H	-1.761392	-0.106748	-1.583273	
8.O	3.194065	-2.846815	-1.056229	
9.C	2.036045	-2.555799	1.086952	
10.H	-5.977503	-2.028347	-0.901051	
11.H	-6.570001	-0.495074	-1.550233	
12.C	-3.303006	-0.676210	0.646491	
13.H	-3.147134	0.401770	0.544535	
14.C	-4.642461	-0.917292	1.356799	
15.H	-4.231354	0.362095	-1.768042	
16.C	-5.775173	-0.947068	-0.943130	
17.H	-4.630862	-0.435469	2.343687	
18.H	-4.775021	-1.999157	1.515128	
19.C	-4.405412	-0.716756	-1.630655	
20.H	-4.382700	-1.189544	-2.621581	
21.H	-3.411878	-2.387186	-0.664881	
22.C	-5.801507	-0.364360	0.489157	
23.H	-6.759154	-0.592814	0.974117	
24.H	-5.719184	0.732026	0.438322	
25.C	2.156629	-2.493828	-0.485434	
26.O	1.109414	-1.991214	-1.115787	
27.C	-3.285961	-1.300061	-0.754353	
28.N	-1.894419	-1.093129	-1.315710	
29.H	-1.779180	-1.649174	-2.169000	
30.Pt	0.489538	1.580450	0.143381	
31.O	-1.109379	1.991421	-1.115720	
32.O	-3.194047	2.846650	-1.056466	
33.N	1.894550	1.093508	-1.315742	
34.H	1.760726	0.106816	-1.581450	
35.H	1.778408	1.648355	-2.169731	
36.H	2.356896	2.063640	1.903840	
37.O	-2.975199	2.977265	1.773119	
38.C	-2.156860	2.493846	-0.485359	
39.H	5.719384	-0.731859	0.438444	
40.H	6.759218	0.593033	0.974193	
41.C	3.285906	1.300072	-0.754132	
42.H	3.411694	2.386990	-0.663031	
43.C	4.405360	0.717150	-1.630593	
44.H	4.774307	1.999235	1.514638	
45.C	5.801551	0.364529	0.489183	
46.H	4.382892	1.190245	-2.621394	
47.H	4.231374	-0.361642	-1.768381	
48.C	4.642361	0.917293	1.356667	
49.H	4.630613	0.435171	2.343365	
50.H	3.146757	-0.402009	0.544912	
51.C	5.775159	0.947341	-0.943007	
52.H	6.569842	0.495283	-1.550228	
53.H	5.978204	2.028501	-0.900810	
54.C	-2.036588	2.555412	1.087023	
55.O	-0.912101	2.084725	1.589773	
56.C	3.302810	0.675979	0.646578	
57.N	2.101730	1.197764	1.414956	
58.H	1.839006	0.518491	2.136896	

```
E-test:            old,new=      -12.24309,      -12.24307      hartree
max    gradient:                        0.00084906    au/angstrom,radian
max      cart.      step:                         0.00287906      angstrom
Geometry Converged
```

	hartree	eV	kcal/mol	kJ/mol
Total Pauli Repulsion:	46.211966782034757	1257.4916	28998.45	121329.50
Electrostatic Interaction:	-10.059397018174307	-273.7301	-6312.37	-26410.94
Total Orbital Interactions:	-48.180987025301945	-1311.0714	-30234.03	-126499.16
Solvation:	-0.093818462206717	-2.5529	-58.87	-246.32
Dispersion Energy:	-0.120977727418162	-3.2920	-75.91	-317.63
Total Bonding Energy:	-12.243208420914947	-333.1547	-7682.73	-32144.54

α[**1**]$_2$-water-tzp-blyp-d3;C_1

Coordinates in Geometry Cycle 4

Atom	X	Y	Z (Angstrom)
1.Pt	-0.489464	-1.580461	0.143556
2.O	0.911906	-2.085218	1.589808
3.O	2.974861	-2.978491	1.772721
4.N	-2.101410	-1.196766	1.415017
5.H	-2.355924	-2.060403	1.908072
6.H	-1.837441	-0.515588	2.134946
7.H	-1.761392	-0.106748	-1.583273
8.O	3.194065	-2.846815	-1.056229
9.C	2.036045	-2.555799	1.086952
10.H	-5.977503	-2.028347	-0.901051
11.H	-6.570001	-0.495074	-1.550233
12.C	-3.303006	-0.676210	0.646491
13.H	-3.147134	0.401770	0.544535
14.C	-4.642461	-0.917292	1.356799
15.H	-4.231354	0.362095	-1.768042
16.C	-5.775173	-0.947068	-0.943130
17.H	-4.630862	-0.435469	2.343687
18.H	-4.775021	-1.999157	1.515128
19.C	-4.405412	-0.716756	-1.630655
20.H	-4.382700	-1.189544	-2.621581
21.H	-3.411878	-2.387186	-0.664881
22.C	-5.801507	-0.364360	0.489157
23.H	-6.759154	-0.592814	0.974117
24.H	-5.719184	0.732026	0.438322
25.C	2.156629	-2.493828	-0.485434
26.O	1.109414	-1.991214	-1.115787
27.C	-3.285961	-1.300061	-0.754353
28.N	-1.894419	-1.093129	-1.315710
29.H	-1.779180	-1.649174	-2.169000
30.Pt	0.489538	1.580450	0.143381
31.O	-1.109379	1.991421	-1.115720
32.O	-3.194047	2.846650	-1.056466
33.N	1.894550	1.093508	-1.315742
34.H	1.760726	0.106816	-1.581450
35.H	1.778408	1.648355	-2.169731
36.H	2.356896	2.063640	1.903840
37.O	-2.975199	2.977265	1.773119
38.C	-2.156860	2.493846	-0.485359
39.H	5.719384	-0.731859	0.438444
40.H	6.759218	0.593033	0.974193
41.C	3.285906	1.300072	-0.754132
42.H	3.411694	2.386990	-0.663031
43.C	4.405360	0.717150	-1.630593
44.H	4.774307	1.999235	1.514638
45.C	5.801551	0.364529	0.489183
46.H	4.382892	1.190245	-2.621394
47.H	4.231374	-0.361642	-1.768381
48.C	4.642361	0.917293	1.356667
49.H	4.630613	0.435171	2.343365
50.H	3.146757	-0.402009	0.544912
51.C	5.775159	0.947341	-0.943007
52.H	6.569842	0.495283	-1.550228
53.H	5.978204	2.028501	-0.900810
54.C	-2.036588	2.555412	1.087023
55.O	-0.912101	2.084725	1.589773
56.C	3.302810	0.675979	0.646578
57.N	2.101730	1.197764	1.414956
58.H	1.839006	0.518491	2.136896

```
E-test:  old,new= -12.24309, -12.24307 hartree
max gradient:      0.00084906 au/angstrom,radian
max cart. step:    0.00287906 angstrom
Geometry Converged
```

	hartree	eV	kcal/mol	kJ/mol
Total Pauli Repulsion:	46.207651043220721	1257.3742	28995.74	121318.17
Electrostatic Interaction:	-10.057837365422134	-273.6877	-6311.39	-26406.85
Total Orbital Interactions:	-48.178059166884637	-1310.9917	-30232.19	-126491.48
Solvation Energy (el):	-0.093866384899179	-2.5542	-58.90	-246.45
Dispersion Energy:	-0.120919025251182	-3.2904	-75.88	-317.47
Total Bonding Energy:	-12.243022772674317	-333.1496	-7682.61	-32144.05

β[**1**]$_2$-tzp-blyp;C_1

```
 Coordinates       in       Geometry       Cycle       25
   Atom          X            Y            Z    (Angstrom)
   1.Pt          -0.608576     -1.762042      0.144779
   2.O            0.753347     -2.267597      1.590598
   3.O            2.996101     -2.323836      1.817350
   4.N           -2.146168     -1.091148      1.414985
   5.H           -2.438377     -1.838778      2.052605
   6.H           -1.763227     -0.309045      1.972528
   7.H           -1.754422     -0.145241     -1.524113
   8.O            3.179965     -2.351310     -1.039309
   9.C            1.979470     -2.301252      1.110313
  10.H           -6.117375     -1.825651     -0.847391
  11.H           -6.614149     -0.287054     -1.551404
  12.C           -3.325856     -0.552865      0.624284
  13.H           -3.090310      0.507459      0.464424
  14.C           -4.673784     -0.684740      1.353647
  15.H           -4.234075      0.407580     -1.842926
  16.C           -5.841682     -0.762534     -0.932587
  17.H           -4.631186     -0.148562      2.311857
  18.H           -4.866989     -1.747414      1.580386
  19.C           -4.467556     -0.648851     -1.639850
  20.H           -4.492240     -1.170873     -2.608020
  21.H           -3.549012     -2.322884     -0.606934
  22.C           -5.820256     -0.122174      0.475214
  23.H           -6.782889     -0.285059      0.978121
  24.H           -5.693007      0.966380      0.378737
  25.C            2.080469     -2.319892     -0.464391
  26.O            0.927939     -2.306860     -1.100626
  27.C           -3.362686     -1.248024     -0.749160
  28.N           -1.972492     -1.140649     -1.320624
  29.H           -1.885882     -1.675825     -2.189598
  30.Pt           2.479343      1.102522      0.183175
  31.O            0.950245      1.666705     -1.062179
  32.O           -1.301769      1.717215     -1.012757
  33.N            3.855244      0.511562     -1.283877
  34.H            3.638865     -0.479592     -1.508750
  35.H            3.774736      1.063836     -2.142661
  36.H            4.297849      1.150444      2.102708
  37.O           -1.135467      1.636214      1.843606
  38.C           -0.205687      1.672143     -0.432268
  39.H            7.564778     -1.626023      0.405249
  40.H            8.650713     -0.384425      1.031496
  41.C            5.241777      0.607836     -0.701262
  42.H            5.428081      1.679910     -0.539290
  43.C            6.352017      0.022880     -1.594988
  44.H            6.730630      1.067926      1.645191
  45.C            7.691335     -0.539152      0.519837
  46.H            6.383319      0.561028     -2.554079
  47.H            6.118918     -1.029753     -1.817175
  48.C            6.539052      0.009079      1.399899
  49.H            6.490404     -0.542653      2.348959
  50.H            4.962107     -1.168530      0.479710
  51.C            7.721905      0.123442     -0.877570
  52.H            8.497536     -0.343447     -1.499007
  53.H            7.998493      1.184688     -0.774182
  54.C           -0.114351      1.624696      1.142720
  55.O            1.108420      1.579759      1.630287
  56.C            5.195950     -0.111016      0.659487
  57.N            4.010630      0.412795      1.451275
  58.H          3.624871   -0.378451    1.993509
```

```
E-test:            old,new=      -12.07053,      -12.07055      hartree
max    gradient:                        0.00076151    au/angstrom,radian
max      cart.      step:                        0.00109997      angstrom
Geometry Converged
```

	hartree	eV	kcal/mol	kJ/mol
Total Pauli Repulsion:	46.228464831898044	1257.9405	29008.80	121372.82
Electrostatic Interaction:	-10.072113929878626	-274.0762	-6320.35	-26444.33
Total Orbital Interactions:	-48.226893189838798	-1312.3205	-30262.84	-126619.69
Total Bonding Energy:	-12.070550612846919	-328.4564	-7574.39	-31691.23

β[**1**]$_2$-tzp-blyp-d3;C_1

Coordinates in Geometry Cycle 9

Atom	X	Y	Z (Angstrom)
1.Pt	-0.518249	-1.660274	0.140428
2.O	0.824967	-2.136952	1.612333
3.O	3.057270	-2.304919	1.872137
4.N	-2.089191	-1.076130	1.403412
5.H	-2.384706	-1.860599	1.993979
6.H	-1.745436	-0.314468	2.011695
7.H	-1.704151	-0.105509	-1.571280
8.O	3.288559	-2.363563	-0.975581
9.C	2.052750	-2.243068	1.150399
10.H	-6.019564	-1.808235	-0.875997
11.H	-6.536603	-0.276523	-1.583747
12.C	-3.257880	-0.525686	0.607453
13.H	-3.016207	0.534097	0.457470
14.C	-4.607749	-0.666272	1.327030
15.H	-4.150346	0.452300	-1.837804
16.C	-5.759902	-0.740988	-0.962014
17.H	-4.568333	-0.140315	2.290660
18.H	-4.799118	-1.732268	1.539833
19.C	-4.383002	-0.608457	-1.659088
20.H	-4.394407	-1.113917	-2.636033
21.H	-3.472642	-2.289667	-0.630174
22.C	-5.749499	-0.100643	0.445844
23.H	-6.715170	-0.263481	0.942874
24.H	-5.618608	0.987300	0.348997
25.C	2.180425	-2.269941	-0.423094
26.O	1.048729	-2.167546	-1.085763
27.C	-3.285041	-1.214124	-0.767978
28.N	-1.893730	-1.100048	-1.340414
29.H	-1.803256	-1.653342	-2.197725
30.Pt	2.390256	1.004437	0.178011
31.O	0.831415	1.535902	-1.048371
32.O	-1.409757	1.723700	-0.948759
33.N	3.773470	0.465787	-1.304032
34.H	3.584083	-0.524279	-1.553926
35.H	3.688905	1.034325	-2.151906
36.H	4.246765	1.173343	2.043437
37.O	-1.195866	1.612746	1.898914
38.C	-0.304837	1.622648	-0.391227
39.H	7.479748	-1.660531	0.375309
40.H	8.578904	-0.423769	0.993343
41.C	5.161801	0.566898	-0.722002
42.H	5.352108	1.639561	-0.566657
43.C	6.262602	-0.029458	-1.616034
44.H	6.665203	1.045342	1.600225
45.C	7.615250	-0.574773	0.488750
46.H	6.281734	0.490858	-2.585014
47.H	6.026271	-1.086285	-1.812292
48.C	6.471091	-0.016897	1.371672
49.H	6.424413	-0.555997	2.327699
50.H	4.881801	-1.199580	0.474633
51.C	7.636219	0.086104	-0.909452
52.H	8.414046	-0.373017	-1.533753
53.H	7.900608	1.150654	-0.806295
54.C	-0.186524	1.568949	1.182431
55.O	1.039203	1.461883	1.649882
56.C	5.124961	-0.142834	0.642413
57.N	3.952933	0.397983	1.440074
58.H	3.604733	-0.371210	2.035782

```
E-test:            old,new=      -12.19392,      -12.19394      hartree
max    gradient:                        0.00098043    au/angstrom,radian
max      cart.      step:                        0.00649941      angstrom
Geometry Converged
```

	hartree	eV	kcal/mol	kJ/mol
Total Pauli Repulsion:	46.357059251317459	1261.4398	29089.50	121710.44
Electrostatic Energy:	-10.113430568934630	-275.2004	-6346.27	-26552.81
Total Orbital Interactions:	-48.311907162391130	-1314.6339	-30316.18	-126842.89
Dispersion Energy:	-0.125677522920947	-3.4199	-78.86	-329.97
Total Bonding Energy:	-12.193956523414069	-331.8144	-7651.82	-32015.23

Frequency cm-1	Dipole Strength 1e-40 esu2 cm2	Absorption Intensity (degeneracy not counted) km/mole
32.814283	793.652053	6.527865
34.324733	230.918773	1.986756
41.457193	12.692134	0.131890
48.212581	4.683183	0.056595
67.037928	16.169741	0.271708
67.976416	4.013514	0.068385
78.792540	8.797320	0.173746
85.614128	110.820285	2.378169
88.886223	10.997688	0.245027
108.632854	63.235134	1.721859
114.362483	12.516581	0.358796
135.004194	20.869969	0.706232
149.292411	42.794740	1.601423
157.976891	954.269250	37.787013
168.126781	2.445362	0.103052
172.715817	20.824459	0.901538
185.152182	1.727895	0.080191
185.721774	67.578358	3.145926
199.924690	44.933200	2.251707
200.489241	62.123098	3.121923
225.735815	44.219878	2.502051
229.142677	25.649904	1.473227
252.408988	91.270249	5.774470
253.544673	602.465004	38.288150
254.342750	51.760125	3.299839
257.915109	1.257107	0.081269
295.128475	5.813505	0.430058
302.044470	830.837561	62.902091
329.611346	0.323741	0.026747
330.278675	16.267289	1.346709
336.629823	5.243910	0.442472
338.025201	89.905165	7.617488
355.781714	2.065230	0.184175
356.259518	145.990701	13.036762
361.437654	3.069889	0.278121
364.415558	84.411224	7.710369
425.840557	13.610329	1.452759
426.745495	6.900430	0.738114
435.063611	104.049162	11.346696
435.787789	3.152999	0.344411
449.778211	0.475820	0.053644
455.990982	934.689970	106.832135
497.111436	1.025318	0.127759
497.360789	51.546988	6.426180
523.144179	476.625773	62.499564
524.976709	1.910683	0.251424
550.683041	23.748442	3.278045
551.081335	24.185066	3.340728
559.360461	2.257022	0.316450
561.830203	60.937269	8.581558
564.025680	44.027466	6.224445
564.666146	0.151049	0.021379
580.027955	18.041418	2.622996
580.219017	19.491304	2.834725
715.567199	22.012686	3.948222
716.230594	7.229277	1.297854
757.511053	36.495544	6.929580
758.980131	201.394538	38.313883
772.030094	38.341183	7.419554
773.267889	223.318003	43.284438
783.537369	5.050649	0.991939
784.523067	20.475944	4.026500
793.608792	30.680970	6.103144
794.057652	4.683134	0.932109
825.381299	16.917053	3.499914
825.542490	12.239364	2.532657
838.558593	17.680421	3.716243
839.092396	12.571050	2.643988
846.517153	1.451129	0.307907
846.533710	8.769907	1.860875
869.377567	0.178128	0.038817
869.448067	0.102862	0.022417
908.870634	5.891045	1.342062
908.906150	14.137240	3.220785
924.307650	3.655316	0.846875
924.356075	3.617034	0.838050
974.065795	554.663229	135.424032
974.809646	21.144577	5.166505
1022.149082	8.339752	2.136709
1022.416077	51.968248	13.318147
1028.348449	3.403134	0.877198
1028.896823	3.596173	0.927450
1035.067093	65.649875	17.032582
1035.299253	27.598745	7.161983
1041.243484	34.474837	8.997722
1041.848256	29.035320	7.582443

1074.081829		41.320290	11.124456
1074.358173		3.520121	0.947949
1119.021958		33.981927	9.531575
1119.211592		100.729946	28.258485
1133.068278		138.652030	39.378610
1133.619328		108.566315	30.848952
1171.830970		14.233549	4.180770
1173.893537		110.647240	32.557224
1177.952883		35.712120	10.544394
1178.132544		3.152475	0.930945
1188.474174		15.147779	4.512495
1190.839082		21.318567	6.363399
1211.661090		25.196956	7.652570
1212.657737		3.701336	1.125058
1237.951979		22.308674	6.922383
1238.068008		6.081194	1.887172
1258.043053		6.250867	1.971124
1258.268558		7.935977	2.502948
1267.638173		10.125138	3.217172
1279.098058		1809.103447	580.023128
1298.748241		6.435631	2.095049
1299.110867		3.834304	1.248564
1311.083378		0.219783	0.072227
1311.211880		0.077634	0.025516
1334.164732		9.715625	3.249064
1334.313178		8.773252	2.934245
1334.721740		8.959301	2.997388
1334.773598		6.007873	2.010048
1342.798611		18.529960	6.236823
1343.024805		14.401726	4.848157
1355.149675		8.955622	3.042013
1355.472065		11.417134	3.879053
1376.126880		1.800175	0.620942
1376.573788		3.340313	1.152563
1388.815262		23.988191	8.350646
1389.153510		24.572826	8.556249
1407.200597		5.058419	1.784222
1408.635561		5.289558	1.867653
1461.358536		2.848120	1.043261
1461.498897		3.782111	1.385514
1463.165191		8.053315	2.953562
1463.375489		8.500052	3.117851
1468.064880		17.843233	6.565940
1468.123745		20.147681	7.414226
1478.289735		15.428883	5.717052
1478.466432		13.910973	5.155218
1558.576692		389.038736	151.984428
1561.289055		146.690577	57.406835
1574.677035		128.563440	50.744274
1580.009947		1430.760542	566.636891
1615.714406		30.525264	12.362380
1617.978684		32.933867	13.356529
1626.538492		81.945563	33.409337
1630.420146		2991.691579	1222.628239
2908.412747		30.134309	21.968244
2908.673578		29.366851	21.410679
2925.671250		31.915191	23.404591
2925.926186		28.286908	20.745643
2937.375481		11.532092	8.490742
2937.439807		25.973927	19.124261
2942.423629		20.773291	15.321051
2943.262052		28.327036	20.898164
2943.339478	19.612770	14.469628	
2943.797838		21.874063	16.140445
2976.856087		66.396636	49.542964
2977.270559		67.219628	50.164037
2980.869761		0.419523	0.313456
2981.398675		2.378489	1.777458
2984.014441		124.005612	92.751370
2984.152893		27.115452	20.282244
2987.531071		44.619545	33.413013
2987.969373		50.808071	38.052826
2998.670691		5.731959	4.308339
3000.025505		7.074442	5.319799
3149.485406		27.223167	21.490985
3153.487297		387.543843	306.330329
3224.637271		117.327180	94.832581
3230.170024		261.912826	212.060714
3372.814871		30.401523	25.701941
3373.103130		46.428380	39.254660
3389.854609		22.355203	18.994932
3389.973341	34.047334	28.930601	

Zero-Point	Energy	:	0.461544 a.u.
==========	12.559250 eV		

```
Statistical       Thermal       Analysis              ***              ideal       gas       assumed              ***
     Temp                                                                 Transl      Rotat     Vibrat       Total
     ----                                                                 ------      -----     ------       -----

     298.15    Entropy (cal/mole-K):                                     45.894     36.988    110.615     193.498
               Internal Energy (Kcal/mole):                              0.889      0.889    306.854     308.631
               Constant Volume Heat Capacity (cal/mole-K):       2.981    2.981   112.189   118.150
```

β[**1**]$_2$-tzp-blyp-d3bj;C_1

Coordinates in Geometry Cycle 28

Atom	X	Y	Z (Angstrom)
1.Pt	-0.528278	-1.670260	0.144484
2.O	0.816790	-2.164972	1.608948
3.O	3.052519	-2.295229	1.856737
4.N	-2.085343	-1.065069	1.403651
5.H	-2.377451	-1.839398	2.007818
6.H	-1.732927	-0.291329	1.992010
7.H	-1.698248	-0.092205	-1.540776
8.O	3.270847	-2.341665	-0.987148
9.C	2.042903	-2.241549	1.140380
10.H	-6.005626	-1.820760	-0.871804
11.H	-6.523462	-0.291424	-1.583485
12.C	-3.252742	-0.527294	0.605912
13.H	-3.017731	0.532487	0.449997
14.C	-4.598849	-0.671683	1.324791
15.H	-4.143243	0.437726	-1.841306
16.C	-5.747216	-0.753954	-0.960655
17.H	-4.562561	-0.143509	2.286887
18.H	-4.786131	-1.737731	1.538901
19.C	-4.372879	-0.622169	-1.656823
20.H	-4.384116	-1.133245	-2.630346
21.H	-3.453770	-2.295048	-0.624973
22.C	-5.738384	-0.110720	0.443071
23.H	-6.704069	-0.272427	0.939180
24.H	-5.607017	0.976531	0.343539
25.C	2.163138	-2.263263	-0.430091
26.O	1.027324	-2.192603	-1.087276
27.C	-3.275295	-1.219055	-0.764301
28.N	-1.888046	-1.092180	-1.330429
29.H	-1.788517	-1.634408	-2.192787
30.Pt	2.401151	1.018173	0.180301
31.O	0.853273	1.566144	-1.050625
32.O	-1.391532	1.708557	-0.961974
33.N	3.770078	0.465261	-1.295844
34.H	3.576882	-0.528826	-1.529450
35.H	3.680628	1.026579	-2.147025
36.H	4.241340	1.149028	2.056149
37.O	-1.191215	1.603869	1.881461
38.C	-0.287202	1.620647	-0.399647
39.H	7.453514	-1.671692	0.362724
40.H	8.561294	-0.448183	0.990678
41.C	5.154157	0.570419	-0.717083
42.H	5.340377	1.642072	-0.556065
43.C	6.252477	-0.019376	-1.613528
44.H	6.655887	1.027905	1.606366
45.C	7.597204	-0.588328	0.485023
46.H	6.276186	0.511342	-2.576284
47.H	6.012824	-1.072716	-1.821263
48.C	6.458116	-0.031526	1.370045
49.H	6.409104	-0.578159	2.321225
50.H	4.871972	-1.201712	0.460955
51.C	7.623152	0.082941	-0.905308
52.H	8.398532	-0.375656	-1.532119
53.H	7.892828	1.144727	-0.793004
54.C	-0.176948	1.567184	1.170479
55.O	1.046500	1.484515	1.645066
56.C	5.115916	-0.147582	0.639160
57.N	3.947856	0.385484	1.439029
58.H	3.588388	-0.394688	2.014154

```
E-test:            old,new=      -12.25770,      -12.25770      hartree
max    gradient:                        0.00073704    au/angstrom,radian
max      cart.      step:                        0.00045716      angstrom
Geometry Converged
```

	hartree	eV	kcal/mol	kJ/mol
Total Pauli Repulsion:	46.598153247698306	1268.0003	29240.79	122343.43
Electrostatic Energy:	-10.176169539398987	-276.9077	-6385.64	-26717.53
Total Orbital Interactions:	-48.490254027992535	-1319.4869	-30428.10	-127311.14
Dispersion Energy:	-0.189432217662722	-5.1547	-118.87	-497.35
Total Bonding Energy:	-12.257703030905526	-333.5491	-7691.83	-32182.59

β[**1**]$_2$-tz2p-blyp-d3;C_1

Coordinates in Geometry Cycle 26

Atom	X	Y	Z (Angstrom)
1.Pt	-0.511410	-1.670035	0.144782
2.O	0.835880	-2.145030	1.602739
3.O	3.064237	-2.315406	1.858335
4.N	-2.083355	-1.102424	1.407679
5.H	-2.387167	-1.901213	1.972240
6.H	-1.743185	-0.361339	2.038593
7.H	-1.685952	-0.126330	-1.575695
8.O	3.282142	-2.352654	-0.991576
9.C	2.062040	-2.252772	1.142929
10.H	-6.020290	-1.760903	-0.878577
11.H	-6.504932	-0.220839	-1.588560
12.C	-3.240333	-0.531376	0.611382
13.H	-2.983143	0.524244	0.465489
14.C	-4.594151	-0.651016	1.325953
15.H	-4.107412	0.461138	-1.838458
16.C	-5.739954	-0.699858	-0.964900
17.H	-4.548418	-0.130452	2.291348
18.H	-4.807136	-1.713256	1.532545
19.C	-4.359392	-0.594078	-1.658505
20.H	-4.377601	-1.101226	-2.633517
21.H	-3.473138	-2.288987	-0.630659
22.C	-5.720104	-0.059198	0.442374
23.H	-6.690078	-0.199275	0.935854
24.H	-5.562944	1.024371	0.345688
25.C	2.181930	-2.272942	-0.432693
26.O	1.044898	-2.172394	-1.081464
27.C	-3.272808	-1.216119	-0.765233
28.N	-1.880048	-1.116004	-1.334998
29.H	-1.789597	-1.679543	-2.184102
30.Pt	2.382898	1.011323	0.180987
31.O	0.835675	1.538990	-1.045346
32.O	-1.402615	1.713413	-0.967070
33.N	3.759843	0.481286	-1.299696
34.H	3.567501	-0.504358	-1.558216
35.H	3.674702	1.058961	-2.139747
36.H	4.244523	1.211287	2.023526
37.O	-1.203499	1.619540	1.883572
38.C	-0.306124	1.623921	-0.402497
39.H	7.438827	-1.678451	0.373197
40.H	8.557826	-0.458949	0.986873
41.C	5.148590	0.572317	-0.719375
42.H	5.347436	1.642951	-0.566217
43.C	6.241313	-0.034508	-1.615525
44.H	6.665678	1.039528	1.593301
45.C	7.591415	-0.595737	0.485558
46.H	6.263823	0.486811	-2.582926
47.H	5.992379	-1.087443	-1.812232
48.C	6.457962	-0.020469	1.370456
49.H	6.408388	-0.554747	2.328140
50.H	4.855489	-1.188288	0.482366
51.C	7.617708	0.064160	-0.912608
52.H	8.387018	-0.405043	-1.538429
53.H	7.895569	1.124415	-0.810271
54.C	-0.196635	1.573035	1.173482
55.O	1.026911	1.460109	1.639115
56.C	5.108867	-0.134325	0.646047
57.N	3.945627	0.421317	1.444200
58.H	3.602406	-0.329697	2.061095

```
E-test:            old,new=      -12.25726,      -12.25726      hartree
max    gradient:                        0.00097922    au/angstrom,radian
max      cart.      step:                         0.00099627      angstrom
Geometry Converged
```

	hartree	eV	kcal/mol	kJ/mol
Total Pauli Repulsion:	46.599749289950296	1268.0437	29241.79	122347.62
Electrostatic Energy:	-10.166560336471566	-276.6462	-6379.61	-26692.30
Total Orbital Interactions:	-48.564622792846556	-1321.5106	-30474.76	-127506.40
Dispersion Energy:	-0.125833464327307	-3.4241	-78.96	-330.38
Total Bonding Energy:	-12.257276196062048	-333.5375	-7691.56	-32181.47

β[**1**]$_2$-qz4p-blyp-d3;C_1

Coordinates in Geometry Cycle 11

Atom	X	Y	Z (Angstrom)
1.Pt	-0.521905	-1.700006	0.148105
2.O	0.831978	-2.134757	1.608582
3.O	3.062569	-2.230941	1.873656
4.N	-2.107051	-1.161446	1.403847
5.H	-2.426109	-1.967930	1.948031
6.H	-1.769207	-0.439011	2.055612
7.H	-1.670856	-0.176352	-1.598540
8.O	3.289351	-2.289417	-0.976932
9.C	2.063013	-2.204368	1.153411
10.H	-6.051489	-1.657411	-0.952417
11.H	-6.459511	-0.079125	-1.619117
12.C	-3.246132	-0.558560	0.606009
13.H	-2.969603	0.494226	0.480355
14.C	-4.608944	-0.662516	1.302220
15.H	-4.039167	0.509152	-1.822593
16.C	-5.725025	-0.607969	-1.000231
17.H	-4.561562	-0.172789	2.282576
18.H	-4.854941	-1.722432	1.476150
19.C	-4.333250	-0.538384	-1.670982
20.H	-4.356953	-1.018964	-2.658034
21.H	-3.520547	-2.286061	-0.667763
22.C	-5.703753	-0.012107	0.424084
23.H	-6.683737	-0.137070	0.899709
24.H	-5.514883	1.068315	0.363900
25.C	2.187831	-2.229198	-0.418697
26.O	1.051150	-2.153909	-1.071412
27.C	-3.281881	-1.218761	-0.780458
28.N	-1.881730	-1.156563	-1.340260
29.H	-1.799265	-1.734782	-2.179706
30.Pt	2.393592	1.043014	0.184241
31.O	0.827305	1.518752	-1.035588
32.O	-1.411275	1.654037	-0.951122
33.N	3.763729	0.526457	-1.304467
34.H	3.552843	-0.447879	-1.584031
35.H	3.688819	1.121700	-2.132641
36.H	4.286918	1.282883	1.998712
37.O	-1.200600	1.537402	1.899025
38.C	-0.312933	1.582256	-0.387992
39.H	7.380189	-1.735948	0.390064
40.H	8.548346	-0.541077	0.950504
41.C	5.160004	0.574148	-0.733794
42.H	5.401856	1.638618	-0.602258
43.C	6.214718	-0.095766	-1.628284
44.H	6.719006	1.039800	1.538430
45.C	7.571105	-0.656969	0.467008
46.H	6.245723	0.399586	-2.607811
47.H	5.918151	-1.139911	-1.797445
48.C	6.472138	-0.017032	1.347723
49.H	6.417818	-0.520722	2.320610
50.H	4.835679	-1.158268	0.497571
51.C	7.602686	-0.040677	-0.948416
52.H	8.338945	-0.563244	-1.570519
53.H	7.932501	1.006796	-0.883687
54.C	-0.196993	1.526618	1.183918
55.O	1.031438	1.449927	1.644643
56.C	5.113480	-0.108119	0.641501
57.N	3.970298	0.484475	1.441287
58.H	3.627838	-0.246123	2.081024

```
E-test:            old,new=      -12.25274,      -12.25249      hartree
max    gradient:                        0.00080619    au/angstrom,radian
max      cart.      step:                        0.00675619      angstrom
Geometry Converged
```

	hartree	eV	kcal/mol	kJ/mol
Total Pauli Repulsion:	46.748604419054097	1272.0943	29335.20	122738.44
Electrostatic Energy:	-10.188903943973671	-277.2542	-6393.63	-26750.96
Total Orbital Interactions:	-48.727124965583535	-1325.9325	-30576.74	-127933.05
Dispersion Energy:	-0.126231525932954	-3.4349	-79.21	-331.42
Total Bonding Energy:	-12.293653304637559	-334.5273	-7714.38	-32276.98

Na,β[**1**]$_2$-tzp-blyp-d3;C_1

Coordinates in Geometry Cycle 113

Atom	X	Y	Z (Angstrom)
1.Pt	-0.500356	-1.693572	0.131273
2.O	0.863450	-2.097235	1.587342
3.O	3.092000	-2.308377	1.823017
4.N	-2.091093	-1.231544	1.427531
5.H	-2.373890	-2.074454	1.941493
6.H	-1.781445	-0.539366	2.121711
7.H	-1.777839	-0.285931	-1.685518
8.O	3.296513	-2.332304	-1.025994
9.C	2.087893	-2.240123	1.110786
10.H	-6.084625	-1.867176	-0.768182
11.H	-6.562838	-0.336113	-1.496847
12.C	-3.257067	-0.668686	0.646453
13.H	-2.984553	0.380303	0.478695
14.C	-4.601358	-0.751580	1.384405
15.H	-4.169431	0.312229	-1.819149
16.C	-5.790914	-0.812763	-0.880115
17.H	-4.528684	-0.230509	2.349540
18.H	-4.829190	-1.807107	1.603373
19.C	-4.424898	-0.738991	-1.604264
20.H	-4.470276	-1.260280	-2.570120
21.H	-3.503083	-2.424945	-0.589463
22.C	-5.733058	-0.151687	0.515247
23.H	-6.694224	-0.261985	1.031781
24.H	-5.568262	0.933787	0.397903
25.C	2.198107	-2.253963	-0.462465
26.O	1.058055	-2.119751	-1.115017
27.C	-3.313978	-1.351548	-0.732906
28.N	-1.934626	-1.246468	-1.344400
29.H	-1.852048	-1.870852	-2.153473
30.Pt	2.389667	0.949385	0.153777
31.O	0.842218	1.433943	-1.146132
32.O	-1.366943	1.894593	-1.102838
33.N	3.820553	0.472934	-1.275094
34.H	3.657039	-0.519846	-1.540088
35.H	3.745897	1.047507	-2.120816
36.H	4.196387	1.234616	2.033135
37.O	-1.269224	1.862403	1.695037
38.C	-0.269668	1.648639	-0.529040
39.H	7.491546	-1.618827	0.502874
40.H	8.567861	-0.377303	1.146464
41.C	5.200054	0.596019	-0.659625
42.H	5.371476	1.671517	-0.503384
43.C	6.323893	0.009578	-1.529058
44.H	6.635572	1.087944	1.700762
45.C	7.619996	-0.532436	0.616048
46.H	6.368359	0.536183	-2.493068
47.H	6.098697	-1.047356	-1.737053
48.C	6.452899	0.024363	1.470813
49.H	6.383011	-0.513879	2.425669
50.H	4.899914	-1.172205	0.531590
51.C	7.676653	0.128166	-0.780886
52.H	8.468766	-0.332241	-1.384249
53.H	7.938838	1.192304	-0.673705
54.C	-0.216045	1.623462	1.044441
55.O	0.934667	1.381967	1.574732
56.C	5.133399	-0.113701	0.699162
57.N	3.928002	0.427573	1.458540
58.H	3.593174	-0.323880	2.082872
59.Na	-2.729611	2.964956	0.358307

```
E-test:            old,new=      -12.09075,      -12.09076      hartree
max    gradient:                        0.00097561    au/angstrom,radian
max      cart.      step:                       0.00186767      angstrom
Geometry Converged
```

	hartree	eV	kcal/mol	kJ/mol
Total Pauli Repulsion:	46.503921007867987	1265.4361	29181.65	122096.03
Electrostatic Energy:	-10.187437164435920	-277.2143	-6392.71	-26747.11
Total Orbital Interactions:	-48.277826478577339	-1313.7065	-30294.80	-126753.42
Dispersion Energy:	-0.129426145059415	-3.5219	-81.22	-339.81
Total Bonding Energy:	-12.090767691010917	-329.0065	-7587.07	-31744.31

Frequency cm-1	Dipole Strength 1e-40 esu2 cm2	Absorption Intensity (degeneracy not counted) km/mole
24.983552	334.352457	2.093808
30.690248	232.773458	1.790655
39.183574	68.089922	0.668752
45.452869	335.196817	3.818909
55.625272	41.446267	0.577877
60.553220	262.302826	3.981239
66.621750	724.731530	12.102393
68.241154	15.389356	0.263236
79.489835	113.229175	2.256046
88.337029	233.363100	5.167173
99.206448	69.398744	1.725717
112.959111	21.880693	0.619527
120.780714	25.115962	0.760371
122.909954	925.766239	28.521113
151.627188	64.010589	2.432803
162.810617	217.283975	8.867241
172.165032	263.878194	11.387451
176.045842	25.393769	1.120549
186.137865	20.879510	0.974166
195.728884	44.807855	2.198301
197.076331	65.845115	3.252641
202.693829	228.286934	11.598442
213.924268	7.134446	0.382559
225.743840	475.219458	26.889838
230.189376	107.952084	6.228656
239.718756	172.435354	10.361113
250.978388	33.190513	2.087990
257.520383	214.723101	13.860167
261.751041	262.459390	17.219820
298.790824	33.320846	2.495522
305.019646	1114.201554	85.186278
329.964197	8.503578	0.703310
332.247789	12.607691	1.049967
337.037308	45.543396	3.847525
352.253198	14.194212	1.253269
355.290411	78.235008	6.967271
355.305237	38.729517	3.449227
369.303374	38.682592	3.580774
394.583420	212.139454	20.981588
424.081797	9.819074	1.043754
429.842073	6.037285	0.650472
432.578154	46.844290	5.079247
436.386524	35.282615	3.859314
443.287062	160.567675	17.841084
451.057259	915.565757	103.514047
492.755172	38.562535	4.762937
497.742173	4.590214	0.572685
507.766722	188.862732	24.037460
527.969118	222.485074	29.443367
546.309725	14.899927	2.040333
556.537111	28.090508	3.918608
561.134115	9.903010	1.392874
562.684139	19.865775	2.801872
567.062428	13.594530	1.932294
572.930542	44.878185	6.444887
577.132591	16.446822	2.379226
589.691338	18.818448	2.781548
696.701452	9.805010	1.712272
721.916392	23.478345	4.248469
740.179870	84.980653	15.766504
760.548452	25.556375	4.871965
762.291414	233.849738	44.682348
774.203720	0.662917	0.128645
782.765566	87.605043	17.188536
788.266858	4.205164	0.830872
789.278020	44.445525	8.792981
795.617206	53.850184	10.739138
825.479991	14.466633	2.993313
826.612959	10.414386	2.157814
839.166025	18.001928	3.786561
843.335589	6.311278	1.334123
845.467261	1.873421	0.397018
845.936692	1.904732	0.403878
861.310930	0.273290	0.059001
874.494389	1.256332	0.275385
905.016604	4.007207	0.909026
907.163488	10.803590	2.456585
924.280718	3.940009	0.912808
924.688613	4.681731	1.085126
962.930594	261.318029	63.072846
973.903985	246.247728	60.112729
1014.844138	7.581272	1.928499
1022.655844	43.122306	11.053748
1024.849664	7.486422	1.923147
1030.347800	8.065539	2.083029
1033.316849	59.183124	15.328846
1033.423558	46.720375	12.102156
1036.195640	25.957367	6.741871

1046.539929		41.688807	10.935870
1062.139692		25.751305	6.855813
1078.191450		32.510616	8.786161
1105.898317		20.348713	5.640664
1125.621820		50.999217	14.389115
1127.038034		101.629920	28.710333
1140.984457		130.143061	37.220210
1143.902428		71.973413	20.636648
1158.339666		46.752365	13.574304
1173.730401		3.080898	0.906408
1178.082838		25.848212	7.632809
1189.511008		5.767413	1.719601
1195.016728		27.842436	8.339870
1220.710435		44.812311	13.711598
1230.114372		6.164317	1.900678
1246.335770		44.501132	13.902221
1250.644392		102.473559	32.123564
1255.642828		11.748472	3.697648
1259.370280		25.532763	8.059894
1263.791620		947.164279	300.039790
1291.463624		27.190020	8.801765
1301.062906		0.325761	0.106237
1306.454832		1.435815	0.470187
1313.480122		0.072315	0.023808
1329.277259		210.254360	70.054922
1331.453568		2.793040	0.932140
1334.543316		6.826960	2.283695
1335.547138		18.477892	6.185712
1336.186613		3.157456	1.057505
1340.935658		22.219004	7.468108
1346.069467		23.869575	8.053603
1349.876722		12.203298	4.129043
1353.165515		2.519855	0.854682
1356.945704		6.578467	2.237511
1372.009467		4.042334	1.390168
1377.206840		6.905837	2.383930
1386.774894		9.926068	3.450335
1390.044337		29.301488	10.209310
1408.136963		9.896709	3.493122
1460.345954		7.685124	2.813097
1463.012147		4.401790	1.614193
1464.270332		11.356320	4.168089
1464.764205		10.520733	3.862707
1468.625777		27.316267	10.055660
1469.145225		22.573882	8.312833
1478.130669		20.015619	7.415833
1479.216307		13.016121	4.826045
1544.547533		270.208908	104.611399
1559.057077		383.801961	149.984809
1566.153232		2193.909917	861.253723
1583.719383		926.567004	367.818131
1606.028060		169.204774	68.115165
1616.296677		224.265697	90.857755
1626.048281		285.034107	116.173838
1643.594165		1480.546705	609.950755
2896.336240		47.505742	34.488408
2914.568540		23.817573	17.400024
2918.603143		19.398564	14.191317
2932.247317		14.224675	10.454928
2933.638486		22.769784	16.743397
2941.904875	11.296263	8.329933	
2947.377561		23.196239	17.136866
2948.060313		20.784364	15.358584
2950.312050		17.354475	12.833866
2962.805735		3.723335	2.765116
2974.831204		18.729877	13.966106
2984.851459		50.018991	37.422752
2986.489236		8.889153	6.654255
2987.229281		0.767355	0.574570
2994.813439		13.643820	10.241978
2997.116447		44.721630	33.596908
2999.116769		30.071830	22.606395
2999.824817		35.566194	26.743076
3000.786543		29.840287	22.444823
3006.953573		3.604820	2.716992
3123.640903		255.152620	199.774109
3245.173279		125.457046	102.049532
3278.559661		58.345607	47.947871
3313.784141		21.087787	17.515933
3368.750853		53.157564	44.886117
3379.723781		50.674901	42.929140
3383.820361		39.273539	33.310827
3389.017525	46.411446	39.425480	

Zero-Point Energy : 0.462875 a.u.
========== 12.595468 eV

Statistical Thermal Analysis *** ideal gas assumed ***

Temp			Transl	Rotat	Vibrat	Total
298.15	Entropy (cal/mole-K):		45.980	37.236	121.988	205.203
	Internal Energy (Kcal/mole):		0.889	0.889	309.019	310.797
	Constant Volume Heat Capacity (cal/mole-K):	2.981	2.981	117.952	123.913	

β[**1**]$_2$-DMSO-tzp-blyp-d3;C_1

Coordinates in Geometry Cycle 33

Atom	X	Y	Z (Angstrom)
1.Pt	-0.536060	-1.651415	0.143751
2.O	0.850795	-2.103011	1.609921
3.O	3.066949	-2.436181	1.844660
4.N	-2.132356	-1.173424	1.401104
5.H	-2.449547	-2.019372	1.888300
6.H	-1.836055	-0.503039	2.120436
7.H	-1.751926	-0.204788	-1.642324
8.O	3.274070	-2.473101	-0.995080
9.C	2.063674	-2.275906	1.132396
10.H	-6.065330	-1.799085	-0.851830
11.H	-6.546588	-0.263535	-1.581161
12.C	-3.280820	-0.567830	0.614525
13.H	-3.005378	0.483745	0.468647
14.C	-4.632032	-0.671042	1.336352
15.H	-4.154444	0.404921	-1.852579
16.C	-5.783037	-0.739670	-0.952656
17.H	-4.580812	-0.143354	2.298357
18.H	-4.846130	-1.730676	1.550179
19.C	-4.405253	-0.649058	-1.654755
20.H	-4.424198	-1.173635	-2.619697
21.H	-3.522314	-2.331832	-0.609187
22.C	-5.754766	-0.081153	0.446071
23.H	-6.723028	-0.212109	0.946184
24.H	-5.594085	1.002227	0.335433
25.C	2.177418	-2.296238	-0.437831
26.O	1.050156	-2.133072	-1.092859
27.C	-3.323105	-1.261195	-0.752710
28.N	-1.928141	-1.172737	-1.332640
29.H	-1.852414	-1.774925	-2.158598
30.Pt	2.407721	0.993226	0.180702
31.O	0.827670	1.489861	-1.057295
32.O	-1.394881	1.837293	-0.967914
33.N	3.808398	0.539448	-1.294829
34.H	3.635527	-0.424903	-1.617192
35.H	3.735950	1.151227	-2.113968
36.H	4.314674	1.349193	1.933912
37.O	-1.207213	1.735096	1.873187
38.C	-0.303140	1.644751	-0.406349
39.H	7.461219	-1.661342	0.361606
40.H	8.589663	-0.458495	0.995732
41.C	5.200086	0.620529	-0.706122
42.H	5.399471	1.689107	-0.547140
43.C	6.286630	0.019805	-1.610540
44.H	6.712674	1.055367	1.611573
45.C	7.623738	-0.580098	0.488869
46.H	6.311187	0.557657	-2.568003
47.H	6.035069	-1.030893	-1.824211
48.C	6.497657	-0.000768	1.381659
49.H	6.440347	-0.541869	2.335769
50.H	4.872732	-1.140235	0.489680
51.C	7.660577	0.098606	-0.899918
52.H	8.426957	-0.369450	-1.531009
53.H	7.943558	1.156070	-0.782147
54.C	-0.199282	1.593724	1.163875
55.O	1.011110	1.414758	1.645192
56.C	5.149788	-0.091345	0.651827
57.N	3.998748	0.506238	1.440475
58.H	3.701008	-0.167196	2.156278

```
E-test:            old,new=      -12.25143,      -12.25146      hartree
max    gradient:                        0.00092979    au/angstrom,radian
max      cart.      step:                        0.00327721      angstrom
Geometry Converged
```

	hartree	eV	kcal/mol	kJ/mol
Total Pauli Repulsion:	46.248773311524502	1258.4932	29021.55	121426.14
Electrostatic Energy:	-10.077476618737419	-274.2221	-6323.71	-26458.41
Total Orbital Interactions:	-48.220204345710087	-1312.1385	-30258.64	-126602.13
Solvation:	-0.078386876553813	-2.1330	-49.19	-205.80
Dispersion Energy:	-0.124226434763154	-3.3804	-77.95	-326.16
Total Bonding Energy:	-12.251511658182523	-333.3806	-7687.94	-32166.34

Frequency	Dipole Strength	Absorption Intensity (degeneracy not counted)
cm-1	1e-40 esu2 cm2	km/mole
-17.166903	0.000000	0.000000
20.550710	464.041746	2.390353
24.966485	377.337565	2.361378
40.102143	50.662578	0.509252
50.864624	35.519812	0.452861
52.248234	58.768751	0.769655
66.418843	228.186840	3.798918
70.188212	30.059719	0.528843
83.500026	2.180000	0.045627
97.403072	283.026167	6.909988
101.209418	64.622372	1.639389
109.247956	272.343717	7.457766
116.230006	3776.144352	110.013231
128.533218	4.118095	0.132675
142.131127	102.573157	3.654273
142.544206	66.144329	2.363308
180.455226	19.624721	0.887669
182.207587	224.275129	10.242964
191.953763	1.267999	0.061009
195.241807	565.652228	27.682187
205.362131	76.228322	3.923872
207.626307	8.864731	0.461345
228.640703	1279.680124	73.338672
234.479775	34.617479	2.034599
250.201948	191.999061	12.041147
251.435558	10.682908	0.673278
282.675976	27.274755	1.932537
284.855176	1550.089034	110.677370
324.599830	18.105100	1.473083
325.682477	27.208779	2.221169
336.795824	35.467542	2.994166
337.671202	185.778047	15.724125
341.733614	97.088730	8.316385
342.995967	17.897404	1.538711
344.929653	14.835195	1.282631
346.610756	221.521211	19.245776
426.547327	63.844104	6.825997
427.028614	38.871427	4.160692
432.887370	121.750307	13.210615
433.337971	4.442396	0.482527
441.379322	0.185448	0.020517
442.595886	2181.134388	241.973534
490.791448	23.341101	2.871418
491.370921	66.199744	8.153495
512.973907	791.919897	101.825042
514.668095	9.464108	1.220914
551.474008	25.034308	3.460499
551.690693	26.838254	3.711316
561.842055	11.033451	1.553831
562.583967	1.384961	0.195300
565.062541	33.783088	4.784912
566.490762	201.518741	28.614512
580.344887	12.428142	1.807883
580.682385	66.565311	9.688682
692.813735	48.892552	8.490578
693.325952	37.002063	6.430451
744.648377	520.875783	97.221761
746.146046	27.000489	5.049793
757.037836	363.850424	69.042823
757.535321	499.951508	94.931172
776.214764	1.333231	0.259397
776.323091	6.411916	1.247695
787.469110	38.322061	7.564156
788.115935	1.513135	0.298914
821.159434	5.291147	1.089069
821.353675	40.425116	8.322610
841.932581	73.044485	15.414975
842.251476	32.038912	6.763907
842.316257	1.339596	0.282831
842.567317	18.666525	3.942268
863.898043	0.800242	0.173285
864.034557	1.639889	0.355160
899.137362	48.480880	10.926338
899.421524	26.595544	5.995843
919.485385	4.644648	1.070473
919.701827	6.733233	1.552204
965.033171	817.832699	197.826644
965.699207	8.056973	1.950257
1015.038852	0.907954	0.231007
1015.223266	23.014807	5.856619
1025.442751	239.139226	61.466758
1025.595681	2.826072	0.726503
1028.254800	5.066541	1.305841
1028.505652	5.397419	1.391461
1039.469015	20.785372	5.415610
1039.829428	17.178100	4.477291
1068.617519	43.615376	11.682613
1069.329851	37.798552	10.131294

1114.690712		40.484605	11.311556
1115.138358		44.300222	12.382625
1135.855678		199.008289	56.659455
1137.428731		242.883842	69.246988
1152.512544		110.316762	31.868765
1153.172814		49.037993	14.174415
1175.235709		21.507353	6.335633
1177.155756		381.705056	112.626325
1188.159222		33.385795	9.942931
1188.992760		29.565287	8.811288
1201.048108		21.566632	6.492632
1202.184640		5.060841	1.525007
1227.978887		5.219043	1.606423
1228.548764		39.474409	12.155872
1244.528947		7.403596	2.309542
1244.724839		7.453438	2.325456
1269.179656		38.698150	12.310945
1273.637302		4318.480578	1378.652495
1288.583371		2.580154	0.833367
1289.060835		0.817639	0.264188
1303.715943		0.829029	0.270913
1304.049421		2.185827	0.714476
1324.486169		0.557386	0.185047
1324.803558		0.327446	0.108735
1326.738514		2.668833	0.887534
1327.178321		3.026472	1.006802
1333.812324		8.590071	2.871901
1333.939436		12.821149	4.286878
1346.170258		15.473497	5.221155
1347.310217		15.154636	5.117893
1367.947304		0.258215	0.088538
1368.076057		0.243151	0.083380
1381.698177		19.096980	6.613874
1382.055099		15.309867	5.303650
1397.052313		9.216820	3.227541
1397.231528		36.463746	12.770495
1445.130781		23.045385	8.347745
1445.375551		8.902991	3.225483
1445.467337		17.826216	6.458706
1445.748065		22.437359	8.130971
1447.897870		66.484697	24.128909
1448.210399		60.340003	21.903578
1457.720036		7.162274	2.616996
1458.246435		8.049172	2.942119
1546.417759		657.406039	254.822979
1548.531109		1168.355420	453.495500
1553.735807		2208.542353	860.123824
1555.995704		325.060931	126.780143
1587.587261		227.340224	90.467369
1588.737233		165.989428	66.101387
1592.597989		4409.899634	1760.406400
1594.673492		1643.244887	656.828721
2926.235134		32.454353	23.804565
2927.099366		31.361147	23.009515
2931.402596		22.900988	16.827041
2931.935123		24.462107	17.977376
2934.717791		21.764879	16.010344
2935.110818		31.184413	22.942468
2937.484644		145.180435	106.896078
2937.555766		9.603660	7.071328
2965.576761	13.357803	9.929383	
2966.979536		14.653061	10.897352
2980.542256		48.711824	36.392152
2981.131865		98.769319	73.804241
2986.749075		64.769058	48.489130
2987.071834		34.667548	25.956543
2987.667093		24.042215	18.004653
2988.695628		103.681474	77.671362
2989.414523		32.864366	24.625750
2989.588861		92.410126	69.248297
3000.634392		16.647521	12.521049
3001.827835		21.256739	15.994125
3270.158236		81.283794	66.627084
3271.256882		233.760711	191.674456
3324.157191		87.690180	73.065201
3325.406739		54.462751	45.396504
3388.656840		241.942292	205.502662
3389.029251		63.063482	53.571195
3393.572062		147.329483	125.321276
3394.114350	131.547406	111.914621	

Zero-Point Energy :	0.459595	a.u.
==========	12.506218	eV
(imaginary frequencies were excluded from the summation)		

```
Statistical       Thermal       Analysis              ***              ideal       gas       assumed              ***
     Temp                                                                 Transl      Rotat     Vibrat       Total
     ----                                                                 ------      -----     ------       -----

     298.15    Entropy (cal/mole-K):                                     45.894     37.022    113.497     196.413
               Internal Energy (Kcal/mole):                              0.889       0.889    305.669     307.446
               Constant Volume Heat Capacity (cal/mole-K):       2.981    2.981   111.511   117.472
```

γ[**1**]$_2$-tzp-blyp-d3;C_1

```
  Coordinates      in      Geometry      Cycle      125
   Atom         X           Y           Z   (Angstrom)
   1.Pt          -0.628856    -0.148244      2.506780
   2.O            1.030989     0.215309      3.645248
   3.O            3.221993    -0.335010      3.747102
   4.N           -1.984697     0.923391      3.699978
   5.H           -2.090839     0.427378      4.593163
   6.H           -1.617044     1.853370      3.925828
   7.H           -2.420944     0.151034      0.588876
   8.O            2.862283    -1.765393      1.286488
   9.C            2.126241    -0.399995      3.203319
  10.H           -6.204800    -0.735088      3.178948
  11.H           -7.016696     0.144154      1.881104
  12.C           -3.331836     1.037969      3.010427
  13.H           -3.217257     1.831125      2.258330
  14.C           -4.483035     1.378994      3.969299
  15.H           -4.841945     0.502798      0.696595
  16.C           -6.080260     0.082274      2.450322
  17.H           -4.291360     2.345963      4.455839
  18.H           -4.526692     0.616355      4.765404
  19.C           -4.910973    -0.251663      1.492691
  20.H           -5.076144    -1.222646      1.004650
  21.H           -3.602845    -1.102867      3.004298
  22.C           -5.831368     1.407042      3.207716
  23.H           -6.648173     1.604117      3.914602
  24.H           -5.821167     2.240739      2.489752
  25.C            1.923770    -1.209854      1.867075
  26.O            0.695626    -1.201752      1.361749
  27.C           -3.578415    -0.287390      2.264843
  28.N           -2.371634    -0.515134      1.393834
  29.H           -2.380869    -1.461433      1.001367
  30.Pt           0.693152     0.410733     -2.472782
  31.O           -0.757128     1.217628     -3.669055
  32.O           -2.856769     2.049944     -3.528537
  33.N            2.145737     0.157180     -3.965777
  34.H            1.916303    -0.682160     -4.512108
  35.H            2.139938     0.944279     -4.623117
  36.H            2.567565     0.380907     -0.641225
  37.O           -2.836763     1.317479     -0.751263
  38.C           -1.875359     1.532085     -3.013289
  39.H            5.549579    -2.601666     -2.563090
  40.H            6.745921    -1.604686     -1.735971
  41.C            3.510835     0.000090     -3.328676
  42.H            3.792179     1.007285     -2.989140
  43.C            4.583129    -0.543419     -4.287289
  44.H            4.973998    -0.036482     -0.952623
  45.C            5.790827    -1.566233     -2.275585
  46.H            4.687170     0.126642     -5.153314
  47.H            4.255577    -1.524250     -4.671080
  48.C            4.686419    -1.030745     -1.333133
  49.H            4.551040    -1.676390     -0.459315
  50.H            3.025894    -1.898372     -2.426936
  51.C            5.935491    -0.701259     -3.549043
  52.H            6.676640    -1.139138     -4.230497
  53.H            6.309845     0.296525     -3.272345
  54.C           -1.847886     1.159687     -1.485887
  55.O           -0.723841     0.638641     -1.033170
  56.C            3.352136    -0.903077     -2.090021
  57.N            2.215988    -0.365070     -1.253230
  58.H          1.889621   -1.091849   -0.598364
```

```
current energy                                  -12.15498145 Hartree
energy change                    -0.00000059      0.00100000     T
constrained gradient max          0.00076909      0.00100000     T
constrained gradient rms          0.00022509      0.00066667     T
gradient  max                                           0.00076909
gradient  rms                                           0.00022509
cart. step max                    0.00669548      0.01000000     T
cart. step rms                    0.00269901      0.00666667     T
GEOMETRY CONVERGED
```

	hartree	eV	kcal/mol	kJ/mol
Total Pauli Repulsion:	46.168343421658975	1256.3045	28971.08	121214.97
Electrostatic Energy:	-10.051627601704107	-273.5187	-6307.49	-26390.54
Total Orbital Interactions:	-48.172202239534329	-1310.8323	-30228.52	-126476.10
Dispersion Energy:	-0.099503577254732	-2.7076	-62.44	-261.25
Total Bonding Energy:	-12.154985277907436	-330.7540	-7627.37	-31912.91

Frequency cm-1	Dipole Strength 1e-40 esu2 cm2	Absorption Intensity (degeneracy not counted) km/mole
-6.689412	0.000000	0.000000
13.636589	0.000000	0.000000
22.907557	49.999205	0.287091
28.721779	130.499039	0.939500
30.681789	404.067728	3.107513
37.595216	112.177622	1.057102
47.177723	747.319972	8.837341
62.661116	12.541411	0.196980
65.208224	34.725371	0.567580
77.595366	80.310472	1.562018
86.749825	17.631484	0.383385
95.502689	239.046965	5.722383
116.615600	476.711862	13.934477
126.258989	62.928868	1.991546
130.291847	31.141355	1.017028
146.351262	315.096070	11.558927
179.914645	3.351528	0.151143
181.505212	12.954393	0.589365
187.940862	4.331659	0.204058
190.290536	230.230292	10.981400
205.723845	14.169313	0.730654
209.903291	9.200875	0.484090
236.178833	66.407036	3.931272
244.457872	103.859271	6.363959
255.966066	30.660967	1.967190
263.886550	182.793001	12.090796
290.968136	301.356403	21.978797
293.802963	168.391703	12.400949
329.808374	10.289864	0.850647
331.115829	14.317217	1.188274
334.807098	25.908322	2.174263
347.925040	82.932087	7.232465
352.051473	5.999852	0.529450
358.885232	144.953086	13.039506
360.182363	35.525545	3.207312
368.482321	27.785683	2.566350
423.600954	11.430865	1.213708
425.387642	4.609779	0.491522
434.320692	35.101256	3.821301
434.894461	27.768293	3.026991
443.260311	143.502520	15.943969
447.002331	263.804033	29.557608
494.022687	45.817495	5.673568
499.790511	23.420519	2.934017
522.387154	88.071820	11.532077
532.056279	313.323159	41.785744
545.566174	22.382748	3.060828
546.970269	22.163782	3.038685
553.696953	153.963968	21.368267
558.832914	20.452834	2.864927
561.190753	2.395861	0.337016
564.806510	11.177581	1.582434
578.922435	12.674552	1.839209
581.378463	138.318984	20.156671
675.693723	12.865077	2.178915
676.238456	34.439020	5.837525
708.651873	74.258493	13.190375
756.978910	55.773783	10.582589
764.765402	218.947087	41.970629
767.111321	238.370831	45.834191
770.077354	8.143625	1.571919
781.188908	26.167372	5.123825
791.633602	1.760780	0.349388
791.843165	1.263960	0.250871
826.512379	20.134393	4.171248
826.959046	21.060888	4.365548
841.041211	25.492365	5.374097
845.984177	8.159847	1.730304
847.638405	31.168015	6.622132
849.326621	7.496619	1.595946
856.531794	10.182492	2.186128
863.508070	12.007340	2.598910
904.925770	3.539738	0.802901
906.988470	15.190200	3.453372
924.868573	8.738341	2.025756
926.440040	23.003501	5.341821
969.643821	176.992070	43.017396

972.650068		252.605208	61.585290
1019.741359		2.268760	0.579905
1019.777058		21.184379	5.415007
1022.407410		33.912965	8.690961
1026.712625		50.308248	12.946911
1027.191722		9.206654	2.370453
1028.196331		8.666515	2.233565
1035.243778		14.173529	3.677890
1035.724179		28.027292	7.276178
1052.775311		30.836447	8.137258
1064.458326		12.632422	3.370493
1096.149123		72.712625	19.978254
1099.565903		87.434893	24.098173
1116.652173		6.816303	1.907853
1127.555879		86.362637	24.408553
1128.803877		57.547606	16.282603
1139.093852		20.739137	5.921453
1139.882779		156.504343	44.716176
1145.875688		37.277394	10.706835
1167.276907		5.968371	1.746255
1176.673432		3.594834	1.060261
1188.130060		36.632663	10.909643
1215.125384		61.159695	18.627925
1227.421006		26.755132	8.231495
1232.219053		3.791423	1.171030
1252.002627		921.268825	289.114375
1257.113367		107.879922	33.993285
1260.446833		25.718658	8.125515
1270.404625		1007.565883	320.843755
1290.236803		0.404837	0.130927
1299.181526		37.074597	12.073254
1309.128693		9.649019	3.166238
1310.181053		0.978487	0.321340
1333.983071		5.739698	1.919188
1334.102199		7.626491	2.550304
1334.980681		3.123878	1.045315
1335.674814		25.466612	8.526091
1340.469539		11.769526	3.954522
1342.204534		26.513752	8.920064
1349.629185		5.255589	1.777927
1352.917226		6.906269	2.342032
1362.208966		0.867026	0.296042
1366.049881		7.765984	2.659140
1369.730244		0.794615	0.272816
1377.057584		0.920847	0.317847
1390.030841		53.253300	18.554490
1392.308259		43.814273	15.290760
1461.302853		3.348764	1.226600
1461.957216		4.116285	1.508406
1463.260819		11.447568	4.198683
1464.065190		11.370868	4.172844
1470.505473		22.185138	8.177242
1470.556872		23.397087	8.624257
1479.545131		1.987670	0.737141
1481.573524		7.277188	2.702495
1595.523163		915.890910	366.289891
1604.314959		81.438588	32.748992
1608.537994		82.957020	33.447413
1620.702815		1045.488086	424.717880
1634.842624		109.361284	44.814404
1645.088314		262.948935	108.427315
1663.576148		1321.698419	551.128824
1670.243675		1369.321063	573.275253
2913.542202		18.435305	13.463244
2917.205907		22.697563	16.596801
2921.908757		1.444401	1.057870
2924.396907		29.187983	21.395304
2931.022789		20.954495	15.394815
2935.768446		66.185689	48.703925
2936.913347		33.579148	24.719454
2941.761464		20.673200	15.243800
2948.228247	7.803639	5.766819	
2951.922543		18.830703	13.933158
2960.565500		18.164277	13.479409
2965.473051		32.011646	23.794690
2974.729673		35.071810	26.150727
2980.472123		19.363556	14.465993
2986.364655		70.968139	53.123212
2987.383448		72.061139	53.959779
2987.520903		15.356621	11.499652
2990.257005		38.006837	28.487105
2998.782556		38.278921	28.772840
3017.847277		1115.722675	843.978897
3034.429194		5.839454	4.441476
3283.692178		351.543651	289.347522
3321.561784		7.618651	6.343055
3325.231715		6.741538	5.619000
3359.252749		44.618947	37.569903
3386.260795		25.300662	21.474861
3391.063361		23.810933	20.239062
3393.319013		24.319114	20.684761

1063.713461	310.806089	82.869028
1104.335661	31.465676	8.709962
1107.098037	22.673896	6.292023
1149.959730	35.050533	10.103116
1151.584968	32.173524	9.286941
1173.434182	5.882532	1.730219
1177.712348	6.108679	1.803286
1209.407418	301.382988	91.362807
1210.511848	198.081288	60.102227
1222.128629	19.294067	5.910426
1222.796752	136.394499	41.805094
1234.069045	148.228915	45.851174
1236.551099	26.397191	8.181781
1240.924411	347.246915	108.009460
1242.733186	236.158434	73.562999
1242.978989	104.422772	32.533971
1247.519462	24.755319	7.740944
1259.278013	1912.953097	603.815160
1264.280332	1095.697577	347.225933
1374.037533	541.060900	186.347177
1381.216830	5.035922	1.743488
1449.452041	21.814213	7.925405
1450.178091	12.298439	4.470431
1452.197918	5.134460	1.868954
1452.342306	13.984369	5.090846
1474.723708	53.397103	19.738149
1475.083065	34.589057	12.788902
1573.535168	198.117876	78.140860
1581.093149	1502.269808	595.365228
1602.029809	109.669033	44.038516
1607.363702	221.143358	89.097625
1613.323892	42.470718	17.174703
1614.147655	14.517253	5.873619
1629.301227	7.430482	3.034565
1629.419630	100.950585	41.230619
1633.685152	29.058617	11.899299
1636.653243	2058.876940	844.627340
1641.162053	49.006027	20.159467
1644.460653	663.921682	273.664465
2968.734265	38.104524	28.354757
2968.962175	50.911602	37.887810
2975.321082	40.632981	30.303347
2977.868553	67.961634	50.727961
3007.206321	18.483430	13.932334
3007.552433	12.093074	9.116497
3013.372597	27.299586	20.619919
3013.497795	7.279093	5.498272
3029.293501	40.863286	31.027924
3030.583938	32.719571	24.854898
3065.890612	5.705512	4.384593
3066.532236	6.620279	5.088642
3209.817744	401.483533	323.017596
3223.962584	664.354204	536.868287
3278.270022	142.607965	117.183530
3292.130275	8.624293	7.116699
3292.449436	10.997309	9.075773
3298.452294	118.802411	98.223076
3393.489965	32.135615	27.334507
3394.318949	35.822757	30.478229
3407.165530	75.407477	64.399977
3411.035481	90.834071	77.662807
3425.928232	32.299172	27.736248
3427.389953	35.025801	30.090518

Zero-Point Energy :	0.459808	a.u.
==========	12.512002	eV

(imaginary frequencies were excluded from the summation)

Statistical Thermal Analysis *** ideal gas assumed ***

Temp		Transl	Rotat	Vibrat	Total
298.15	Entropy (cal/mole-K):	45.894	37.862	111.274	195.031
	Internal Energy (Kcal/mole):	0.889	0.889	305.314	307.092
	Constant Volume Heat Capacity (cal/mole-K):	2.981	2.981	109.330	115.291

γ[**1**]$_2$-tzp-blyp-d3bj;C_1

Coordinates	in	Geometry	Cycle	25
Atom	X	Y	Z	(Angstrom)
1.Pt	-0.629276	-0.201792	2.460529	
2.O	1.066428	0.189043	3.534720	
3.O	3.252257	-0.384310	3.590986	
4.N	-1.928274	0.965481	3.612467	
5.H	-2.023384	0.530538	4.537414	
6.H	-1.534620	1.899217	3.764592	
7.H	-2.451263	0.027385	0.564170	
8.O	2.795737	-1.940503	1.236584	
9.C	2.135920	-0.466476	3.092312	
10.H	-6.178705	-0.642392	3.279941	
11.H	-7.002592	0.174326	1.950033	
12.C	-3.284275	1.063399	2.945744	
13.H	-3.172441	1.806955	2.145403	
14.C	-4.406189	1.480751	3.905269	
15.H	-4.850605	0.421640	0.703800	
16.C	-6.055880	0.128136	2.502633	
17.H	-4.189418	2.471739	4.328851	
18.H	-4.443881	0.767025	4.745193	
19.C	-4.915946	-0.282224	1.544417	
20.H	-5.109443	-1.277568	1.120113	
21.H	-3.587431	-1.066642	3.073250	
22.C	-5.768413	1.487851	3.174151	
23.H	-6.565271	1.739449	3.885768	
24.H	-5.761274	2.277383	2.408432	
25.C	1.880806	-1.345355	1.815466	
26.O	0.640731	-1.344638	1.345698	
27.C	-3.569657	-0.296482	2.287575	
28.N	-2.392110	-0.592638	1.404701	
29.H	-2.422510	-1.560630	1.072396	
30.Pt	0.669753	0.378858	-2.467377	
31.O	-0.763814	1.208721	-3.663085	
32.O	-2.874559	2.012262	-3.527020	
33.N	2.157040	0.229957	-3.925263	
34.H	1.952061	-0.576943	-4.526371	
35.H	2.155818	1.056268	-4.531673	
36.H	2.504122	0.325695	-0.616810	
37.O	-2.909058	1.152641	-0.797461	
38.C	-1.898115	1.479433	-3.017289	
39.H	5.523624	-2.578308	-2.588460	
40.H	6.702440	-1.627314	-1.686594	
41.C	3.504195	0.051107	-3.265525	
42.H	3.770153	1.041418	-2.869897	
43.C	4.598904	-0.436749	-4.224401	
44.H	4.913833	-0.095398	-0.868859	
45.C	5.759703	-1.559726	-2.243387	
46.H	4.723336	0.280083	-5.048755	
47.H	4.282837	-1.394992	-4.668948	
48.C	4.637122	-1.071077	-1.301320	
49.H	4.483075	-1.756652	-0.461914	
50.H	3.006599	-1.889397	-2.470314	
51.C	5.932051	-0.632683	-3.465597	
52.H	6.687663	-1.036397	-4.151588	
53.H	6.299698	0.349159	-3.130381	
54.C	-1.901607	1.036818	-1.514456	
55.O	-0.784336	0.509723	-1.057042	
56.C	3.322996	-0.910750	-2.080570	
57.N	2.171810	-0.413847	-1.246772	
58.H	1.843921	-1.160731	-0.615715	

current energy		-12.22315477 Hartree	
energy change	-0.00000556	0.00100000	T
constrained gradient max	0.00087882	0.00100000	T
constrained gradient rms	0.00017912	0.00066667	T
gradient max		0.00087882	
gradient rms		0.00017912	
cart. step max	0.00741290	0.01000000	T
cart. step rms	0.00232675	0.00666667	T
GEOMETRY CONVERGED			

	hartree	eV	kcal/mol	kJ/mol
Total Pauli Repulsion:	46.405701097622973	1262.7634	29120.02	121838.15
Electrostatic Interaction:	-10.114581570324718	-275.2318	-6347.00	-26555.83
Total Orbital Interactions:	-48.346020902598561	-1315.5622	-30337.59	-126932.46
Dispersion Energy:	-0.168264559977216	-4.5787	-105.59	-441.78
Total Bonding Energy:	-12.223154756739504	-332.6090	-7670.15	-32091.89

α,α[**1**]$_3$-tzp-blyp-d3;C_1

Coordinates	in	Geometry	Cycle	153
Atom	X	Y	Z	(Angstrom)
1.Pt	-0.820168	-1.698177	0.201498	
2.O	0.528106	-2.057390	1.690148	
3.O	2.716031	-2.530643	1.960838	
4.N	-2.470840	-1.349967	1.452376	
5.H	-2.684957	-2.215385	1.961812	
6.H	-2.246236	-0.636199	2.155392	
7.H	-2.146611	-0.395086	-1.666260	
8.O	2.980211	-2.499915	-0.881953	
9.C	1.744153	-2.343539	1.235469	
10.H	-6.353321	-2.297100	-0.868805	
11.H	-6.911301	-0.780833	-1.581631	
12.C	-3.670951	-0.896865	0.645067	
13.H	-3.549836	0.179415	0.506383	
14.C	-5.013772	-1.131122	1.346965	
15.H	-4.567314	0.028402	-1.829793	
16.C	-6.127960	-1.222192	-0.951977	
17.H	-5.006323	-0.623745	2.321920	
18.H	-5.158135	-2.209291	1.531672	
19.C	-4.752356	-1.038135	-1.639225	
20.H	-4.730847	-1.560816	-2.606740	
21.H	-3.725907	-2.660073	-0.608469	
22.C	-6.155372	-0.584086	0.456561	
23.H	-7.124177	-0.765195	0.939482	
24.H	-6.035587	0.505765	0.367167	
25.C	1.890356	-2.342110	-0.337472	
26.O	0.780589	-2.058280	-1.018616	
27.C	-3.625308	-1.572075	-0.738042	
28.N	-2.239243	-1.357306	-1.310806	
29.H	-2.083522	-1.982977	-2.107349	
30.Pt	0.824781	1.443855	0.039868	
31.O	-0.792866	1.607684	-1.257624	
32.O	-3.027027	1.877759	-1.193819	
33.N	2.253332	0.821813	-1.345515	
34.H	2.105106	-0.174823	-1.565921	
35.H	2.169620	1.347420	-2.221625	
36.H	2.738290	2.267768	1.592564	
37.O	-2.844461	2.170842	1.622528	
38.C	-1.930436	1.818388	-0.625687	
39.H	5.936484	-0.957072	0.605373	
40.H	7.040710	0.335509	1.102193	
41.C	3.641879	1.044777	-0.767469	
42.H	3.775343	2.127328	-0.788884	
43.C	4.769168	0.386837	-1.569316	
44.H	5.142105	1.874943	1.519118	
45.C	6.083570	0.133525	0.604892	
46.H	4.786408	0.811572	-2.583421	
47.H	4.578802	-0.693091	-1.645861	
48.C	4.942628	0.799386	1.413998	
49.H	4.879171	0.363258	2.421301	
50.H	3.364018	-0.486525	0.725491	
51.C	6.116627	0.652790	-0.851119	
52.H	6.925936	0.164925	-1.409533	
53.H	6.319391	1.734169	-0.856940	
54.C	-1.827625	2.022294	0.941615	
55.O	-0.598874	2.066986	1.425938	
56.C	3.606361	0.578052	0.691995	
57.N	2.443525	1.308299	1.351671	
58.H	2.181670	0.823590	2.216974	
59.Pt	1.674963	4.749656	-0.226004	
60.C	4.421563	4.360455	0.406102	
61.C	4.328966	4.354607	-1.172608	
62.O	3.242749	4.427649	1.044827	
63.O	5.487768	4.222260	0.988262	
64.O	3.093600	4.474268	-1.669172	
65.O	5.320872	4.168288	-1.865523	
66.N	0.182637	5.046113	1.237333	
67.H	0.529240	5.584019	2.037514	
68.H	-0.110083	4.119401	1.587781	
69.N	0.041040	5.024277	-1.526912	
70.H	0.009134	4.250259	-2.199761	
71.H	0.150177	5.892285	-2.064220	
72.C	-1.003553	5.743585	0.603878	
73.C	-3.482531	6.303170	0.717977	
74.C	-2.266706	5.728993	1.486270	
75.C	-1.252473	5.042814	-0.742422	

76.C	-2.449464	5.616712	-1.509012
77.C	-3.711663	5.556241	-0.615281
78.H	-0.686128	6.780033	0.415139
79.H	-3.319010	7.373799	0.514485
80.H	-4.376628	6.233699	1.351011
81.H	-2.484179	4.694018	1.788861
82.H	-2.078144	6.309047	2.401402
83.H	-1.457978	3.994655	-0.529958
84.H	-4.566294	5.986593	-1.153834
85.H	-2.601547	5.034812	-2.428901
86.H	-2.240128	6.659655	-1.801568
87.H	-3.950556	4.501012	-0.415098

```
E-test:            old,new=      -18.29127,      -18.29140      hartree
max    gradient:                        0.00093604    au/angstrom,radian
max      cart.      step:                        0.00685308      angstrom
Geometry Converged
```

	hartree	eV	kcal/mol	kJ/mol
Total Pauli Repulsion:	69.595767715170993	1893.7972	43672.01	182723.66
Electrostatic Energy:	-15.153682357890023	-412.3527	-9509.08	-39785.99
Total Orbital Interactions:	-72.521802529899446	-1973.4187	-45508.12	-190405.97
Dispersion Energy:	-0.211842348420472	-5.7645	-132.93	-556.19
Total Bonding Energy:	-18.291548974587837	-497.7384	-11478.12	-48024.46

Na,α,α[**1**]$_3$-tzp-blyp-d3;C$_1$

Coordinates in Geometry Cycle 162

Atom	X	Y	Z (Angstrom)
1.Pt	-1.184643	-1.638021	0.247368
2.O	0.197078	-1.702373	1.752756
3.O	2.427863	-1.552706	2.019867
4.N	-2.853972	-1.268413	1.459040
5.H	-3.047725	-2.092325	2.040072
6.H	-2.656940	-0.481677	2.090434
7.H	-2.564232	-0.571611	-1.691509
8.O	2.693606	-1.901140	-0.805933
9.C	1.435883	-1.714497	1.302268
10.H	-6.666031	-2.590712	-0.779184
11.H	-7.303654	-1.175975	-1.617592
12.C	-4.061403	-0.918163	0.610407
13.H	-3.936937	0.143460	0.367907
14.C	-5.398329	-1.143597	1.331029
15.H	-4.996356	-0.258867	-1.917925
16.C	-6.500993	-1.515733	-0.950731
17.H	-5.426861	-0.547695	2.253870
18.H	-5.482914	-2.204569	1.621548
19.C	-5.131334	-1.317116	-1.644950
20.H	-5.077983	-1.906242	-2.571669
21.H	-4.064724	-2.799349	-0.462628
22.C	-6.574206	-0.763050	0.398110
23.H	-7.526562	-0.975878	0.899775
24.H	-6.544650	0.321518	0.213948
25.C	1.580107	-1.897038	-0.259579
26.O	0.451334	-1.979213	-0.931972
27.C	-3.991717	-1.726929	-0.696735
28.N	-2.613097	-1.520379	-1.284653
29.H	-2.436553	-2.194202	-2.036375
30.Pt	1.294054	1.424342	-0.048874
31.O	-0.299775	1.587982	-1.356969
32.O	-2.546749	1.409570	-1.313323
33.N	2.753170	0.882958	-1.439665
34.H	2.663645	-0.140641	-1.599818
35.H	2.639316	1.368766	-2.334624
36.H	3.117053	2.169968	1.676999
37.O	-2.425585	1.758847	1.512481
38.C	-1.458808	1.505488	-0.730082
39.H	6.549974	-0.724450	0.536902
40.H	7.571043	0.640456	0.987822
41.C	4.121042	1.159551	-0.862697
42.H	4.231513	2.248615	-0.871131
43.C	5.267754	0.526685	-1.665848
44.H	5.560981	2.070949	1.387745
45.C	6.621632	0.372337	0.505387
46.H	5.264951	0.915533	-2.694024
47.H	5.110531	-0.560825	-1.716913
48.C	5.438741	0.979521	1.300344
49.H	5.414719	0.567922	2.318199
50.H	3.945358	-0.422380	0.584589
51.C	6.618184	0.826495	-0.972141
52.H	7.436275	0.348580	-1.524958
53.H	6.799607	1.917569	-1.023107
54.C	-1.396217	1.690561	0.837107
55.O	-0.182101	1.899893	1.328364
56.C	4.116544	0.659700	0.587656
57.N	2.899298	1.245666	1.284748
58.H	2.640108	0.603206	2.048137
59.Pt	1.576750	4.714134	-0.225557
60.C	4.370266	4.637618	0.301335
61.C	4.221646	4.642481	-1.270344
62.O	3.261032	4.626357	0.983871
63.O	5.508767	4.582799	0.811895
64.O	3.005594	4.625467	-1.729883
65.O	5.248064	4.602106	-1.981719
66.N	0.141059	4.836573	1.278987
67.H	0.481854	5.341791	2.103399
68.H	-0.079282	3.865948	1.572080
69.N	-0.118729	4.763455	-1.447323
70.H	-0.143447	3.892505	-1.995877
71.H	-0.061672	5.550291	-2.103950
72.C	-1.093696	5.517165	0.719220
73.C	-3.532682	6.126807	0.946788
74.C	-2.321784	5.452971	1.643294
75.C	-1.400390	4.847771	-0.627560

76.C	-2.564268	5.534920	-1.352366
77.C	-3.818217	5.507317	-0.441058
78.H	-0.806509	6.564187	0.546185
79.H	-3.333866	7.203913	0.833607
80.H	-4.417501	6.035276	1.588779
81.H	-2.551391	4.399703	1.865079
82.H	-2.098519	5.954459	2.595590
83.H	-1.686374	3.812808	-0.432256
84.H	-4.639778	6.042241	-0.933480
85.H	-2.766861	5.018304	-2.300466
86.H	-2.289849	6.576519	-1.588716
87.H	-4.140072	4.462837	-0.318308
88.Na	7.128279	4.478506	-0.752876
77.C	-3.711663	5.556241	-0.615281
78.H	-0.686128	6.780033	0.415139
79.H	-3.319010	7.373799	0.514485
80.H	-4.376628	6.233699	1.351011
81.H	-2.484179	4.694018	1.788861
82.H	-2.078144	6.309047	2.401402
83.H	-1.457978	3.994655	-0.529958
84.H	-4.566294	5.986593	-1.153834
85.H	-2.601547	5.034812	-2.428901
86.H	-2.240128	6.659655	-1.801568
87.H	-3.950556	4.501012	-0.415098

```
E-test:            old,new=      -18.22383,      -18.22391      hartree
max    gradient:                        0.00088945    au/angstrom,radian
max      cart.      step:                       0.00783620      angstrom
Geometry Converged
```

	hartree	eV	kcal/mol	kJ/mol
Total Pauli Repulsion:	69.858059919839874	1900.9345	43836.60	183412.31
Electrostatic Energy:	-15.276870262645163	-415.7048	-9586.38	-40109.42
Total Orbital Interactions:	-72.590880806101794	-1975.2984	-45551.47	-190587.33
Dispersion Energy:	-0.214275015643038	-5.8307	-134.46	-562.58
Total Bonding Energy:	-18.223964834156032	-495.8993	-11435.71	-47847.01

Frequency cm-1	Dipole Strength 1e-40 esu2 cm2	Absorption Intensity (degeneracy not counted) km/mole
11.157409	0.000000	0.000000
16.783245	0.000000	0.000000
19.882547	0.000000	0.000000
25.702946	203.742595	1.312631
30.173838	137.878789	1.042812
33.366277	515.315884	4.309822
36.494987	206.154780	1.885839
45.268361	75.556541	0.857324
47.716722	179.925968	2.152001
51.914967	29.806880	0.387871
58.666819	311.105377	4.574863
62.315496	655.316181	10.235876
67.639510	40.912866	0.693647
72.532612	71.179045	1.294087
79.102467	273.804968	5.428870
81.416331	680.595054	13.889237
82.091351	242.732376	4.994628
91.421308	64.508352	1.478228
101.562408	277.254934	7.058141
110.660023	149.017552	4.133389
119.981150	33.222352	0.999129
122.678415	87.191367	2.681141
131.890081	72.550386	2.398446
144.717016	672.747379	24.403363
149.890516	149.071428	5.600756
153.343035	99.813807	3.836478
155.037876	728.420385	28.307269
165.078174	38.166392	1.579243
180.280314	149.486015	6.755025
183.145513	225.739149	10.362898
186.070435	99.574215	4.644108
189.536680	7.120892	0.338303
194.744624	348.739679	17.023345
197.771321	228.587823	11.331685
200.408845	112.864003	5.669574
209.944737	21.362048	1.124154
220.322320	29.986989	1.656035
225.243210	114.474107	6.463043
228.152742	290.141749	16.592583
246.788861	808.802076	50.031771

247.822241	24.171423	1.501484
251.652738	41.966156	2.647152
254.045177	69.210451	4.407179
254.927772	10.101502	0.645478
261.370400	28.033568	1.836593
275.837075	223.806176	15.474007
299.464333	350.877388	26.337743
311.015525	799.786503	62.349677
326.811482	31.507414	2.581001
327.241417	30.739285	2.521390
328.242893	9.573198	0.787645
337.687838	24.905230	2.108065
338.935313	49.954015	4.243901
344.346674	27.174024	2.345459
353.630514	13.327380	1.181334
355.715067	78.760506	7.022453
357.940168	43.843233	3.933608
361.574839	87.341747	7.915861
368.031502	46.819915	4.319104
396.967656	353.799498	35.203870
425.500788	21.406641	2.283111
426.069251	30.145996	3.219496
426.602494	5.655885	0.604786
433.971694	62.745654	6.825322
434.973494	44.739234	4.877861
435.171133	4.688441	0.511407
441.164453	74.346286	8.221250
441.763656	472.755408	52.348538
452.123597	739.071644	83.757129
493.115312	46.088013	5.696584
494.557035	24.849366	3.080419
500.301844	9.021912	1.131381
508.294200	110.875172	14.126271
513.694152	415.094991	53.447843
525.151147	203.033946	26.725820
548.491146	140.483355	19.314015
550.790359	10.390325	1.434477
552.319338	11.186314	1.548657
556.425145	11.471167	1.599898
562.661483	61.182802	8.628884
562.977152	21.665358	3.057276
563.602739	0.140772	0.019887
564.172760	2.053729	0.290425
572.131122	29.284895	4.199691
579.219184	15.563671	2.259608
579.631173	8.608059	1.250648
587.335503	17.625665	2.594836
705.039003	28.301240	5.001459
705.893836	28.061044	4.965023
725.872919	6.823139	1.241432
750.931725	95.589782	17.992437
756.598520	150.368220	28.516723
760.506714	145.652561	27.765100
764.984894	142.586547	27.340691
771.424724	144.516077	27.943950
780.307918	3.079770	0.602369
783.541339	210.473153	41.336784
785.922622	48.465713	9.547562
788.726132	29.787602	5.888977
789.688920	22.088266	4.372157
794.715568	11.764687	2.343528
796.673498	0.598271	0.119469
823.548538	14.323506	2.956764
824.151299	17.257638	3.565056
825.509684	3.308551	0.684602
826.577376	17.241647	3.572238
841.511363	16.282222	3.434407
842.041202	2.814653	0.594068
843.951174	3.132174	0.662585
845.819865	2.061511	0.437060
846.343349	3.763660	0.798427
867.387558	0.092067	0.020017
870.562314	0.972498	0.212210
874.194918	0.122156	0.026767
905.728419	4.972319	1.128847
907.373820	7.721235	1.756108
907.787476	5.795922	1.318818
920.572873	7.586182	1.750490
922.671827	8.093650	1.871845
925.380319	4.357021	1.010620
962.696078	152.702394	36.847932
970.157633	431.280032	104.876872
970.858205	35.021480	8.522527
1013.876889	6.549414	1.664431
1020.244786	23.224122	5.939115
1021.072708	8.090352	2.070628
1027.033783	2.830129	0.728566
1028.068568	9.976018	2.570735
1030.117936	4.782015	1.234741
1030.839754	18.129813	4.684493
1034.874713	53.264503	13.816681

1035.459739		49.750513	12.912456
1038.055404		26.964262	7.015961
1041.754997		61.732996	16.119851
1046.176996		12.240761	3.209901
1070.515978		31.748352	8.519074
1071.694194		6.887644	1.850204
1080.740559		1.878912	0.508986
1116.344827		26.388297	7.383934
1117.413796		23.002491	6.442686
1118.670116		15.816288	4.434909
1132.268756		143.539223	40.737857
1137.497752		82.655471	23.566779
1143.873448		78.665476	22.554865
1147.009393		75.003431	21.563844
1155.093248		49.667551	14.380297
1167.119547		16.105276	4.711526
1169.524772		37.012419	10.850131
1171.417583	35.597273	10.452172	
1182.972715		17.265128	5.119442
1184.126608		10.184688	3.022901
1192.796572		17.181250	5.136877
1204.274280		40.492124	12.222894
1205.713537		28.918784	8.739815
1217.705701		13.722471	4.188444
1227.982570		79.902743	24.594158
1233.677867		26.477342	8.187555
1234.079066		96.356085	29.805760
1238.740817		125.374195	38.928411
1242.390386		356.900774	111.143391
1256.229049		6.945359	2.186964
1258.906183		13.864905	4.375104
1259.395102		6.914377	2.182695
1272.801187		1286.197214	410.342223
1294.598719		0.256897	0.083363
1296.802876		16.460891	5.350636
1298.972667		4.708084	1.532930
1305.751700		1.457193	0.476931
1309.781529		9.094116	2.985640
1311.169046		0.640901	0.210634
1313.375095		478.130992	157.403267
1322.190800		3.473015	1.151010
1332.975506		6.921587	2.312629
1335.572026		5.863786	1.963015
1335.942434		5.035183	1.686091
1336.628380		9.098361	3.048259
1340.659759		15.794998	5.307820
1342.052122		17.972701	6.045898
1342.747025		7.763051	2.612791
1344.969634		15.491586	5.222596
1354.449188		4.965041	1.685635
1354.501897		21.357798	7.251271
1355.023279		9.582814	3.254752
1358.506501		0.897069	0.305468
1370.854927		12.397254	4.259857
1373.318036		1.620569	0.557849
1377.929414		5.311572	1.834544
1388.856202		23.083166	8.035830
1389.808998		19.051284	6.636780
1392.484118		24.295512	8.479971
1409.279170		7.450641	2.631896
1417.535093		5.210599	1.851397
1443.394462		10.296034	3.725058
1462.239889		4.818644	1.766125
1462.584694		3.322693	1.218118
1462.818237		7.888848	2.892558
1463.835873		10.468326	3.841030
1465.294648		12.090542	4.440673
1469.303098		21.793051	8.026154
1470.675475		18.666984	6.881278
1471.612932		16.337135	6.026256
1478.978656		19.839273	7.354713
1479.223205		43.974808	16.304810
1481.465483		27.538658	10.226155
1560.367862		217.081091	84.903787
1567.818047		31.685161	12.451728
1576.938568		395.061594	156.155634
1582.420601		410.329138	162.754257
1583.795992		646.909930	256.815438
1593.610604		122.088488	48.768006
1605.531279		3044.979398	1225.409378
1618.949840		318.948958	129.429315
1622.790486		57.357115	23.330703
1624.205427		238.586895	97.132734
1635.538836		142.807634	58.545073
1637.170808		2114.724715	867.812504
2858.990462		135.358880	97.001294
2915.929330		24.069603	17.592356
2922.754679		20.497416	15.016529
2934.299210		17.759709	13.062260
2934.908383		30.203658	22.219391
2936.787527		7.260547	5.344658

2936.836890	13.059939	9.613888
2943.112948	24.348881	17.962386
2943.621524	11.225587	8.282646
2947.420507	10.741813	7.935929
2950.094529	26.164909	19.347873
2950.674830	13.331800	9.860257
2951.331980	15.396342	11.389736
2958.152204	8.738366	6.479311
2977.962526	39.913938	29.793524
2982.228438	24.175584	18.071572
2984.718503	18.493419	13.835621
2986.178854	28.578533	21.391135
2988.547003	5.901787	4.421012
2989.588679	18.096703	13.560914
2991.467894	49.803194	37.343895
2993.195708	42.949393	32.223315
2995.070475	36.649597	27.514037
2995.805726	47.292011	35.512357
2998.249614	32.340105	24.304533
3001.602588	28.043303	21.098930
3008.966572	48.331592	36.452434
3011.237389	4.857286	3.666205
3026.749410	3.654934	2.772899
3059.763063	0.049808	0.038200
3129.747193	282.739345	221.806146
3166.774852	318.278604	252.640343
3229.189805	145.087302	117.435945
3269.771028	62.425096	51.162838
3296.091029	44.528212	36.788538
3312.172010	21.342299	17.718712
3360.599837	91.300781	76.907619
3378.019965	68.627733	58.108536
3380.804842	61.144673	51.815155
3383.444371	49.462334	41.948044
3386.816839	28.603328	24.282106
3388.490792	44.656823	37.929070

Zero-Point	Energy	:	0.694080 a.u.
==========	18.886887 eV		

Statistical Thermal Analysis *** ideal gas assumed ***

Temp		Transl	Rotat	Vibrat	Total
298.15	Entropy (cal/mole-K):	47.160	39.641	178.711	265.512
	Internal Energy (Kcal/mole):	0.889	0.889	462.779	464.557
	Constant Volume Heat Capacity (cal/mole-K): 2.981	2.981	174.284	180.246	

α,Na,α[**1**]$_3$-tzp-blyp-d3;C_1

Coordinates	in	Geometry	Cycle	188
Atom	X	Y	Z	(Angstrom)
1.Pt	-1.239079	-1.678548	0.245714	
2.O	0.129181	-1.710142	1.744328	
3.O	2.360077	-1.583804	2.017897	
4.N	-2.930507	-1.447329	1.477793	
5.H	-3.108353	-2.321713	1.986495	
6.H	-2.757456	-0.716056	2.178265	
7.H	-2.631681	-0.652966	-1.725794	
8.O	2.624316	-1.905781	-0.821148	
9.C	1.379247	-1.722277	1.292913	
10.H	-6.774508	-2.587192	-0.825534	
11.H	-7.352094	-1.135915	-1.639968	
12.C	-4.119383	-1.068858	0.630843	
13.H	-3.950262	-0.009068	0.410023	
14.C	-5.476561	-1.256118	1.323916	
15.H	-5.015410	-0.296892	-1.913905	
16.C	-6.567338	-1.517286	-0.974906	
17.H	-5.491419	-0.698763	2.271612	
18.H	-5.612375	-2.319910	1.575105	
19.C	-5.186000	-1.354808	-1.651249	
20.H	-5.146336	-1.922877	-2.590436	
21.H	-4.134159	-2.895200	-0.528183	
22.C	-6.624218	-0.799198	0.391773	
23.H	-7.591412	-0.972506	0.878333	
24.H	-6.557128	0.293712	0.231441	
25.C	1.522027	-1.883264	-0.270323	
26.O	0.382704	-1.935151	-0.947142	
27.C	-4.051506	-1.815447	-0.716854	
28.N	-2.675024	-1.589161	-1.297015	
29.H	-2.479075	-2.271172	-2.037053	
30.Pt	1.248060	1.404718	-0.021282	
31.O	-0.420031	1.481267	-1.308574	
32.O	-2.679080	1.552631	-1.225910	
33.N	2.706645	0.941251	-1.420387	
34.H	2.622559	-0.068387	-1.638410	
35.H	2.589874	1.478813	-2.285626	
36.H	3.094999	2.296981	1.549803	
37.O	-2.525108	1.813262	1.547467	
38.C	-1.538355	1.528322	-0.673044	
39.H	6.497290	-0.735058	0.500176	
40.H	7.522798	0.619872	0.985747	
41.C	4.092604	1.200179	-0.847813	
42.H	4.208927	2.284593	-0.851909	
43.C	5.227202	0.573899	-1.667485	
44.H	5.552902	2.045819	1.432946	
45.C	6.575026	0.362962	0.496261	
46.H	5.225077	0.990181	-2.684750	
47.H	5.066829	-0.512757	-1.739982	
48.C	5.403586	0.963730	1.317204	
49.H	5.369476	0.516616	2.320437	
50.H	3.872004	-0.388494	0.588657	
51.C	6.575005	0.876480	-0.961927	
52.H	7.391524	0.410208	-1.527906	
53.H	6.748533	1.962647	-0.974840	
54.C	-1.456521	1.694239	0.886896	
55.O	-0.271258	1.818051	1.386272	
56.C	4.078524	0.686207	0.591829	
57.N	2.870389	1.326967	1.272095	
58.H	2.637747	0.773465	2.106787	
59.Pt	1.705328	4.751046	-0.201287	
60.C	4.454412	4.502803	0.463025	
61.C	4.388154	4.586892	-1.112011	
62.O	3.257618	4.412173	1.077819	
63.O	5.512383	4.415467	1.062170	
64.O	3.149108	4.628786	-1.624908	
65.O	5.395883	4.516270	-1.797116	
66.N	0.167870	4.909748	1.249041	
67.H	0.490464	5.425836	2.073878	
68.H	-0.086653	3.962125	1.564897	
69.N	0.103951	5.114926	-1.528861	
70.H	0.115418	4.431089	-2.293097	
71.H	0.226206	6.041446	-1.955084	
72.C	-1.020703	5.605910	0.627842	
73.C	-3.505187	6.150108	0.722986	
74.C	-2.314193	5.485886	1.456428	
75.C	-1.212170	5.037717	-0.793735	

76.C	-2.372855	5.724425	-1.533159
77.C	-3.678833	5.610606	-0.714460
78.H	-0.737755	6.664996	0.541078
79.H	-3.338481	7.235913	0.669897
80.H	-4.427072	6.009502	1.303442
81.H	-2.519036	4.419454	1.644663
82.H	-2.166230	5.953269	2.439383
83.H	-1.426761	3.966861	-0.712655
84.H	-4.493893	6.133758	-1.228973
85.H	-2.496886	5.275906	-2.528194
86.H	-2.134387	6.789764	-1.681299
87.H	-3.972743	4.543295	-0.687443
88.Na	-4.278091	2.319015	0.210396

```
E-test:            old,new=      -18.18391,      -18.18395      hartree
max    gradient:                        0.00099004    au/angstrom,radian
max      cart.      step:                      0.00938141      angstrom
Geometry Converged
```

	hartree	eV	kcal/mol	kJ/mol
Total Pauli Repulsion:	69.848284115084383	1900.6685	43830.46	183386.64
Electrostatic Energy:	-15.267465383872670	-415.4489	-9580.48	-40084.72
Total Orbital Interactions:	-72.546638450673029	-1974.0945	-45523.71	-190471.17
Dispersion Energy:	-0.218170624603983	-5.9367	-136.90	-572.81
Total Bonding Energy:	-18.183985970346082	-494.8114	-11410.62	-47742.05

Frequency	Dipole Strength	Absorption Intensity (degeneracy not counted)
cm-1	1e-40 esu2 cm2	km/mole
-10.521390	0.000000	0.000000
9.819101	0.000000	0.000000
16.479352	0.000000	0.000000
23.110101	363.112846	2.103398
26.172488	102.327706	0.671299
31.463395	362.819599	2.861372
37.795442	332.897600	3.153756
42.633595	356.486983	3.809550
49.369577	53.848195	0.666360
53.580180	80.319533	1.078707
56.272641	41.523329	0.585690
58.703518	89.044281	1.310232
64.919442	19.525953	0.317735
68.990702	23.706890	0.409962
73.168470	156.470171	2.869681
77.686239	117.137659	2.280965
89.885267	74.191133	1.671547
94.495188	234.591186	5.556476
102.703169	141.852517	3.651733
107.689102	280.737250	7.577917
114.405306	21.868359	0.627105
119.396088	98.877921	2.959154
121.700176	11.888147	0.362646
126.444337	2226.229557	70.558184
135.544243	39.626909	1.346323
147.433798	17.890595	0.661150
160.465485	242.803051	9.765935
171.097020	502.548325	21.552534
177.818609	6.012971	0.268006
183.122666	70.495171	3.235784
184.451350	19.328936	0.893651
191.403333	226.125897	10.848704
195.673546	4.764739	0.233695
197.063521	75.481862	3.728438
199.104169	92.379388	4.610346
204.823519	7.488471	0.384460
209.534902	6.014572	0.315892
224.837916	94.835986	5.344669
232.717885	290.094062	16.921804
235.079676	150.523409	8.869460
237.924110	231.702014	13.818036
247.448087	154.413824	9.577416
247.900261	177.156699	11.008107
250.074800	28.873542	1.809873
256.347599	37.639404	2.418522
298.479288	76.815018	5.746963
300.681712	256.280451	19.315260
304.609229	798.124125	60.938473
324.118500	66.986887	5.442165
328.193738	8.305110	0.683209
329.828493	23.190585	1.917246
330.190128	8.578163	0.709964
334.089053	3.919238	0.328203

336.272737	56.106455	4.729144
350.577674	47.045013	4.134052
356.288012	38.525615	3.440558
357.190063	70.877363	6.345780
362.423462	41.189613	3.741813
373.432764	39.009356	3.651399
390.872338	193.067343	18.915674
418.675184	20.329089	2.133404
422.636817	12.814927	1.357568
429.481621	32.660358	3.515957
429.692710	31.276635	3.368652
431.505097	48.237043	5.217286
435.199553	19.325274	2.108105
437.412457	284.746482	31.219618
441.957205	9.416032	1.043101
448.395608	1264.531974	142.124593
490.690805	36.046141	4.433480
491.768326	37.555436	4.629259
499.792080	1.924587	0.241104
510.910046	227.859419	29.180283
524.858883	204.420694	26.893386
530.423679	206.902639	27.508506
536.810985	5.875395	0.790563
544.531228	9.350370	1.276232
552.871910	3.638943	0.504287
558.800477	34.829940	4.878514
560.807619	18.308682	2.573647
561.093696	3.168028	0.445556
561.794784	6.729852	0.947679
568.540017	6.196758	0.883087
571.825009	26.218391	3.757918
576.464844	18.263434	2.638963
581.799872	17.299244	2.522777
588.217557	26.414919	3.894622
669.227563	10.044353	1.684899
691.662862	9.802570	1.699466
718.110747	134.062796	24.131136
734.875483	56.235265	10.358588
735.554099	37.267652	6.871075
752.835905	39.130116	7.383963
754.228107	198.984543	37.618383
763.750294	109.248272	20.914334
769.473723	2.373730	0.457829
772.345717	0.441739	0.085518
783.186219	29.255701	5.743196
784.116450	3.338622	0.656184
784.982495	0.678710	0.133543
793.133588	95.139891	18.914160
802.245460	214.071453	43.047119
822.016983	14.432801	2.973784
822.755069	43.541086	8.979412
826.480047	9.295014	1.925575
826.580428	9.497023	1.967663
837.337813	22.263259	4.672696
839.871267	1.539565	0.324107
843.089401	3.798873	0.802798
844.821224	3.161693	0.669519
846.803361	0.539631	0.114540
856.938314	0.406815	0.087382
859.038425	0.250615	0.053963
883.593220	1.532699	0.339459
903.486575	3.897972	0.882752
905.273785	3.081150	0.699151
907.491245	11.527803	2.622207
919.174780	5.920166	1.363986
924.205414	4.708343	1.090723
924.531885	10.968931	2.541934
950.755844	161.781512	38.554579
973.179767	190.105078	46.372964
977.388171	249.173116	61.044471
1007.286685	0.709828	0.179219
1018.850117	68.939262	17.605769
1021.675413	54.797980	14.033163
1022.242498	5.153433	1.320470
1025.440457	26.170494	6.726675
1026.062940	46.829756	12.044089
1027.494633	28.968474	7.460763
1030.491476	24.453879	6.316409
1036.363056	12.764099	3.315738
1037.440164	37.851783	9.843000
1038.107640	14.172238	3.687728
1050.223726	17.306870	4.555945
1056.798003	7.346610	1.946064
1060.421088	18.645072	4.955877
1077.037361	46.318308	12.504362
1089.403634	1.863652	0.508899
1099.293820	10.584403	2.916475
1100.348813	17.293769	4.769777
1119.556610	91.080337	25.559288
1122.932668	145.782035	41.033238
1126.311284	18.034984	5.091577

1133.352597		6.251161	1.775840
1139.504640		79.000753	22.564484
1141.278620		34.317358	9.817109
1155.117612		27.079008	7.840378
1157.013849	19.792423	5.740049	
1166.211527		9.672182	2.827352
1166.370858		6.384147	1.866455
1187.717509		79.882036	23.781561
1188.674701		5.203873	1.550486
1199.855479		968.612219	291.311046
1207.603594		208.944119	63.245935
1216.730150		92.681140	28.265958
1224.283365		15.529450	4.765584
1227.577631		8.447088	2.599166
1244.808226		137.601419	42.934206
1245.095628		5.996017	1.871301
1246.880757		964.332173	301.390563
1252.103622		16.040741	5.034343
1254.124484		11.962887	3.760579
1259.578955		39.724395	12.541826
1288.460763		1.273838	0.411399
1290.533045		13.640983	4.412583
1303.629045		13.061991	4.268168
1303.913046		1.947079	0.636371
1304.808615		3.837120	1.254961
1311.210305		191.259892	62.859993
1314.555262		4.868900	1.604308
1321.079625		4.670932	1.546716
1328.583841		3.692504	1.229668
1334.265956		6.459425	2.160301
1334.885302		2.755270	0.921905
1336.642340		10.960875	3.672303
1338.616989		8.304255	2.786346
1339.710884		6.672737	2.240749
1340.806561		16.647047	5.594759
1345.523272		27.293707	9.205170
1347.934521		4.569723	1.543962
1350.344173		3.673759	1.243464
1350.792512		3.894538	1.318629
1356.138655		1.699122	0.577573
1358.274409		2.215902	0.754425
1369.091796		24.569494	8.431539
1374.561754		1.741189	0.599913
1375.606021		6.919478	2.385863
1384.858469		8.831649	3.065669
1390.995758		15.004704	5.231561
1392.765752		23.265012	8.121933
1411.590437		5.841098	2.066718
1441.582949		9.594417	3.466860
1457.036501		8.902823	3.251444
1461.887436		9.443707	3.460465
1462.413767		4.126918	1.512774
1463.570634		12.808931	4.698991
1469.063763		14.549760	5.357652
1470.085701		25.039339	9.226640
1471.196691		15.547170	5.733240
1471.538356		18.316860	6.756172
1478.128437		10.328654	3.826784
1478.195694		68.535679	25.393743
1483.558009		27.943367	10.391096
1529.707420		461.502212	176.953937
1550.615843		2055.421112	798.882854
1564.584854		425.382896	166.823495
1582.452405		211.674654	83.960997
1604.215795		128.791097	51.787709
1604.718037		78.560566	31.599587
1613.696505		111.542522	45.117018
1627.797807		50.307557	20.526351
1638.127442		427.641485	175.592347
1656.750416		1143.474675	474.855759
1673.543516		340.872709	142.990542
1684.949239		1344.750370	567.945371
2863.455986		233.975307	167.933990
2865.576651		9.898470	7.109813
2915.894504		20.055429	14.658240
2929.815144		4.257625	3.126696
2935.900866		14.760882	10.862550
2936.180855		12.671075	9.325547
2938.465601		30.314069	22.327645
2940.497042		14.648278	10.796560
2947.738258		25.148303	18.581282
2949.630650		10.012823	7.402906
2950.717102		21.198652	15.678838
2957.301304		20.278892	15.032038
2958.819368		5.110109	3.789891
2965.673467		4.632094	3.443331
2974.892339		17.172173	12.804853
2983.857779		32.244347	24.116250
2984.428450		20.670553	15.462914
2986.455032		7.103093	5.317182
2988.487034		17.114369	12.820068

2990.114104		19.688502	14.756335
2994.825184		35.829844	26.896419
2997.715767		30.923113	23.235485
2999.629150		9.756793	7.335889
2999.749735		34.916616	26.253986
3001.734290		38.368979	28.868922
3004.430498		7.855976	5.916167
3010.161509		18.121972	13.673299
3020.978120		6.173798	4.674962
3029.297668		19.278384	14.638300
3073.657117		0.151654	0.116839
3191.301129		172.235842	137.774673
3230.813564		100.327514	81.247502
3274.851328		127.665775	104.795865
3283.212593		54.895043	45.176252
3318.187428		14.431562	12.003070
3326.690727		11.870013	9.897869
3351.765899		104.335060	87.656075
3383.492666		49.356604	41.858974
3384.221077		40.094890	34.011503
3389.215087		72.809349	61.853510
3389.776566		42.000351	35.686345
3394.600991	33.921271	28.862830	

Zero-Point Energy :	0.693034	a.u.
==========	18.858428	eV
(imaginary frequencies were excluded from the summation)		

Statistical Thermal Analysis *** ideal gas assumed ***

Temp			Transl	Rotat	Vibrat	Total
----			------	-----	------	-----
298.15	Entropy (cal/mole-K):		47.160	39.603	181.130	267.893
	Internal Energy (Kcal/mole):		0.889	0.889	462.360	464.137
	Constant Volume Heat Capacity (cal/mole-K):	2.981	2.981	175.128	181.089	

α,β[**1**]$_3$-tzp-blyp-d3;C_1

Coordinates	in	Geometry	Cycle	102
Atom	X	Y	Z	(Angstrom)
1.Pt	-0.648512	-1.648861	0.160019	
2.O	0.709957	-2.050290	1.633628	
3.O	2.897534	-2.535071	1.876368	
4.N	-2.232801	-1.105610	1.434320	
5.H	-2.484627	-1.892707	2.041806	
6.H	-1.901915	-0.340831	2.036090	
7.H	-1.881096	-0.235554	-1.647456	
8.O	3.135166	-2.451175	-0.970981	
9.C	1.920040	-2.335963	1.161112	
10.H	-6.188768	-1.960766	-0.812283	
11.H	-6.722752	-0.432962	-1.516625	
12.C	-3.436047	-0.634604	0.641398	
13.H	-3.289334	0.434391	0.476726	
14.C	-4.771641	-0.814057	1.375851	
15.H	-4.352819	0.314461	-1.805791	
16.C	-5.937380	-0.892082	-0.902005	
17.H	-4.728875	-0.293275	2.342559	
18.H	-4.939438	-1.885029	1.580470	
19.C	-4.569407	-0.746894	-1.614983	
20.H	-4.584640	-1.264973	-2.584894	
21.H	-3.606427	-2.406413	-0.586700	
22.C	-5.922544	-0.251769	0.506157	
23.H	-6.883799	-0.418190	1.010069	
24.H	-5.788723	0.836078	0.411943	
25.C	2.046891	-2.323699	-0.415609	
26.O	0.916994	-2.091219	-1.081124	
27.C	-3.448566	-1.327983	-0.734202	
28.N	-2.064390	-1.199726	-1.328523	
29.H	-1.968987	-1.811101	-2.145102	
30.Pt	0.755333	1.409640	0.077932	
31.O	-0.810249	1.616344	-1.274949	
32.O	-2.924584	2.372346	-1.375464	
33.N	2.270768	1.035744	-1.303868	
34.H	2.170985	0.073704	-1.658211	
35.H	2.186405	1.691785	-2.090174	
36.H	2.568866	2.236009	1.720467	
37.O	-2.850980	2.721045	1.448867	
38.C	-1.888778	2.128966	-0.732836	
39.H	5.906129	-0.826091	0.709591	
40.H	6.993647	0.460258	1.252074	
41.C	3.637642	1.231798	-0.664352	
42.H	3.771177	2.317558	-0.610028	
43.C	4.778316	0.593752	-1.470556	
44.H	5.036890	1.989962	1.627886	
45.C	6.047901	0.264612	0.729181	
46.H	4.821897	1.053122	-2.468600	
47.H	4.579347	-0.480600	-1.595588	
48.C	4.876707	0.906310	1.516901	
49.H	4.805547	0.465772	2.521477	
50.H	3.392435	-0.414884	0.707372	
51.C	6.118777	0.799525	-0.720748	
52.H	6.925294	0.296052	-1.270437	
53.H	6.361451	1.873287	-0.703802	
54.C	-1.854058	2.287776	0.836805	
55.O	-0.778312	1.834316	1.426786	
56.C	3.566891	0.661738	0.754139	
57.N	2.346096	1.269739	1.425652	
58.H	2.096528	0.714010	2.250526	
59.Pt	-0.714533	5.183680	-0.138774	
60.C	1.956330	4.495746	0.468030	
61.C	1.828124	4.417285	-1.103754	
62.O	0.900391	4.982492	1.098849	
63.O	2.982519	4.122954	1.048334	
64.O	0.661860	4.811518	-1.592286	
65.O	2.755454	4.016412	-1.809040	
66.N	-2.186964	5.514462	1.333134	
67.H	-1.862156	6.118993	2.093458	
68.H	-2.414173	4.585044	1.731485	
69.N	-2.376845	5.313673	-1.418201	
70.H	-2.378824	4.497953	-2.043999	
71.H	-2.315576	6.157987	-1.998395	
72.C	-3.429387	6.083577	0.687743	
73.C	-5.928274	6.521111	0.827956	
74.C	-4.678649	6.006844	1.585414	
75.C	-3.660008	5.302187	-0.616722	

76.C	-4.871536	5.832993	-1.395529
77.C	-6.137661	5.771118	-0.508170
78.H	-3.202204	7.133562	0.447782
79.H	-5.812933	7.597466	0.625024
80.H	-6.815723	6.413250	1.465398
81.H	-4.826771	4.957474	1.883345
82.H	-4.516996	6.590528	2.503096
83.H	-3.818372	4.248623	-0.359990
84.H	-6.994771	6.190804	-1.051201
85.H	-5.008497	5.236870	-2.308792
86.H	-4.685862	6.875201	-1.707191
87.H	-6.374265	4.716189	-0.302220

```
E-test:            old,new=      -18.30590,      -18.30597      hartree
max    gradient:                        0.00073167    au/angstrom,radian
max      cart.      step:                        0.00378570      angstrom
Geometry Converged
```

	hartree	eV	kcal/mol	kJ/mol
Total Pauli Repulsion:	69.587357387527248	1893.5683	43666.73	182701.58
Electrostatic Energy:	-15.169087315197078	-412.7719	-9518.75	-39826.43
Total Orbital Interactions:	-72.512371426992402	-1973.1620	-45502.20	-190381.20
Dispersion Energy:	-0.211912239830897	-5.7664	-132.98	-556.38
Total Bonding Energy:	-18.306004116986124	-498.1317	-11487.19	-48062.41

β,β[**1**]$_3$-tzp-blyp-d3;C_1

Coordinates	in	Geometry	Cycle	106
Atom	X	Y	Z	(Angstrom)
1.Pt	-2.394622	-1.042764	0.211519	
2.O	-1.023432	-1.414152	1.675244	
3.O	1.204484	-1.653446	1.905085	
4.N	-3.932764	-0.353554	1.478854	
5.H	-4.256324	-1.116798	2.083391	
6.H	-3.559039	0.389137	2.084239	
7.H	-3.591850	0.362357	-1.633124	
8.O	1.373963	-1.836660	-0.951549	
9.C	0.199532	-1.583138	1.194840	
10.H	-7.967703	-0.968564	-0.653466	
11.H	-8.399288	0.546287	-1.447654	
12.C	-5.081610	0.217089	0.672876	
13.H	-4.780266	1.246708	0.443728	
14.C	-6.418376	0.211822	1.432259	
15.H	-5.974426	1.090246	-1.801205	
16.C	-7.638419	0.070085	-0.814988	
17.H	-6.318325	0.789293	2.362097	
18.H	-6.671480	-0.824208	1.716089	
19.C	-6.274981	0.061393	-1.549495	
20.H	-6.348345	-0.499501	-2.492380	
21.H	-5.447043	-1.608539	-0.431892	
22.C	-7.548316	0.794476	0.548428	
23.H	-8.507312	0.723672	1.079236	
24.H	-7.354519	1.865039	0.380413	
25.C	0.289044	-1.696573	-0.377202	
26.O	-0.870620	-1.637579	-1.014181	
27.C	-5.190092	-0.561284	-0.651447	
28.N	-3.817001	-0.585133	-1.275009	
29.H	-3.785976	-1.239099	-2.062690	
30.Pt	0.598521	1.523488	0.048615	
31.O	-0.934765	1.834455	-1.308374	
32.O	-3.148047	2.223375	-1.361601	
33.N	2.081048	1.053771	-1.332010	
34.H	1.900967	0.089499	-1.655761	
35.H	2.054010	1.702117	-2.127284	
36.H	2.437357	2.093357	1.784264	
37.O	-3.061813	2.609038	1.451166	
38.C	-2.070127	2.084714	-0.732959	
39.H	5.632067	-1.086165	0.620566	
40.H	6.736162	0.148928	1.236017	
41.C	3.441579	1.136170	-0.672042	
42.H	3.649607	2.206300	-0.562816	
43.C	4.556170	0.475160	-1.494227	
44.H	4.833501	1.700054	1.675373	
45.C	5.792274	0.000512	0.693870	
46.H	4.626696	0.963200	-2.476924	
47.H	4.310808	-0.585761	-1.660957	
48.C	4.628102	0.632370	1.499375	
49.H	4.528680	0.142835	2.478434	
50.H	3.020699	-0.550633	0.616869	
51.C	5.897031	0.597572	-0.729412	
52.H	6.694839	0.096531	-1.294361	
53.H	6.171556	1.661392	-0.660776	
54.C	-2.034299	2.243104	0.830527	
55.O	-0.896441	1.998594	1.404770	
56.C	3.311238	0.502605	0.716579	
57.N	2.140483	1.179035	1.409463	
58.H	1.811021	0.572570	2.170574	
59.Pt	-0.637972	5.175892	-0.115082	
60.C	2.013887	4.475674	0.541242	
61.C	1.927589	4.439362	-1.035444	
62.O	0.957059	4.987357	1.153164	
63.O	3.009094	4.052132	1.138144	
64.O	0.778755	4.859193	-1.544906	
65.O	2.868796	4.044739	-1.725326	
66.N	-2.148805	5.461710	1.327660	
67.H	-1.842480	6.070786	2.092184	
68.H	-2.385421	4.539954	1.734341	
69.N	-2.274666	5.267627	-1.432180	
70.H	-2.248658	4.452770	-2.058365	
71.H	-2.208498	6.108522	-2.016877	
72.C	-3.378139	6.028107	0.652917	
73.C	-5.881325	6.450619	0.732360	
74.C	-4.647794	5.943633	1.519880	
75.C	-3.575358	5.250325	-0.659767	

```
  76.C            -4.772414      5.770661     -1.466200
  77.C            -6.056042      5.695576     -0.605962
  78.H            -3.147055      7.079177      0.422704
  79.H            -5.764660      7.526585      0.527567
  80.H            -6.783043      6.342935      1.349634
  81.H            -4.794800      4.893057      1.813912
  82.H            -4.510932      6.528909      2.440658
  83.H            -3.746567      4.198922     -0.407301
  84.H            -6.907028      6.103958     -1.166992
  85.H            -4.881770      5.170487     -2.380631
  86.H            -4.590608      6.814191     -1.775553
  87.H         -6.283325    4.637846   -0.401604
```

```
E-test:            old,new=      -18.31516,      -18.31526      hartree
max    gradient:                        0.00046731    au/angstrom,radian
max      cart.      step:                        0.00534678      angstrom
Geometry Converged
```

	hartree	eV	kcal/mol	kJ/mol
Total Pauli Repulsion:	69.621221310046735	1894.4898	43687.98	182790.49
Electrostatic Energy:	-15.191215137416751	-413.3740	-9532.63	-39884.53
Total Orbital Interactions:	-72.528770293403298	-1973.6083	-45512.50	-190424.26
Dispersion Energy:	-0.216539025134750	-5.8923	-135.88	-568.52
Total Bonding Energy:	-18.315296494223812	-498.3846	-11493.02	-48086.80

2-tzp-blyp-d3;C_1

Coordinates in Geometry Cycle 7			
Atom	X	Y	Z (Angstrom)
1.Pd	-0.907590	2.476053	0.483312
2.O	-1.646261	3.842974	-0.802643
3.O	-2.688790	3.915523	-2.796498
4.N	-0.159897	3.877079	1.917621
5.H	0.690551	4.315264	1.540754
6.H	-0.829992	4.637009	2.080877
7.H	-0.900365	0.625739	2.386894
8.O	-2.692569	1.054697	-2.802352
9.C	-2.200650	3.272229	-1.878112
10.H	2.978569	1.925153	4.638111
11.H	2.154992	1.189860	6.014178
12.C	0.150366	3.150097	3.198558
13.H	-0.820040	2.958630	3.678437
14.C	1.049088	3.952139	4.160685
15.H	0.140710	0.725200	4.624047
16.C	1.990384	1.773433	5.099258
17.H	0.558909	4.903192	4.411721
18.H	1.988800	4.201347	3.640010
19.C	1.092712	0.974321	4.126153
20.H	1.568688	0.023374	3.848773
21.H	1.718865	1.976393	2.304757
22.C	1.366710	3.144544	5.440690
23.H	2.042546	3.722333	6.084198
24.H	0.438064	2.992323	6.012219
25.C	-2.187620	1.693017	-1.889610
26.O	-1.590626	1.116367	-0.840414
27.C	0.784478	1.784647	2.851393
28.N	-0.118091	1.065619	1.885072
29.H	0.384286	0.307772	1.409216

```
E-test:          old,new=          -5.97411,          -5.97394     hartree
max    gradient:                        0.00070103    au/angstrom,radian
max      cart.      step:                        0.00155294      angstrom
Geometry Converged
```

	hartree	eV	kcal/mol	kJ/mol
Total Pauli Repulsion:	22.396737936130222	609.4462	14054.17	58802.63
Electrostatic Energy:	-4.827219781984139	-131.3553	-3029.13	-12673.86
Total Orbital Interactions:	-23.507079829150264	-639.6602	-14750.92	-61717.83
Dispersion Energy:	-0.036337847443805	-0.9888	-22.80	-95.41
Total Bonding Energy:	-5.973896929864079	-162.5580	-3748.68	-15684.46

Frequency cm-1	Dipole Strength 1e-40 esu2 cm2	Absorption Intensity (degeneracy not counted) km/mole
17.600269	0.000000	0.000000
53.785806	1.658688	0.022362
61.311322	29.701467	0.456454
84.941428	242.295636	5.158735
122.084866	0.257707	0.007886
150.644234	21.000463	0.792975
172.511033	1.228608	0.053126
176.587279	0.262810	0.011633
210.195330	71.252644	3.754068
239.437581	18.784848	1.127400
309.637040	89.007956	6.908119
325.062246	41.628627	3.391850
329.721627	51.891339	4.288648
345.900619	13.130909	1.138477
362.782935	34.417272	3.129690
408.850701	28.301698	2.900383
417.695974	122.015040	12.774730
438.507329	197.302558	21.686409
465.275426	145.861939	17.011013
504.665741	9.741501	1.232275
511.306868	15.161181	1.943089
517.223842	182.991849	23.724024
551.154623	18.374306	2.538414
559.941335	5.794950	0.813337
597.642519	1.883219	0.282111
637.215383	67.961945	10.855007
737.702263	112.266362	20.759115
759.830822	0.180349	0.034349
785.170710	0.005413	0.001065
801.775743	2.827791	0.568301

828.529970		3.394295	0.704914
846.901207		3.991542	0.847328
852.208409		1.401608	0.299399
905.681191		5.483979	1.244942
920.642339		1.095890	0.252892
977.273109		586.390721	143.641889
991.988452		129.177871	32.119798
1005.814603		20.364113	5.134067
1024.125876		1.550264	0.397958
1037.576919		51.219729	13.320964
1042.347977		2.282896	0.596454
1065.285300		23.855500	6.369899
1088.003431		78.487972	21.404813
1101.120652		23.791878	6.566617
1115.189715		0.105694	0.029544
1142.896467		3.114664	0.892270
1181.973059		19.113394	5.662699
1218.463059		1060.938746	324.026663
1223.443996		3.208350	0.983884
1258.775280		8.546585	2.696615
1291.061543		1.302967	0.421656
1304.558490		4.108579	1.343486
1332.844454		12.180724	4.069402
1334.942619		7.211192	2.412947
1338.765326		4.940023	1.657721
1350.622513		6.287361	2.128533
1351.956899		12.399884	4.202024
1369.068368		0.716869	0.246004
1390.504547		33.652281	11.729108
1459.888085		1.637156	0.599084
1461.699103		8.780648	3.217086
1467.118799		23.223834	8.540381
1476.926175		8.598558	3.183189
1609.505027		122.694994	49.499094
1611.614783		3.557053	1.436910
1656.977830		238.350627	98.994500
1661.219621		1231.410084	512.752549
2919.406897		29.010161	21.228673
2920.939528		0.497849	0.364500
2933.519616		17.914302	13.172462
2940.018710		32.634096	24.049151
2949.007347		1.176571	0.869705
2962.668169		18.531328	13.761558
2979.852110		0.081103	0.060578
2982.324956		54.011506	40.375631
2990.702025		56.501995	42.356005
2993.190934		40.161816	30.131852
3327.882278		1.597938	1.332925
3328.328012		12.537490	10.459593
3400.258168		0.869125	0.740751
3400.388314	44.379015	37.825462	

Zero-Point Energy : 0.227776 a.u.
========== 6.198104 eV

Statistical Thermal Analysis *** ideal gas assumed ***

Temp		Transl	Rotat	Vibrat	Total
298.15	Entropy (cal/mole-K):	43.071	32.824	43.646	119.541
	Internal Energy (Kcal/mole):	0.889	0.889	150.119	151.897
	Constant Volume Heat Capacity (cal/mole-K):	2.981	2.981	50.198	56.160

2-tzp-blyp-d3bj;C_1

```
 Coordinates      in      Geometry      Cycle      27
   Atom         X           Y           Z   (Angstrom)
   1.Pd          -0.037448    -0.060528    -0.001956
   2.O           -1.578056     0.336884    -1.243752
   3.O           -3.758028     0.884335    -1.132760
   4.N            1.419827    -0.423850    -1.517487
   5.H            1.243615    -1.347592    -1.931718
   6.H            1.342135     0.258872    -2.278911
   7.H            1.927633     0.410417     1.706453
   8.O           -3.555768     0.771931     1.711212
   9.C           -2.703994     0.608671    -0.576806
  10.H            5.014239    -2.721808     0.160983
  11.H            6.167559    -1.556551     0.811137
  12.C            2.785590    -0.382143    -0.894640
  13.H            3.001949     0.680516    -0.718948
  14.C            3.884971    -0.991309    -1.781890
  15.H            4.329945     0.002846     1.420448
  16.C            5.201541    -1.646237     0.299006
  17.H            3.924475    -0.452429    -2.738367
  18.H            3.615347    -2.035543    -2.010061
  19.C            4.087651    -1.046206     1.184048
  20.H            4.019625    -1.584098     2.139465
  21.H            2.426173    -2.129932     0.304605
  22.C            5.258566    -0.954721    -1.077997
  23.H            6.012929    -1.433653    -1.714463
  24.H            5.570939     0.092686    -0.949317
  25.C           -2.590880     0.554824     0.991538
  26.O           -1.377275     0.261305     1.469460
  27.C            2.722566    -1.085802     0.475254
  28.N            1.614252    -0.470608     1.280318
  29.H          1.334429   -1.085931    2.051537
```

```
E-test:          old,new=          -6.01056,          -6.01056     hartree
max    gradient:                          0.00095857    au/angstrom,radian
max      cart.      step:                         0.00165279      angstrom
Geometry Converged
```

	hartree	eV	kcal/mol	kJ/mol
Total Pauli Repulsion:	22.495464088286443	612.1327	14116.12	59061.83
Electrostatic Energy:	-4.850672886855492	-131.9935	-3043.84	-12735.44
Total Orbital Interactions:	-23.582511869656390	-641.7128	-14798.25	-61915.88
Dispersion Energy:	-0.072840736998126	-1.9821	-45.71	-191.24
Total Bonding Energy:	-6.010563907691035	-163.5558	-3771.69	-15780.73

2-DMSO-tzp-blyp-d3;C_1

Coordinates	in	Geometry	Cycle	21
Atom	X	Y	Z	(Angstrom)
1.Pd	0.009962	0.043121	0.011787	
2.O	1.407188	-0.327775	1.479179	
3.O	3.557891	-0.972610	1.679755	
4.N	-1.606337	0.442889	1.282565	
5.H	-1.890281	-0.436496	1.735597	
6.H	-1.350387	1.089690	2.038444	
7.H	-1.275816	1.356009	-1.843450	
8.O	3.743202	-1.022468	-1.141065	
9.C	2.574969	-0.678369	0.984353	
10.H	-5.517996	-0.363095	-0.920283	
11.H	-6.064176	1.129935	-1.691946	
12.C	-2.761687	1.004838	0.485923	
13.H	-2.523493	2.062623	0.313552	
14.C	-4.111339	0.884373	1.215014	
15.H	-3.703493	1.884320	-1.998884	
16.C	-5.278479	0.702899	-1.055537	
17.H	-4.068745	1.440513	2.161003	
18.H	-4.284302	-0.175589	1.461514	
19.C	-3.910949	0.826632	-1.770669	
20.H	-3.914755	0.277250	-2.721591	
21.H	-2.948205	-0.787879	-0.689809	
22.C	-5.263174	1.405238	0.320993	
23.H	-6.219954	1.251396	0.836644	
24.H	-5.145895	2.490126	0.176669	
25.C	2.678649	-0.705696	-0.590805	
26.O	1.586606	-0.374246	-1.245185	
27.C	-2.790861	0.283900	-0.867383	
28.N	-1.415093	0.404933	-1.474872	
29.H	-1.319166	-0.232889	-2.274181	

E-test:	old,new=	-6.03572,	-6.03564 hartree
max gradient:		0.00078051	au/angstrom,radian
max cart. step:		0.00943475	angstrom
Geometry Converged			

	hartree	eV	kcal/mol	kJ/mol
Total Pauli Repulsion:	22.422689668344418	610.1524	14070.45	58870.76
Electrostatic Energy:	-4.839541407032186	-131.6906	-3036.86	-12706.21
Total Orbital Interactions:	-23.495020201010199	-639.3320	-14743.35	-61686.17
Solvation:	-0.087529557091809	-2.3818	-54.93	-229.81
Dispersion Energy:	-0.036246712897243	-0.9863	-22.75	-95.17
Total Bonding Energy:	-6.035647834531554	-164.2383	-3787.43	-15846.59

Frequency	Dipole Strength	Absorption Intensity (degeneracy not counted)
cm-1	1e-40 esu2 cm2	km/mole
-0.562775	0.000000	0.000000
42.862481	2.592129	0.027849
67.445193	125.635762	2.123941
76.196687	823.960767	15.736955
117.745632	0.404449	0.011937
166.234600	587.601181	24.483988
169.413812	62.552863	2.656281
175.214567	11.499639	0.505048
206.300436	210.631314	10.891837
246.331023	96.244790	5.942571
300.078837	603.463891	45.390475
324.635079	133.635657	10.874164
334.120109	96.642689	8.093748
336.546028	67.427106	5.687967
347.238390	92.770985	8.074543
418.881406	59.200938	6.215810
424.875821	119.844395	12.763148
441.268776	520.467177	57.567135
476.063429	127.355103	15.197048
493.399306	331.229983	40.964367
527.544144	285.875682	37.801940
535.747434	22.272507	2.990937
553.478479	16.715876	2.319038
567.294213	47.093863	6.696544
634.844890	12.610834	2.006733
673.509314	262.205481	44.265303
746.763748	441.341556	82.610665
765.845259	2.310969	0.443622
798.292600	0.022456	0.004493

822.447419		16.080222	3.314960
826.914112		16.582479	3.437066
843.371445		21.590069	4.564056
853.520179		2.771498	0.592934
898.506237		31.797380	7.161278
918.543958		6.142122	1.414153
972.250069		312.123260	76.064530
1014.639093		5.715568	1.453614
1020.915025		12.107949	3.098406
1023.062373		304.459332	78.074547
1030.024160		2.556891	0.660142
1050.582075		28.426297	7.485630
1093.266981		28.864434	7.909834
1113.905909		152.668910	42.626255
1118.224758		49.243265	13.802381
1153.181165		27.377672	7.913564
1169.709138		193.853647	56.836841
1176.943905		51.239346	15.116018
1217.956322		0.074224	0.022660
1242.977333		8.791734	2.739150
1269.145770		2476.116752	787.699728
1282.815433		15.952750	5.129533
1300.545709		2.493187	0.812753
1323.674179		0.072669	0.024111
1325.076072		0.763942	0.253734
1333.462538		15.224687	5.088705
1343.480596		11.830014	3.983774
1349.130872		0.770400	0.260524
1365.974978		0.666315	0.228140
1386.570844		67.326542	23.399493
1443.810333		3.175236	1.149117
1444.490102		18.466312	6.686099
1445.907827		61.407403	22.255605
1456.363947		5.552750	2.027011
1560.351884		258.997906	101.297067
1563.873176		125.233797	49.090918
1575.198758		535.724601	211.521745
1582.190618		4406.319049	1747.482420
2928.389242		41.575838	30.517425
2929.510007		9.581715	7.035846
2934.060975		31.324289	23.037133
2938.207968		75.380914	55.516490
2966.358951		1.001685	0.744788
2977.562562		44.094652	32.909773
2986.382805		62.359939	46.679826
2987.983313		48.849864	36.586394
2989.001186		18.718642	14.024213
2993.409005		105.542926	79.190532
3322.667203		102.635158	85.479323
3324.402390		69.494024	57.908073
3395.348537		179.657355	152.899982
3395.807901	38.179703	32.497782	

Zero-Point Energy :	0.227703	a.u.
==========	6.196127	eV

(imaginary frequencies were excluded from the summation)

Statistical Thermal Analysis *** ideal gas assumed ***

Temp		Transl	Rotat	Vibrat	Total
298.15	Entropy (cal/mole-K):	43.071	32.815	43.839	119.725
	Internal Energy (Kcal/mole):	0.889	0.889	150.061	151.838
	Constant Volume Heat Capacity (cal/mole-K):	2.981	2.981	49.832	55.793

α[**2**]$_2$-tzp-blyp;C_1

Coordinates	in	Geometry	Cycle	25
Atom	X	Y	Z	(Angstrom)
1.Pd	-0.633064	-1.559808	0.142284	
2.O	0.693158	-2.072243	1.603225	
3.O	2.819421	-2.788895	1.821657	
4.N	-2.273774	-1.167455	1.427975	
5.H	-2.485325	-2.015289	1.968649	
6.H	-2.012702	-0.435777	2.101720	
7.H	-1.941219	-0.049222	-1.553716	
8.O	3.079378	-2.647980	-1.001848	
9.C	1.863871	-2.467456	1.119075	
10.H	-6.092339	-2.254464	-0.929251	
11.H	-6.759521	-0.760073	-1.587686	
12.C	-3.486443	-0.723579	0.634467	
13.H	-3.402123	0.363286	0.530754	
14.C	-4.824399	-1.040396	1.328238	
15.H	-4.482876	0.227960	-1.812005	
16.C	-5.944513	-1.163387	-0.972718	
17.H	-4.853701	-0.542714	2.307335	
18.H	-4.892955	-2.127261	1.507612	
19.C	-4.586632	-0.856045	-1.652181	
20.H	-4.534239	-1.342235	-2.637642	
21.H	-3.469615	-2.440717	-0.672498	
22.C	-6.015278	-0.574698	0.454373	
23.H	-6.958131	-0.862800	0.937938	
24.H	-6.006915	0.523478	0.398781	
25.C	2.009057	-2.395862	-0.452085	
26.O	0.942772	-1.945167	-1.108242	
27.C	-3.418946	-1.346698	-0.772507	
28.N	-2.052018	-1.055642	-1.339689	
29.H	-1.906390	-1.572356	-2.214335	
30.Pd	0.633064	1.559808	0.142284	
31.O	-0.942772	1.945167	-1.108242	
32.O	-3.079378	2.647980	-1.001848	
33.N	2.052018	1.055642	-1.339689	
34.H	1.941219	0.049222	-1.553716	
35.H	1.906390	1.572356	-2.214335	
36.H	2.485325	2.015289	1.968649	
37.O	-2.819421	2.788895	1.821657	
38.C	-2.009057	2.395862	-0.452085	
39.H	6.006915	-0.523478	0.398781	
40.H	6.958131	0.862800	0.937938	
41.C	3.418946	1.346698	-0.772507	
42.H	3.469615	2.440717	-0.672498	
43.C	4.586632	0.856045	-1.652181	
44.H	4.892955	2.127261	1.507612	
45.C	6.015278	0.574698	0.454373	
46.H	4.534239	1.342235	-2.637642	
47.H	4.482876	-0.227960	-1.812005	
48.C	4.824399	1.040396	1.328238	
49.H	4.853701	0.542714	2.307335	
50.H	3.402123	-0.363286	0.530754	
51.C	5.944513	1.163387	-0.972718	
52.H	6.759521	0.760073	-1.587686	
53.H	6.092339	2.254464	-0.929251	
54.C	-1.863871	2.467456	1.119075	
55.O	-0.693158	2.072243	1.603225	
56.C	3.486443	0.723579	0.634467	
57.N	2.273774	1.167455	1.427975	
58.H	2.012702	0.435777	2.101720	

E-test:	old,new=	-11.91949,	-11.91938 hartree
max gradient:		0.00087491	au/angstrom,radian
max cart. step:		0.00671654	angstrom
Geometry Converged			

	hartree	eV	kcal/mol	kJ/mol
Total Pauli Repulsion:	44.938686622560787	1222.8439	28199.45	117986.51
Electrostatic Interaction:	-9.696708782026548	-263.8609	-6084.78	-25458.71
Total Orbital Interactions:	-47.161458340137337	-1283.3286	-29594.27	-123822.39
Total Bonding Energy:	-11.919470131961990	-324.3453	-7479.58	-31294.56

Frequency cm-1	Dipole Strength 1e-40 esu2	Absorption Intensity (degeneracy not counted) cm2	km/mole
-20.980679	55.843186		-0.293676
15.823497	0.000000		0.000000
16.268500	0.000000		0.000000
22.563609	1014.961411		5.740321
41.335700	271.890813		2.817072
44.222406	17.342230		0.192232
53.132451	195.757160		2.607087
61.699856	10.651381		0.164728
62.471229	124.222106		1.945168
64.067386	63.496868		1.019688
67.108710	11.457449		0.192728
67.242375	93.767182		1.580418
93.595234	0.815034		0.019121
98.321424	2170.569109		53.493356
120.571777	4.272196		0.129114
122.258077	15.578055		0.477385
169.514738	0.417514		0.017740
169.813262	74.683856		3.178897
173.202146	47.215630		2.049827
175.007579	0.018421		0.000808
180.753010	19.868970		0.900200
186.119191	81.652364		3.809237
216.363923	31.050017		1.683933
220.696450	123.593001		6.837027
244.221583	20.257362		1.240067
244.349157	24.644181		1.509396
304.736867	191.382049		14.618549
306.691737	2.294081		0.176355
315.037427	0.008109		0.000640
315.476371	138.972088		10.989362
327.616715	0.052609		0.004320
328.092037	95.789614		7.877568
342.601692	0.711371		0.061089
343.484410	68.975585		5.938551
351.435355	72.809219		6.413718
352.220647	7.791242		0.687859
409.300707	12.735659		1.306598
410.601172	24.119017		2.482321
421.241345	116.313467		12.281151
421.342935	2.807650		0.296522
444.177376	1.007321		0.112151
444.497132	557.041794		62.063293
476.427309	0.018292		0.002184
477.385682	120.803077		14.455245
506.966926	1.983578		0.252062
510.232605	255.324044		32.654121
514.631982	312.813950		40.351618
515.627509	0.047147		0.006094
524.179583	18.635502		2.448495
524.236245	49.043654		6.444481
545.428206	10.259408		1.402613
546.685776	0.148889		0.020402
565.826621	5.766946		0.817913
565.932034	16.173858		2.294330
639.436336	67.536211		10.824605
639.758545	0.014661		0.002351
696.033737	3.610271		0.629866
696.322268	298.158513		52.039794
743.671150	3.755348		0.700018
744.016632	223.337756		41.650754
765.430366	0.477516		0.091616
765.565641	0.246243		0.047252
794.274131	2.587005		0.515046
794.281350	0.043582		0.008677
816.361183	13.609535		2.784862
816.514947	0.732725		0.149963
820.658923	17.696240		3.640171
820.759289	0.146415		0.030122
839.130200	0.068565		0.014422
839.170323	6.370624		1.340017
850.895034	0.267355		0.057022
851.002930	0.414434		0.088403
898.739371	4.196397		0.945341
898.825041	6.105946		1.375644
914.876183	5.146667		1.180229
914.959280	3.959140		0.907989
970.098248	497.273613		120.917513
970.227016	1.566280		0.380909
1004.730039	211.695815		53.313811
1005.233861	1.517870		0.382454
1012.840003	0.565547		0.143578
1013.135929	26.364345		6.695188
1023.511224	81.737203		20.969615
1024.099707	0.130166		0.033413
1031.964864	52.912417		13.686758
1032.039573	1.570389		0.406239
1049.257949	42.020862		11.051603
1050.267083	3.998141		1.052533

1075.666072		45.194693	12.185490
1077.568113		18.613019	5.027356
1098.015111		130.918185	36.031834
1099.996634		0.367604	0.101356
1119.556416		52.870833	14.836799
1120.550809		10.594370	2.975670
1130.075818		0.514406	0.145711
1130.218429		38.220468	10.827706
1142.206157		8.547875	2.447263
1148.317697		0.510074	0.146816
1181.082312		0.040128	0.011880
1182.022833		28.188731	8.351788
1220.202022		19.252036	5.888253
1220.565016		0.464612	0.142144
1239.749486		3.441478	1.069441
1239.853044		1854.539528	576.347451
1252.346171		20.122813	6.316713
1252.388692		18.838698	5.913820
1285.370539		2.755592	0.887813
1285.444667		0.128791	0.041497
1302.051631		2.572893	0.839707
1302.112805		0.783531	0.255731
1327.697661		13.720839	4.566231
1327.776994		0.947530	0.315353
1333.847401		12.243635	4.093498
1333.875923		7.765216	2.596253
1338.600612		21.892662	7.345607
1338.629084		2.011589	0.674959
1346.667396		9.601619	3.241029
1346.667648		17.599980	5.940879
1347.592684		0.492304	0.166292
1347.646781		4.799332	1.621194
1368.607864		4.070059	1.396233
1368.717671		0.007770	0.002666
1389.735354		6.564986	2.286883
1389.942769		65.170506	22.705239
1458.179411		3.461121	1.265045
1458.182680		0.454232	0.166023
1461.239875		7.299508	2.673580
1461.249528		11.070034	4.054632
1464.182946		5.000448	1.835196
1464.189412		31.128056	11.424240
1474.738002		50.236637	18.570068
1474.761820		2.075521	0.767233
1600.332178		67.569196	27.104223
1600.750249		122.747758	49.251019
1619.539924		4.040862	1.640377
1623.935132		126.922557	51.663706
1631.172453		133.127320	54.430853
1632.418707		275.706778	112.812462
1638.881027		2629.187885	1080.058105
1640.923313		57.192189	23.523561
2912.820697		20.407824	14.900077
2912.821719		31.898328	23.289485
2926.734608		72.847082	53.440877
2926.762609		1.585790	1.163352
2939.606550		2.732226	2.013186
2939.647165		35.048566	25.825190
2949.054911		20.467387	15.129457
2949.059457		6.086244	4.498948
2951.152724	33.653660	24.894423	
2951.155810		3.755043	2.777699
2980.580103		21.681188	16.198021
2980.612244		73.103993	54.616599
2983.080507		5.512415	4.121781
2983.102393		0.987336	0.738263
2987.937144		121.095387	90.693702
2988.010265		0.595309	0.445865
2992.955548		6.643446	4.983928
2992.966639		58.025635	43.531120
3019.278136		0.130055	0.098426
3019.292519		0.904037	0.684179
3245.301739		1.436271	1.168340
3248.623040		217.630275	177.213458
3322.710981		17.597444	14.656161
3322.991486		10.130874	8.438286
3388.667656		15.077644	12.806797
3388.708187		42.736675	36.300531
3391.511654		0.489946	0.416505
3391.538382	86.319274	73.380824	

Zero-Point Energy : 0.456758 a.u.
==========
12.429022 eV
(imaginary frequencies were excluded from the summation)

```
Statistical       Thermal       Analysis              ***              ideal       gas       assumed              ***
     Temp                                                                 Transl      Rotat     Vibrat       Total
     ----                                                                 ------      -----     ------       -----

     298.15    Entropy (cal/mole-K):                                     45.137     35.336    110.472     190.945
               Internal Energy (Kcal/mole):                              0.889       0.889    303.440     305.217
               Constant Volume Heat Capacity (cal/mole-K):       2.981    2.981   109.559   115.521
```

α[**2**]$_2$-tzp-blyp;C_2

Coordinates	in	Geometry	Cycle	25
Atom	X	Y	Z	(Angstrom)
1.Pd	-0.633064	-1.559808	0.142284	
2.O	0.693158	-2.072243	1.603225	
3.O	2.819421	-2.788895	1.821657	
4.N	-2.273774	-1.167455	1.427975	
5.H	-2.485325	-2.015289	1.968649	
6.H	-2.012702	-0.435777	2.101720	
7.H	-1.941219	-0.049222	-1.553716	
8.O	3.079378	-2.647980	-1.001848	
9.C	1.863871	-2.467456	1.119075	
10.H	-6.092339	-2.254464	-0.929251	
11.H	-6.759521	-0.760073	-1.587686	
12.C	-3.486443	-0.723579	0.634467	
13.H	-3.402123	0.363286	0.530754	
14.C	-4.824399	-1.040396	1.328238	
15.H	-4.482876	0.227960	-1.812005	
16.C	-5.944513	-1.163387	-0.972718	
17.H	-4.853701	-0.542714	2.307335	
18.H	-4.892955	-2.127261	1.507612	
19.C	-4.586632	-0.856045	-1.652181	
20.H	-4.534239	-1.342235	-2.637642	
21.H	-3.469615	-2.440717	-0.672498	
22.C	-6.015278	-0.574698	0.454373	
23.H	-6.958131	-0.862800	0.937938	
24.H	-6.006915	0.523478	0.398781	
25.C	2.009057	-2.395862	-0.452085	
26.O	0.942772	-1.945167	-1.108242	
27.C	-3.418946	-1.346698	-0.772507	
28.N	-2.052018	-1.055642	-1.339689	
29.H	-1.906390	-1.572356	-2.214335	
30.Pd	0.633064	1.559808	0.142284	
31.O	-0.942772	1.945167	-1.108242	
32.O	-3.079378	2.647980	-1.001848	
33.N	2.052018	1.055642	-1.339689	
34.H	1.941219	0.049222	-1.553716	
35.H	1.906390	1.572356	-2.214335	
36.H	2.485325	2.015289	1.968649	
37.O	-2.819421	2.788895	1.821657	
38.C	-2.009057	2.395862	-0.452085	
39.H	6.006915	-0.523478	0.398781	
40.H	6.958131	0.862800	0.937938	
41.C	3.418946	1.346698	-0.772507	
42.H	3.469615	2.440717	-0.672498	
43.C	4.586632	0.856045	-1.652181	
44.H	4.892955	2.127261	1.507612	
45.C	6.015278	0.574698	0.454373	
46.H	4.534239	1.342235	-2.637642	
47.H	4.482876	-0.227960	-1.812005	
48.C	4.824399	1.040396	1.328238	
49.H	4.853701	0.542714	2.307335	
50.H	3.402123	-0.363286	0.530754	
51.C	5.944513	1.163387	-0.972718	
52.H	6.759521	0.760073	-1.587686	
53.H	6.092339	2.254464	-0.929251	
54.C	-1.863871	2.467456	1.119075	
55.O	-0.693158	2.072243	1.603225	
56.C	3.486443	0.723579	0.634467	
57.N	2.273774	1.167455	1.427975	
58.H	2.012702	0.435777	2.101720	

```
E-test:            old,new=      -11.91949,      -11.91938      hartree
max    gradient:                       0.00087491    au/angstrom,radian
max      cart.      step:                        0.00671654      angstrom
Geometry Converged
```

	hartree	eV	kcal/mol	kJ/mol
Total Pauli Repulsion:	44.947923529402459	1223.0952	28205.25	118010.76
Electrostatic Interaction:	-9.699219051932502	-263.9292	-6086.35	-25465.30
Total Orbital Interactions:	-47.168125699704767	-1283.5100	-29598.45	-123839.90
Total Bonding Energy:	-11.919407259541725	-324.3436	-7479.54	-31294.40

Frequency	Dipole Strength	Absorption Intensity (degeneracy not counted)
cm-1	1e-40 esu2 cm2	km/mole
-20.980679	55.843186	-0.293676
15.823497	0.000000	0.000000
16.268500	0.000000	0.000000
22.563609	1014.961411	5.740321
41.335700	271.890813	2.817072
44.222406	17.342230	0.192232
53.132451	195.757160	2.607087
61.699856	10.651381	0.164728
62.471229	124.222106	1.945168
64.067386	63.496868	1.019688
67.108710	11.457449	0.192728
67.242375	93.767182	1.580418
93.595234	0.815034	0.019121
98.321424	2170.569109	53.493356
120.571777	4.272196	0.129114
122.258077	15.578055	0.477385
169.514738	0.417514	0.017740
169.813262	74.683856	3.178897
173.202146	47.215630	2.049827
175.007579	0.018421	0.000808
180.753010	19.868970	0.900200
186.119191	81.652364	3.809237
216.363923	31.050017	1.683933
220.696450	123.593001	6.837027
244.221583	20.257362	1.240067
244.349157	24.644181	1.509396
304.736867	191.382049	14.618549
306.691737	2.294081	0.176355
315.037427	0.008109	0.000640
315.476371	138.972088	10.989362
327.616715	0.052609	0.004320
328.092037	95.789614	7.877568
342.601692	0.711371	0.061089
343.484410	68.975585	5.938551
351.435355	72.809219	6.413718
352.220647	7.791242	0.687859
409.300707	12.735659	1.306598
410.601172	24.119017	2.482321
421.241345	116.313467	12.281151
421.342935	2.807650	0.296522
444.177376	1.007321	0.112151
444.497132	557.041794	62.063293
476.427309	0.018292	0.002184
477.385682	120.803077	14.455245
506.966926	1.983578	0.252062
510.232605	255.324044	32.654121
514.631982	312.813950	40.351618
515.627509	0.047147	0.006094
524.179583	18.635502	2.448495
524.236245	49.043654	6.444481
545.428206	10.259408	1.402613
546.685776	0.148889	0.020402
565.826621	5.766946	0.817913
565.932034	16.173858	2.294330
639.436336	67.536211	10.824605
639.758545	0.014661	0.002351
696.033737	3.610271	0.629866
696.322268	298.158513	52.039794
743.671150	3.755348	0.700018
744.016632	223.337756	41.650754
765.430366	0.477516	0.091616
765.565641	0.246243	0.047252
794.274131	2.587005	0.515046
794.281350	0.043582	0.008677
816.361183	13.609535	2.784862
816.514947	0.732725	0.149963
820.658923	17.696240	3.640171
820.759289	0.146415	0.030122
839.130200	0.068565	0.014422
839.170323	6.370624	1.340017
850.895034	0.267355	0.057022
851.002930	0.414434	0.088403
898.739371	4.196397	0.945341
898.825041	6.105946	1.375644
914.876183	5.146667	1.180229
914.959280	3.959140	0.907989
970.098248	497.273613	120.917513
970.227016	1.566280	0.380909
1004.730039	211.695815	53.313811
1005.233861	1.517870	0.382454
1012.840003	0.565547	0.143578
1013.135929	26.364345	6.695188
1023.511224	81.737203	20.969615
1024.099707	0.130166	0.033413
1031.964864	52.912417	13.686758
1032.039573	1.570389	0.406239
1049.257949	42.020862	11.051603
1050.267083	3.998141	1.052533

1075.666072		45.194693	12.185490
1077.568113		18.613019	5.027356
1098.015111		130.918185	36.031834
1099.996634		0.367604	0.101356
1119.556416		52.870833	14.836799
1120.550809		10.594370	2.975670
1130.075818		0.514406	0.145711
1130.218429		38.220468	10.827706
1142.206157		8.547875	2.447263
1148.317697		0.510074	0.146816
1181.082312		0.040128	0.011880
1182.022833		28.188731	8.351788
1220.202022		19.252036	5.888253
1220.565016		0.464612	0.142144
1239.749486		3.441478	1.069441
1239.853044		1854.539528	576.347451
1252.346171		20.122813	6.316713
1252.388692		18.838698	5.913820
1285.370539		2.755592	0.887813
1285.444667		0.128791	0.041497
1302.051631		2.572893	0.839707
1302.112805		0.783531	0.255731
1327.697661		13.720839	4.566231
1327.776994		0.947530	0.315353
1333.847401		12.243635	4.093498
1333.875923		7.765216	2.596253
1338.600612		21.892662	7.345607
1338.629084		2.011589	0.674959
1346.667396		9.601619	3.241029
1346.667648		17.599980	5.940879
1347.592684		0.492304	0.166292
1347.646781		4.799332	1.621194
1368.607864		4.070059	1.396233
1368.717671		0.007770	0.002666
1389.735354		6.564986	2.286883
1389.942769		65.170506	22.705239
1458.179411		3.461121	1.265045
1458.182680		0.454232	0.166023
1461.239875		7.299508	2.673580
1461.249528		11.070034	4.054632
1464.182946		5.000448	1.835196
1464.189412		31.128056	11.424240
1474.738002		50.236637	18.570068
1474.761820		2.075521	0.767233
1600.332178		67.569196	27.104223
1600.750249		122.747758	49.251019
1619.539924		4.040862	1.640377
1623.935132		126.922557	51.663706
1631.172453		133.127320	54.430853
1632.418707		275.706778	112.812462
1638.881027		2629.187885	1080.058105
1640.923313		57.192189	23.523561
2912.820697		20.407824	14.900077
2912.821719		31.898328	23.289485
2926.734608		72.847082	53.440877
2926.762609		1.585790	1.163352
2939.606550		2.732226	2.013186
2939.647165		35.048566	25.825190
2949.054911		20.467387	15.129457
2949.059457		6.086244	4.498948
2951.152724	33.653660	24.894423	
2951.155810		3.755043	2.777699
2980.580103		21.681188	16.198021
2980.612244		73.103993	54.616599
2983.080507		5.512415	4.121781
2983.102393		0.987336	0.738263
2987.937144		121.095387	90.693702
2988.010265		0.595309	0.445865
2992.955548		6.643446	4.983928
2992.966639		58.025635	43.531120
3019.278136		0.130055	0.098426
3019.292519		0.904037	0.684179
3245.301739		1.436271	1.168340
3248.623040		217.630275	177.213458
3322.710981		17.597444	14.656161
3322.991486		10.130874	8.438286
3388.667656		15.077644	12.806797
3388.708187		42.736675	36.300531
3391.511654		0.489946	0.416505
3391.538382	86.319274	73.380824	

Zero-Point Energy :	0.456758	a.u.
==========	12.429022	eV
(imaginary frequencies were excluded from the summation)		

Statistical Thermal Analysis *** ideal gas assumed ***					
Temp			Transl	Rotat	Vibrat	Total
----			------	-----	------	-----
298.15	Entropy (cal/mole-K):		45.137	35.336	110.472	190.945
	Internal Energy (Kcal/mole):		0.889	0.889	303.440	305.217
	Constant Volume Heat Capacity (cal/mole-K):	2.981	2.981	109.559	115.521	

α[**2**]$_2$-tzp-blyp-d3;C_2

Coordinates in Geometry Cycle 32

Atom	X	Y	Z	(Angstrom)
1.Pd	-0.567316	-1.471062	0.140812	
2.O	0.787607	-1.911307	1.601554	
3.O	2.912792	-2.634414	1.799761	
4.N	-2.179078	-1.018310	1.429990	
5.H	-2.379415	-1.830428	2.026085	
6.H	-1.902415	-0.240075	2.045389	
7.H	-1.877036	-0.020612	-1.585483	
8.O	3.130694	-2.556218	-1.028331	
9.C	1.941626	-2.342200	1.106697	
10.H	-6.033632	-2.143338	-0.873670	
11.H	-6.687591	-0.649493	-1.550878	
12.C	-3.405285	-0.622952	0.633885	
13.H	-3.343959	0.457286	0.492413	
14.C	-4.731290	-0.923576	1.349934	
15.H	-4.389137	0.303180	-1.793903	
16.C	-5.872797	-1.055039	-0.937221	
17.H	-4.738403	-0.417091	2.324472	
18.H	-4.810225	-2.008860	1.534176	
19.C	-4.516395	-0.778031	-1.631851	
20.H	-4.477824	-1.271284	-2.614208	
21.H	-3.424511	-2.372764	-0.632100	
22.C	-5.920328	-0.443516	0.481704	
23.H	-6.866093	-0.701461	0.976072	
24.H	-5.880985	0.652903	0.408690	
25.C	2.059551	-2.319188	-0.474294	
26.O	0.977096	-1.907601	-1.127590	
27.C	-3.354357	-1.282185	-0.754670	
28.N	-1.989745	-1.019893	-1.341411	
29.H	-1.854495	-1.563263	-2.201443	
30.Pd	0.567316	1.471062	0.140812	
31.O	-0.977096	1.907601	-1.127590	
32.O	-3.130694	2.556218	-1.028331	
33.N	1.989745	1.019893	-1.341411	
34.H	1.877036	0.020612	-1.585483	
35.H	1.854495	1.563263	-2.201443	
36.H	2.379415	1.830428	2.026085	
37.O	-2.912792	2.634414	1.799761	
38.C	-2.059551	2.319188	-0.474294	
39.H	5.880985	-0.652903	0.408690	
40.H	6.866093	0.701461	0.976072	
41.C	3.354357	1.282185	-0.754670	
42.H	3.424511	2.372764	-0.632100	
43.C	4.516395	0.778031	-1.631851	
44.H	4.810225	2.008860	1.534176	
45.C	5.920328	0.443516	0.481704	
46.H	4.477824	1.271284	-2.614208	
47.H	4.389137	-0.303180	-1.793903	
48.C	4.731290	0.923576	1.349934	
49.H	4.738403	0.417091	2.324472	
50.H	3.343959	-0.457286	0.492413	
51.C	5.872797	1.055039	-0.937221	
52.H	6.687591	0.649493	-1.550878	
53.H	6.033632	2.143338	-0.873670	
54.C	-1.941626	2.342200	1.106697	
55.O	-0.787607	1.911307	1.601554	
56.C	3.405285	0.622952	0.633885	
57.N	2.179078	1.018310	1.429990	
58.H	1.902415	0.240075	2.045389	

```
E-test:            old,new=      -12.03251,      -12.03217      hartree
max    gradient:                       0.00096232    au/angstrom,radian
max      cart.      step:                        0.00678989      angstrom
Geometry Converged
```

	hartree	eV	kcal/mol	kJ/mol
Total Pauli Repulsion:	45.151122883172086	1228.6246	28332.76	118544.26
Electrostatic Energy:	-9.764166840544309	-265.6965	-6127.11	-25635.82
Total Orbital Interactions:	-47.303746036522305	-1287.2004	-29683.55	-124195.97
Dispersion Energy:	-0.115422033298285	-3.1408	-72.43	-303.04
Total Bonding Energy:	-12.032200095489218	-327.4128	-7550.32	-31590.54

Frequency	Dipole Strength	Absorption Intensity (degeneracy not counted)
cm-1	1e-40 esu2 cm2	km/mole
-21.764093	49.416880	-0.269584
17.196922	0.000000	0.000000
23.154208	1065.557723	6.184221
54.554194	65.106130	0.890283
55.103436	24.306460	0.335721
61.220286	15.670716	0.240471
67.645609	77.158820	1.308288
69.525183	0.012886	0.000225
71.020007	81.795491	1.456090
77.608030	59.227283	1.152143
78.612588	156.564837	3.085066
89.420592	0.560585	0.012565
109.333044	0.103138	0.002826
124.635295	36.361089	1.135942
139.072700	1686.123478	58.777259
145.404718	16.882615	0.615313
171.427367	150.686806	6.474906
173.260226	0.386661	0.016792
183.747142	1.477860	0.068066
191.378161	71.984442	3.453099
192.795574	38.378412	1.854651
202.573334	3.218779	0.163437
232.010573	21.958184	1.276975
232.361987	170.484026	9.929488
248.173574	25.053228	1.558466
249.175034	15.520564	0.969371
306.591136	264.737206	20.344764
308.926797	2.457120	0.190265
329.424314	0.129377	0.010683
330.281455	140.265794	11.612187
331.574883	0.141414	0.011753
332.009380	14.436057	1.201371
350.170514	69.575715	6.106823
350.450958	1.510810	0.132714
363.845632	1.292777	0.117901
364.956878	82.484732	7.545590
414.216186	27.339169	2.838510
415.589722	22.639475	2.358355
426.440479	122.327091	13.075525
426.539186	2.159841	0.230919
448.197560	0.371259	0.041708
448.392807	559.805765	62.917879
487.672602	0.017293	0.002114
488.858934	101.805089	12.474729
502.492187	1.721913	0.216880
505.852013	311.952519	39.553967
522.491817	222.658590	29.160638
523.002666	0.780947	0.102377
530.944761	18.362908	2.443818
531.207738	84.749665	11.284451
556.409438	6.361582	0.887233
558.787528	0.033189	0.004649
569.198883	3.039280	0.433623
570.238383	23.207842	3.317182
651.435392	82.166715	13.416689
651.462944	0.158907	0.025948
705.472653	2.399930	0.424382
705.899524	344.393239	60.936229
744.609305	3.588791	0.669815
744.815971	237.327318	44.307249
775.018798	0.273862	0.053201
775.141032	0.192995	0.037498
796.060270	0.051200	0.010216
796.061564	3.958886	0.789947
814.659350	17.734316	3.621334
814.817490	0.439575	0.089778
825.817071	20.301557	4.202341
825.908753	0.191614	0.039668
845.367293	0.073918	0.015663
845.388072	5.010405	1.061713
861.045074	0.292742	0.063181
861.153043	0.214563	0.046314
907.435508	3.097356	0.704506
907.538760	6.607295	1.503028
919.650097	5.469222	1.260742
919.731147	3.862605	0.890470
975.347850	447.853215	109.489708
975.465566	0.822527	0.201113
1010.030335	190.679517	48.274361
1010.587527	3.284975	0.832116
1019.567727	0.859743	0.219717
1019.832567	25.798706	6.594849
1030.244829	49.988634	12.908916
1030.820081	0.627319	0.162087
1034.221164	109.318647	28.339080
1034.442503	1.763833	0.457343

1058.680627		23.920307	6.347603
1059.537363		2.456989	0.652526
1083.422671		53.349944	14.488051
1086.994994		29.031739	7.910040
1106.309075		101.461483	28.135572
1108.103178		0.079771	0.022156
1127.229730		10.258958	2.898637
1130.558004		47.773661	13.538154
1134.475685		46.076170	13.102363
1135.405422		0.539865	0.153644
1148.729918		11.863284	3.415867
1154.950821		0.026452	0.007658
1188.997473		0.005928	0.001767
1190.041096		25.079756	7.481063
1225.942002		221.629834	68.104564
1226.854865		0.343777	0.105718
1236.495106		4.600250	1.425778
1237.014318		1675.563928	519.533790
1258.042006		10.460929	3.298705
1258.098771		18.773274	5.920152
1294.804908		3.484166	1.130788
1295.078241		0.695235	0.225687
1305.789112		2.733474	0.894677
1305.841868		0.199354	0.065252
1332.175702		7.640502	2.551300
1332.223788		5.582042	1.864011
1333.652463		14.605522	4.882450
1333.721593		3.994889	1.335513
1344.318851		18.767885	6.324056
1344.358291		0.438180	0.147654
1353.427072		5.989512	2.031910
1353.716672		2.243770	0.761350
1358.243504		12.915710	4.397178
1358.424966		4.825681	1.643131
1377.991168		1.692331	0.584534
1378.204697		0.301902	0.104294
1398.984289		7.740290	2.714239
1399.416585		73.050795	25.624184
1460.825431		4.370020	1.600147
1460.828787		0.162055	0.059339
1464.994732		15.609034	5.731789
1465.003701		7.072565	2.597130
1468.808159		9.612464	3.538978
1468.815033		25.111329	9.245169
1480.161015		65.968534	24.475066
1480.208898		3.775229	1.400698
1601.328250		121.148421	48.626856
1602.511156		89.444140	35.927833
1623.688436		23.439280	9.539487
1628.537658		156.553976	63.905756
1633.259256		216.670308	88.701834
1634.497500		251.323636	102.966432
1640.981206		2575.969237	1059.552181
1643.003894		67.833853	27.935931
2911.215997		33.841083	24.694302
2911.216141		21.422573	15.632346
2923.971446		79.157606	58.015475
2924.001660		1.099274	0.805679
2937.906196		5.838311	4.299354
2937.952210		37.127602	27.341334
2948.510030		22.859272	16.894412
2948.517596		5.003800	3.698126
2949.630678	32.263487	23.853769	
2949.639219		5.872090	4.341499
2981.836891		23.338819	17.443790
2981.890533		69.541866	51.977586
2984.924902		0.470298	0.351872
2984.931939		6.217087	4.651569
2987.995221		117.783123	88.214715
2988.059009		0.013459	0.010080
2994.215155		65.490346	49.151679
2994.220713		4.426840	3.322429
3063.457716		0.006092	0.004678
3063.466382		12.773023	9.808100
3239.017057		1.587957	1.289229
3242.801968		221.288585	179.869493
3305.201254		17.201153	14.250613
3306.381755		49.870630	41.331001
3384.323510		0.916283	0.777284
3384.435749		70.670943	59.952215
3386.153548		13.430083	11.398913
3386.235539	73.302441	62.217659	

Zero-Point	Energy	:	0.459065 a.u.
==========			12.491782 eV
(imaginary frequencies were excluded from the summation)			

Statistical Thermal Analysis *** ideal gas assumed ***					
Temp			Transl	Rotat	Vibrat	Total
----			------	-----	------	-----
298.15	Entropy (cal/mole-K):		45.137	35.192	108.549	188.878
	Internal Energy (Kcal/mole):		0.889	0.889	304.947	306.724
	Constant Volume Heat Capacity (cal/mole-K):	2.981	2.981	110.440	116.402	

Na,α[**2**]$_2$-tzp-blyp-d3;C_1

Coordinates in Geometry Cycle 116

Atom	X	Y	Z (Angstrom)
1.Pd	-0.621738	-1.369788	0.081539
2.O	0.806914	-1.860558	1.506654
3.O	2.863075	-2.788863	1.593258
4.N	-2.224297	-1.079419	1.398041
5.H	-2.353138	-1.939996	1.946573
6.H	-2.011454	-0.320927	2.063601
7.H	-2.055441	-0.000029	-1.603781
8.O	3.024128	-2.623080	-1.182812
9.C	1.876693	-2.344261	0.961205
10.H	-6.050106	-2.390712	-0.863351
11.H	-6.792771	-0.920672	-1.496471
12.C	-3.498638	-0.740547	0.637106
13.H	-3.504118	0.344723	0.522540
14.C	-4.783497	-1.144270	1.374479
15.H	-4.560244	0.161670	-1.763171
16.C	-5.949698	-1.294748	-0.902651
17.H	-4.806955	-0.658680	2.359035
18.H	-4.793670	-2.235750	1.534809
19.C	-4.622999	-0.926829	-1.616043
20.H	-4.571025	-1.405059	-2.604657
21.H	-3.419526	-2.467786	-0.659157
22.C	-6.011380	-0.717588	0.529652
23.H	-6.930852	-1.043990	1.031141
24.H	-6.041537	0.380378	0.482948
25.C	1.963573	-2.267904	-0.618452
26.O	0.942722	-1.754308	-1.232525
27.C	-3.426409	-1.372650	-0.757166
28.N	-2.083060	-1.003869	-1.354486
29.H	-1.914905	-1.533425	-2.218682
30.Pd	0.701200	1.560516	0.142012
31.O	-0.875414	1.924546	-1.086854
32.O	-3.092833	2.252063	-0.931433
33.N	2.112973	1.219117	-1.387080
34.H	1.994696	0.251028	-1.722639
35.H	1.968556	1.836487	-2.194511
36.H	2.575046	2.008071	1.938675
37.O	-2.835310	2.242142	1.893643
38.C	-1.987898	2.164434	-0.400585
39.H	6.004287	-0.613491	0.258618
40.H	7.012138	0.704233	0.857707
41.C	3.486952	1.422519	-0.801403
42.H	3.589982	2.505340	-0.645015
43.C	4.626071	0.917713	-1.707267
44.H	5.003434	2.030473	1.483276
45.C	6.055468	0.483109	0.368711
46.H	4.585653	1.437221	-2.674437
47.H	4.467654	-0.154823	-1.906361
48.C	4.888797	0.955499	1.268750
49.H	4.899551	0.429088	2.233173
50.H	3.404745	-0.347698	0.404540
51.C	5.999770	1.137720	-1.029361
52.H	6.796823	0.740138	-1.669954
53.H	6.185758	2.217719	-0.929743
54.C	-1.844419	2.147658	1.175249
55.O	-0.629654	1.881075	1.638668
56.C	3.535462	0.726238	0.572714
57.N	2.350012	1.161352	1.400783
58.H	2.101811	0.430242	2.079748
59.Na	4.461794	-3.643140	0.254965

```
E-test:            old,new=      -11.93526,      -11.93528      hartree
max    gradient:                        0.00090917    au/angstrom,radian
max      cart.      step:                       0.00450976      angstrom
Geometry Converged
```

	hartree	eV	kcal/mol	kJ/mol
Total Pauli Repulsion:	45.314844653507542	1233.0797	28435.50	118974.11
Electrostatic Energy:	-9.838677848133711	-267.7240	-6173.86	-25831.45
Total Orbital Interactions:	-47.294894252556333	-1286.9596	-29678.00	-124172.73
Dispersion Energy:	-0.116581080725826	-3.1723	-73.16	-306.08
Total Bonding Energy:	-11.935305790479692	-324.7762	-7489.52	-31336.14

Frequency cm-1	Dipole Strength 1e-40 esu2	Absorption Intensity (degeneracy not counted) cm2	km/mole
-28.683957	138.911614		-0.998747
13.167234	0.000000		0.000000
22.714625	407.811054		2.321895
37.779361	395.046855		3.740945
51.283480	39.719702		0.510577
55.385535	95.446453		1.325056
56.487799	72.505338		1.026603
59.856072	70.440977		1.056846
61.712354	21.492298		0.332455
80.576836	249.757614		5.044371
82.396758	42.375884		0.875199
88.496681	107.269886		2.379484
93.535802	60.386740		1.415786
111.333183	1428.176202		39.855154
126.117646	0.436644		0.013803
139.273439	785.387028		27.417642
150.338871	132.328843		4.986592
161.049336	39.194556		1.582205
171.875396	62.147321		2.677406
182.189006	31.641278		1.444955
186.244267	13.407817		0.625920
190.252747	328.768929		15.678329
192.489744	96.969741		4.678664
210.401734	18.087225		0.953892
225.923119	117.388686		6.647602
235.712952	203.420981		12.018694
239.573240	678.468893		40.742373
246.981136	19.700332		1.219594
257.439899	52.012672		3.356318
308.979519	594.635445		46.053067
311.685775	41.461020		3.239180
329.863880	13.498149		1.116059
331.088852	110.401035		9.162116
331.784670	8.123461		0.675578
347.037645	12.283292		1.068487
357.535941	34.062478		3.052629
359.336061	22.731404		2.047412
363.407902	49.040076		4.467078
393.619041	423.024794		41.736881
414.811742	22.362776		2.325171
417.569679	20.145053		2.108509
424.028633	69.920496		7.431522
428.710322	42.618815		4.579767
445.471295	282.252168		31.516290
450.896818	277.891261		31.407266
483.207501	42.739042		5.176504
491.347500	17.674308		2.176753
493.943352	199.896092		24.749106
513.076453	145.377544		18.696378
524.373811	96.638922		12.701972
528.471273	26.641247		3.529019
529.682982	123.148942		16.350264
542.592419	33.463190		4.551129
556.173216	8.781424		1.224202
560.240003	4.294539		0.603071
566.681429	13.971169		1.984494
577.565069	13.204875		1.911672
641.804784	18.795880		3.023735
680.828662	21.880248		3.733947
686.179970	169.897771		29.221586
729.122816	169.893038		31.049481
747.080895	104.180823		19.508932
754.077013	164.395665		31.073068
769.751785	0.590412		0.113916
777.872271	0.918487		0.179085
799.134259	4.208371		0.842969
804.236081	0.230493		0.046464
817.224386	6.976819		1.429147
824.987121	11.444927		2.366673
826.470053	7.089213		1.468599
831.411111	0.159695		0.033280
840.804197	2.932985		0.618134
843.524769	2.151376		0.454875
855.867284	0.392352		0.084171
860.467734	0.699901		0.150956
904.161011	6.529602		1.479826
905.447385	3.117341		0.707499
919.018752	6.273748		1.445205
920.636947	3.583492		0.826938
962.630170	164.369418		39.660534
978.554469	226.428967		55.538617
1009.573563	31.274948		7.914302
1010.103071	146.410076		37.069329
1017.699126	16.439775		4.193661
1022.742226	10.478785		2.686304
1026.163128	21.524164		5.536315
1029.887497	14.038851		3.624094
1036.076378	141.036229		36.626931

1036.272763		2.837838	0.737123
1051.441432		13.644711	3.596065
1054.378226		25.339699	6.696933
1080.811694		33.484796	9.071430
1097.949317		21.227231	5.841894
1104.537238		74.605508	20.655196
1117.000918		23.816018	6.668079
1125.139641		23.023234	6.493081
1126.021928		73.781911	20.824511
1133.170958		21.083127	5.988369
1147.264820		5.333802	1.533835
1158.895671		7.549078	2.192887
1184.466015		4.588817	1.362390
1185.815903		16.638632	4.945531
1226.795925		4.154305	1.277464
1230.111025		113.504372	34.997335
1231.651966		92.204088	28.465332
1241.573434		763.346985	237.559541
1255.939865		13.858843	4.362886
1256.318379		27.740889	8.735709
1291.538722		0.226699	0.073390
1292.431206		10.792748	3.496371
1304.743529		2.350394	0.768677
1308.232890		0.800422	0.262472
1320.181240		335.894081	111.151155
1330.629670		4.782799	1.595208
1332.147113		6.701706	2.237771
1334.076128		5.786979	1.935132
1334.760298		5.711472	1.910862
1339.552404		23.000836	7.722917
1347.718491		15.624235	5.278081
1348.146345		2.604085	0.879975
1353.763673		6.963143	2.362796
1355.133840		1.811560	0.615337
1360.041763		11.176627	3.810141
1373.312744		16.158228	5.562132
1383.851835		7.999965	2.774954
1392.809122		27.771243	9.695383
1410.991221		36.284946	12.833020
1457.089155		8.779544	3.206536
1462.047065		2.512187	0.920643
1462.939181		7.936296	2.910196
1465.370939		13.134362	4.824304
1469.233090		20.278608	7.468045
1469.511829		25.290376	9.315506
1477.513785		36.728655	13.602372
1480.296621		27.708691	10.281177
1564.980590		205.866506	80.755613
1586.270436		2966.966919	1179.690289
1600.833746		124.191541	49.832918
1607.674582		166.684593	67.169432
1614.218070		145.849573	59.012693
1622.220051		51.961494	21.128539
1638.771202		223.887211	91.965657
1643.882615		1067.716609	439.951569
2902.777483		51.882619	37.749718
2916.299868		25.838880	18.887911
2926.659372		10.588585	7.767624
2930.174648		14.210087	10.436823
2933.223372		30.589645	22.490424
2944.468292	16.105359	11.886538	
2944.853019		25.037535	18.481332
2953.128224		12.413145	9.188449
2955.293341		13.000074	9.629960
2960.965565		5.314396	3.944258
2982.281618		20.818649	15.562497
2986.515555		18.620075	13.938765
2989.381734		34.880359	26.136076
2990.951286		1.063614	0.797391
2996.979422		20.840178	15.655367
2997.736630		46.396325	34.862227
2998.934964		29.061764	21.845756
3003.359759		26.043994	19.606182
3020.727991		6.472460	4.900711
3062.137438		25.771145	19.780464
3260.433426		90.338891	73.829200
3293.648758		29.552623	24.397840
3297.274122		54.389307	44.951755
3321.027406		13.378347	11.136609
3370.772127		50.864182	42.975361
3377.626108		47.853431	40.513776
3388.710247		34.237984	29.081760
3390.321019	54.803350	46.572119	

Zero-Point Energy :	0.460706	a.u.
==========	12.536441	eV
(imaginary frequencies were excluded from the summation)		

Statistical Thermal Analysis *** ideal gas assumed ***				
Temp	Transl	Rotat	Vibrat	Total
298.15 Entropy (cal/mole-K):	45.247	36.915	117.630	199.792
Internal Energy (Kcal/mole):	0.889	0.889	307.124	308.901
Constant Volume Heat Capacity (cal/mole-K): 2.981	2.981	115.713	121.675	

β[**2**]$_2$-tzp-blyp;C_1

Coordinates in Geometry Cycle 26

Atom	X	Y	Z (Angstrom)
1.Pd	-0.618931	-1.554909	0.139382
2.O	0.714546	-2.058048	1.598373
3.O	2.837341	-2.789241	1.809554
4.N	-2.254666	-1.151267	1.431343
5.H	-2.463416	-1.992419	1.983192
6.H	-1.988046	-0.411390	2.094306
7.H	-1.935646	-0.050946	-1.557471
8.O	3.084065	-2.661562	-1.016500
9.C	1.880246	-2.465431	1.110204
10.H	-6.090527	-2.240756	-0.908993
11.H	-6.753031	-0.743670	-1.566473
12.C	-3.471707	-0.713612	0.640905
13.H	-3.389129	0.372740	0.531379
14.C	-4.806687	-1.026332	1.342167
15.H	-4.473874	0.232916	-1.802949
16.C	-5.937719	-1.150514	-0.954212
17.H	-4.830154	-0.525848	2.319881
18.H	-4.876564	-2.112549	1.524705
19.C	-4.581177	-0.850393	-1.639914
20.H	-4.534720	-1.339095	-2.624378
21.H	-3.463852	-2.435928	-0.660018
22.C	-6.000241	-0.559534	0.472413
23.H	-6.941626	-0.844399	0.960593
24.H	-5.989195	0.538470	0.415196
25.C	2.017080	-2.404469	-0.462611
26.O	0.946340	-1.959909	-1.115817
27.C	-3.411229	-1.342391	-0.763662
28.N	-2.045767	-1.055997	-1.337839
29.H	-1.904866	-1.577023	-2.210712
30.Pd	0.618959	1.554910	0.139359
31.O	-0.946332	1.959961	-1.115827
32.O	-3.084156	2.661312	-1.016355
33.N	2.045708	1.055792	-1.337849
34.H	1.935582	0.050781	-1.557553
35.H	1.904833	1.576942	-2.210666
36.H	2.463056	1.991937	1.983405
37.O	-2.837277	2.789160	1.809631
38.C	-2.017087	2.404395	-0.462540
39.H	5.989459	-0.537787	0.415789
40.H	6.941668	0.845436	0.960668
41.C	3.411147	1.342219	-0.763633
42.H	3.463685	2.435761	-0.659960
43.C	4.581134	0.850353	-1.639844
44.H	4.876112	2.113367	1.524253
45.C	6.000330	0.560240	0.472590
46.H	4.534620	1.338993	-2.624336
47.H	4.473950	-0.232978	-1.802827
48.C	4.806642	1.027057	1.342168
49.H	4.830275	0.526976	2.320092
50.H	3.389624	-0.372866	0.531656
51.C	5.937697	1.150665	-0.954256
52.H	6.752969	0.743580	-1.566406
53.H	6.090542	2.240916	-0.909429
54.C	-1.880197	2.465351	1.110257
55.O	-0.714502	2.057911	1.598413
56.C	3.471755	0.713538	0.640997
57.N	2.254524	1.150819	1.431349
58.H	1.987902	0.410840	2.094131

```
E-test:            old,new=      -11.91943,      -11.91944      hartree
max    gradient:                       0.00086541    au/angstrom,radian
max      cart.      step:                        0.00722744      angstrom
Geometry Converged
```

	hartree	eV	kcal/mol	kJ/mol
Total Pauli Repulsion:	44.938686622560787	1222.8439	28199.45	117986.51
Electrostatic Interaction:	-9.696708782026548	-263.8609	-6084.78	-25458.71
Total Orbital Interactions:	-47.161458340137337	-1283.3286	-29594.27	-123822.39
Total Bonding Energy:	-11.919470131961990	-324.3453	-7479.58	-31294.56

β[**2**]$_2$-tzp-blyp-d3;C_1

Coordinates in Geometry Cycle 52

Atom	X	Y	Z (Angstrom)
1.Pd	-0.482927	-1.651832	0.132519
2.O	0.839031	-2.143296	1.604160
3.O	3.068514	-2.376475	1.833902
4.N	-2.035139	-1.025023	1.418352
5.H	-2.313423	-1.791262	2.042632
6.H	-1.673615	-0.243324	1.991261
7.H	-1.678764	-0.072771	-1.547962
8.O	3.288171	-2.404286	-0.992814
9.C	2.052868	-2.293817	1.127734
10.H	-5.952239	-1.918806	-0.804725
11.H	-6.541753	-0.422428	-1.530770
12.C	-3.214110	-0.511623	0.623004
13.H	-3.001225	0.551749	0.456778
14.C	-4.557426	-0.679956	1.356176
15.H	-4.189176	0.402380	-1.820688
16.C	-5.738221	-0.843022	-0.911560
17.H	-4.526024	-0.136599	2.310434
18.H	-4.705545	-1.748326	1.591702
19.C	-4.375995	-0.664868	-1.625814
20.H	-4.378331	-1.181151	-2.596974
21.H	-3.398307	-2.292890	-0.581605
22.C	-5.735452	-0.179032	0.484492
23.H	-6.684749	-0.378007	1.000160
24.H	-5.657794	0.912218	0.368219
25.C	2.173329	-2.313861	-0.449930
26.O	1.049296	-2.187458	-1.114243
27.C	-3.239449	-1.216631	-0.744204
28.N	-1.868128	-1.075440	-1.344418
29.H	-1.787483	-1.604738	-2.219485
30.Pd	2.471281	0.965610	0.142595
31.O	0.942061	1.507996	-1.105312
32.O	-1.296944	1.726974	-0.988334
33.N	3.861840	0.401555	-1.333965
34.H	3.671548	-0.599034	-1.546447
35.H	3.785823	0.938655	-2.204674
36.H	4.292831	1.078066	2.063379
37.O	-1.089733	1.659997	1.836350
38.C	-0.183977	1.629009	-0.443042
39.H	7.642657	-1.606652	0.370284
40.H	8.666865	-0.325597	1.025186
41.C	5.230179	0.536084	-0.725494
42.H	5.387289	1.610354	-0.548640
43.C	6.371696	-0.003034	-1.608464
44.H	6.685459	1.037681	1.624687
45.C	7.720182	-0.517151	0.501957
46.H	6.378616	0.526675	-2.572374
47.H	6.186642	-1.067609	-1.818977
48.C	6.538072	-0.027431	1.374419
49.H	6.501797	-0.583309	2.321255
50.H	4.985215	-1.246747	0.453035
51.C	7.730056	0.166119	-0.884619
52.H	8.537092	-0.245172	-1.505475
53.H	7.942729	1.240415	-0.761444
54.C	-0.070131	1.589318	1.134599
55.O	1.141616	1.436049	1.615333
56.C	5.198241	-0.185631	0.632817
57.N	4.016017	0.319921	1.428646
58.H	3.651474	-0.467573	1.991639

```
E-test:            old,new=      -12.04314,      -12.04322      hartree
max    gradient:                        0.00098184    au/angstrom,radian
max      cart.      step:                        0.01000000      angstrom
Geometry Converged
```

	hartree	eV	kcal/mol	kJ/mol
Total Pauli Repulsion:	45.233360196630372	1230.8624	28384.37	118760.17
Electrostatic Energy:	-9.785488287476614	-266.2767	-6140.49	-25691.80
Total Orbital Interactions:	-47.380815372129049	-1289.2976	-29731.91	-124398.31
Dispersion Energy:	-0.110363466971154	-3.0031	-69.25	-289.76
Total Bonding Energy:	-12.043297641068367	-327.7148	-7557.28	-31619.67

Frequency cm-1	Dipole Strength 1e-40 esu2 cm2	Absorption Intensity (degeneracy not counted) km/mole
25.273009	1238.388604	7.844982
32.471972	90.424143	0.735989
37.796810	0.242387	0.002296
44.434879	12.787716	0.142428
60.774453	4.045234	0.061623
61.329937	3.165007	0.048655
71.248108	6.445705	0.115112
81.008464	34.946432	0.709596
81.998103	82.585608	1.697408
99.978350	60.825217	1.524290
107.369928	30.427465	0.818892
122.488487	24.031210	0.737818
139.278402	29.417702	1.027000
154.389618	834.999302	32.313372
158.678420	1.361749	0.054162
164.267516	52.526925	2.162777
172.179402	175.913028	7.592019
178.633857	1.232283	0.055176
188.781200	56.846804	2.689942
192.544981	0.079038	0.003815
209.432882	108.339598	5.687353
215.609758	21.125939	1.141728
240.239980	34.329893	2.067263
243.057553	725.061643	44.173532
251.257438	10.112246	0.636861
255.791438	21.771409	1.395888
309.744662	13.022768	1.011079
314.904851	540.193846	42.639004
329.925273	0.921173	0.076179
330.444399	63.033981	5.220970
333.801185	10.694579	0.894808
334.723242	131.174843	11.005619
356.265129	11.750683	1.049336
356.765714	71.583672	6.401403
359.108758	39.773167	3.580092
363.708526	75.088805	6.845525
417.294761	16.045236	1.678290
418.185429	14.236238	1.492252
427.290728	166.653764	17.849114
428.112920	22.117155	2.373371
450.291174	0.482522	0.054461
455.217032	907.560742	103.555287
486.611448	7.078078	0.863328
487.534871	138.278314	16.898098
508.895850	111.760420	14.255912
510.165971	334.030204	42.714497
527.529295	0.327888	0.043356
527.836573	204.372120	27.039534
533.986577	26.005413	3.480745
534.738105	15.224918	2.040676
559.355839	20.889829	2.928877
559.602593	2.530481	0.354945
571.059137	9.560927	1.368545
571.980211	25.886423	3.711343
676.796241	73.322371	12.438629
677.049625	3.164435	0.537025
732.164167	96.748269	17.755371
732.627205	196.063104	36.004517
747.759645	171.984175	32.235067
748.304489	74.796354	14.029327
774.179213	0.920145	0.178557
774.421602	0.846123	0.164244
796.662744	8.796637	1.756585
797.309583	5.225723	1.044363
822.688354	5.865563	1.209548
822.848890	0.804420	0.165913
825.984904	7.999874	1.656278
826.224848	18.670186	3.866562
845.086004	3.439608	0.728598
845.388730	4.254220	0.901477
863.799889	0.081891	0.017731
863.916858	0.736707	0.159531
908.248966	9.768604	2.223901
908.462510	10.363599	2.359911
922.782052	3.158485	0.730560
922.862656	2.892021	0.668985
981.182103	581.608246	143.040244
981.968622	1.957265	0.481754
1014.709174	109.608797	27.878222
1015.179746	59.550198	15.153195
1023.991025	46.993997	12.061924
1024.326603	12.395283	3.182533
1034.497302	1.180095	0.306002
1035.150419	3.619132	0.939044
1037.706237	105.627147	27.474389
1038.388866	86.826027	22.598938

1068.503944		44.440284	11.902304
1068.791242		8.997964	2.410545
1107.094504		131.057260	36.368371
1107.520852		64.112260	17.797995
1120.528443		98.674677	27.714476
1120.905028		106.581369	29.945266
1158.961357		11.902339	3.457637
1159.444916		37.788951	10.982293
1170.671171		36.601690	10.740244
1171.218851		6.063634	1.780119
1181.234781		3.923637	1.161724
1185.648719		75.299846	22.378357
1199.290510		2.701582	0.812121
1200.591095		12.256823	3.688511
1229.755852		3.163692	0.975194
1230.048269		2.392808	0.737748
1257.248969		9.383772	2.957173
1257.681786		9.736491	3.069385
1275.942525		6.006202	1.920919
1284.982265		1511.387493	486.800514
1296.069300		5.005495	1.626123
1296.482775		4.377532	1.422572
1311.157002		0.109043	0.035837
1311.233584		0.138170	0.045412
1333.314009		6.089097	2.034995
1333.736670		5.678181	1.898267
1333.976704		7.428675	2.483920
1334.179452		9.924957	3.319105
1342.497868		18.634818	6.270712
1342.733223		15.202546	5.116631
1354.038155		11.103525	3.768512
1354.457806		14.900215	5.058667
1370.902089		1.288245	0.442673
1371.905220		2.052962	0.705965
1385.292847		25.003942	8.682167
1385.485260		27.994118	9.721802
1401.329006		11.262990	3.956142
1402.448929		15.303879	5.379806
1459.898407		5.448833	1.993904
1460.566985		4.450487	1.629323
1462.922635		5.594859	2.051581
1463.445722		4.454829	1.634127
1467.693434		20.195104	7.429499
1467.873448		20.877860	7.681617
1477.880850		16.143742	5.980283
1477.921899		10.237454	3.792465
1552.948690		360.828374	140.454565
1557.081682		137.464424	53.651242
1569.541179		120.830697	47.536595
1576.205274		1661.814888	656.558596
1609.202326		60.292864	24.319500
1611.336735		29.165739	11.779785
1616.926635		52.223582	21.165817
1618.173123		2238.868507	908.095746
2906.784970		28.163646	20.520118
2906.979473		27.574855	20.092468
2924.099451		31.333312	22.965532
2924.341467		27.656684	20.272451
2936.309643		12.318243	9.066271
2936.485946		15.028731	11.061864
2940.599387		24.187371	17.827999
2941.541215		27.860534	20.541987
2941.916570	27.210069	20.064949	
2942.096940		28.320913	20.885376
2976.295163		61.086426	45.572073
2976.535171		67.585519	50.424633
2979.969383		21.975822	16.414777
2980.547056		22.160218	16.555721
2981.260879		72.745004	54.360222
2981.675191		43.436638	32.463445
2985.239159		39.729131	29.728039
2985.833407		46.930916	35.123895
2996.676989		7.522393	5.650333
2997.884943		7.236396	5.437701
3134.656133		4.727035	3.714127
3139.906420		485.930590	382.445024
3224.228149		33.499465	27.073332
3228.433281		382.281994	309.352571
3375.824445		3.793138	3.209642
3375.858876		81.577855	69.029485
3387.219053		31.616220	26.843015
3387.418755	27.936490	23.720225	

Zero-Point Energy : 0.459373 a.u.
========== 12.500186 eV

Statistical Thermal Analysis *** ideal gas assumed ***					
Temp			Transl	Rotat	Vibrat	Total
----			------	-----	------	-----
298.15	Entropy (cal/mole-K):		45.137	36.716	114.786	196.639
	Internal Energy (Kcal/mole):		0.889	0.889	305.851	307.628
	Constant Volume Heat Capacity (cal/mole-K):	2.981	2.981	113.411	119.372	

β[**2**]$_2$-tzp-blyp-d3bj;C_1

Coordinates in Geometry Cycle 13

Atom	X	Y	Z (Angstrom)
1.Pd	-0.528351	-1.662555	0.141592
2.O	0.793753	-2.138719	1.619034
3.O	3.027839	-2.297175	1.862402
4.N	-2.089486	-1.068413	1.413773
5.H	-2.383931	-1.850793	2.009392
6.H	-1.733645	-0.302421	2.010734
7.H	-1.695991	-0.092991	-1.546600
8.O	3.261670	-2.340690	-0.960081
9.C	2.014600	-2.239495	1.150219
10.H	-6.010426	-1.824372	-0.854945
11.H	-6.522393	-0.301532	-1.585133
12.C	-3.242746	-0.528311	0.606201
13.H	-3.000227	0.527975	0.443777
14.C	-4.594740	-0.657685	1.320955
15.H	-4.143035	0.418677	-1.849210
16.C	-5.747958	-0.759687	-0.956654
17.H	-4.554316	-0.124309	2.279919
18.H	-4.786444	-1.721436	1.542896
19.C	-4.373763	-0.639117	-1.653481
20.H	-4.385350	-1.158743	-2.622313
21.H	-3.441817	-2.299204	-0.611532
22.C	-5.734032	-0.099913	0.438219
23.H	-6.698818	-0.251917	0.939354
24.H	-5.598440	0.985708	0.326058
25.C	2.143438	-2.260716	-0.422041
26.O	1.021550	-2.165553	-1.093053
27.C	-3.266451	-1.224535	-0.761692
28.N	-1.889781	-1.094644	-1.345054
29.H	-1.797942	-1.630288	-2.214396
30.Pd	2.399971	1.004760	0.176531
31.O	0.857564	1.529036	-1.058422
32.O	-1.382995	1.705330	-0.937745
33.N	3.772271	0.466596	-1.310798
34.H	3.578763	-0.530459	-1.533966
35.H	3.687539	1.019857	-2.169876
36.H	4.244066	1.160996	2.058712
37.O	-1.168908	1.606194	1.885264
38.C	-0.268722	1.613249	-0.393557
39.H	7.463553	-1.653535	0.348191
40.H	8.563786	-0.430427	0.990216
41.C	5.145349	0.582428	-0.715676
42.H	5.322123	1.653775	-0.544659
43.C	6.256924	0.010344	-1.610476
44.H	6.651246	1.034584	1.606228
45.C	7.601813	-0.570518	0.480263
46.H	6.276617	0.547650	-2.569538
47.H	6.024285	-1.042920	-1.827264
48.C	6.458418	-0.024776	1.364994
49.H	6.410387	-0.574236	2.314502
50.H	4.867471	-1.191300	0.455764
51.C	7.627024	0.113548	-0.902778
52.H	8.403744	-0.336507	-1.534259
53.H	7.892799	1.175255	-0.780739
54.C	-0.150870	1.560883	1.178840
55.O	1.066500	1.448417	1.653924
56.C	5.110711	-0.138622	0.639216
57.N	3.953036	0.388640	1.448336
58.H	3.592902	-0.386625	2.030373

```
E-test:            old,new=      -12.11579,      -12.11578      hartree
max    gradient:                        0.00098331    au/angstrom,radian
max      cart.      step:                        0.00407485      angstrom
Geometry Converged
```

	hartree	eV	kcal/mol	kJ/mol
Total Pauli Repulsion:	45.472170055115413	1237.3607	28534.22	119387.17
Electrostatic Energy:	-9.848003708250744	-267.9778	-6179.72	-25855.93
Total Orbital Interactions:	-47.556510719557551	-1294.0785	-29842.16	-124859.60
Dispersion Energy:	-0.183438957604284	-4.9916	-115.11	-481.62
Total Bonding Energy:	-12.115776971452773	-329.6871	-7602.77	-31809.97

β[**2**]$_2$-tz2p-blyp-d3;C_1

Coordinates in Geometry Cycle 51

Atom	X	Y	Z	(Angstrom)
1.Pd	-0.501743	-1.648534	0.130788	
2.O	0.814054	-2.127845	1.596641	
3.O	3.038424	-2.351593	1.836403	
4.N	-2.043518	-1.024894	1.412821	
5.H	-2.316984	-1.797600	2.032845	
6.H	-1.679207	-0.249401	1.986000	
7.H	-1.686069	-0.075341	-1.547224	
8.O	3.260364	-2.399372	-0.988596	
9.C	2.029346	-2.278550	1.131195	
10.H	-5.954866	-1.937346	-0.804127	
11.H	-6.553440	-0.446454	-1.531194	
12.C	-3.224129	-0.516143	0.619861	
13.H	-3.013858	0.547266	0.453566	
14.C	-4.565895	-0.689262	1.353138	
15.H	-4.206444	0.391065	-1.823317	
16.C	-5.747760	-0.861373	-0.912618	
17.H	-4.536926	-0.145489	2.306377	
18.H	-4.708592	-1.757382	1.589279	
19.C	-4.386756	-0.676335	-1.627844	
20.H	-4.387118	-1.192818	-2.598091	
21.H	-3.401937	-2.297499	-0.582742	
22.C	-5.747386	-0.195396	0.482049	
23.H	-6.694325	-0.398391	0.998643	
24.H	-5.675170	0.895171	0.364332	
25.C	2.151284	-2.308434	-0.448988	
26.O	1.026187	-2.180079	-1.107605	
27.C	-3.247897	-1.221733	-0.746980	
28.N	-1.877256	-1.079606	-1.346651	
29.H	-1.791178	-1.607189	-2.218159	
30.Pd	2.488529	0.957303	0.145191	
31.O	0.966761	1.497913	-1.094741	
32.O	-1.267851	1.716824	-0.983913	
33.N	3.868735	0.401681	-1.332557	
34.H	3.679895	-0.599179	-1.543708	
35.H	3.783707	0.939692	-2.198954	
36.H	4.298309	1.087720	2.055285	
37.O	-1.058227	1.647076	1.841343	
38.C	-0.161068	1.621440	-0.440039	
39.H	7.664525	-1.582487	0.366600	
40.H	8.679838	-0.295058	1.019355	
41.C	5.237285	0.542232	-0.727448	
42.H	5.388132	1.616521	-0.551213	
43.C	6.380366	0.009653	-1.610937	
44.H	6.690386	1.054206	1.619427	
45.C	7.734925	-0.493324	0.497385	
46.H	6.382609	0.537843	-2.574930	
47.H	6.203019	-1.055718	-1.819771	
48.C	6.549782	-0.011284	1.370637	
49.H	6.518899	-0.566093	2.317415	
50.H	5.001791	-1.239747	0.453461	
51.C	7.738465	0.189159	-0.889153	
52.H	8.547214	-0.216464	-1.509944	
53.H	7.942774	1.264222	-0.767186	
54.C	-0.046015	1.580389	1.140172	
55.O	1.167542	1.426475	1.610276	
56.C	5.210696	-0.177986	0.631545	
57.N	4.027186	0.322518	1.426817	
58.H	3.662237	-0.460551	1.990981	

```
E-test:            old,new=      -12.10416,      -12.10425      hartree
max    gradient:                        0.00098287    au/angstrom,radian
max      cart.      step:                       0.01000000      angstrom
Geometry Converged
```

	hartree	eV	kcal/mol	kJ/mol
Total Pauli Repulsion:	45.488774536220539	1237.8125	28544.64	119430.76
Electrostatic Energy:	-9.843244242372588	-267.8483	-6176.73	-25843.43
Total Orbital Interactions:	-47.639644861407135	-1296.3407	-29894.33	-125077.87
Dispersion Energy:	-0.110193218565270	-2.9985	-69.15	-289.31
Total Bonding Energy:	-12.104302541730107	-329.3748	-7595.57	-31779.84

β[**2**]$_2$-DMSO-tzp-blyp-d3;C_1

Coordinates in Geometry Cycle 45

Atom	X	Y	Z	(Angstrom)
1.Pd	-0.562542	-1.622461	0.130446	
2.O	0.796340	-2.088723	1.605297	
3.O	3.009108	-2.455311	1.827541	
4.N	-2.133697	-1.080518	1.407481	
5.H	-2.410082	-1.903417	1.958462	
6.H	-1.819411	-0.356753	2.067461	
7.H	-1.795488	-0.135072	-1.598400	
8.O	3.215746	-2.520398	-0.994465	
9.C	1.998255	-2.291821	1.122939	
10.H	-6.025525	-2.013604	-0.790780	
11.H	-6.635136	-0.534969	-1.541343	
12.C	-3.312220	-0.556792	0.615832	
13.H	-3.097291	0.505892	0.443956	
14.C	-4.653132	-0.726866	1.352844	
15.H	-4.300767	0.314570	-1.847431	
16.C	-5.828682	-0.937298	-0.914568	
17.H	-4.628598	-0.172723	2.300764	
18.H	-4.785184	-1.793316	1.597632	
19.C	-4.469711	-0.752881	-1.633906	
20.H	-4.459996	-1.288473	-2.592882	
21.H	-3.472957	-2.350169	-0.566517	
22.C	-5.833765	-0.250614	0.469968	
23.H	-6.779027	-0.454508	0.990137	
24.H	-5.769662	0.839999	0.336370	
25.C	2.111954	-2.328095	-0.452198	
26.O	0.994456	-2.152855	-1.114962	
27.C	-3.332366	-1.275025	-0.739194	
28.N	-1.959425	-1.123264	-1.341842	
29.H	-1.875320	-1.684045	-2.197600	
30.Pd	2.552432	0.940137	0.153002	
31.O	0.999919	1.473266	-1.096352	
32.O	-1.224097	1.826334	-0.986128	
33.N	3.946975	0.445265	-1.322539	
34.H	3.780389	-0.539600	-1.589321	
35.H	3.863832	1.016363	-2.171615	
36.H	4.403797	1.198719	1.985790	
37.O	-1.031266	1.762185	1.834527	
38.C	-0.121725	1.639590	-0.438925	
39.H	7.750230	-1.545030	0.341317	
40.H	8.763880	-0.258001	1.003628	
41.C	5.320187	0.586051	-0.718938	
42.H	5.465386	1.659471	-0.539208	
43.C	6.455036	0.064975	-1.617569	
44.H	6.774270	1.082496	1.622068	
45.C	7.817810	-0.455562	0.482390	
46.H	6.446708	0.606159	-2.573444	
47.H	6.282091	-1.000597	-1.837404	
48.C	6.638981	0.018327	1.368822	
49.H	6.612563	-0.542777	2.312563	
50.H	5.077057	-1.201968	0.452140	
51.C	7.814738	0.240285	-0.897604	
52.H	8.619751	-0.160487	-1.527233	
53.H	8.015066	1.315247	-0.767062	
54.C	-0.015885	1.598949	1.136416	
55.O	1.182872	1.392336	1.625611	
56.C	5.297010	-0.141315	0.631045	
57.N	4.121120	0.383077	1.427047	
58.H	3.802549	-0.345192	2.080150	

```
E-test:            old,new=      -12.09949,      -12.09952      hartree
max    gradient:                       0.00085306    au/angstrom,radian
max      cart.      step:                        0.01000000      angstrom
Geometry                                                      Converged
```

	hartree	eV	kcal/mol	kJ/mol
Total Pauli Repulsion:	45.092932222998918	1227.0411	28296.25	118391.48
Electrostatic Energy:	-9.744712624611054	-265.1671	-6114.90	-25584.74
Total Orbital Interactions:	-47.262288250376585	-1286.0723	-29657.54	-124087.12
Solvation:	-0.078460389757880	-2.1350	-49.23	-206.00
Dispersion Energy:	-0.107308967300171	-2.9200	-67.34	-281.74
Total Bonding Energy:	-12.099836555934967	-329.2533	-7592.76	-31768.12

Frequency cm-1	Dipole Strength 1e-40 esu2 cm2	Absorption Intensity (degeneracy not counted) km/mole
-18.497468	0.000000	0.000000
-9.935909	0.000000	0.000000
19.871190	0.000000	0.000000
33.316293	226.211833	1.889079
36.920184	3.506265	0.032448
47.403281	209.494983	2.489202
67.597330	242.487181	4.108624
71.470051	34.800423	0.623429
75.679893	25.872883	0.490799
85.738776	43.923082	0.943948
94.056530	248.056606	5.848141
96.599618	192.277226	4.655661
108.082636	4462.456804	120.894913
121.315806	0.837976	0.025482
131.501417	71.540510	2.358091
137.323877	111.869316	3.850659
168.029788	714.527943	30.094253
170.173799	86.403377	3.685543
180.001746	9.381034	0.423258
182.106332	64.597455	2.948618
184.404709	201.124453	9.296403
187.479323	81.775742	3.842872
215.938886	903.430148	48.899397
221.016590	52.972638	2.934638
246.852012	147.490120	9.125941
248.499483	15.228224	0.948534
301.645291	195.256314	14.763173
302.703787	1199.404752	91.004253
324.577282	75.599269	6.150548
325.782437	120.998827	9.880681
334.237711	70.455771	5.902692
334.750877	83.436335	7.000918
343.033832	8.204990	0.705494
343.222909	177.092691	15.235439
347.253558	6.046943	0.526333
349.967616	201.454867	17.671918
419.997351	48.823967	5.139936
420.260488	63.831592	6.724071
425.713527	204.923405	21.866893
426.004655	24.679414	2.635283
444.693506	173.118385	19.296656
445.190477	1807.739697	201.725050
482.035199	54.475358	6.581985
482.322437	127.053732	15.360415
495.401361	453.271728	56.285159
496.599622	400.517637	49.854699
532.228690	99.087605	13.218911
532.837203	274.685678	36.686698
539.119565	29.188148	3.944298
539.778705	21.476694	2.905770
556.282056	31.462595	4.387000
556.469577	2.542879	0.354687
569.327713	66.922144	9.550151
569.932928	27.977421	3.996773
654.693559	139.349511	22.867653
655.764212	40.000943	6.575004
709.157171	657.320510	116.841669
711.002211	26.545686	4.730891
747.395270	261.473229	48.984158
748.016660	504.966219	94.678565
769.690258	3.240522	0.625186
769.791873	1.765097	0.340581
792.709902	14.318534	2.845056
792.892393	7.034335	1.398026
821.885928	7.163791	1.475817
821.968499	25.546354	5.263349
827.639715	22.957548	4.762609
828.131975	8.297417	1.722347
841.600112	23.558002	4.969610
841.810592	17.986486	3.795236
858.224654	1.976679	0.425221
858.371509	0.640794	0.137871
899.215267	38.449906	8.666366
899.290827	33.394489	7.527539
917.895497	9.885803	2.274486
918.082581	1.059322	0.243774
972.940689	752.268346	183.458241
973.723169	11.356870	2.771866
1015.800809	8.322609	2.119074
1016.040102	117.039600	29.807239
1020.952077	6.476521	1.657392
1021.058770	16.641753	4.259199
1027.371378	394.215498	101.517105
1027.782405	41.848250	10.780938
1030.771700	42.239892	10.913483
1030.900982	13.143079	3.396191
1061.903805	51.682585	13.756485
1062.473071	67.892286	18.080750

1101.794872		69.206591	19.112886
1102.368248		67.720434	18.712185
1119.686232		0.734909	0.206257
1120.284259		548.032779	153.890864
1145.074038		54.688634	15.696713
1145.768747		46.979586	13.492245
1157.151649		28.869271	8.373445
1157.934871		72.368687	21.004527
1182.086256		9.710242	2.877116
1182.675719		159.681297	47.336681
1186.097097		25.683804	7.635855
1186.489137		184.113952	54.755599
1219.515968		0.254885	0.077913
1219.727126		9.131664	2.791841
1242.966147		13.798353	4.298972
1243.100840		9.287097	2.893773
1275.837683		62.436191	19.966866
1279.960861		3815.028336	1223.974946
1286.442362		4.890266	1.576888
1287.146602		3.010609	0.971316
1302.765289		2.181888	0.712487
1303.000899		1.728038	0.564386
1323.949268		0.163915	0.054396
1323.978096		0.025922	0.008603
1325.281893		3.108443	1.032593
1325.461976		1.109766	0.368703
1333.904354		20.867634	6.977116
1333.962514		1.778403	0.594637
1346.371148		23.813357	8.036436
1346.774527		17.812898	6.013226
1358.653325		1.632812	0.556061
1359.059495		2.100506	0.715551
1375.087100		10.568022	3.642520
1375.766808		9.896247	3.412663
1393.049273		25.808238	9.011621
1393.256865		84.433151	29.486434
1443.908694		16.881245	6.109734
1444.351615		19.160386	6.936737
1445.248694		14.052541	5.090677
1445.753890		12.630539	4.577141
1447.169930		59.422971	21.555195
1447.607124		57.490497	20.860506
1456.952616		6.038320	2.205157
1457.109244		3.409739	1.245350
1536.849636		586.686210	226.003585
1537.958597		1326.573843	511.392252
1549.669846		3114.241617	1209.677372
1550.948400		253.222045	98.441207
1578.277383		382.949423	151.496578
1579.105877		143.636706	56.853179
1582.024351		4087.015307	1620.680842
1582.709285		486.593773	193.039315
2925.204949		37.235118	27.301538
2926.037833		24.183919	17.737185
2929.511694		29.691876	21.802734
2930.544833		15.260438	11.209686
2932.384658		46.623630	34.269289
2933.212329		33.749982	24.813905
2937.112977		13.744927	10.119083
2937.297622		117.681275	86.642982
2963.810635	7.132125	5.298433	
2964.530568		11.614904	8.630771
2976.787878		65.184493	48.637389
2977.440971		37.359986	27.882258
2984.318142		75.135425	56.204092
2984.555799		48.607068	36.362790
2986.112572		48.042275	35.959017
2986.345635		41.835184	31.315534
2986.714281		5.945589	4.451092
2987.586628		66.487495	49.789590
2992.648964		100.505084	75.391412
2992.864401		55.706911	41.790175
3249.665150		129.340499	105.354045
3252.750819		239.482063	195.254861
3311.715807		97.702427	81.102919
3313.346669		66.075359	54.876257
3382.681496		179.187825	151.931448
3384.470934		157.625521	133.719700
3389.129889		135.111879	114.778308
3389.384440	123.753798	105.137450	

Zero-Point Energy : 0.457173 a.u.
==========
12.440323 eV
(imaginary frequencies were excluded from the summation)

```
Statistical       Thermal       Analysis              ***              ideal       gas       assumed              ***
     Temp                                                                 Transl      Rotat     Vibrat       Total
     ----                                                                 ------      -----     ------       -----

     298.15    Entropy (cal/mole-K):                                     45.137     36.782    115.752     197.672
               Internal Energy (Kcal/mole):                              0.889       0.889    304.540     306.317
               Constant Volume Heat Capacity (cal/mole-K):       2.981    2.981   112.669   118.631
```

Na,β[**2**]$_2$-tzp-blyp-d3;C_1

Coordinates in Geometry Cycle 156

Atom	X	Y	Z	(Angstrom)
1.Pd	-0.449789	-1.726577	0.115355	
2.O	0.885285	-2.123606	1.585572	
3.O	3.113528	-2.334242	1.819644	
4.N	-2.029994	-1.222016	1.424523	
5.H	-2.321909	-2.059823	1.945543	
6.H	-1.704691	-0.530912	2.113486	
7.H	-1.704418	-0.274499	-1.679854	
8.O	3.334448	-2.363388	-1.009744	
9.C	2.103743	-2.275826	1.109679	
10.H	-6.017960	-1.878491	-0.751061	
11.H	-6.511768	-0.361260	-1.497787	
12.C	-3.182487	-0.655391	0.636222	
13.H	-2.905459	0.391572	0.459950	
14.C	-4.530630	-0.726239	1.373933	
15.H	-4.123112	0.303217	-1.834037	
16.C	-5.732943	-0.823190	-0.878420	
17.H	-4.454552	-0.196146	2.333719	
18.H	-4.753599	-1.780284	1.606663	
19.C	-4.370832	-0.747631	-1.607932	
20.H	-4.416132	-1.277423	-2.568984	
21.H	-3.433801	-2.415944	-0.582942	
22.C	-5.671595	-0.143517	0.506876	
23.H	-6.627983	-0.255573	1.032094	
24.H	-5.516505	0.941525	0.374604	
25.C	2.224058	-2.294968	-0.465367	
26.O	1.097193	-2.158127	-1.131656	
27.C	-3.245378	-1.344697	-0.740472	
28.N	-1.878645	-1.243856	-1.367572	
29.H	-1.810584	-1.846698	-2.195567	
30.Pd	2.471131	0.927225	0.123320	
31.O	0.928014	1.403529	-1.179512	
32.O	-1.278285	1.873492	-1.098177	
33.N	3.892504	0.439072	-1.318114	
34.H	3.711906	-0.556052	-1.567853	
35.H	3.823957	1.005981	-2.171436	
36.H	4.281641	1.191263	2.008283	
37.O	-1.141831	1.898210	1.684725	
38.C	-0.161796	1.644730	-0.545872	
39.H	7.537805	-1.696213	0.431249	
40.H	8.624991	-0.481213	1.107281	
41.C	5.261847	0.555160	-0.688974	
42.H	5.434955	1.627459	-0.516285	
43.C	6.392510	-0.017214	-1.562311	
44.H	6.709516	0.994923	1.682797	
45.C	7.677370	-0.614079	0.570035	
46.H	6.441375	0.527683	-2.515807	
47.H	6.163866	-1.068896	-1.792417	
48.C	6.514884	-0.061835	1.432364	
49.H	6.436088	-0.616254	2.376991	
50.H	4.939211	-1.218391	0.481707	
51.C	7.743817	0.078682	-0.809423	
52.H	8.534739	-0.371351	-1.422133	
53.H	8.010994	1.138674	-0.676397	
54.C	-0.089429	1.648047	1.035026	
55.O	1.056954	1.395334	1.561873	
56.C	5.188531	-0.166457	0.662302	
57.N	4.003939	0.384144	1.434238	
58.H	3.653094	-0.362661	2.057507	
59.Na	-2.605298	2.981411	0.355542	

```
E-test:            old,new=      -11.94170,      -11.94171      hartree
max    gradient:                        0.00069254    au/angstrom,radian
max      cart.      step:                       0.00230668      angstrom
Geometry Converged
```

	hartree	eV	kcal/mol	kJ/mol
Total Pauli Repulsion:	45.378756487418670	1234.8188	28475.60	119141.91
Electrostatic Energy:	-9.861011815947661	-268.3318	-6187.88	-25890.08
Total Orbital Interactions:	-47.344767817371512	-1288.3167	-29709.29	-124303.67
Dispersion Energy:	-0.114668054272822	-3.1203	-71.96	-301.06
Total Bonding Energy:	-11.941686516159526	-324.9498	-7493.52	-31352.89

Frequency cm-1	Dipole Strength 1e-40 esu2	Absorption Intensity (degeneracy not counted) cm2 km/mole
22.100630	273.248154	1.513701
25.558580	168.229437	1.077747
35.812137	83.041344	0.745423
42.021259	436.403793	4.596589
50.684989	29.550953	0.375430
57.002672	223.521421	3.193688
63.812190	148.983779	2.382982
65.699113	580.048741	9.552171
75.157606	105.640259	1.990126
84.843960	180.647754	3.841772
89.103975	72.630237	1.622156
105.950673	62.614511	1.662864
111.422052	10.909065	0.304675
116.141259	1042.636992	30.352728
142.721144	52.054099	1.862179
153.493122	116.212771	4.471167
156.618720	276.351171	10.848834
166.068222	92.637201	3.856115
174.056856	32.076247	1.399435
186.349358	41.603415	1.943278
188.165903	28.072199	1.324023
192.823143	16.313050	0.788447
202.770232	308.836946	15.696814
213.542783	91.152024	4.878983
223.238174	170.068344	9.516341
235.286136	605.603290	35.715985
244.074579	503.369991	30.795548
247.951779	28.949535	1.799231
259.348094	56.495157	3.672589
309.648863	320.079828	24.843104
315.465536	428.244729	33.862734
331.314118	57.055145	4.738194
332.192950	39.314270	3.273548
333.778607	71.917686	6.016893
353.145726	17.018020	1.506403
354.553630	9.387758	0.834299
355.592732	87.437884	7.793465
367.146113	37.919918	3.489670
392.302313	293.067726	28.818205
416.102954	15.508516	1.617518
422.587658	17.531878	1.857049
424.079891	90.351254	9.604172
428.878126	61.404531	6.601040
446.156060	123.588858	13.821150
451.480816	838.809334	94.925004
481.683587	88.918526	10.735745
486.081746	29.356575	3.576784
490.562429	173.265595	21.305155
516.394997	175.177933	22.674593
524.878632	109.920326	14.461554
529.424443	16.956067	2.250128
538.503580	106.142870	14.327074
546.559966	20.753238	2.843163
557.572219	13.378798	1.869805
561.876326	14.006392	1.972627
567.991388	14.043188	1.999335
579.015625	17.434064	2.530271
657.477800	17.819828	2.936721
696.444036	23.832701	4.160424
700.641254	135.693116	23.830414
747.498204	64.882819	12.156763
750.333401	199.251011	37.474244
756.220331	183.836015	34.846328
767.214384	1.273859	0.244972
780.154690	2.444583	0.478039
794.660126	6.726856	1.339898
795.880045	0.506244	0.100992
822.531900	3.263545	0.672853
826.666350	12.523189	2.594916
827.587485	9.917257	2.057233
830.824860	1.730120	0.360300
845.252148	3.824963	0.810385
845.400250	2.950063	0.625132
857.184012	0.534883	0.114924
867.782682	0.377454	0.082102
905.317019	3.354973	0.761321
906.263348	9.167057	2.082392
923.174666	2.627719	0.608052
924.144032	3.130821	0.725230
969.858261	218.049312	53.007956
981.798658	257.273204	63.313316
1013.699184	34.502142	8.766641
1014.777272	146.357606	37.227519
1020.829906	45.604822	11.669230
1025.851637	6.352379	1.633424
1027.350273	6.980880	1.797657
1033.136527	36.387696	9.423025
1037.377784	56.143044	14.598592

1040.801670		102.852924	26.832596
1056.849943		24.058272	6.373175
1070.443318		38.898427	10.436954
1089.643224		26.472709	7.230374
1112.682000		151.476469	42.246848
1116.526103		71.186944	19.922659
1128.613386		88.772661	25.113226
1132.708971		7.779787	2.208839
1151.256692		22.317326	6.440097
1168.085730		41.909240	12.270509
1171.144218		36.048932	10.582319
1172.327023		6.663660	1.958122
1184.628915		3.986473	1.183721
1203.912711		20.971427	6.328504
1227.175213		1.210142	0.372238
1236.037653		3.669028	1.136739
1251.476845		121.674640	38.168137
1255.728961		11.240750	3.538093
1257.271274		30.526859	9.620313
1272.343442		768.174304	244.986527
1291.811993		25.046141	8.109950
1298.380443		0.563844	0.183501
1305.831213		1.078942	0.353153
1312.660626		0.146191	0.048101
1332.272154		2.765777	0.923609
1334.333437		4.794912	1.603700
1334.479912		1.269085	0.424503
1335.192154		6.764628	2.263944
1336.521883		111.887159	37.483004
1340.327733		34.237397	11.502436
1345.257980		24.695221	8.327153
1350.227076		12.440001	4.210225
1350.647494		4.525937	1.532246
1354.666996		6.085571	2.066388
1370.110170		4.137779	1.421022
1373.355445		3.914513	1.347531
1387.396232		14.924150	5.190010
1388.154781		34.942621	12.158260
1408.827696		16.144028	5.700958
1459.259469		7.348281	2.687796
1462.442104		2.637050	0.966663
1464.147659		7.994453	2.933943
1464.156800		11.267068	4.135010
1467.960590		27.169580	9.997131
1468.685600		23.213653	8.545754
1477.967881		20.910913	7.746688
1478.783521		11.813446	4.378842
1534.313790		363.071306	139.631751
1550.701716		444.101560	172.619016
1558.979099		2113.296203	825.807334
1577.756739		1035.654093	409.574434
1603.148708		165.876595	66.655654
1613.452547		236.024540	95.453405
1616.143079		47.891999	19.400854
1624.677906		1270.328562	517.322547
2898.508991		43.935900	31.920688
2914.765754		24.623165	17.989770
2917.551918		19.520641	14.275481
2928.968094		14.375943	10.554291
2933.362058		23.074439	16.965821
2941.481257	10.183107	7.508004	
2945.266326		24.535020	18.112945
2947.441926		24.802816	18.324170
2949.720431		18.128015	13.403221
2959.402538		4.880107	3.620024
2972.505030		15.189496	11.317332
2985.436650		44.661991	33.421352
2985.778911		2.562945	1.918117
2988.717804		5.566434	4.170038
2990.719314		29.728731	22.285896
2996.092693		46.709247	35.078109
2996.820185		35.187756	26.432018
2998.683979		27.274462	20.500524
2999.395528		31.318115	23.545473
3009.976155		6.373524	4.808623
3126.521773		258.264669	202.397212
3242.122825		123.372678	100.259729
3269.372646		68.730014	56.323408
3312.596538		15.578615	12.935269
3361.266148		60.324317	50.824532
3380.687597		43.336708	36.723074
3381.536855		47.605073	40.350176
3390.386737	45.307622	38.503356	

Zero-Point Energy : 0.460869 a.u.
========== 12.540871 eV

Statistical Thermal Analysis *** ideal gas assumed ***				
Temp	Transl	Rotat	Vibrat	Total
298.15 Entropy (cal/mole-K):	45.247	36.983	126.147	208.377
Internal Energy (Kcal/mole):	0.889	0.889	308.116	309.894
Constant Volume Heat Capacity (cal/mole-K): 2.981	2.981	119.118	125.079	

3-tzp-blyp-d3;C_1

Coordinates in Geometry Cycle 29				
Atom	X	Y	Z	(Angstrom)
1.Pt	0.006528	-0.001468	0.013418	
2.C	-4.028558	0.062832	-2.488295	
3.C	-1.882858	0.059135	-2.961676	
4.C	-2.735437	0.068721	-1.612862	
5.C	-3.178454	-0.341476	-3.734878	
6.C	-2.516894	1.342131	-0.769662	
7.H	-3.219822	-1.419543	-3.927912	
8.H	2.030486	-1.783267	-0.434972	
9.O	-1.325555	1.502640	-0.156985	
10.H	-4.441404	1.072517	-2.559874	
11.H	-1.529900	1.068163	-3.205389	
12.H	0.638997	2.450600	0.295458	
13.H	2.037322	1.797583	-0.319360	
14.H	1.716934	1.691074	1.305125	
15.H	-3.375527	0.200219	-4.667145	
16.H	-4.800366	-0.639029	-2.165826	
17.N	1.279425	-1.694168	0.254927	
18.H	-1.033222	-0.632251	-2.983804	
19.C	-2.522624	-1.275988	-0.872924	
20.O	-3.350128	2.242432	-0.716119	
21.O	-1.339428	-1.478665	-0.258841	
22.N	1.295335	1.659298	0.372424	
23.H	0.619216	-2.472529	0.108847	
24.H	1.687188	-1.801102	1.188275	
25.O	-3.350052	-2.182278	-0.903853	

current energy		-5.14525797 Hartree	
energy change	-0.00006255	0.00100000	T
constrained gradient max	0.00056291	0.00100000	T
constrained gradient rms	0.00016950	0.00066667	T
gradient max		0.00056291	
gradient rms		0.00016950	
cart. step max	0.00885878	0.01000000	T
cart. step rms	0.00275727	0.00666667	T
GEOMETRY CONVERGED			

	hartree	eV	kcal/mol	kJ/mol
Total Pauli Repulsion:	19.181145306307940	521.9455	12036.35	50360.09
Electrostatic Energy:	-4.158872559353545	-113.1687	-2609.73	-10919.12
Total Orbital Interactions:	-20.132487626063824	-547.8329	-12633.33	-52857.84
Dispersion Energy:	-0.035049853163866	-0.9538	-21.99	-92.02
Total Bonding Energy:	-5.145259055334192	-140.0096	-3228.70	-13508.88

Frequency cm-1	Dipole Strength 1e-40 esu2 cm2	Absorption Intensity (degeneracy not counted) km/mole
54.159101	1114.650802	15.131722
56.104088	15.906695	0.223693
77.451322	120.748890	2.344175
108.125705	23.091038	0.625821
146.349224	15.438073	0.566320
167.443821	7.657064	0.321373
168.753036	216.938900	9.176289
169.876951	167.640165	7.138231
184.585572	602.420127	27.872460
190.445068	33.804979	1.613721
205.042965	49.120152	2.524542
218.989910	11.968262	0.656951
258.510753	7.027115	0.455338
323.198477	133.985359	10.854372
338.786257	180.457032	15.324195
349.193689	109.117068	9.550743
405.724086	17.958075	1.826285
406.507857	76.883646	7.833953
451.764130	33.552593	3.799408
476.306692	1.044176	0.124663
540.427165	60.243837	8.160709
645.312844	5.213676	0.843320
672.580874	6.749327	1.137845
676.177214	2.125102	0.360179
688.775870	69.935242	12.074025
720.010660	5.260637	0.949413
724.538817	9.786769	1.777375
739.120790	368.427887	68.256809
743.710316	42.769519	7.972899

795.567256	6.970482	1.390009
815.636731	84.884592	17.354165
844.716123	38.163648	8.080509
857.154541	57.557363	12.366252
900.526652	14.645300	3.305772
917.914782	18.438731	4.242399
972.003791	21.668570	5.279299
1041.288552	84.326696	22.009706
1056.660230	387.061829	102.516502
1083.058197	12.351525	3.353130
1149.635158	6.894510	1.986742
1173.367329	4.925953	1.448780
1205.752474	526.663198	159.172927
1222.596692	231.564583	70.963238
1228.224406	453.508405	139.617910
1228.496600	432.470097	133.170525
1235.066761	120.440573	37.285615
1241.951118	280.912402	87.448726
1250.818542	568.555757	178.256528
1449.400025	20.380394	7.404213
1451.503240	5.954500	2.166414
1474.605026	37.403161	13.824903
1607.642807	1.364083	0.549678
1613.235532	11.750002	4.751315
1626.779663	841.485658	343.125917
1630.144506	2.482078	1.014191
1635.073872	95.583168	39.173905
1650.513202	865.142541	357.918989
2965.504951	40.186010	29.871127
2974.277716	64.373220	47.991555
3006.200850	9.043767	6.814679
3011.968733	15.161689	11.446590
3026.819305	40.329705	30.597759
3067.330617	5.435875	4.179344
3281.555856	17.712467	14.569241
3282.630279	21.987748	18.091759
3392.321996	15.086213	12.827895
3393.101450	48.441711	41.199732
3432.737115	0.182800	0.157288
3433.371933	56.590254	48.701301

Zero-Point Energy : 0.190307 a.u.
========== 5.178518 eV

Statistical Thermal Analysis *** ideal gas assumed ***

Temp			Transl	Rotat	Vibrat	Total
298.15	Entropy (cal/mole-K):		43.626	32.160	48.676	124.462
	Internal Energy (Kcal/mole):		0.889	0.889	127.190	128.968
	Constant Volume Heat Capacity (cal/mole-K):	2.981	2.981	49.747	55.709	

3–tzp-blyp-d3bj;C_1

Coordinates in Geometry Cycle 34

Atom	X	Y	Z (Angstrom)
1.Pt	0.000623	-0.001147	0.009652
2.C	-3.997855	0.059107	-2.484571
3.C	-1.849963	0.061371	-2.941640
4.C	-2.712950	0.064115	-1.601025
5.C	-3.139026	-0.323101	-3.729752
6.C	-2.510985	1.337329	-0.758534
7.H	-3.180261	-1.396022	-3.946488
8.H	1.997197	-1.789001	-0.471890
9.O	-1.327013	1.505810	-0.137532
10.H	-4.418221	1.065630	-2.542456
11.H	-1.488570	1.069481	-3.173472
12.H	0.605168	2.438953	0.265644
13.H	2.003284	1.798382	-0.370289
14.H	1.712275	1.697443	1.261724
15.H	-3.327562	0.238526	-4.651362
16.H	-4.760863	-0.656302	-2.173691
17.N	1.260314	-1.693667	0.231000
18.H	-1.006316	-0.636352	-2.963091
19.C	-2.514229	-1.278436	-0.859933
20.O	-3.352958	2.229490	-0.711079
21.O	-1.340656	-1.484584	-0.232634
22.N	1.276989	1.660249	0.336542
23.H	0.582355	-2.458412	0.095135
24.H	1.679569	-1.801011	1.158151
25.O	-3.348961	-2.177992	-0.895767

current energy		-5.17277705 Hartree	
energy change	-0.00000628	0.00100000	T
constrained gradient max	0.00012805	0.00100000	T
constrained gradient rms	0.00003012	0.00066667	T
gradient max	0.00012805		
gradient rms	0.00003012		
cart. step max	0.00484835	0.01000000	T
cart. step rms	0.00121378	0.00666667	T
GEOMETRY CONVERGED			

	hartree	eV	kcal/mol	kJ/mol
Total Pauli Repulsion:	19.277808509272660	524.5759	12097.01	50613.88
Electrostatic Energy:	-4.185494038280275	-113.8931	-2626.44	-10989.01
Total Orbital Interactions:	-20.202280674926996	-549.7320	-12677.12	-53041.08
Dispersion Energy:	-0.062817928848733	-1.7094	-39.42	-164.93
Total Bonding Energy:	-5.172777061888317	-140.7584	-3245.97	-13581.12

3-water-tzp-blyp-d3;C_1

```
 Coordinates      in      Geometry      Cycle      43
   Atom         X           Y           Z   (Angstrom)
   1.Pt          -0.002689    -0.000322     0.010190
   2.C           -3.960697     0.075246    -2.590831
   3.C           -1.788612     0.049895    -2.918435
   4.C           -2.729841     0.070068    -1.629924
   5.C           -3.032814    -0.342891    -3.775732
   6.C           -2.562607     1.314549    -0.734947
   7.H           -3.068613    -1.421067    -3.971199
   8.H            2.162058    -1.458406    -0.511020
   9.O           -1.418270     1.482749    -0.086333
  10.H           -4.353399     1.089691    -2.703299
  11.H           -1.411084     1.054381    -3.140360
  12.H            0.992761     2.410925     0.254803
  13.H            2.152625     1.482047    -0.460629
  14.H            1.925984     1.406956     1.171966
  15.H           -3.164268     0.198206    -4.719164
  16.H           -4.770721    -0.607418    -2.322551
  17.N            1.409827    -1.528556     0.181526
  18.H           -0.947042    -0.648944    -2.884617
  19.C           -2.573105    -1.250783    -0.836287
  20.O           -3.460881     2.174227    -0.653384
  21.O           -1.442341    -1.454211    -0.174818
  22.N            1.438014     1.486931     0.274002
  23.H            0.954843    -2.437156     0.041343
  24.H            1.851032    -1.552538     1.106743
  25.O        -3.458972   -2.126243   -0.848471
```

```
E-test:          old,new=          -5.20774,          -5.20772     hartree
max    gradient:                        0.00084988    au/angstrom,radian
max      cart.      step:                       0.00459139      angstrom
Geometry Converged
```

	hartree	eV	kcal/mol	kJ/mol
Total Pauli Repulsion:	19.164005772773894	521.4791	12025.60	50315.09
Electrostatic Energy:	-4.159952185062642	-113.1981	-2610.41	-10921.95
Total Orbital Interactions:	-20.083847548928201	-546.5093	-12602.81	-52730.13
Solvation:	-0.092190565878860	-2.5086	-57.85	-242.05
Dispersion Energy:	-0.035741675777484	-0.9726	-22.43	-93.84
Total Bonding Energy:	-5.207724825365864	-141.7094	-3267.90	-13672.88

α[**3**]$_2$-tzp-blyp-d3;C_1

Coordinates in Geometry Cycle 65				
Atom	X	Y	Z	(Angstrom)
1.Pt	0.868744	-0.426223	-1.513729	
2.C	-3.353931	0.884692	-3.321235	
3.C	-1.437191	0.150562	-4.139713	
4.C	-1.984588	0.479980	-2.692877	
5.C	-2.898098	0.266768	-4.684529	
6.C	-1.216210	1.608210	-1.956433	
7.H	-3.350715	-0.713568	-4.875444	
8.H	2.287625	-2.710847	-1.699318	
9.O	0.083420	1.444597	-1.793743	
10.H	-3.465293	1.972428	-3.345769	
11.H	-0.766269	0.937557	-4.500582	
12.H	3.186507	0.804972	-1.988795	
13.H	3.241919	0.133237	-0.462681	
14.H	2.393919	1.522824	-0.705458	
15.H	-3.031895	0.897239	-5.570639	
16.H	-4.230688	0.438807	-2.844046	
17.N	1.649812	-2.306634	-1.008564	
18.H	-0.934018	-0.815980	-4.240230	
19.C	-2.042758	-0.751188	-1.780764	
20.O	-1.809962	2.625380	-1.568825	
21.O	-0.931982	-1.441442	-1.612336	
22.N	2.642380	0.617645	-1.142172	
23.H	0.847019	-2.936618	-0.912223	
24.H	2.130333	-2.240848	-0.080698	
25.O	-3.103715	-1.082986	-1.200071	
26.Pt	-0.903775	-0.013972	1.544649	
27.C	3.525737	0.688875	3.190417	
28.C	1.517727	0.481307	4.087047	
29.C	2.092381	0.474407	2.613171	
30.C	2.982295	0.377152	4.624063	
31.C	1.549366	1.609534	1.706761	
32.H	3.231712	-0.637347	4.957246	
33.H	-2.744561	-1.917710	2.049177	
34.O	0.240353	1.684541	1.555222	
35.H	3.847360	1.725780	3.057878	
36.H	1.028993	1.433876	4.318600	
37.H	-2.927416	1.707112	1.791975	
38.H	-3.133139	0.838652	0.382307	
39.H	-2.024862	2.054185	0.430227	
40.H	3.257697	1.086893	5.412044	
41.H	4.289799	0.015677	2.792833	
42.N	-2.050489	-1.755840	1.314757	
43.H	0.829823	-0.335621	4.325339	
44.C	1.889087	-0.867622	1.899979	
45.O	2.325662	2.420041	1.179455	
46.O	0.660526	-1.340412	1.822308	
47.N	-2.441479	1.291509	0.992557	
48.H	-1.390721	-2.540156	1.324075	
49.H	-2.523751	-1.734199	0.380999	
50.O	2.853342	-1.488455	1.392216	

current energy		-10.38371450 Hartree	
energy change	0.00003262	0.00100000	T
constrained gradient max	0.00050599	0.00100000	T
constrained gradient rms	0.00009978	0.00066667	T
gradient max		0.00050599	
gradient rms		0.00009978	
cart. step max	0.00794118	0.01000000	T
cart. step rms	0.00198225	0.00666667	T
GEOMETRY CONVERGED			

	hartree	eV	kcal/mol	kJ/mol
Total Pauli Repulsion:	38.875425500419723	1057.8542	24394.70	102067.42
Electrostatic Interaction:	-8.459141822624311	-230.1850	-5308.19	-22209.47
Total Orbital Interactions:	-40.682834048801432	-1107.0362	-25528.87	-106812.77
Dispersion Energy:	-0.117186989078369	-3.1888	-73.54	-307.67
Total Bonding Energy:	-10.383720558946042	-282.5554	-6515.88	-27262.45

Frequency	Dipole Strength	Absorption Intensity (degeneracy not counted)	
cm-1	1e-40 esu2 cm2		km/mole
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23.138429	98.676570	0.572303
39.155591	216.965109	2.129422
53.233297	128.776466	1.718296
66.242735	19.698351	0.327074
67.381579	18.803552	0.317584
75.043503	0.416653	0.007837
85.910266	171.477093	3.692574
93.831609	46.192518	1.086423
106.845125	92.423186	2.475219
113.009604	108.254991	3.066489
127.311400	5.648067	0.180238
138.331970	344.423268	11.942441
148.198644	11.769969	0.437218
158.377476	1.355512	0.053811
161.008122	165.536606	6.680668
161.396366	488.892345	19.778122
172.188985	74.852764	3.230660
177.327706	152.715871	6.787953
190.945035	16.236585	0.777108
191.832273	229.164083	11.019104
219.041336	37.824348	2.076709
221.587307	119.810370	6.654530
229.009731	49.876521	2.863045
230.235430	199.522562	11.514425
232.996070	39.867992	2.328365
235.896190	260.891190	15.426181
249.377871	864.704869	54.051019
252.434625	4.056682	0.256684
275.873713	0.361057	0.024967
287.282717	203.644961	14.664297
307.958978	56.453288	4.357729
310.239691	62.982419	4.897729
324.707559	2.033435	0.165501
328.386967	178.992937	14.733295
340.763315	139.741804	11.935957
349.002133	173.523247	15.179722
365.151817	1075.572477	98.444445
365.766283	22.949564	2.104051
440.633179	5.450864	0.602033
443.460863	135.340268	15.043899
451.482226	4.854389	0.549355
452.439343	5.415415	0.614144
461.070665	0.173612	0.020064
463.280087	32.511701	3.775386
475.351670	8.662367	1.032119
476.446982	32.466274	3.877262
556.179849	21.117887	2.944041
556.453669	88.549246	12.350711
637.884248	26.913058	4.303115
638.280811	11.700832	1.872003
682.040680	25.068274	4.285611
683.596405	65.943064	11.299181
725.178922	9.165433	1.666005
726.238095	75.688290	13.777988
745.080808	60.241070	11.250560
745.757618	83.147572	15.542660
766.847107	12.247197	2.354093
769.231121	1.296164	0.249916
772.771189	179.461783	34.761697
773.650430	0.026790	0.005195
795.663801	3.799784	0.757821
796.088792	3.651234	0.728583
807.731422	52.744704	10.678836
809.565955	30.031654	6.094100
823.675417	10.194529	2.104754
824.013318	43.860642	9.059147
837.002052	6.695462	1.404705
838.006604	9.858264	2.070742
851.184541	68.843144	14.687994
851.747035	103.675156	22.134178
864.052854	97.988710	21.222396
866.025008	303.763446	65.939252
901.008766	7.801824	1.761989
901.077449	9.286080	2.097358
914.486735	11.359323	2.603802
914.574009	24.773881	5.679250
1009.214670	17.259023	4.365941
1010.213105	14.966044	3.789641
1044.945276	3.537920	0.926658
1045.714562	3.540481	0.928012
1071.083411	24.373821	6.543724
1071.810669	270.994234	72.804160
1131.228327	2.692166	0.763361
1131.487436	0.671518	0.190452
1168.500681	46.772102	13.699160
1169.526523	67.066160	19.660366
1178.795811	16.777455	4.957272
1179.929525	12.860196	3.803485
1214.413270	98.955661	30.122098
1214.649420	51.809934	15.774008
1218.297499	52.136724	15.921177

1218.867817		48.068241	14.685641
1229.563834		15.588058	4.804201
1229.844021		44.811652	13.813988
1239.859620		1.131144	0.351535
1240.252433		1.003967	0.312110
1295.538329		123.891672	40.231891
1295.717771		104.599181	33.971660
1299.213931		2282.055145	743.164360
1300.450324		404.009488	131.693216
1314.994609		75.375400	24.844581
1315.696688		618.549385	203.989696
1453.507851		3.533579	1.287390
1453.977791		3.825628	1.394243
1457.806435		14.130015	5.163219
1458.252310		22.303961	8.152536
1480.008994		19.706570	7.310607
1480.612691		83.461050	30.974434
1520.415929		556.381239	212.037638
1524.168174		475.440779	181.638283
1574.349335		592.560708	233.836351
1589.327401		1369.292200	545.490982
1608.767618		199.254285	80.348737
1612.512096		55.204271	22.312783
1623.281878		32.071666	13.049490
1625.800299		3.788401	1.543836
1640.893541		233.327525	95.967559
1643.371159		70.714746	29.128875
1653.340031		27.599486	11.437767
1656.695848		271.523078	112.752869
2970.548664		163.871136	122.016119
2970.680218		4.588734	3.416858
2982.515503		12.249010	9.157180
2983.501610		82.498271	61.694890
2985.232506		39.515812	29.568354
2993.629394		1410.710942	1058.556735
3001.968178		14.767533	11.111997
3002.081204		26.159807	19.684983
3012.007275		16.641251	12.563772
3012.538427		17.824215	13.459257
3036.325673		11.810603	8.988733
3036.374138		20.805118	15.834470
3054.795163		8.108521	6.208717
3055.120434		8.471710	6.487502
3225.693600		84.778127	68.546455
3228.338351		225.807434	182.723898
3346.682825		25.619852	21.491624
3346.891940		24.940119	20.922727
3363.797382		22.599190	19.054641
3364.183660		40.766816	34.376730
3423.346638		15.648294	13.427524
3423.643939		88.444183	75.898979
3431.286643		31.298443	26.918931
3431.732702	8.214349	7.065855	

Zero-Point Energy : 0.461544 a.u.
========== 12.559250 eV

Statistical Thermal Analysis *** ideal gas assumed ***

Temp		Transl	Rotat	Vibrat	Total
298.15	Entropy (cal/mole-K):	45.894	36.988	110.615	193.498
	Internal Energy (Kcal/mole):	0.889	0.889	306.854	308.631
	Constant Volume Heat Capacity (cal/mole-K): 2.981	2.981	112.189	118.150	

$\alpha[\mathbf{3}]_2$-tzp-blyp-d3bj;C_1

Coordinates in Geometry Cycle 39

Atom	X	Y	Z (Angstrom)
1.Pt	0.825682	-0.180942	-1.538754
2.C	-3.457562	0.029925	-3.518650
3.C	-1.369149	-0.217876	-4.183672
4.C	-2.082231	-0.011214	-2.790802
5.C	-2.768620	-0.504629	-4.815259
6.C	-1.691936	1.248093	-2.008827
7.H	-2.940126	-1.576262	-4.967658
8.H	2.869898	-1.933672	-1.698596
9.O	-0.412734	1.447182	-1.762209
10.H	-3.821334	1.057198	-3.609252
11.H	-0.911609	0.711441	-4.539227
12.H	1.803655	2.162634	-1.742345
13.H	3.109955	1.172763	-1.987679
14.H	2.579767	1.507322	-0.426610
15.H	-2.996626	0.028414	-5.744352
16.H	-4.231405	-0.595499	-3.068764
17.N	1.995744	-1.875089	-1.172434
18.H	-0.622837	-1.016139	-4.218747
19.C	-1.912182	-1.205697	-1.831709
20.O	-2.563400	2.043753	-1.603464
21.O	-0.684109	-1.579232	-1.536171
22.N	2.278952	1.315927	-1.410190
23.H	1.402782	-2.664693	-1.450988
24.H	2.208462	-2.006779	-0.157332
25.O	-2.901500	-1.771643	-1.324883
26.Pt	-0.810003	0.216621	1.530423
27.C	3.447897	-0.127964	3.535686
28.C	1.357179	0.144799	4.183488
29.C	2.086173	-0.005150	2.791654
30.C	2.676414	-0.315240	4.881658
31.C	1.946393	1.174362	1.822618
32.H	2.632497	-1.364467	5.195030
33.H	-3.156568	-1.054198	1.925185
34.O	0.729710	1.582557	1.523728
35.H	4.009383	0.808778	3.480669
36.H	1.096372	1.188816	4.387080
37.H	-1.306471	2.711207	1.373065
38.H	-2.778458	2.042399	1.736717
39.H	-2.210853	2.033943	0.153397
40.H	3.012906	0.295146	5.726435
41.H	4.078269	-0.954391	3.201036
42.N	-2.296858	-1.248678	1.407992
43.H	0.467245	-0.475612	4.319882
44.C	1.674062	-1.272567	2.017341
45.O	2.954265	1.711055	1.319877
46.O	0.393126	-1.436945	1.758138
47.N	-1.941961	1.934265	1.159530
48.H	-1.866236	-2.088730	1.810002
49.H	-2.547694	-1.486753	0.421481
50.O	2.526675	-2.090438	1.616931

current energy		-10.43623218 Hartree	
energy change	0.00003636	0.00100000	T
constrained gradient max	0.00058278	0.00100000	T
constrained gradient rms	0.00015267	0.00066667	T
gradient max		0.00058278	
gradient rms		0.00015267	
cart. step max	0.00970471	0.01000000	T
cart. step rms	0.00259866	0.00666667	T

GEOMETRY CONVERGED

	hartree	eV	kcal/mol	kJ/mol
Total Pauli Repulsion:	39.108604367496937	1064.1993	24541.02	102679.63
Electrostatic Energy:	-8.515633322695622	-231.7222	-5343.64	-22357.79
Total Orbital Interactions:	-40.867941967768147	-1112.0733	-25645.02	-107298.77
Dispersion Energy:	-0.161263730306676	-4.3882	-101.19	-423.40
Total Bonding Energy:	-10.436232197768113	-283.9843	-6548.84	-27400.32

α[**3**]$_2$-water-tzp-blyp-d3;C_1

Coordinates in Geometry Cycle 25			
Atom	X	Y	Z (Angstrom)
1.Pt	0.974143	-0.485541	-1.492943
2.C	-3.334005	1.136497	-2.950979
3.C	-1.564749	0.387017	-4.016820
4.C	-1.929181	0.637352	-2.488099
5.C	-3.087740	0.483821	-4.349879
6.C	-1.019351	1.684076	-1.807773
7.H	-3.549743	-0.507442	-4.428881
8.H	2.393633	-2.740043	-1.705393
9.O	0.270203	1.435017	-1.744166
10.H	-3.355326	2.228586	-2.996737
11.H	-0.985117	1.225204	-4.419269
12.H	3.410180	0.465782	-1.979372
13.H	3.364675	-0.111926	-0.428604
14.H	2.678458	1.351316	-0.776008
15.H	-3.359930	1.079603	-5.227717
16.H	-4.183906	0.774978	-2.366758
17.N	1.695158	-2.386909	-1.044982
18.H	-1.042224	-0.549688	-4.233704
19.C	-1.979947	-0.713584	-1.750676
20.O	-1.492439	2.774875	-1.427493
21.O	-0.868125	-1.404244	-1.638326
22.N	2.827809	0.399738	-1.139078
23.H	0.913785	-3.050188	-1.036152
24.H	2.114473	-2.375895	-0.097399
25.O	-3.063800	-1.176641	-1.320243
26.Pt	-1.015206	-0.052158	1.524149
27.C	3.533651	0.882744	2.833277
28.C	1.648519	0.664284	3.940915
29.C	2.058260	0.607085	2.404381
30.C	3.159675	0.510441	4.304734
31.C	1.377306	1.697952	1.549020
32.H	3.416253	-0.528126	4.545268
33.H	-2.855785	-1.913199	2.061208
34.O	0.063922	1.703860	1.486571
35.H	3.773242	1.943294	2.717800
36.H	1.245148	1.650040	4.198163
37.H	-3.191020	1.448162	1.828069
38.H	-3.315985	0.613835	0.403706
39.H	-2.338031	1.943563	0.490118
40.H	3.542685	1.167892	5.092638
41.H	4.295378	0.277012	2.336095
42.N	-2.108789	-1.816658	1.367454
43.H	0.950430	-0.108917	4.275727
44.C	1.837478	-0.818929	1.867019
45.O	2.059162	2.600535	1.021033
46.O	0.610781	-1.286499	1.831161
47.N	-2.662834	1.118851	1.014373
48.H	-1.477871	-2.616926	1.478095
49.H	-2.528950	-1.871387	0.421856
50.O	2.805672	-1.540148	1.524436

current energy		-10.43990908 Hartree	
energy change	0.00002359	0.00100000	T
constrained gradient max	0.00065081	0.00100000	T
constrained gradient rms	0.00014198	0.00066667	T
gradient max		0.00065081	
gradient rms		0.00014198	
cart. step max	0.00766569	0.01000000	T
cart. step rms	0.00166031	0.00666667	T
GEOMETRY CONVERGED			

	hartree	eV	kcal/mol	kJ/mol
Total Pauli Repulsion:	38.807103168372187	1055.9950	24351.83	101888.03
Electrostatic Energy:	-8.442457568734044	-229.7310	-5297.72	-22165.67
Total Orbital Interactions:	-40.607922411109016	-1104.9978	-25481.86	-106616.09
Solvation:	-0.078262591355347	-2.1296	-49.11	-205.48
Dispersion Energy:	-0.118383024236657	-3.2214	-74.29	-310.81
Total Bonding Energy:	-10.439917122962951	-284.0846	-6551.15	-27410.00

β[**3**]$_2$-tzp-blyp-d3;C_S

Coordinates in Geometry Cycle 109

Atom	X	Y	Z (Angstrom)
1.C	-4.081625	0.920404	0.000000
2.C	-3.768026	2.483765	0.000000
3.H	-3.220641	2.815560	0.889243
4.C	-5.302713	2.780303	0.000000
5.H	-5.654098	3.314733	0.890969
6.C	-5.609415	1.246819	0.000000
7.H	-6.114784	0.876502	-0.895175
8.C	-3.582047	0.249027	-1.304549
9.N	0.423646	0.581865	-1.631616
10.O	-2.257281	0.167758	-1.496802
11.O	-4.357172	-0.125249	-2.185303
12.Pt	-0.917117	0.453545	0.000000
13.H	-0.197973	0.647434	-2.448042
14.H	1.049301	1.390836	-1.648077
15.H	0.991327	-0.276234	-1.748917
16.H	-3.220641	2.815560	-0.889243
17.H	-5.654098	3.314733	-0.890969
18.H	-6.114784	0.876502	0.895175
19.C	-3.582047	0.249027	1.304549
20.O	-2.257281	0.167758	1.496802
21.O	-4.357172	-0.125249	2.185303
22.N	0.423646	0.581865	1.631616
23.H	-0.197973	0.647434	2.448042
24.H	1.049301	1.390836	1.648077
25.H	0.991327	-0.276234	1.748917
26.C	1.763178	-3.092036	0.000000
27.C	1.500615	-4.665493	0.000000
28.H	1.892445	-5.170290	-0.889678
29.C	-0.036763	-4.400082	0.000000
30.H	-0.555200	-4.771407	-0.890024
31.C	0.217054	-2.860512	0.000000
32.H	-0.145974	-2.336841	0.884907
33.C	2.513111	-2.604890	1.258745
34.N	5.779939	-4.882186	1.660126
35.O	3.736510	-3.103542	1.481110
36.O	2.022505	-1.811659	2.068691
37.Pt	4.752417	-4.045656	0.000000
38.H	5.308883	-4.447022	2.466278
39.H	5.686830	-5.897585	1.756632
40.H	6.775190	-4.646966	1.719215
41.H	1.892445	-5.170290	0.889678
42.H	-0.555200	-4.771407	0.890024
43.H	-0.145974	-2.336841	-0.884907
44.C	2.513111	-2.604890	-1.258745
45.O	3.736510	-3.103542	-1.481110
46.O	2.022505	-1.811659	-2.068691
47.N	5.779939	-4.882186	-1.660126
48.H	5.308883	-4.447022	-2.466278
49.H	5.686830	-5.897585	-1.756632
50.H	6.775190	-4.646966	-1.719215

current energy		-10.32562156 Hartree	
energy change	-0.00000360	0.00100000	T
constrained gradient max	0.00070739	0.00100000	T
constrained gradient rms	0.00018566	0.00066667	T
gradient max		0.00070739	
gradient rms		0.00018566	
cart. step max	0.00774298	0.01000000	T
cart. step rms	0.00275253	0.00666667	T
GEOMETRY CONVERGED			

	hartree	eV	kcal/mol	kJ/mol
Total Pauli Repulsion:	38.604377823487447	1050.4786	24224.62	101355.78
Electrostatic Energy:	-8.358915215414626	-227.4577	-5245.30	-21946.33
Total Orbital Interactions:	-40.485744037672724	-1101.6731	-25405.19	-106295.31
Dispersion Energy:	-0.085356375740241	-2.3227	-53.56	-224.10
Total Bonding Energy:	-10.325622449708721	-280.9745	-6479.43	-27109.92

Frequency cm-1	Dipole Strength 1e-40 esu2 cm2	Absorption Intensity (degeneracy not counted) km/mole
-38.116660	14.401525	-0.137595
-16.411366	0.000000	0.000000
13.688065	0.000000	0.000000
24.724976	44.673939	0.276865
29.326351	720.269826	5.294578
36.714751	16.476044	0.151625
40.342446	603.189775	6.099500
47.312670	87.356019	1.035973
69.367674	843.752595	14.670683
74.346688	48.943441	0.912083
83.985481	303.887727	6.397281
99.632694	103.880537	2.594264
110.702240	16.312712	0.452648
127.981952	3.700004	0.118694
134.641444	304.615305	10.280365
139.071064	0.538008	0.018754
143.422634	8.231707	0.295928
164.812491	496.132388	20.495842
171.598197	899.387265	38.684548
171.773921	8.434136	0.363142
177.861971	46.881950	2.090099
178.885639	443.246591	19.874625
186.585500	521.532494	24.391434
190.657554	0.037724	0.001803
212.774106	19.329179	1.030885
215.496978	5.726783	0.309336
221.603212	7.397658	0.410912
227.799039	980.595823	55.991229
258.622551	38.382525	2.488158
261.477551	92.047816	6.032898
269.738774	4.003338	0.270672
277.962699	8.138253	0.567017
295.967847	51.201828	3.798464
312.790760	128.017059	10.036905
343.034488	700.540801	60.235052
343.522847	5.552238	0.478081
345.939028	291.956252	25.316019
350.408873	95.707761	8.406212
417.395149	2.244152	0.234789
419.817305	114.215389	12.018853
436.474372	121.307500	13.271636
438.218276	18.652690	2.048849
449.283395	5.958644	0.671036
461.152924	100.674523	11.637042
476.930500	3.306853	0.395319
478.324700	4.222126	0.506212
547.894937	84.968880	11.669043
550.554594	90.419023	12.477807
636.982000	13.345005	2.130708
657.652464	6.469448	1.066453
687.855048	0.931894	0.160673
701.675283	59.950203	10.543988
706.767887	22.883318	4.053908
712.313134	24.397694	4.356100
715.023298	5.003919	0.896827
719.607661	9.118345	1.644712
737.013437	0.005375	0.000993
738.307387	2.781575	0.514762
747.618981	38.963226	7.301520
753.650994	396.801379	74.958609
757.604938	95.465034	18.128639
759.556577	28.720156	5.467956
785.462954	9.006454	1.773200
786.613563	32.209017	6.350632
788.501598	71.696931	14.170371
790.973711	3.667080	0.727044
799.959925	4.593332	0.921031
806.590911	264.094707	53.393832
820.475253	188.317395	38.728796
828.938631	14.379658	2.987783
850.739883	102.470764	21.851177
852.836967	60.757257	12.987999
906.629748	21.206946	4.819325
915.181025	11.248360	2.580324
915.541534	25.292908	5.804367
932.906665	4.915990	1.149548
977.731441	19.331410	4.737631
984.764187	22.240859	5.489868
1048.727933	1.778950	0.467632
1055.898854	737.081165	195.081328
1057.996732	173.671076	46.056390
1059.898898	0.738058	0.196080
1097.597704	11.452011	3.150671
1099.273160	0.689570	0.190004
1141.108261	16.494480	4.717844
1143.081216	6.877318	1.970490
1200.163689	248.829400	74.854902
1204.544541	1.421785	0.429274

1209.010714		263.776937	79.936484
1210.301048		0.858584	0.260468
1221.224128		465.069336	142.361040
1226.731706		515.555493	158.526941
1228.241601		7.969130	2.453425
1237.825543		19.604068	6.082522
1243.725036		120.322804	37.510287
1247.728285		2057.083713	643.354075
1247.977046		350.698190	109.702921
1253.036826		1137.075655	357.134056
1255.211830		16.688689	5.250701
1268.032383		321.829342	102.290206
1290.514671		227.535292	73.602028
1296.047057		108.732909	35.323184
1442.623394		118.681815	42.915603
1444.313021		8.810105	3.189485
1447.698464		2.550846	0.925636
1449.512733		17.247567	6.266542
1471.155926		74.411595	27.439575
1471.477179		36.001449	13.278579
1589.296095		501.198474	199.660717
1608.503638		530.382169	213.840043
1611.024114		54.855407	22.151317
1614.062593		171.366980	69.330700
1617.827086		415.359911	168.435934
1619.755026		226.640898	92.016495
1627.080314		1575.780419	642.662206
1629.722461		0.154966	0.063304
1635.198387		72.652068	29.778067
1637.480824		847.510026	347.855711
1655.336588		11.774855	4.885623
1660.981906		71.806853	29.895709
2961.815767		92.414275	68.608065
2970.939096		36.172887	26.937357
2974.198378		42.528042	31.704681
2988.319298		45.479548	34.066005
2998.198409		7.140333	5.366077
3008.927380		39.559922	29.836316
3014.215988		0.585243	0.442170
3023.441364		22.779051	17.262960
3035.175126		13.534660	10.296964
3035.632178		16.282221	12.389131
3061.864895		2.346500	1.800879
3086.632921		0.029074	0.022494
3184.685358		0.195806	0.156305
3195.170076		1635.441527	1309.806290
3294.452970		14.343381	11.844396
3294.522686		7.532433	6.220222
3339.827871		7.410905	6.204023
3341.159151		344.905869	288.852292
3394.820417		6.770906	5.761581
3395.724136		73.950209	62.943353
3425.492565		4.790162	4.112930
3425.959366		39.625360	34.027771
3430.683140		0.064909	0.055816
3431.527680	65.153311	56.040509	

Zero-Point Energy : 0.382496 a.u.
==========
10.408252 eV
(imaginary frequencies were excluded from the summation)

Statistical Thermal Analysis *** ideal gas assumed ***

Temp		Transl	Rotat	Vibrat	Total
298.15	Entropy (cal/mole-K):	45.693	37.411	111.776	194.879
	Internal Energy (Kcal/mole):	0.889	0.889	256.819	258.597
	Constant Volume Heat Capacity (cal/mole-K):	2.981	2.981	104.082	110.043

β[**3**]$_2$-tzp-blyp-d3bj;C_1

Coordinates in Geometry Cycle 25

Atom	X	Y	Z (Angstrom)
1.C	-4.050539	0.930579	0.000000
2.C	-3.728955	2.492288	0.000000
3.H	-3.182561	2.821939	0.889633
4.C	-5.260102	2.795317	0.000000
5.H	-5.608152	3.330585	0.890767
6.C	-5.574284	1.265467	0.000000
7.H	-6.076547	0.896393	-0.896238
8.C	-3.567312	0.257881	-1.305972
9.N	0.399327	0.572347	-1.637559
10.O	-2.247209	0.146998	-1.502182
11.O	-4.353796	-0.094751	-2.185731
12.Pt	-0.917346	0.428666	0.000000
13.H	-0.244865	0.594135	-2.438449
14.H	0.982172	1.410766	-1.674871
15.H	1.002185	-0.261597	-1.745891
16.H	-3.182561	2.821939	-0.889633
17.H	-5.608152	3.330585	-0.890767
18.H	-6.076547	0.896393	0.896238
19.C	-3.567312	0.257881	1.305972
20.O	-2.247209	0.146998	1.502182
21.O	-4.353796	-0.094751	2.185731
22.N	0.399327	0.572347	1.637559
23.H	-0.244865	0.594135	2.438449
24.H	0.982172	1.410766	1.674871
25.H	1.002185	-0.261597	1.745891
26.C	1.783334	-3.081880	0.000000
27.C	1.529479	-4.654157	0.000000
28.H	1.922054	-5.156537	-0.889581
29.C	-0.007885	-4.395934	0.000000
30.H	-0.523503	-4.769482	-0.889871
31.C	0.237956	-2.857007	0.000000
32.H	-0.125442	-2.333732	0.884032
33.C	2.523116	-2.591489	1.259145
34.N	5.747210	-4.865085	1.661949
35.O	3.745410	-3.085960	1.486242
36.O	2.023779	-1.800222	2.065417
37.Pt	4.738878	-4.037126	0.000000
38.H	5.267843	-4.413877	2.453699
39.H	5.646546	-5.877825	1.766506
40.H	6.741794	-4.631322	1.721709
41.H	1.922054	-5.156537	0.889581
42.H	-0.523503	-4.769482	0.889871
43.H	-0.125442	-2.333732	-0.884032
44.C	2.523116	-2.591489	-1.259145
45.O	3.745410	-3.085960	-1.486242
46.O	2.023779	-1.800222	-2.065417
47.N	5.747210	-4.865085	-1.661949
48.H	5.267843	-4.413877	-2.453699
49.H	5.646546	-5.877825	-1.766506
50.H	6.741794	-4.631322	-1.721709

current energy			-10.38023437 Hartree
energy change	0.00000126	0.00100000	T
constrained gradient max	0.00089684	0.00100000	T
constrained gradient rms	0.00018500	0.00066667	T
gradient max			0.00089684
gradient rms			0.00018500
cart. step max	0.00362967	0.01000000	T
cart. step rms	0.00147072	0.00666667	T
GEOMETRY CONVERGED			

	hartree	eV	kcal/mol	kJ/mol
Total Pauli Repulsion:	38.812143176377866	1056.1322	24354.99	101901.27
Electrostatic Interaction:	-8.415269775372115	-228.9911	-5280.66	-22094.29
Total Orbital Interactions:	-40.637067447337216	-1105.7909	-25500.15	-106692.61
Dispersion Energy:	-0.140022437460090	-3.8102	-87.87	-367.63
Total Bonding Energy:	-10.380234380187822	-282.4605	-6513.70	-27253.30

Na,β[**3**]$_2$-tzp-blyp-d3;C_s

Coordinates in Geometry Cycle 53			
Atom	X	Y	Z (Angstrom)
1.C	-3.920781	1.093028	0.000000
2.C	-3.366321	2.567717	0.000000
3.H	-2.777679	2.812718	0.889059
4.C	-4.833634	3.109654	0.000000
5.H	-5.098722	3.688803	0.889976
6.C	-5.386320	1.647058	0.000000
7.H	-5.955771	1.376493	-0.896164
8.C	-3.533290	0.186903	-1.193931
9.N	0.496848	0.527489	-1.570456
10.O	-2.264522	0.122338	-1.514009
11.O	-4.409187	-0.525451	-1.741031
12.Pt	-0.870906	0.423587	0.000000
13.H	-0.050633	0.644585	-2.431570
14.H	1.157704	1.308095	-1.522557
15.H	1.043269	-0.357530	-1.678611
16.H	-2.777679	2.812718	-0.889059
17.H	-5.098722	3.688803	-0.889976
18.H	-5.955771	1.376493	0.896164
19.C	-3.533290	0.186903	1.193931
20.O	-2.264522	0.122338	1.514009
21.O	-4.409187	-0.525451	1.741031
22.N	0.496848	0.527489	1.570456
23.H	-0.050633	0.644585	2.431570
24.H	1.157704	1.308095	1.522557
25.H	1.043269	-0.357530	1.678611
26.C	1.783293	-3.117725	0.000000
27.C	1.568372	-4.696536	0.000000
28.H	1.973101	-5.189913	-0.889459
29.C	0.023097	-4.478291	0.000000
30.H	-0.481976	-4.866552	-0.890725
31.C	0.231225	-2.931087	0.000000
32.H	-0.143521	-2.420219	0.888851
33.C	2.523236	-2.599821	1.251943
34.N	5.886796	-4.775086	1.634117
35.O	3.747613	-3.062953	1.479713
36.O	2.007101	-1.795529	2.043080
37.Pt	4.805265	-3.976261	0.000000
38.H	5.430494	-4.371044	2.463905
39.H	5.838144	-5.794900	1.721880
40.H	6.874530	-4.503034	1.666541
41.H	1.973101	-5.189913	0.889459
42.H	-0.481976	-4.866552	0.890725
43.H	-0.143521	-2.420219	-0.888851
44.C	2.523236	-2.599821	-1.251943
45.O	3.747613	-3.062953	-1.479713
46.O	2.007101	-1.795529	-2.043080
47.N	5.886796	-4.775086	-1.634117
48.H	5.430494	-4.371044	-2.463905
49.H	5.838144	-5.794900	-1.721880
50.H	6.874530	-4.503034	-1.666541
51.Na	-5.549190	-1.496284	0.000000

current energy		-10.25137548 Hartree	
energy change	-0.00000394	0.00100000	T
constrained gradient max	0.00068242	0.00100000	T
constrained gradient rms	0.00016294	0.00066667	T
gradient max		0.00068242	
gradient rms		0.00016294	
cart. step max	0.00637717	0.01000000	T
cart. step rms	0.00227985	0.00666667	T
GEOMETRY CONVERGED			

	hartree	eV	kcal/mol	kJ/mol
Total Pauli Repulsion:	38.890720847053828	1058.2704	24404.30	102107.57
Electrostatic Energy:	-8.484909113736727	-230.8861	-5324.36	-22277.13
Total Orbital Interactions:	-40.567383716046464	-1103.8947	-25456.42	-106509.65
Dispersion Energy:	-0.089826058604480	-2.4443	-56.37	-235.84
Total Bonding Energy:	-10.251374609092448	-278.9541	-6432.84	-26914.98

Frequency	Dipole Strength	Absorption Intensity (degeneracy not counted)
cm-1	1e-40 esu2 cm2	km/mole
-18.801748	0.000000	0.000000
11.569564	0.000000	0.000000
17.044480	0.000000	0.000000
31.693327	908.791214	7.219548
43.988852	404.680751	4.462038
49.044567	1310.888564	16.115165
56.458508	0.064961	0.000919
57.313106	1.848154	0.026550
60.570516	729.334124	11.073015
81.059743	14.000543	0.284465
83.825347	598.005400	12.564886
105.129357	325.110274	8.567079
110.599884	114.894537	3.185166
120.032557	456.462547	13.733533
122.596928	0.007956	0.000244
129.172108	0.508522	0.016465
141.063565	8.737297	0.308937
147.341729	242.207027	8.945211
156.755632	61.041341	2.398420
165.685232	157.363887	6.535321
174.124524	885.829296	38.662332
175.208785	29.470555	1.294262
181.377405	482.598141	21.940519
189.817932	323.397696	15.386939
194.048716	51.576435	2.508651
204.424603	236.170117	12.101416
212.801921	122.484162	6.533314
216.123371	6.695801	0.362729
222.544134	19.870055	1.108392
230.477059	1579.630487	91.255969
240.931885	603.415947	36.440903
261.775263	112.049836	7.352210
268.402357	345.880896	23.269710
277.253514	13.496614	0.937951
285.045731	32.317563	2.309039
290.135516	29.668795	2.157639
301.039518	46.159343	3.483062
337.273187	29.436071	2.488512
348.976604	1374.908056	120.267432
353.293658	42.869969	3.796357
354.378708	99.470124	8.835647
426.822925	0.130117	0.013921
429.834891	116.331135	12.533596
443.047068	110.172200	12.234887
458.556543	121.333048	13.946013
471.868956	14.762980	1.746118
475.030173	1.537486	0.183067
480.209094	3.715246	0.447194
485.483719	47.681859	5.802377
552.740952	132.631278	18.375775
555.639978	64.769831	9.020785
603.913328	10.820087	1.637885
636.151876	12.792278	2.039796
701.631080	1.021559	0.179660
710.791918	22.708938	4.045921
713.697122	1.212831	0.216966
716.746304	89.141171	16.014813
717.640958	6.446853	1.159666
721.559572	51.160128	9.252986
748.105932	0.061836	0.011595
758.183051	26.791434	5.091528
762.658031	38.953146	7.446470
768.189964	325.922743	62.756883
781.947361	5.419391	1.062199
790.450630	46.330189	9.179455
793.885742	6.787587	1.350677
795.137039	10.245082	2.041905
800.279870	2.682034	0.538003
806.503499	75.535235	15.269820
828.923731	165.990920	34.488712
835.825249	155.052995	32.484315
836.037029	34.803004	7.293237
844.243748	2.401292	0.508149
856.945774	69.985915	15.032875
858.957604	105.552544	22.725765
913.094438	13.493820	3.088365
918.488908	22.704819	5.227211
921.074339	3.794845	0.876127
931.500648	2.801952	0.654217
989.478988	23.487677	5.825386
1040.486961	18.158717	4.735871
1053.799913	0.267369	0.070623
1062.648603	171.221863	45.606523
1063.105181	2.465065	0.656875
1065.222607	278.937112	74.477441
1118.641986	3.334847	0.935072
1120.332256	3.946398	1.108220
1156.644462	33.094339	9.594706

1184.080351	93.771572	27.831105
1204.220782	28.977783	8.746803
1210.590119	7.569689	2.296959
1213.184751	70.337238	21.388992
1213.702503	0.634245	0.192951
1220.834334	63.288813	19.366973
1232.556367	202.724712	62.631318
1234.780823	35.148156	10.878537
1239.571327	27.982365	8.694288
1240.855742	0.548300	0.170537
1258.959490	105.800969	33.387159
1268.890873	309.998082	98.596466
1272.862852	732.678875	233.761697
1282.805499	1783.183780	573.370030
1312.223315	1404.724024	462.037080
1346.066806	121.700893	41.061844
1355.839852	135.788796	46.147736
1448.463632	71.624023	26.004253
1449.241687	10.532462	3.826034
1451.479170	2.397659	0.872321
1455.834743	12.787511	4.666338
1473.956123	87.344921	32.270098
1479.609977	42.959038	15.932351
1520.365547	477.414546	181.937296
1565.669126	2438.164798	956.843948
1568.019592	574.538023	225.812683
1605.567779	1696.419529	682.715837
1613.705833	69.362063	28.055915
1615.840540	77.690908	31.466379
1621.829839	340.996024	138.622163
1624.856984	163.259186	66.492221
1630.143936	0.605799	0.247533
1636.422563	105.053204	43.090629
1655.564323	15.756474	6.538576
1662.781079	59.595063	24.838389
2973.623903	33.284068	24.808500
2979.451243	30.479535	22.762643
2988.404155	62.633069	46.916013
2988.747485	37.620854	28.183566
2998.125835	35.152633	26.417139
3018.939506	18.767951	14.201994
3019.699516	0.231769	0.175427
3020.041763	0.481209	0.364271
3020.368921	0.399654	0.302568
3034.217442	0.726562	0.552583
3039.519801	12.055743	9.184955
3044.124686	3482.351315	2657.131755
3050.556992	15.005307	11.473663
3072.174099	0.955051	0.735446
3302.367189	15.619876	12.929479
3302.476592	1.390386	1.150941
3352.209921	23.013255	19.336921
3352.678618	144.485504	121.421130
3395.083852	8.392812	7.142267
3396.132411	89.137523	75.879288
3422.946685	7.968496	6.836826
3423.855533	40.140651	34.449103
3425.474824	0.038887	0.033389
3426.605593	79.856283	68.588496

Zero-Point Energy :	0.384900	a.u.
==========	10.473674	eV

(imaginary frequencies were excluded from the summation)

Statistical Thermal Analysis *** ideal gas assumed ***

Temp		Transl	Rotat	Vibrat	Total
298.15	Entropy (cal/mole-K):	45.783	37.673	115.293	198.749
	Internal Energy (Kcal/mole):	0.889	0.889	259.199	260.976
	Constant Volume Heat Capacity (cal/mole-K):	2.981	2.981	108.650	114.611

γ[**3**]$_2$-tzp-blyp-d3;C_1

Coordinates in Geometry Cycle 30

Atom	X	Y	Z (Angstrom)
1.Pt	0.843027	-0.381651	-1.651823
2.C	-3.592179	-0.261524	-3.371828
3.C	-1.602334	-0.840841	-4.114429
4.C	-2.163634	-0.251241	-2.743763
5.C	-3.070645	-1.166558	-4.533575
6.C	-1.603793	1.129942	-2.396226
7.H	-3.316036	-2.222534	-4.375722
8.H	2.449542	-2.551937	-1.750033
9.O	-0.295269	1.233167	-2.115958
10.H	-3.877141	0.741624	-3.700783
11.H	-1.139231	-0.054186	-4.721768
12.H	2.827055	0.693924	-3.086678
13.H	3.296912	0.844466	-1.495891
14.H	2.174115	1.827717	-2.053792
15.H	-3.357900	-0.877362	-5.550837
16.H	-4.368719	-0.682156	-2.729765
17.N	1.900956	-2.089482	-1.019162
18.H	-0.898654	-1.674300	-4.017196
19.C	-1.994990	-1.311884	-1.614270
20.O	-2.302013	2.154587	-2.428778
21.O	-0.763722	-1.514204	-1.127928
22.N	2.485050	0.843672	-2.133163
23.H	1.158912	-2.737734	-0.718694
24.H	2.517103	-1.917961	-0.218671
25.O	-2.941302	-1.994788	-1.228706
26.Pt	1.204158	5.012678	-1.160682
27.C	5.567130	4.689308	0.687449
28.C	3.543461	5.121109	1.423718
29.C	4.173348	4.798992	-0.005786
30.C	4.863273	4.606607	2.079422
31.C	4.024536	5.957907	-1.028171
32.H	4.765409	3.572833	2.431406
33.H	-0.785607	3.802701	0.136238
34.O	2.802363	6.219351	-1.512186
35.H	6.128806	5.616183	0.545620
36.H	3.392272	6.199819	1.544941
37.H	-0.453675	7.120089	-0.837518
38.H	-0.456292	6.688045	-2.438975
39.H	0.864699	7.462896	-1.791087
40.H	5.280147	5.222021	2.884572
41.H	6.173081	3.833500	0.382261
42.N	-0.428782	3.730814	-0.821377
43.H	2.610346	4.600201	1.663462
44.C	3.644681	3.442476	-0.502328
45.O	4.982144	6.666495	-1.330709
46.O	2.362320	3.366711	-0.880910
47.N	0.129447	6.766679	-1.601825
48.H	-0.111090	2.756250	-0.969309
49.H	-1.234950	3.774411	-1.461974
50.O	4.342707	2.415871	-0.501392

```
E-test:            old,new=      -10.34937,       -10.34940      hartree
max    gradient:                        0.00095914    au/angstrom,radian
max      cart.      step:                         0.00350400      angstrom
Geometry Converged
```

	hartree	eV	kcal/mol	kJ/mol
Total Pauli Repulsion:	38.610897166242637	1050.6560	24228.71	101372.90
Electrostatic Energy:	-8.386460536485622	-228.2072	-5262.58	-22018.65
Total Orbital Interactions:	-40.493676256351286	-1101.8890	-25410.17	-106316.13
Dispersion Energy:	-0.087159960961464	-2.3717	-54.69	-228.84
Total Bonding Energy:	-10.349459083795317	-281.6231	-6494.38	-27172.50

Frequency cm-1	Dipole Strength 1e-40 esu2	Absorption Intensity (degeneracy not counted) cm2 km/mole
-55.156699	16.206669	-0.224063
-38.939329	150.096913	-1.465002
23.668768	822.586468	4.880174
26.611713	506.746495	3.380194
32.546558	433.180141	3.533879
49.519229	27.308594	0.338962

57.100997	182.429417	2.611059
60.730125	710.218659	10.811210
83.627621	51.831894	1.086488
86.431976	18.186012	0.393994
92.062471	24.117173	0.556528
100.267053	131.213122	3.297719
116.911917	1328.641706	38.935408
123.025832	66.304764	2.044651
127.266020	216.922102	6.919813
132.480838	43.554704	1.446326
155.810439	3.007207	0.117446
158.854342	18.245676	0.726503
161.299273	10.817291	0.437350
168.269007	111.284319	4.693709
176.608543	623.961481	27.621519
180.750492	31.156877	1.411599
187.298671	285.862697	13.420548
192.299163	21.962914	1.058633
194.183573	148.202980	7.213524
209.235289	159.017711	8.339855
217.879925	94.292448	5.149585
220.104754	110.760228	6.110705
249.770244	174.729636	10.939194
251.413883	29.894252	1.883888
267.241866	1.430457	0.095820
269.469679	360.395404	24.342614
320.783436	377.673570	30.367329
324.484482	207.034579	16.838945
333.443284	159.049746	13.293307
344.200289	35.291165	3.044776
353.719322	339.163863	30.070900
363.029540	189.886412	17.278814
431.321837	8.602290	0.930023
434.076461	41.474918	4.512631
446.597528	0.400144	0.044793
454.348884	47.416457	5.400036
468.126971	118.331505	13.884880
473.977420	2.819974	0.335028
485.309915	70.353462	8.558205
488.420173	18.655276	2.283880
542.017307	69.465052	9.437514
543.384106	37.409220	5.095228
643.547146	3.547218	0.572198
648.314325	25.493432	4.142781
675.686840	8.517495	1.442565
678.632737	23.860439	4.058741
702.816282	27.635837	4.868470
702.986174	26.547532	4.677879
727.075204	31.434020	5.728716
729.117560	18.235331	3.332647
729.867325	10.007499	1.830828
737.364426	7.251308	1.340222
745.793447	37.975628	7.099072
753.231849	133.089629	25.127597
757.950597	54.664614	10.385448
758.546748	290.963366	55.322110
793.029844	221.705495	44.070102
794.795500	14.662997	2.921166
796.209697	22.659805	4.522324
802.105589	3.297725	0.663016
819.512515	148.770879	30.559876
821.598676	35.598110	7.331026
840.226567	66.795313	14.067615
848.878483	18.555700	3.948216
858.401570	98.998407	21.300842
865.024253	167.826383	36.388704
900.250700	13.729238	3.098047
903.125549	13.222784	2.993292
917.110049	20.208885	4.645601
920.885439	21.847604	5.042983
975.310247	24.203541	5.916975
978.285631	27.767776	6.809024
1044.402337	31.250277	8.180875
1045.654873	38.124220	9.992345
1061.420217	392.652060	104.465601
1063.713461	310.806089	82.869028
1104.335661	31.465676	8.709962
1107.098037	22.673896	6.292023
1149.959730	35.050533	10.103116
1151.584968	32.173524	9.286941
1173.434182	5.882532	1.730219
1177.712348	6.108679	1.803286
1209.407418	301.382988	91.362807
1210.511848	198.081288	60.102227
1222.128629	19.294067	5.910426
1222.796752	136.394499	41.805094
1234.069045	148.228915	45.851174
1236.551099	26.397191	8.181781
1240.924411	347.246915	108.009460
1242.733186	236.158434	73.562999
1242.978989	104.422772	32.533971

1247.519462		24.755319	7.740944
1259.278013		1912.953097	603.815160
1264.280332		1095.697577	347.225933
1374.037533		541.060900	186.347177
1381.216830		5.035922	1.743488
1449.452041		21.814213	7.925405
1450.178091		12.298439	4.470431
1452.197918		5.134460	1.868954
1452.342306		13.984369	5.090846
1474.723708		53.397103	19.738149
1475.083065		34.589057	12.788902
1573.535168		198.117876	78.140860
1581.093149		1502.269808	595.365228
1602.029809		109.669033	44.038516
1607.363702		221.143358	89.097625
1613.323892		42.470718	17.174703
1614.147655		14.517253	5.873619
1629.301227		7.430482	3.034565
1629.419630		100.950585	41.230619
1633.685152		29.058617	11.899299
1636.653243		2058.876940	844.627340
1641.162053		49.006027	20.159467
1644.460653		663.921682	273.664465
2968.734265		38.104524	28.354757
2968.962175		50.911602	37.887810
2975.321082		40.632981	30.303347
2977.868553		67.961634	50.727961
3007.206321		18.483430	13.932334
3007.552433		12.093074	9.116497
3013.372597		27.299586	20.619919
3013.497795		7.279093	5.498272
3029.293501		40.863286	31.027924
3030.583938		32.719571	24.854898
3065.890612		5.705512	4.384593
3066.532236		6.620279	5.088642
3209.817744		401.483533	323.017596
3223.962584		664.354204	536.868287
3278.270022		142.607965	117.183530
3292.130275		8.624293	7.116699
3292.449436		10.997309	9.075773
3298.452294		118.802411	98.223076
3393.489965		32.135615	27.334507
3394.318949		35.822757	30.478229
3407.165530		75.407477	64.399977
3411.035481		90.834071	77.662807
3425.928232		32.299172	27.736248
3427.389953	35.025801	30.090518	

```
 Zero-Point        Energy        :                                    0.382761        a.u.
 ====================                                             10.415465          eV
 (imaginary frequencies were excluded from the summation)
```

```
Statistical       Thermal       Analysis              ***              ideal       gas       assumed              ***
     Temp                                                                 Transl      Rotat     Vibrat      Total
     ----                                                                 ------      -----     ------      -----

     298.15    Entropy (cal/mole-K):                                     45.693     37.275    115.252    198.220
               Internal Energy (Kcal/mole):                              0.889       0.889    257.442    259.219
               Constant Volume Heat Capacity (cal/mole-K):       2.981     2.981   105.741   111.703
```

γ[**3**]$_2$-tzp-blyp-d3bj;C_1

Coordinates in Geometry Cycle 10

Atom	X	Y	Z (Angstrom)
1.Pt	0.835161	-0.383050	-1.671318
2.C	-3.560283	-0.239415	-3.421423
3.C	-1.574737	-0.853764	-4.135590
4.C	-2.138986	-0.232261	-2.782551
5.C	-3.041323	-1.181755	-4.551690
6.C	-1.572596	1.146645	-2.448951
7.H	-3.294358	-2.230084	-4.361415
8.H	2.393394	-2.573453	-1.720048
9.O	-0.267255	1.242418	-2.166725
10.H	-3.824604	0.758446	-3.780198
11.H	-1.111223	-0.081213	-4.759410
12.H	2.772314	0.713484	-3.126154
13.H	3.314142	0.776746	-1.549625
14.H	2.187307	1.808850	-2.007775
15.H	-3.321825	-0.923146	-5.578467
16.H	-4.346400	-0.631932	-2.774397
17.N	1.855788	-2.084614	-0.999422
18.H	-0.874260	-1.686537	-4.018379
19.C	-2.001845	-1.271883	-1.633432
20.O	-2.266088	2.175179	-2.488643
21.O	-0.778889	-1.495734	-1.140198
22.N	2.479773	0.825686	-2.152025
23.H	1.094694	-2.704165	-0.687118
24.H	2.472853	-1.903706	-0.202710
25.O	-2.968164	-1.918537	-1.235448
26.Pt	1.193339	4.953523	-1.116074
27.C	5.565457	4.642465	0.650618
28.C	3.559759	5.116899	1.409238
29.C	4.160838	4.742425	-0.017913
30.C	4.894177	4.639570	2.059112
31.C	4.010499	5.876085	-1.063151
32.H	4.807742	3.630247	2.476978
33.H	-0.805215	3.752063	0.175886
34.O	2.782212	6.149616	-1.519056
35.H	6.139420	5.549367	0.447686
36.H	3.403670	6.198041	1.490609
37.H	-0.379021	7.098358	-0.741061
38.H	-0.495327	6.637838	-2.331983
39.H	0.890725	7.378912	-1.779186
40.H	5.329051	5.303652	2.813975
41.H	6.144650	3.759228	0.375249
42.N	-0.435103	3.676969	-0.775055
43.H	2.636761	4.599494	1.688967
44.C	3.623211	3.380907	-0.480351
45.O	4.974326	6.555946	-1.408139
46.O	2.336772	3.301809	-0.841691
47.N	0.141809	6.715595	-1.534492
48.H	-0.102860	2.707826	-0.917169
49.H	-1.227320	3.712505	-1.434731
50.O	4.321647	2.355104	-0.479977

```
E-test:            old,new=      -10.40263,      -10.40266      hartree
max    gradient:                        0.00091639    au/angstrom,radian
max      cart.      step:                        0.00614873      angstrom
Geometry Converged
```

	hartree	eV	kcal/mol	kJ/mol
Total Pauli Repulsion:	38.797827188446739	1055.7426	24346.01	101863.68
Electrostatic Interaction:	-8.437408943396141	-229.5936	-5294.55	-22152.41
Total Orbital Interactions:	-40.622362517639047	-1105.3907	-25490.92	-106654.00
Dispersion Energy:	-0.140808806028363	-3.8316	-88.36	-369.69
Total Bonding Energy:	-10.402752595018608	-283.0733	-6527.83	-27312.42

β[1,2]-tzp-blyp-d3;C_1

```
  Coordinates      in      Geometry      Cycle      24
   Atom         X           Y           Z   (Angstrom)
   1.Pt          -0.506842    -1.674087      0.145730
   2.O            0.836310    -2.160362      1.615225
   3.O            3.068724    -2.352776      1.868545
   4.N           -2.082186    -1.101749      1.410017
   5.H           -2.386845    -1.895468      1.983522
   6.H           -1.738395    -0.354534      2.034449
   7.H           -1.684650    -0.113765     -1.564869
   8.O            3.298700    -2.363490     -0.975836
   9.C            2.063406    -2.280370      1.151229
  10.H           -6.021097    -1.759296     -0.879404
  11.H           -6.506310    -0.216546     -1.585982
  12.C           -3.240845    -0.531037      0.613975
  13.H           -2.983334     0.525498      0.469999
  14.C           -4.594746    -0.652911      1.328725
  15.H           -4.108319     0.467337     -1.835094
  16.C           -5.740427    -0.697136     -0.963033
  17.H           -4.549171    -0.133393      2.295675
  18.H           -4.807515    -1.716363      1.534186
  19.C           -4.359793    -0.589134     -1.656790
  20.H           -4.377945    -1.094611     -2.633649
  21.H           -3.471827    -2.286854     -0.633188
  22.C           -5.721039    -0.059763      0.446017
  23.H           -6.691891    -0.201381      0.939395
  24.H           -5.564610     1.025061      0.351867
  25.C            2.189760    -2.287375     -0.423571
  26.O            1.059003    -2.167187     -1.086182
  27.C           -3.272373    -1.212526     -0.764837
  28.N           -1.878766    -1.108093     -1.334378
  29.H           -1.790299    -1.662162     -2.191354
  30.Pd           2.373274     1.035215      0.176739
  31.O            0.838765     1.559484     -1.066627
  32.O           -1.404651     1.708471     -0.962834
  33.N            3.753995     0.495100     -1.314632
  34.H            3.551281    -0.492952     -1.562642
  35.H            3.682606     1.062772     -2.166326
  36.H            4.247200     1.218040      2.033300
  37.O           -1.205547     1.613191      1.869694
  38.C           -0.294073     1.629367     -0.409236
  39.H            7.406381    -1.705754      0.350112
  40.H            8.536614    -0.507432      0.988587
  41.C            5.132020     0.578619     -0.715576
  42.H            5.335132     1.646937     -0.548733
  43.C            6.232152    -0.021194     -1.611613
  44.H            6.658987     1.005309      1.605848
  45.C            7.570167    -0.625679      0.480513
  46.H            6.259263     0.512000     -2.573293
  47.H            5.976329    -1.070548     -1.823269
  48.C            6.439862    -0.050305      1.368294
  49.H            6.380653    -0.595360      2.320216
  50.H            4.818910    -1.185609      0.472428
  51.C            7.607518     0.056889     -0.905720
  52.H            8.374988    -0.408271     -1.538427
  53.H            7.894034     1.114029     -0.785327
  54.C           -0.184719     1.575456      1.167451
  55.O            1.032138     1.471503      1.649161
  56.C            5.084571    -0.136265      0.645787
  57.N            3.938751     0.427008      1.455003
  58.H          3.588377   -0.317417    2.078145
```

```
E-test:            old,new=      -12.11923,      -12.11923      hartree
max    gradient:                        0.00075197    au/angstrom,radian
max      cart.      step:                        0.00268719      angstrom
Geometry Converged
```

	hartree	eV	kcal/mol	kJ/mol
Total Pauli Repulsion:	45.792541623205103	1246.0785	28735.26	120228.30
Electrostatic Energy:	-9.949107334799606	-270.7290	-6243.16	-26121.38
Total Orbital Interactions:	-47.844371680379773	-1301.9116	-30022.80	-125615.38
Dispersion Energy:	-0.118299443921444	-3.2191	-74.23	-310.60
Total Bonding Energy:	-12.119238763220343	-329.7813	-7604.94	-31819.06

Frequency cm-1	Dipole Strength 1e-40 esu2 cm2	Absorption Intensity (degeneracy not counted) km/mole
34.460436	111.665382	0.964534
36.251045	724.363781	6.581961
41.008384	33.893064	0.348387
48.290235	9.969825	0.120677
66.469622	14.084861	0.234668
67.695748	1.581726	0.026839
80.151603	11.564928	0.232345
86.885585	51.692131	1.125771
87.519664	86.256611	1.892240
105.687298	39.352713	1.042499
111.423599	16.209549	0.452716
128.489998	30.157402	0.971273
146.350403	83.080717	3.047700
153.473418	895.097944	34.433550
162.293935	5.552817	0.225888
168.747019	79.073199	3.344595
178.351466	87.504209	3.911864
183.532291	19.149338	0.880936
193.228737	21.184230	1.026036
198.757474	59.755645	2.977011
213.505790	36.221372	1.938441
224.693813	38.724844	2.181016
242.485396	263.233049	15.999414
250.796334	118.340388	7.439303
253.180234	315.896239	20.047135
256.972570	40.535139	2.610938
297.488345	298.104957	22.228862
316.911499	320.961970	25.495859
330.394994	5.276930	0.437012
332.075246	44.938219	3.740507
335.345752	71.815513	6.036555
338.703158	71.858324	6.100626
356.457247	55.260917	4.937460
357.341443	54.850712	4.912966
361.613338	18.797974	1.703859
365.320075	78.329305	7.172588
420.045107	18.321708	1.929034
425.994301	13.591598	1.451284
427.784141	88.596802	9.499939
435.660731	48.660119	5.313732
448.400751	139.770117	15.709369
456.078631	733.005763	83.796366
487.425183	68.741830	8.398604
496.852112	26.458922	3.295166
513.261818	233.776124	30.075800
522.495958	229.140498	30.009783
530.971666	95.319780	12.686226
537.305857	24.712539	3.328258
550.419058	25.753473	3.553099
559.453513	40.090439	5.621897
561.440925	10.371452	1.459559
564.908151	21.018770	2.976208
572.508539	15.328826	2.199728
579.833497	15.786421	2.294378
680.532318	27.399837	4.673850
714.691583	14.060916	2.518897
730.694386	157.485938	28.844009
749.137764	95.580802	17.947767
759.205996	141.074257	26.846364
772.439379	132.262661	25.608240
774.453015	10.137091	1.967825
783.914274	8.828560	1.734748
794.823586	11.759814	2.342876
796.005754	10.809839	2.156818
824.473578	4.658743	0.962772
825.596314	14.250137	2.948933
826.847498	13.595192	2.817662
838.669280	16.676981	3.505793
847.193489	4.700220	0.998111
847.969446	4.213492	0.895572
863.758117	0.354695	0.076794
869.772963	0.178789	0.038979
908.615997	7.526225	1.714098
908.887458	10.099560	2.300862
923.666546	3.193187	0.739295
924.602869	3.798283	0.880280
973.953585	311.753091	76.107437
981.138091	252.123763	62.004326
1015.969595	99.718801	25.394276
1022.255898	33.714338	8.638778
1025.247030	16.703825	4.292621
1028.459578	3.760886	0.969517
1035.044862	48.095323	12.477859
1035.753688	41.022369	10.650139
1036.360256	48.924020	12.708988
1042.116839	29.320603	7.658917

1067.205761	27.677400	7.403746
1074.261636	21.682570	5.838468
1106.685650	68.310611	18.949184
1118.735009	145.849260	40.898702
1119.613474	38.483882	10.800032
1133.219998	126.038301	35.800974
1156.664865	17.458664	5.061702
1164.739175	19.690235	5.748541
1171.161360	55.192124	16.202122
1175.971697	16.391791	4.831715
1183.683545	36.286650	10.766153
1188.354668	27.226318	8.109854
1199.222977	1.732693	0.520834
1214.015956	14.636830	4.453993
1229.810338	0.908233	0.279971
1237.412059	11.728681	3.637823
1257.759067	8.056106	2.539807
1258.437259	7.791636	2.457753
1269.986783	270.433776	86.087125
1283.861705	1419.607030	456.840351
1296.631566	6.464816	2.101120
1298.956296	2.343921	0.763160
1310.931243	0.338669	0.111284
1311.561577	0.122504	0.040273
1333.737595	4.753202	1.589040
1334.299815	6.179055	2.066586
1334.728501	11.000085	3.680163
1335.139654	10.602492	3.548238
1342.664061	17.709564	5.960097
1343.083169	15.155255	5.102044
1354.498461	9.364454	3.179355
1355.781864	10.970586	3.728187
1372.775922	1.026393	0.353176
1377.338132	3.777342	1.304082
1387.860015	27.986542	9.735830
1389.750032	25.772010	8.977658
1408.906185	3.721997	1.314426
1410.797085	7.053806	2.494400
1460.880445	1.572821	0.575933
1461.536742	3.371230	1.235026
1463.120985	7.397819	2.713076
1463.321320	8.252460	3.026922
1467.807427	19.045456	7.007103
1468.115230	19.688256	7.245118
1478.338026	20.235025	7.498175
1478.393713	10.987248	4.071525
1556.041629	324.410494	126.530195
1564.631457	120.287773	47.174968
1569.149784	531.471950	209.036834
1579.719524	1152.881987	456.502236
1611.045358	18.668087	7.538512
1617.705280	507.843787	205.924309
1618.281695	486.705361	197.423261
1630.784348	1798.130545	735.014358
2905.888252	31.944854	23.267937
2907.785695	31.053806	22.633687
2924.633494	33.016401	24.203560
2925.417472	29.395993	21.555299
2937.044650	15.858173	11.674594
2937.646409	18.821402	13.858925
2940.632413	26.284646	19.374074
2942.229430	24.335673	17.947252
2942.554236	25.592964	18.876573
2943.199246	23.689228	17.476266
2976.962668	67.666489	50.492294
2977.413425	66.539008	49.658493
2980.572933	0.766393	0.572571
2981.988702	18.624675	13.921074
2983.542672	65.514942	48.994878
2984.219683	68.627486	51.334218
2987.616998	49.442079	37.025396
2987.852305	54.958198	41.159461
3000.804257	6.977022	5.247904
3005.795937	11.572934	8.719288
3143.018174	208.348910	164.140668
3168.058874	227.622881	180.753714
3240.494067	156.834002	127.388295
3266.794267	110.906067	90.814492
3372.401294	37.085011	31.348426
3372.788042	51.164130	43.254641
3385.617068	30.285275	25.700846
3389.805595	28.566363	24.272125
1074.081829	41.320290	11.124456
1074.358173	3.520121	0.947949
1119.021958	33.981927	9.531575
1119.211592	100.729946	28.258485
1133.068278	138.652030	39.378610
1133.619328	108.566315	30.848952
1171.830970	14.233549	4.180770
1173.893537	110.647240	32.557224
1177.952883	35.712120	10.544394

1178.132544	3.152475	0.930945
1188.474174	15.147779	4.512495
1190.839082	21.318567	6.363399
1211.661090	25.196956	7.652570
1212.657737	3.701336	1.125058
1237.951979	22.308674	6.922383
1238.068008	6.081194	1.887172
1258.043053	6.250867	1.971124
1258.268558	7.935977	2.502948
1267.638173	10.125138	3.217172
1279.098058	1809.103447	580.023128
1298.748241	6.435631	2.095049
1299.110867	3.834304	1.248564
1311.083378	0.219783	0.072227
1311.211880	0.077634	0.025516
1334.164732	9.715625	3.249064
1334.313178	8.773252	2.934245
1334.721740	8.959301	2.997388
1334.773598	6.007873	2.010048
1342.798611	18.529960	6.236823
1343.024805	14.401726	4.848157
1355.149675	8.955622	3.042013
1355.472065	11.417134	3.879053
1376.126880	1.800175	0.620942
1376.573788	3.340313	1.152563
1388.815262	23.988191	8.350646
1389.153510	24.572826	8.556249
1407.200597	5.058419	1.784222
1408.635561	5.289558	1.867653
1461.358536	2.848120	1.043261
1461.498897	3.782111	1.385514
1463.165191	8.053315	2.953562
1463.375489	8.500052	3.117851
1468.064880	17.843233	6.565940
1468.123745	20.147681	7.414226
1478.289735	15.428883	5.717052
1478.466432	13.910973	5.155218
1558.576692	389.038736	151.984428
1561.289055	146.690577	57.406835
1574.677035	128.563440	50.744274
1580.009947	1430.760542	566.636891
1615.714406	30.525264	12.362380
1617.978684	32.933867	13.356529
1626.538492	81.945563	33.409337
1630.420146	2991.691579	1222.628239
2908.412747	30.134309	21.968244
2908.673578	29.366851	21.410679
2925.671250	31.915191	23.404591
2925.926186	28.286908	20.745643
2937.375481	11.532092	8.490742
2937.439807	25.973927	19.124261
2942.423629	20.773291	15.321051
2943.262052	28.327036	20.898164
2943.339478	19.612770	14.469628
2943.797838	21.874063	16.140445
2976.856087	66.396636	49.542964
2977.270559	67.219628	50.164037
2980.869761	0.419523	0.313456
2981.398675	2.378489	1.777458
2984.014441	124.005612	92.751370
2984.152893	27.115452	20.282244
2987.531071	44.619545	33.413013
2987.969373	50.808071	38.052826
2998.670691	5.731959	4.308339
3000.025505	7.074442	5.319799
3149.485406	27.223167	21.490985
3153.487297	387.543843	306.330329
3224.637271	117.327180	94.832581
3230.170024	261.912826	212.060714
3372.814871	30.401523	25.701941
3373.103130	46.428380	39.254660
3389.854609	22.355203	18.994932
3389.973341	34.047334	28.930601

Zero-Point Energy :	0.460822	a.u.
==========	12.539596 eV	

Statistical Thermal Analysis *** ideal gas assumed ***				
Temp	Transl	Rotat	Vibrat	Total
----	------	-----	------	-----
298.15 Entropy (cal/mole-K):	45.540	36.838	111.470	193.848
Internal Energy (Kcal/mole):	0.889	0.889	306.528	308.306
Constant Volume Heat Capacity (cal/mole-K):	2.981	2.981	112.727	118.689

β[1,2]-tzp-blyp-d3bj;C_1

Coordinates in Geometry Cycle 12				
Atom	X	Y	Z	(Angstrom)
1.Pt	-0.513666	-1.664773	0.146027	
2.O	0.829295	-2.149334	1.614856	
3.O	3.062518	-2.317370	1.865640	
4.N	-2.077445	-1.083167	1.405424	
5.H	-2.373849	-1.867225	1.994933	
6.H	-1.728425	-0.319383	2.008047	
7.H	-1.687988	-0.102675	-1.548556	
8.O	3.290256	-2.345277	-0.973057	
9.C	2.055179	-2.250439	1.148846	
10.H	-6.008318	-1.784587	-0.870974	
11.H	-6.501296	-0.247493	-1.583847	
12.C	-3.237988	-0.531876	0.607684	
13.H	-2.990060	0.525135	0.453870	
14.C	-4.586178	-0.659595	1.325405	
15.H	-4.111860	0.444839	-1.841679	
16.C	-5.733007	-0.722062	-0.960191	
17.H	-4.542440	-0.134149	2.288710	
18.H	-4.790162	-1.723136	1.536681	
19.C	-4.356553	-0.611410	-1.656025	
20.H	-4.374872	-1.123528	-2.628874	
21.H	-3.452087	-2.296102	-0.627564	
22.C	-5.714975	-0.078497	0.443209	
23.H	-6.683974	-0.222655	0.938213	
24.H	-5.563555	1.006137	0.343675	
25.C	2.180362	-2.263422	-0.422135	
26.O	1.049890	-2.162840	-1.085655	
27.C	-3.265529	-1.220948	-0.763512	
28.N	-1.877122	-1.100976	-1.330233	
29.H	-1.778976	-1.649963	-2.188538	
30.Pd	2.381724	1.021364	0.178146	
31.O	0.849444	1.554689	-1.063152	
32.O	-1.393831	1.699641	-0.960957	
33.N	3.755041	0.484419	-1.309558	
34.H	3.557504	-0.507932	-1.546474	
35.H	3.675589	1.048029	-2.162393	
36.H	4.237703	1.179459	2.046892	
37.O	-1.198006	1.592513	1.867288	
38.C	-0.283555	1.613232	-0.406941	
39.H	7.404723	-1.699275	0.338395	
40.H	8.530637	-0.502450	0.985940	
41.C	5.129402	0.580636	-0.713303	
42.H	5.320430	1.649294	-0.540389	
43.C	6.231373	-0.005434	-1.611017	
44.H	6.647054	0.998203	1.610820	
45.C	7.565639	-0.620113	0.476156	
46.H	6.259689	0.536151	-2.567403	
47.H	5.980367	-1.053475	-1.832122	
48.C	6.434010	-0.056164	1.364697	
49.H	6.375708	-0.609621	2.311305	
50.H	4.825454	-1.191537	0.453134	
51.C	7.602925	0.070756	-0.903200	
52.H	8.371592	-0.389386	-1.537232	
53.H	7.886845	1.127156	-0.775726	
54.C	-0.175478	1.555473	1.165963	
55.O	1.040271	1.462913	1.649020	
56.C	5.084887	-0.143460	0.638759	
57.N	3.936139	0.401015	1.449299	
58.H	3.579716	-0.362832	2.046948	

```
E-test:            old,new=      -12.18701,      -12.18700      hartree
max    gradient:                        0.00098866    au/angstrom,radian
max      cart.      step:                        0.00110327      angstrom
Geometry Converged
```

	hartree	eV	kcal/mol	kJ/mol
Total Pauli Repulsion:	46.035768901320679	1252.6970	28887.88	120866.89
Electrostatic Energy:	-10.013356743695322	-272.4773	-6283.48	-26290.06
Total Orbital Interactions:	-48.022618692783581	-1306.7619	-30134.65	-126083.37
Dispersion Energy:	-0.186798375756437	-5.0830	-117.22	-490.44
Total Bonding Energy:	-12.187004086611452	-331.6253	-7647.46	-31996.97

CB7-tzp-blyp-d3;C_1

Coordinates in Geometry Cycle 8

Atom	X	Y	Z (Angstrom)
1.H	-6.693196	0.496077	2.175741
2.C	-4.437263	-1.589316	-1.862146
3.C	-3.429336	-3.575017	-2.991732
4.H	-3.997834	-4.490495	-3.230305
5.H	-3.494443	-2.870261	-3.825744
6.C	-1.068637	-3.435187	-3.753755
7.C	1.295579	-3.982148	-4.359978
8.H	1.000788	-3.376025	-5.221442
9.H	1.644141	-4.971643	-4.697928
10.C	2.858010	-2.047751	-4.192323
11.C	4.841504	-0.584324	-3.810590
12.H	5.871991	-0.916760	-4.009154
13.H	4.408375	-0.149082	-4.715432
14.C	4.052935	1.593938	-2.860265
15.C	3.880083	3.744079	-1.644410
16.H	3.248396	3.919598	-2.520184
17.H	4.760767	4.411861	-1.682430
18.C	1.806226	4.636176	-0.618652
19.C	0.182902	5.841803	0.852938
20.H	0.384036	6.757791	1.433229
21.H	-0.220562	6.105890	-0.128763
22.C	-2.111645	4.900840	0.940332
23.C	-4.369824	4.120878	1.685505
24.H	-4.957202	4.583589	2.492532
25.H	-4.612861	4.590846	0.728599
26.C	-4.939857	2.082029	0.346974
27.C	-5.823816	-0.101329	-0.426333
28.H	-6.876360	-0.340955	-0.192350
29.H	-5.773999	0.475869	-1.354414
30.O	-3.255080	-3.991075	2.619172
31.O	0.027071	-5.287095	0.993388
32.O	3.659686	-3.660882	0.708404
33.O	5.335474	-0.231568	1.821974
34.O	3.639547	2.370560	3.699057
35.O	-0.147674	1.924894	4.747040
36.O	-3.198568	-0.795782	4.278880
37.O	-4.296030	-0.805369	-2.788837
38.O	-1.249431	-2.591227	-4.619021
39.O	2.374414	-1.395886	-5.106527
40.O	3.289099	1.881762	-3.768770
41.O	1.161683	4.725740	-1.652639
42.O	-2.436003	5.224718	-0.192892
43.O	-4.883689	2.609451	-0.753498
44.N	-4.770383	-2.627479	1.459032
45.N	-3.539795	-4.115802	0.291976
46.N	-1.561482	-5.160304	-0.725691
47.N	0.626774	-5.038539	-1.265167
48.N	2.919748	-4.188633	-1.454593
49.N	4.542746	-2.641845	-1.211106
50.N	5.341943	-0.429991	-0.521884
51.N	5.435380	1.629672	0.400664
52.N	4.194430	3.365400	1.650626
53.N	2.276729	3.986335	2.669227
54.N	0.002883	3.963774	3.600492
55.N	-2.007101	2.943094	3.730292
56.N	-3.792058	1.300582	3.391580
57.N	-4.957707	-0.527587	2.752543
58.N	-5.097964	-1.339205	-0.648208
59.N	-4.043257	-2.936810	-1.842143
60.N	-2.020019	-3.915106	-2.836192
61.N	0.109655	-4.168942	-3.542693
62.N	2.399333	-3.285983	-3.716157
63.N	4.024802	-1.740820	-3.474199
64.N	4.896240	0.469572	-2.811050
65.N	4.324460	2.359138	-1.711108
66.N	3.084943	4.067359	-0.469531
67.N	1.443196	5.158972	0.632864
68.N	-0.843775	5.056310	1.528304
69.N	-2.959394	4.378640	1.930110
70.N	-4.764129	2.725137	1.584932
71.N	-5.276526	0.745461	0.626138
72.C	-3.771218	-3.606125	1.580285
73.C	-2.743102	-5.320142	0.101069
74.H	-2.403300	-5.633887	1.092328
75.H	-3.376381	-6.105116	-0.344747
76.C	-0.265913	-5.150625	-0.185337

77.C	2.049451	-5.287527	-1.076668
78.H	2.201893	-5.467769	-0.008450
79.H	2.339773	-6.184050	-1.652067
80.C	3.684772	-3.496823	-0.502151
81.C	5.573101	-1.869981	-0.542834
82.H	6.543132	-2.077594	-1.027283
83.H	5.601797	-2.200636	0.499613
84.C	5.341316	0.260593	0.704018
85.C	5.444825	2.656116	1.430237
86.H	5.694780	2.159429	2.371703
87.H	6.222050	3.391474	1.174384
88.C	3.385174	3.126978	2.773515
89.C	1.414807	4.204011	3.826430
90.H	1.537486	5.240639	4.183384
91.H	1.745024	3.504098	4.599271
92.C	-0.651117	2.819584	4.084583
93.C	-3.009057	2.082780	4.339082
94.H	-3.690602	2.699011	4.953959
95.H	-2.478898	1.371138	4.978933
96.C	-3.877699	-0.095805	3.543745
97.C	-5.309089	-1.932746	2.618086
98.H	-4.915790	-2.447417	3.499071
99.H	-6.406723	-2.006044	2.598118
100.C	-5.332341	-2.554213	0.120750
101.H	-6.415956	-2.761402	0.163666
102.C	-4.528908	-3.650676	-0.675139
103.H	-5.160474	-4.498070	-0.994621
104.C	-1.570717	-5.139800	-2.174952
105.H	-2.150044	-5.999700	-2.554169
106.C	-0.045318	-5.215107	-2.551321
107.H	0.242166	-6.186797	-2.989727
108.C	3.349715	-3.929084	-2.819158
109.H	3.714410	-4.865430	-3.277010
110.C	4.484719	-2.848122	-2.648644
111.H	5.467292	-3.196697	-3.012531
112.C	5.732053	0.449941	-1.629974
113.H	6.778274	0.247424	-1.916628
114.C	5.527751	1.881952	-1.022126
115.H	6.371982	2.562517	-1.227299
116.C	3.691850	4.433878	0.810893
117.H	4.486528	5.182156	0.645427
118.C	2.478228	5.000818	1.631966
119.H	2.694067	5.975829	2.102396
120.C	-0.900283	4.912207	2.983166
121.H	-0.783491	5.901606	3.459121
122.C	-2.318555	4.279181	3.226942
123.H	-2.912014	4.830142	3.977524
124.C	-4.974800	1.837454	2.709003
125.H	-5.646455	2.315639	3.442406
126.C	-5.599348	0.559961	2.045430

current energy		-29.92083518 Hartree	
energy change	-0.00009261	0.00100000	T
constrained gradient max	0.00081435	0.00100000	T
constrained gradient rms	0.00017859	0.00066667	T
gradient max	0.00081435		
gradient rms	0.00017859		
cart. step max	0.00968254	0.01000000	T
cart. step rms	0.00272179	0.00666667	T
GEOMETRY CONVERGED			

	hartree	eV	kcal/mol	kJ/mol
Total Pauli Repulsion:	139.822842174499101	3804.7731	87740.17	367104.82
Electrostatic Interaction:	-30.819827899133145	-838.6502	-19339.74	-80917.45
Total Orbital Interactions:	-138.669988075931030	-3773.4024	-87016.74	-364078.00
Dispersion Energy:	-0.253801177781737	-6.9063	-159.26	-666.35
Total Bonding Energy:	-29.920835730675584	-814.1874	-18775.61	-78557.14

CB7-water-tzp-blyp-d3;C_1

Coordinates in Geometry Cycle 41

Atom	X	Y	Z	(Angstrom)
1.H	-6.582004	0.364124	2.282754	
2.C	-4.588381	-1.813251	-1.798644	
3.C	-3.578232	-3.816198	-2.904577	
4.H	-4.110487	-4.768819	-3.015936	
5.H	-3.762153	-3.186926	-3.776732	
6.C	-1.233261	-3.476184	-3.707076	
7.C	1.137984	-3.852037	-4.409654	
8.H	0.791288	-3.226329	-5.233151	
9.H	1.500916	-4.810170	-4.800650	
10.C	2.630035	-1.865487	-4.108804	
11.C	4.632971	-0.405950	-3.768779	
12.H	5.649645	-0.716088	-4.037640	
13.H	4.166870	0.100986	-4.614675	
14.C	4.103125	1.800839	-2.717359	
15.C	4.255413	3.947167	-1.444957	
16.H	3.793755	4.301862	-2.367936	
17.H	5.202629	4.475015	-1.277774	
18.C	2.072642	4.783750	-0.555535	
19.C	0.322179	5.919335	0.827536	
20.H	0.509317	6.809570	1.439739	
21.H	-0.003683	6.219285	-0.169276	
22.C	-1.910749	4.795578	0.734014	
23.C	-4.215641	4.004031	1.295843	
24.H	-4.875999	4.541862	1.986734	
25.H	-4.377263	4.362077	0.277965	
26.C	-4.880671	1.866903	0.179311	
27.C	-5.978132	-0.316916	-0.352888	
28.H	-6.965572	-0.601273	0.030039	
29.H	-6.086912	0.190616	-1.312286	
30.O	-2.813559	-3.809719	2.614413	
31.O	0.213397	-5.294541	0.898750	
32.O	3.713757	-3.826867	0.535804	
33.O	5.076245	-0.503588	1.792376	
34.O	3.252016	2.153588	3.720362	
35.O	-0.378669	2.166895	4.900337	
36.O	-3.072500	-0.482398	4.400901	
37.O	-4.518380	-1.055179	-2.774148	
38.O	-1.479941	-2.563585	-4.504855	
39.O	2.019180	-1.103146	-4.867734	
40.O	3.342832	2.208690	-3.604120	
41.O	1.503317	4.907432	-1.647290	
42.O	-2.094195	4.930117	-0.481709	
43.O	-4.782099	2.270583	-0.986077	
44.N	-4.528611	-2.618161	1.547998	
45.N	-3.437150	-4.207203	0.388900	
46.N	-1.478045	-5.176235	-0.721562	
47.N	0.666810	-5.173565	-1.399317	
48.N	2.918902	-4.234840	-1.632794	
49.N	4.511024	-2.671579	-1.343547	
50.N	5.375505	-0.525134	-0.534188	
51.N	5.237559	1.458512	0.517698	
52.N	4.055540	3.198064	1.781121	
53.N	2.228933	4.047677	2.784434	
54.N	-0.092339	4.075441	3.568038	
55.N	-2.155857	3.204664	3.774324	
56.N	-3.890101	1.501556	3.454932	
57.N	-4.688796	-0.461260	2.701475	
58.N	-5.197730	-1.528297	-0.579097	
59.N	-4.106084	-3.117970	-1.737319	
60.N	-2.144413	-4.083653	-2.846917	
61.N	-0.002795	-4.105734	-3.536335	
62.N	2.248961	-3.160023	-3.764312	
63.N	3.841502	-1.596449	-3.477486	
64.N	4.711409	0.549310	-2.669588	
65.N	4.534489	2.524523	-1.608965	
66.N	3.345134	4.256663	-0.347154	
67.N	1.572476	5.184723	0.680127	
68.N	-0.761054	5.151467	1.435849	
69.N	-2.830482	4.293130	1.651206	
70.N	-4.559191	2.586395	1.327309	
71.N	-5.369217	0.626304	0.579185	
72.C	-3.508208	-3.562330	1.620872	
73.C	-2.613548	-5.390747	0.168651	
74.H	-2.220381	-5.704378	1.136719	
75.H	-3.243445	-6.183960	-0.250740	
76.C	-0.158580	-5.211105	-0.278470	

77.C	2.105073	-5.405059	-1.321897
78.H	2.336942	-5.706888	-0.299584
79.H	2.369808	-6.211380	-2.016057
80.C	3.706078	-3.593886	-0.679487
81.C	5.600104	-1.959191	-0.684111
82.H	6.520643	-2.113983	-1.259865
83.H	5.714787	-2.382176	0.315000
84.C	5.203114	0.079838	0.708494
85.C	5.271713	2.407594	1.625560
86.H	5.414720	1.837688	2.544711
87.H	6.116878	3.090219	1.477913
88.C	3.179720	3.030249	2.849761
89.C	1.308656	4.324323	3.883972
90.H	1.421278	5.373406	4.182115
91.H	1.580059	3.673127	4.715852
92.C	-0.824715	3.045425	4.151800
93.C	-3.240472	2.432534	4.371229
94.H	-3.994878	3.127275	4.759797
95.H	-2.819703	1.849316	5.191435
96.C	-3.796177	0.119683	3.598009
97.C	-5.004515	-1.885638	2.715840
98.H	-4.527555	-2.321544	3.594707
99.H	-6.092215	-2.004349	2.787452
100.C	-5.277255	-2.700286	0.293059
101.H	-6.325622	-2.948606	0.495518
102.C	-4.517273	-3.808132	-0.513973
103.H	-5.141778	-4.674608	-0.761891
104.C	-1.581142	-5.257856	-2.178017
105.H	-2.136450	-6.157759	-2.467371
106.C	-0.087295	-5.266520	-2.650422
107.H	0.194547	-6.176833	-3.192501
108.C	3.281485	-3.859590	-2.999591
109.H	3.629301	-4.740197	-3.552345
110.C	4.389858	-2.770598	-2.797965
111.H	5.355968	-3.043648	-3.238199
112.C	5.688461	0.442971	-1.586760
113.H	6.685872	0.244591	-1.996207
114.C	5.576924	1.824731	-0.856716
115.H	6.507293	2.404042	-0.873849
116.C	3.799340	4.428169	1.034615
117.H	4.682120	5.077412	1.062307
118.C	2.550593	5.040937	1.755566
119.H	2.748000	6.014017	2.220502
120.C	-0.942067	5.049912	2.885023
121.H	-0.832100	6.037215	3.348735
122.C	-2.379891	4.446355	3.034148
123.H	-3.070106	5.093743	3.586224
124.C	-4.969654	1.897075	2.550725
125.H	-5.712900	2.496289	3.089392
126.C	-5.528927	0.529926	2.029664

current energy		-30.14406883 Hartree	
energy change	0.00032288	0.00100000	T
constrained gradient max	0.00088874	0.00100000	T
constrained gradient rms	0.00025362	0.00066667	T
gradient max		0.00088874	
gradient rms		0.00025362	
cart. step max	0.00557700	0.01000000	T
cart. step rms	0.00173116	0.00666667	T
GEOMETRY CONVERGED			

	hartree	eV	kcal/mol	kJ/mol
Total Pauli Repulsion:	139.454320097318742	3794.7451	87508.92	366137.27
Electrostatic Interaction:	-30.683020827985935	-834.9275	-19253.89	-80558.26
Total Orbital Interactions:	-138.339006185243136	-3764.3959	-86809.05	-363209.01
Solvation Energy (el):	-0.321024833840324	-8.7355	-201.45	-842.85
Dispersion Energy:	-0.255207134994591	-6.9445	-160.14	-670.05
Total Bonding Energy:	-30.144031212368748	-820.2608	-18915.67	-79143.14

1@CB7-tzp-blyp-d3(AE tight);C_1

Coordinates in Geometry Cycle 27

Atom	X	Y	Z (Angstrom)
1.Pt	16.438456	6.945434	11.377175
2.O	15.707898	5.498205	12.618379
3.O	17.317617	7.628834	13.087347
4.O	15.663484	4.952046	14.807170
5.O	17.371374	7.199722	15.301431
6.N	15.515171	6.267755	9.606697
7.H	16.018053	5.457269	9.223350
8.H	14.555851	5.952133	9.795276
9.N	17.130719	8.477473	10.108325
10.H	16.639658	9.338034	10.386581
11.H	18.131823	8.668291	10.227785
12.C	15.500816	7.386229	8.592294
13.H	14.710860	8.072906	8.926283
14.C	15.209841	6.914071	7.154600
15.H	14.230826	6.415156	7.117744
16.H	15.963498	6.163098	6.871783
17.C	15.253285	8.098279	6.158552
18.H	14.414271	8.779023	6.369549
19.H	15.106555	7.729924	5.134489
20.C	16.582752	8.882917	6.261332
21.H	16.561349	9.754337	5.593776
22.H	17.413761	8.242980	5.924259
23.C	16.860651	9.336054	7.715125
24.H	17.822268	9.861925	7.779386
25.H	16.085055	10.051001	8.035490
26.C	16.853278	8.126559	8.667922
27.H	17.644885	7.422598	8.380048
28.C	16.043390	5.683094	13.894778
29.C	16.983661	6.923777	14.167853
30.O	12.577891	4.695169	9.416479
31.O	15.336202	3.320784	7.888125
32.O	18.454892	5.040377	7.789148
33.O	20.186784	8.563316	9.042246
34.O	18.900107	11.214894	10.754160
35.O	15.685506	10.791983	11.425972
36.O	12.876088	7.833829	10.818617
37.O	11.224473	7.862074	4.234562
38.O	14.271607	6.081791	2.475504
39.O	17.692537	7.189378	1.994723
40.O	18.596875	10.562889	3.388619
41.O	16.586592	13.426513	5.435261
42.O	13.110589	13.941912	6.786870
43.O	10.585120	11.265202	6.231505
44.N	10.936946	6.031669	8.408184
45.N	11.903061	4.406660	7.190810
46.N	13.782546	3.217567	6.136912
47.N	15.964644	3.450683	5.629761
48.N	18.277595	4.262900	5.587033
49.N	19.536999	6.087603	5.987394
50.N	20.393431	8.252942	6.724182
51.N	20.705422	10.315695	7.574463
52.N	19.589736	12.182776	8.736411
53.N	17.779155	13.027813	9.768682
54.N	15.516836	13.015933	10.721578
55.N	13.688305	11.703057	10.599988
56.N	12.033381	9.948733	10.229909
57.N	10.832138	8.113569	9.708765
58.N	10.374968	7.288952	6.344980
59.N	11.431963	5.706329	5.137493
60.N	13.412227	4.658113	4.136962
61.N	15.485854	4.266118	3.325333
62.N	17.723763	5.299575	3.391955
63.N	19.324356	6.870257	3.645793
64.N	20.107312	9.083040	4.400397
65.N	19.652388	11.036883	5.436343
66.N	18.554745	12.890340	6.598115
67.N	16.946035	14.059518	7.664486
68.N	14.655742	13.922166	8.561542
69.N	12.563103	13.154167	8.927016
70.N	10.879596	11.371540	8.555837
71.N	10.332530	9.385376	7.625298
72.C	11.902186	5.021073	8.449993
73.C	12.592480	3.148595	6.964745
74.H	12.908423	2.777200	7.943287
75.H	11.893951	2.437802	6.500381
76.C	15.059501	3.350996	6.697751

77.C	17.374296	3.164422	5.858469
78.H	17.480765	2.913428	6.917353
79.H	17.679136	2.307552	5.238321
80.C	18.707523	5.132793	6.595995
81.C	20.518255	6.805317	6.783179
82.H	21.531606	6.510647	6.454668
83.H	20.373992	6.514522	7.827261
84.C	20.384566	8.994871	7.914183
85.C	20.784137	11.379610	8.562752
86.H	20.988190	10.906877	9.527075
87.H	21.618250	12.038064	8.283604
88.C	18.757270	12.028062	9.854114
89.C	16.922157	13.332032	10.902020
90.H	16.999557	14.400837	11.145907
91.H	17.284462	12.731118	11.740689
92.C	15.042654	11.717334	10.949313
93.C	12.821733	10.696532	11.192754
94.H	12.147111	11.182538	11.921710
95.H	13.466011	9.980188	11.711858
96.C	12.031825	8.544359	10.297445
97.C	10.499613	6.707000	9.618078
98.H	10.991275	6.201706	10.453811
99.H	9.408181	6.609657	9.711121
100.C	10.214873	6.084824	7.144635
101.H	9.143775	5.889203	7.317895
102.C	10.917633	4.970616	6.281446
103.H	10.225946	4.180753	5.944239
104.C	13.786517	3.352165	4.693623
105.H	13.173275	2.556856	4.240486
106.C	15.309875	3.241497	4.334093
107.H	15.589573	2.257374	3.925205
108.C	18.712834	4.662678	4.264418
109.H	19.171001	3.803627	3.747244
110.C	19.730621	5.822272	4.561800
111.H	20.778860	5.537431	4.372575
112.C	20.913771	9.042013	5.599073
113.H	21.941934	8.726832	5.357131
114.C	20.824295	10.505597	6.144874
115.H	21.715725	11.113157	5.918742
116.C	19.177792	13.266685	7.863108
117.H	20.027534	13.944931	7.680539
118.C	18.000586	13.946737	8.656035
119.H	18.258412	14.946086	9.042543
120.C	14.549217	13.836287	10.024602
121.H	14.524572	14.845656	10.465296
122.C	13.212145	13.037693	10.217639
123.H	12.566821	13.452935	11.008479
124.C	10.775440	10.468527	9.684596
125.H	10.172253	10.927310	10.485181
126.C	10.113572	9.189848	9.066784
127.H	9.035603	9.106928	9.280790
128.C	11.054569	7.059021	5.139273
129.C	12.021280	5.075935	3.974056
130.H	11.413242	4.198434	3.694408
131.H	12.002691	5.813151	3.166090
132.C	14.384362	5.135912	3.239593
133.C	16.731639	4.543429	2.633248
134.H	16.483416	5.146174	1.755301
135.H	17.166715	3.582834	2.318307
136.C	18.172852	6.544908	2.914503
137.C	20.105656	8.063104	3.365783
138.H	21.148657	7.768049	3.176643
139.H	19.676252	8.513684	2.466941
140.C	19.340663	10.256219	4.307301
141.C	19.314805	12.456154	5.440703
142.H	18.695268	12.637149	4.557571
143.H	20.242754	13.051732	5.373067
144.C	17.266401	13.434751	6.449805
145.C	15.670139	14.721025	7.881106
146.H	15.856626	15.644297	8.452013
147.H	15.262019	14.968985	6.897150
148.C	13.413973	13.680496	7.941016
149.C	11.179386	12.792040	8.655429
150.H	10.550669	13.220715	9.449269
151.H	10.920138	13.238155	7.691567
152.C	10.619968	10.733682	7.331278
153.C	9.696624	8.544269	6.616160
154.H	8.660032	8.322525	6.922939
155.H	9.691599	9.119320	5.685830

current energy		-36.04466143 Hartree	
energy change	0.00015693	0.00100000	T
constrained gradient max	0.00097973	0.00100000	T
constrained gradient rms	0.00010903	0.00066667	T
gradient max		0.00097973	
gradient rms		0.00010903	
cart. step max	0.00969089	0.01000000	T
cart. step rms	0.00224255	0.00666667	T
GEOMETRY CONVERGED			

	hartree	eV	kcal/mol	kJ/mol
Total Pauli Repulsion:	163.409252006621898	4446.5920	102540.86	429030.93
Electrostatic Energy:	-35.936771776875062	-977.8893	-22550.67	-94351.98
Total Orbital Interactions:	-163.156099004846283	-4439.7033	-102382.01	-428366.28
Dispersion Energy:	-0.361037569867288	-9.8243	-226.55	-947.90
Total Bonding Energy:	-36.044663834819708	-980.8252	-22618.37	-94635.25

Frequency cm-1	Dipole Strength 1e-40 esu2 cm2	Absorption Intensity (degeneracy not counted) km/mole
-39.190585	6.265498	-0.061548
-25.268220	36.751839	-0.232773
-15.857311	49.767414	-0.197812
-5.218913	4325.309801	-5.658161
10.111702	307.020302	0.778161
11.600743	212.067382	0.616649
18.036272	444.372006	2.008961
21.411792	41.226591	0.221263
27.991742	85.403928	0.599219
30.876770	84.174270	0.651462
33.291005	29.114621	0.242950
34.496339	29.716160	0.256947
37.499344	31.686199	0.297832
41.631119	41.656901	0.434693
45.279634	15.879048	0.180221
52.631791	56.586436	0.746515
56.993136	11.493107	0.164187
62.460380	3.478143	0.054454
66.373712	7.878603	0.131076
70.482023	8.884302	0.156957
72.476559	28.850427	0.524117
73.871363	86.341272	1.598721
76.021446	30.878975	0.588406
86.667370	404.864177	8.795146
89.015628	20.901206	0.466354
91.137932	22.255738	0.508416
93.422937	73.508486	1.721350
94.867207	156.974383	3.732699
96.706022	140.647182	3.409280
99.278217	78.891884	1.963199
100.763555	372.657434	9.412204
103.456934	60.550068	1.570190
108.834683	82.972309	2.263490
110.347484	246.808184	6.826531
118.046270	428.055535	12.665737
118.991221	171.074175	5.102435
130.947019	130.484372	4.282843
134.769379	97.322313	3.287621
138.977366	9.262344	0.322658
144.418202	88.179491	3.192035
145.094172	42.199832	1.534754
150.157781	5.682734	0.213886
153.196025	3.317520	0.127391
155.504866	26.737400	1.042176
159.592986	26.804793	1.072270
164.974444	11.270798	0.466068
169.099287	32.400653	1.373326
173.349345	20.988083	0.911954
176.275047	19.011131	0.839995
177.560642	1.980827	0.088160
181.899433	15.415588	0.702861
182.998294	0.761574	0.034933
185.684935	69.234138	3.222367
186.763213	17.414350	0.815223
188.897111	4.965144	0.235091
201.509552	8.513000	0.429988
203.986212	4.414736	0.225727
208.951935	0.502860	0.026337
214.557916	49.722578	2.674091
223.575599	50.769860	2.845171
227.954312	62.031386	3.544356
231.856767	52.381836	3.044238
233.969266	145.632673	8.540744
235.222023	26.259483	1.548254

247.792500	33.973363	2.110108
250.460244	41.001215	2.574030
253.477531	15.841788	1.006518
259.183367	2.963824	0.192547
260.155716	123.617186	8.061025
280.435616	0.285000	0.020033
281.142650	2.054669	0.144793
286.439985	4.757954	0.341611
287.841176	2.450411	0.176795
290.188750	397.293506	28.898155
319.209284	33.632352	2.690982
323.073469	12.411715	1.005104
325.117691	2.131766	0.173723
329.041524	3.819409	0.315010
329.636920	6.421096	0.530546
332.393395	2.930840	0.244187
333.118647	13.721476	1.145718
346.413732	125.543312	10.901010
348.779293	32.499704	2.841242
352.661025	87.447602	7.730070
353.831835	344.947310	30.593399
355.578681	112.773683	10.051284
358.004118	78.507814	7.044967
359.460799	152.033607	13.698380
359.912170	123.950132	11.182054
360.677279	145.293371	13.135380
362.764748	274.691183	24.977437
364.231356	56.926673	5.197221
364.799567	89.306194	8.166086
368.821695	61.457549	5.681588
371.100965	44.196229	4.111075
374.847593	5.108697	0.480002
377.318434	1.866563	0.176534
404.489237	8.486064	0.860382
406.631635	4.900014	0.499432
408.145207	0.747914	0.076515
416.936760	5.211564	0.544649
419.536100	124.545361	13.097095
420.099461	119.726204	12.607222
422.226384	15.629286	1.654103
430.369682	4.168047	0.449627
432.488296	7.562646	0.819835
433.781897	3.550182	0.386011
433.884913	13.700128	1.489969
438.124967	8.605557	0.945051
441.735444	146.558631	16.227504
442.413570	28.624088	3.174228
445.489794	7.940831	0.886710
493.054032	36.609896	4.524505
498.008708	1.732125	0.216219
500.050373	0.245069	0.030717
520.977361	209.378865	27.341967
545.350144	6.415283	0.876939
551.285578	51.733175	7.148647
556.662186	3.567090	0.497719
560.563559	46.129227	6.481554
562.744988	19.412457	2.738232
575.033248	16.581382	2.389966
585.125137	6.830679	1.001822
586.030365	15.134196	2.223092
594.220850	9.637495	1.435457
595.321320	25.717757	3.837626
601.860739	113.732133	17.157629
604.505438	20.589299	3.119750
604.562261	43.507734	6.593038
609.019424	69.313967	10.581079
609.821336	53.611341	8.194781
615.027921	3.127152	0.482083
626.928495	10.000437	1.571502
630.077200	7.993759	1.262475
630.925699	15.955060	2.523218
635.284134	90.475689	14.407147
638.066076	50.076608	8.009006
639.879456	34.105688	5.470198
645.093642	40.670152	6.576224
649.764444	354.751611	57.777453
649.915734	305.720662	49.803505
653.514552	178.398812	29.223033
658.494284	3.618646	0.597278
665.963087	5.274511	0.880462
673.556699	145.086626	24.495122
673.703023	150.983907	25.496304
678.159160	7.663471	1.302672
684.034279	2.304974	0.395205
686.445341	3.277230	0.563885
689.802748	7.049926	1.218955
690.445447	2.355224	0.407605
696.454498	5.597261	0.977117
697.526158	0.041215	0.007206
700.836075	1.953176	0.343112
701.816976	9.882490	1.738475

702.515327	7.754461	1.365480
704.844272	13.826653	2.442802
705.208071	2.578604	0.455806
706.961167	35.679822	6.322609
708.138266	13.984003	2.482148
710.199869	22.789143	4.056829
711.153274	6.140837	1.094634
711.981500	2.006428	0.358072
714.238071	35.428062	6.342617
716.572635	465.133790	83.544176
723.552224	33.394739	6.056560
749.359243	23.651675	4.442527
750.791301	31.896974	6.002702
756.443066	4.445142	0.842830
757.547182	4.142441	0.786582
759.525716	38.086264	7.250850
759.915624	88.689978	16.893436
763.678883	501.090363	95.919057
767.598911	303.841127	58.460022
770.291175	104.570440	20.190261
770.915533	3253.451241	628.679312
772.358194	1491.138132	288.678676
774.457548	1272.073161	246.937915
775.039561	1352.626484	262.772449
787.328220	536.800763	105.936840
789.825802	512.338533	101.429996
790.145747	0.677508	0.134184
793.802512	8.809732	1.752884
801.562464	47.795636	9.602928
802.090482	145.689445	29.290685
802.921805	90.951715	18.304683
804.985300	46.858450	9.454835
807.773402	345.858421	70.027073
810.481986	100.863634	20.490665
812.209348	110.301502	22.455746
822.639217	1.352352	0.278854
830.813850	40.005652	8.331115
843.263449	0.350750	0.074138
855.147630	4.868329	1.043516
870.718342	2.654807	0.579414
871.342456	49.690090	10.852673
875.268502	58.160582	12.759925
884.389355	0.799641	0.177262
886.152722	1.832776	0.407095
900.700136	1.781340	0.402166
902.661367	5.991519	1.355626
903.598220	4.044621	0.916076
918.300810	5.833203	1.342673
920.580053	2.214506	0.510995
922.065975	3.909640	0.903601
930.515586	101.667713	23.712906
933.817675	4.786884	1.120452
940.757052	55.419995	13.068389
941.595364	506.607504	119.567734
943.794645	1314.695664	311.014624
946.454449	182.455950	43.284840
946.781179	816.003259	193.650927
948.653468	51.781259	12.312841
949.234827	19.668344	4.679716
951.401738	134.137957	31.988487
952.182705	61.979557	14.792679
959.257530	65.863946	15.836567
960.992267	79.554604	19.162990
965.956837	19.348465	4.684706
966.720580	13.505783	3.272644
971.862766	10.166694	2.476639
976.074169	193.046090	47.230430
978.971811	19.029987	4.669676
983.435663	4.870983	1.200717
988.959709	6.987845	1.732208
993.938292	4.329866	1.078728
996.524477	0.921174	0.230095
1001.476005	8.693392	2.182267
1008.395490	9.305715	2.352116
1012.158340	1.516416	0.384720
1015.624696	0.472128	0.120191
1016.199352	2.094060	0.533391
1019.123295	2.479883	0.633485
1026.813434	26.020022	6.696953
1029.230921	22.519194	5.809567
1031.330351	53.632099	13.864387
1041.547395	6.023309	1.572506
1043.709523	3.239729	0.847552
1055.607574	8.978411	2.375637
1059.159568	28.789839	7.643261
1062.184960	18.727977	4.986193
1062.573691	11.565732	3.080422
1069.309334	104.903538	28.117167
1072.392400	61.249616	16.463993
1080.100568	50.913999	13.784134
1081.871083	9.171971	2.487232

1086.652997	29.069079	7.917722
1091.179371	24.846434	6.795764
1102.228686	7.021302	1.939847
1103.891557	20.902887	5.783767
1109.078086	51.292374	14.259129
1117.551166	9.643693	2.701400
1125.701227	15.576035	4.394992
1135.942162	62.105774	17.683420
1140.159978	1254.701163	358.578431
1141.918855	1453.323547	415.983040
1143.619185	1607.345397	460.753575
1146.478996	63.662395	18.294778
1146.996214	236.187361	67.904211
1148.507862	56.401577	16.236906
1149.778477	221.907446	63.953471
1151.705438	938.680704	270.980087
1157.629084	267.024894	77.481720
1162.854258	102.007193	29.732687
1167.559955	8.057680	2.358127
1169.623957	18.773229	5.503808
1177.033023	546.602546	161.264349
1177.816298	883.950606	260.965819
1179.600655	1168.549434	345.509637
1181.008085	756.742819	224.016109
1182.722653	1963.235501	582.013936
1184.434709	839.643123	249.277988
1186.213740	409.940886	121.888366
1187.262076	237.176946	70.582516
1187.988265	14.263802	4.247423
1190.803783	455.140716	135.851352
1194.047886	264.442377	79.146346
1194.729195	401.852622	120.341204
1195.966226	321.023155	96.235065
1198.726177	447.521744	134.465912
1200.729862	331.259742	99.699284
1204.457130	164.065602	49.532124
1207.117057	612.169135	185.224694
1209.485970	286.547380	86.871105
1214.517591	1210.941022	368.642049
1225.071525	0.619459	0.190218
1227.554933	25.429778	7.824590
1227.958926	13.641984	4.198938
1231.348133	20.981692	6.475889
1233.763804	58.512987	18.095157
1238.247299	257.704291	79.984735
1239.482020	1830.978831	568.855059
1239.730115	236.189993	73.395041
1241.448119	282.987679	88.059086
1243.401327	78.542376	24.478986
1245.404439	172.532024	53.858989
1245.862326	113.041348	35.300873
1246.802077	65.885229	20.590346
1247.982321	202.532899	63.355173
1249.850308	123.225381	38.604350
1250.653563	32.174199	10.086090
1251.592005	228.677594	71.740511
1272.523944	95.954595	30.606228
1274.359893	21.534835	6.878785
1278.757952	28.726816	9.207758
1280.827462	200.447630	64.353123
1283.357876	1160.914215	373.444424
1285.813679	1022.797585	329.644478
1288.714921	948.691113	306.450094
1288.874597	923.290356	298.281991
1293.393732	8.903594	2.886517
1294.798845	417.150199	135.385711
1296.499391	403.740452	131.205685
1296.960026	102.362678	33.277164
1299.502630	242.423946	78.964292
1299.799825	87.587630	28.536277
1300.545792	81.090736	26.434735
1300.615456	61.868477	20.169559
1319.751586	16.668615	5.514038
1328.676130	12.464177	4.151077
1331.945830	19.175539	6.401949
1339.210309	11.512569	3.864552
1340.283859	98.802169	33.192605
1343.245783	1446.059678	486.877575
1343.504618	1555.452792	523.810342
1350.469335	37.594342	12.725806
1352.961585	531.364430	180.200510
1355.715658	119.550018	40.625276
1358.546515	23.113803	7.870893
1358.971866	172.265369	58.679515
1361.325131	54.834962	18.711021
1365.709805	17.954355	6.146195
1367.167869	5.980079	2.049306
1370.770824	44.141111	15.166528
1373.211889	180.785042	62.226893
1375.035574	20.478337	7.058082
1375.226241	16.475702	5.679317

1375.580771	8.813135	3.038747
1376.803973	91.528428	31.586840
1377.944487	9.958669	3.439625
1378.786173	8.114584	2.804408
1380.638791	84.289411	29.169646
1381.435576	2.902887	1.005168
1382.644437	19.324363	6.697208
1383.977519	43.087284	14.947075
1385.736974	95.253983	33.085829
1388.930067	248.791719	86.615251
1390.583500	13.715596	4.780682
1391.224495	179.150752	62.473224
1393.024078	16.328485	5.701414
1395.026339	36.162180	12.644891
1396.517738	4.099741	1.435096
1397.246242	27.269725	9.550625
1398.037430	4.351088	1.524736
1399.352612	4.155290	1.457493
1402.699783	37.466903	13.173179
1404.584821	4.536621	1.597197
1405.589360	129.227917	45.529499
1407.541295	140.478930	49.562181
1408.315565	99.079149	34.975209
1409.571813	177.941463	62.869852
1410.031682	575.255948	203.314362
1411.355917	441.793903	156.291132
1412.366313	160.972449	56.987155
1415.549985	107.434574	38.119513
1417.039243	185.822929	66.002327
1419.414763	7.876800	2.802446
1429.340477	363.970729	130.400790
1430.386134	277.495380	99.491761
1431.061442	196.473552	70.475870
1431.229949	8.660341	3.106866
1431.576896	147.071027	52.773984
1431.719677	220.435645	79.107541
1432.128792	15.490467	5.560639
1432.635192	63.660093	22.860249
1433.175938	30.960787	11.122171
1433.489285	48.504195	17.428171
1434.415891	26.340981	9.470766
1435.938722	19.886264	7.157596
1440.573604	22.654216	8.180174
1441.681357	36.031004	13.020382
1452.013502	5.926990	2.157163
1458.135430	7.138541	2.609068
1466.763883	19.378834	7.124689
1474.222026	0.804556	0.297302
1606.290652	155.440853	62.584584
1611.956553	61.603341	24.890617
1638.569897	293.924101	120.719726
1651.928323	2940.450312	1217.539654
1698.143255	12.562089	5.347050
1700.712639	52.229564	22.265139
1704.889018	11.704538	5.001825
1707.121470	7.574966	3.241329
1708.834807	57.017864	24.422443
1712.773981	86.214979	37.013560
1718.485075	50.266348	21.652157
1718.860177	142.328696	61.321263
1724.936443	590.479035	255.302843
1727.615623	38.259759	16.567899
1736.178696	1311.804455	570.875749
1738.364577	906.806567	395.124165
1741.213353	6216.787661	2713.289243
1748.796322	29.213482	12.805620
2867.184971	73.567852	52.871527
2870.913892	74.257779	53.436769
2877.059312	77.023553	55.545698
2888.089924	19.803287	14.335936
2889.342425	89.400788	64.746818
2892.740642	27.210714	19.730019
2895.832957	15.766287	11.444083
2898.448792	15.682062	11.393230
2902.493771	9.152306	6.658553
2903.177278	8.584562	6.246975
2907.075974	3.051836	2.223800
2908.711264	97.969753	71.428363
2909.159231	20.884888	15.229222
2910.773771	67.440703	49.204929
2912.689997	23.097181	16.862863
2916.121257	79.748029	58.291282
2917.446113	175.616995	128.424373
2917.486617	65.671839	48.024861
2921.135925	53.873684	39.446322
2921.382387	29.940888	21.924573
2923.420169	45.794406	33.556893
2923.567088	80.793852	59.206508
2927.487998	93.932607	68.927031
2930.092013	141.443366	103.882385
2930.314658	98.991460	72.709315

2935.261861	85.240755	62.715113
2936.892215	10.929534	8.045772
2938.893401	64.307171	47.371955
2939.080506	26.511268	19.530801
2941.089956	115.913069	85.451322
2947.418462	47.867138	35.363670
2948.459601	115.814775	85.592797
2965.811376	5.191540	3.859383
2980.540247	22.002575	16.437909
2986.478295	5.010181	3.750514
2986.956150	9.731882	7.286245
2991.220991	15.145320	11.355468
3000.737163	15.576624	11.716000
3036.178673	23.071663	17.558374
3039.706998	7.730585	5.890093
3041.867710	5.220022	3.980070
3042.055611	12.716891	9.696749
3042.696788	14.780289	11.272485
3045.605006	3.767143	2.875834
3045.867949	8.197814	6.258744
3046.969002	15.722940	12.008254
3047.803730	5.737968	4.383522
3048.173098	3.644744	2.784740
3048.774174	12.940374	9.888950
3050.160853	10.253698	7.839373
3051.635312	7.944797	6.077059
3052.401025	8.374501	6.407352
3298.322614	158.964140	131.422694
3315.602525	51.464092	42.770551
3375.851937	69.111760	58.480815
3380.188312	100.328435	85.004713

Zero-Point Energy : 1.162114 a.u.
==========
31.622742 eV
(imaginary frequencies were excluded from the summation)

Statistical Thermal Analysis *** ideal gas assumed ***

Temp		Transl	Rotat	Vibrat	Total
298.15	Entropy (cal/mole-K):	47.906	42.255	282.977	373.138
	Internal Energy (Kcal/mole):	0.889	0.889	773.453	775.231
	Constant Volume Heat Capacity (cal/mole-K):	2.981	2.981	297.773	303.735

2@CB7-tzp-blyp-d3;C_1

Coordinates in Geometry Cycle 13				
Atom	X	Y	Z	(Angstrom)
1.Pd	16.406974	6.945085	11.348395	
2.O	15.667514	5.495187	12.570665	
3.O	17.242097	7.662662	13.059104	
4.O	15.603866	4.967049	14.761410	
5.O	17.253446	7.237832	15.272663	
6.N	15.507031	6.249202	9.554769	
7.H	16.028418	5.448316	9.172463	
8.H	14.549558	5.918372	9.730310	
9.N	17.114213	8.489182	10.078242	
10.H	16.600542	9.338195	10.353404	
11.H	18.110348	8.702287	10.209664	
12.C	15.499597	7.378862	8.560140	
13.H	14.711876	8.065981	8.897130	
14.C	15.205835	6.922117	7.115350	
15.H	14.224361	6.427904	7.077474	
16.H	15.954745	6.166926	6.830086	
17.C	15.256276	8.106291	6.120685	
18.H	14.422473	8.793466	6.332298	
19.H	15.106363	7.739600	5.096369	
20.C	16.591757	8.878648	6.226510	
21.H	16.579827	9.752037	5.560972	
22.H	17.418054	8.232089	5.890295	
23.C	16.866979	9.326507	7.681437	
24.H	17.830716	9.847777	7.751125	
25.H	16.094325	10.046373	7.998527	
26.C	16.849931	8.122280	8.645005	
27.H	17.642454	7.416426	8.366952	
28.C	15.983522	5.695424	13.844028	
29.C	16.897957	6.955827	14.127943	
30.O	12.577774	4.668325	9.431103	
31.O	15.338435	3.294271	7.890430	
32.O	18.438833	5.050538	7.790323	
33.O	20.198603	8.564650	9.049193	
34.O	18.913113	11.229611	10.766395	
35.O	15.683977	10.805409	11.458658	
36.O	12.901445	7.843507	10.835850	
37.O	11.232258	7.867778	4.251909	
38.O	14.279979	6.088186	2.486553	
39.O	17.710297	7.181720	1.986788	
40.O	18.611573	10.560990	3.380709	
41.O	16.582702	13.412997	5.433727	
42.O	13.104083	13.924592	6.796695	
43.O	10.569941	11.272453	6.257782	
44.N	10.958730	6.029764	8.422347	
45.N	11.907583	4.397336	7.201334	
46.N	13.783777	3.211571	6.138722	
47.N	15.966408	3.439122	5.633441	
48.N	18.274023	4.265224	5.590248	
49.N	19.533060	6.090189	5.991322	
50.N	20.395096	8.252414	6.730370	
51.N	20.706390	10.316578	7.576805	
52.N	19.590210	12.183832	8.737617	
53.N	17.778757	13.028358	9.769228	
54.N	15.519881	13.022889	10.731593	
55.N	13.688230	11.713473	10.624711	
56.N	12.038774	9.953992	10.255192	
57.N	10.857714	8.110432	9.721440	
58.N	10.387915	7.292226	6.363905	
59.N	11.447435	5.712850	5.154527	
60.N	13.417944	4.660049	4.142798	
61.N	15.492642	4.270520	3.334284	
62.N	17.733886	5.295472	3.389023	
63.N	19.336114	6.863433	3.644035	
64.N	20.109881	9.077094	4.404698	
65.N	19.655469	11.033887	5.435028	
66.N	18.553491	12.885118	6.596581	
67.N	16.941606	14.050713	7.661902	
68.N	14.654380	13.915611	8.566597	
69.N	12.561171	13.155104	8.944454	
70.N	10.877954	11.371307	8.580178	
71.N	10.338537	9.385949	7.645505	
72.C	11.909796	5.006025	8.463144	
73.C	12.593567	3.138985	6.966478	
74.H	12.908809	2.760595	7.942551	
75.H	11.893263	2.432974	6.497636	
76.C	15.061219	3.335383	6.700600	

77.C	17.376817	3.161127	5.861882
78.H	17.483382	2.910604	6.920895
79.H	17.687568	2.306320	5.241803
80.C	18.698696	5.138492	6.598081
81.C	20.514664	6.804770	6.790048
82.H	21.527850	6.505531	6.464775
83.H	20.366454	6.515438	7.833995
84.C	20.389820	8.995444	7.919817
85.C	20.785449	11.382035	8.563438
86.H	20.991494	10.910865	9.528097
87.H	21.618377	12.041127	8.282091
88.C	18.762378	12.033931	9.859580
89.C	16.926184	13.338099	10.904902
90.H	17.006106	14.407887	11.144051
91.H	17.290857	12.739909	11.744404
92.C	15.042942	11.727322	10.972894
93.C	12.819587	10.709239	11.218077
94.H	12.138424	11.198936	11.938113
95.H	13.461369	9.998151	11.747106
96.C	12.051701	8.549126	10.316280
97.C	10.527777	6.703355	9.635768
98.H	11.027788	6.199360	10.467327
99.H	9.437258	6.602973	9.738137
100.C	10.230582	6.086995	7.162046
101.H	9.160044	5.892092	7.339977
102.C	10.927686	4.973338	6.293985
103.H	10.231007	4.190047	5.951669
104.C	13.789182	3.352006	4.695451
105.H	13.175007	2.559105	4.239228
106.C	15.312852	3.239814	4.336167
107.H	15.590592	2.257633	3.921044
108.C	18.716820	4.659712	4.268646
109.H	19.176094	3.798134	3.756879
110.C	19.734669	5.818816	4.567454
111.H	20.783623	5.531515	4.386217
112.C	20.915658	9.039137	5.604029
113.H	21.943982	8.723304	5.362967
114.C	20.825888	10.503754	6.146842
115.H	21.717795	11.110526	5.920307
116.C	19.175495	13.264487	7.861315
117.H	20.023908	13.944080	7.677317
118.C	17.997144	13.943797	8.652998
119.H	18.252625	14.945248	9.035798
120.C	14.552032	13.840035	10.030548
121.H	14.530594	14.852565	10.464052
122.C	13.213974	13.046052	10.233590
123.H	12.572141	13.469033	11.023233
124.C	10.779120	10.465445	9.707575
125.H	10.171098	10.919455	10.507279
126.C	10.127089	9.183110	9.086848
127.H	9.050656	9.088803	9.304095
128.C	11.065916	7.064172	5.156924
129.C	12.028863	5.084246	3.985980
130.H	11.416050	4.210292	3.705644
131.H	12.010066	5.824471	3.180710
132.C	14.391489	5.140245	3.248441
133.C	16.736274	4.541719	2.635829
134.H	16.486852	5.144174	1.758023
135.H	17.166321	3.578984	2.320523
136.C	18.186124	6.538841	2.910129
137.C	20.116258	8.058199	3.369028
138.H	21.160954	7.765637	3.184596
139.H	19.689947	8.508080	2.468241
140.C	19.348107	10.253013	4.304924
141.C	19.315160	12.452448	5.439539
142.H	18.696283	12.632423	4.555754
143.H	20.242100	13.049844	5.373041
144.C	17.263227	13.425150	6.447942
145.C	15.665418	14.711416	7.877690
146.H	15.851981	15.638587	8.442211
147.H	15.254233	14.952277	6.893240
148.C	13.410455	13.671008	7.951735
149.C	11.176571	12.792110	8.679736
150.H	10.551698	13.220086	9.476901
151.H	10.912205	13.238735	7.717402
152.C	10.615339	10.736718	7.355124
153.C	9.704829	8.544724	6.635615
154.H	8.668956	8.319189	6.941931
155.H	9.698062	9.120637	5.705744

current energy		-35.97264197 Hartree	
energy change	0.00018605	0.00100000	T
constrained gradient max	0.00072622	0.00100000	T
constrained gradient rms	0.00014213	0.00066667	T
gradient max		0.00072622	
gradient rms		0.00014213	
cart. step max	0.00882269	0.01000000	T
cart. step rms	0.00245400	0.00666667	T
GEOMETRY CONVERGED			

	hartree	eV	kcal/mol	kJ/mol
Total Pauli Repulsion:	162.867951378920822	4431.8625	102201.19	427609.75
Electrostatic Energy:	-35.777775168142725	-973.5628	-22450.90	-93934.54
Total Orbital Interactions:	-162.706217948501433	-4427.4615	-102099.70	-427185.11
Dispersion Energy:	-0.356595543030683	-9.7035	-223.77	-936.24
Total Bonding Energy:	-35.972642690019704	-978.8654	-22573.18	-94446.16

Frequency cm-1	Dipole Strength 1e-40 esu2	Absorption Intensity (degeneracy not counted) cm2 km/mole
-38.339600	6.648601	-0.063893
-24.450229	15.581860	-0.095495
-16.143555	88.990773	-0.360099
-11.642274	2201.122234	-6.423327
7.515673	246.462352	0.464298
11.995459	265.655377	0.798755
16.635511	399.570386	1.666125
20.155470	62.377616	0.315137
28.687568	27.243584	0.195901
30.701317	69.539962	0.535143
33.360352	32.367595	0.270657
34.513136	28.188478	0.243856
38.070414	35.455350	0.338335
40.521409	51.790122	0.526029
45.356365	16.121174	0.183279
52.279187	50.968800	0.667900
55.975241	9.121065	0.127973
61.542029	5.073015	0.078256
65.574483	11.695515	0.192235
68.064766	15.876716	0.270870
71.031086	6.480113	0.115374
72.961770	64.178402	1.173714
75.096927	28.886302	0.543741
86.402255	394.773109	8.549697
88.627910	57.720172	1.282260
90.047582	24.330539	0.549164
92.964928	79.962204	1.863296
94.316720	165.321208	3.908367
96.662865	124.250566	3.010483
98.963730	81.476343	2.021090
100.385245	327.013323	8.228362
103.369687	76.887799	1.992181
108.209300	132.424800	3.591799
109.759936	225.212530	6.196044
118.058609	391.650747	11.589767
119.092271	110.009937	3.283928
124.647817	188.119285	5.877546
134.205742	115.232678	3.876366
138.371871	11.702439	0.405884
144.209894	73.613767	2.660922
144.916254	61.150209	2.221228
149.536292	0.249989	0.009370
149.945938	69.431868	2.609586
152.205727	1.798349	0.068609
154.736815	21.601181	0.837817
159.604733	23.764374	0.950715
164.312006	7.295902	0.300487
169.072493	29.302868	1.241827
172.379570	8.957721	0.387045
173.812847	3.845112	0.167521
175.742462	25.639538	1.129445
179.833974	1.671265	0.075335
182.550995	1.691050	0.077378
185.340252	13.755759	0.639046
187.021858	19.429757	0.910831
188.358779	13.728415	0.648163
203.308630	5.486287	0.279584
208.993530	0.312194	0.016354
214.283773	25.927698	1.392616
216.844709	151.608137	8.240421
223.872785	57.854679	3.246518
227.832010	61.837918	3.531406
232.588397	13.283880	0.774446
235.184456	11.216455	0.661214

244.510624	44.134929	2.704944
248.139367	29.272776	1.820697
253.303468	16.090794	1.021637
259.036825	1.955819	0.126990
259.972065	126.197101	8.223451
280.364571	0.138385	0.009725
281.257473	2.135340	0.150539
286.361449	5.113119	0.367011
287.858163	2.630335	0.189788
302.146887	228.373156	17.295824
321.517707	107.661636	8.676487
322.865511	14.594015	1.181067
325.001550	2.072008	0.168793
328.473765	29.775520	2.451535
328.572166	0.988234	0.081390
329.604555	5.559653	0.459324
331.875447	0.612804	0.050977
346.372283	112.064251	9.729450
348.409660	40.586364	3.544446
352.216640	23.937358	2.113315
353.576078	341.954274	30.306025
355.170178	206.634512	18.395747
356.372323	31.448485	2.809194
358.456340	60.177981	5.406945
359.614050	332.915067	30.008768
360.973194	91.880663	8.313371
362.702017	295.970883	26.907728
364.201251	51.294881	4.682670
364.891355	48.789484	4.462394
368.918465	56.614053	5.235193
371.145850	41.965049	3.904005
374.882582	3.964708	0.372550
377.061007	2.025748	0.191459
404.418938	6.830579	0.692416
406.388007	6.258459	0.637509
408.238732	0.809062	0.082789
412.938636	14.821946	1.534154
416.426260	2.596001	0.270970
419.203610	126.957637	13.340187
419.641290	132.345679	13.920860
424.122651	59.868128	6.364514
430.071766	4.395146	0.473797
432.110994	4.452172	0.482220
433.427602	3.046161	0.330939
437.603884	8.124169	0.891124
442.348836	9.667835	1.071944
444.922107	161.336029	17.992579
445.509616	9.333097	1.042224
473.587986	62.476027	7.416383
498.157507	0.684505	0.085472
499.454534	119.242124	14.928072
500.142528	0.374438	0.046941
517.366888	192.627823	24.980189
525.479840	20.906974	2.753755
551.720548	6.717619	0.928993
560.598830	47.817420	6.719182
562.506327	20.823253	2.935986
563.526925	12.503501	1.766137
585.213509	5.649716	0.828741
586.086932	14.035791	2.061945
594.327081	7.892610	1.175775
595.309748	27.307244	4.074731
601.822729	118.817703	17.923706
604.389667	15.308234	2.319104
604.456120	41.834486	6.338366
608.918675	72.854654	11.119741
609.383003	51.408141	7.852362
614.919544	2.037282	0.314013
627.118940	8.270681	1.300078
630.060582	7.190369	1.135564
631.145572	13.382195	2.117069
633.688012	2.038018	0.323714
635.187887	85.798517	13.660294
638.067662	44.113159	7.055259
639.917440	37.589008	6.029244
645.199165	45.654027	7.383307
649.285278	493.089537	80.248960
649.816948	167.836641	27.337317
652.953809	178.333531	29.187274
658.656409	4.889661	0.807264
666.194731	3.910015	0.652917
673.659978	134.773963	22.757514
673.897765	139.793644	23.613454
676.472084	94.605057	16.041401
684.232348	2.836035	0.486400
686.554202	4.030317	0.693573
689.653660	5.811365	1.004586
690.354903	1.677451	0.290269
696.301334	5.481367	0.956674
697.485585	0.345808	0.060457
700.846582	2.596700	0.456166

701.623312	10.923382	1.921052
702.506718	7.021319	1.236367
704.763241	12.499051	2.207996
705.085533	2.148940	0.379791
707.065912	39.209510	6.949113
707.672395	11.412244	2.024330
710.017985	28.963905	5.154714
711.151087	6.658322	1.186874
712.065694	6.494305	1.159127
714.271155	53.274288	9.538033
716.606880	425.470343	76.423749
742.463007	82.790396	15.407524
749.411374	20.173085	3.789402
750.671533	33.769950	6.354164
756.350259	3.928149	0.744713
757.285881	2.747232	0.521475
759.936643	92.099180	17.543297
763.770316	444.883315	85.170062
763.903190	1.460661	0.279683
767.355892	266.208906	51.203245
770.872055	3269.556141	631.755703
771.947405	1573.777174	304.515234
774.196264	1254.757143	243.494311
775.009450	1433.311835	278.436236
787.270980	519.286343	102.472944
789.707283	499.697206	98.912490
792.483523	0.076797	0.015255
793.737289	8.563887	1.703828
801.599389	45.952824	9.233102
802.135870	131.635930	26.466740
803.145715	108.904351	21.923892
805.022595	63.952926	12.904660
807.973720	302.863474	61.336954
810.435588	101.473128	20.613305
811.105491	2.851628	0.579760
812.610895	119.223533	24.284138
823.801682	2.059141	0.425194
843.076148	0.278815	0.058920
851.556994	5.814989	1.241197
870.860406	3.514096	0.767079
871.386495	48.050066	10.495011
875.456771	58.077496	12.744437
884.578198	0.656751	0.145618
886.062530	2.036660	0.452336
900.760513	1.639430	0.370152
902.492195	5.171409	1.169851
903.907198	5.195390	1.177118
918.326466	4.677806	1.076756
920.476347	1.791900	0.413432
921.327883	7.570660	1.748341
930.535122	86.766935	20.237884
933.796914	4.475396	1.047519
940.933432	38.970522	9.191221
941.704078	489.426538	115.526079
943.889749	1353.667547	320.266384
946.395246	361.966221	85.865492
946.782573	647.102445	153.568226
948.771278	69.719123	16.580267
949.303586	19.460303	4.630552
951.514637	91.595100	21.845691
952.164397	83.877001	20.018563
959.453227	65.900268	15.848533
961.194125	79.106529	19.059061
966.013474	14.867831	3.600053
966.684215	15.988884	3.874189
972.136045	3.581894	0.872806
978.979799	7.817240	1.918250
982.564058	211.569255	52.106452
983.641435	2.755822	0.679463
988.972824	7.227696	1.791688
994.111781	3.528558	0.879246
996.735494	1.363124	0.340560
1001.435744	8.606599	2.160393
1008.418120	7.582774	1.916668
1012.089188	1.603711	0.406839
1014.412591	4.620775	1.174918
1015.805330	2.194075	0.558650
1016.320137	2.043005	0.520449
1019.844447	133.418901	34.105888
1027.280022	4.063919	1.046434
1032.218918	45.071460	11.661422
1041.573386	6.300416	1.644891
1043.894800	3.648999	0.954792
1054.299679	5.419257	1.432128
1055.873773	5.494174	1.454094
1060.068518	28.177649	7.487154
1062.339417	26.290419	7.000658
1069.391289	105.139788	28.182649
1072.854820	64.575068	17.365364
1080.213259	50.162331	13.582049
1081.632541	9.312125	2.524682

1086.328727		30.924855	8.420677
1091.017258		26.606831	7.276170
1093.294127		4.276053	1.171813
1103.847337		20.218560	5.594191
1108.988864		51.394249	14.286300
1117.560890		8.675219	2.430131
1118.971070		67.796516	19.015349
1133.008759		1.800349	0.511291
1136.306250		63.710888	18.146260
1140.764842		1081.277325	309.179929
1141.988405		1440.345712	412.293520
1143.499996		1764.788843	505.832800
1146.463961		65.975730	18.959317
1147.125130		223.210058	64.180430
1148.804917		25.200929	7.256729
1151.337716		1011.275062	291.843550
1155.038098		136.447840	39.503997
1157.779982		244.502502	70.955720
1163.254330		106.585972	31.077981
1167.868891		15.677475	4.589319
1169.910867		23.232893	6.812933
1177.731840		14.532390	4.290042
1179.122419		2358.401918	697.035322
1180.116301		1018.440992	301.258113
1181.408924		10.104784	2.992302
1182.226906		2322.189888	688.139740
1184.740875		444.276282	131.933344
1186.739924		629.868358	187.362820
1187.631310		85.267011	25.382871
1190.784031		442.386716	132.042321
1194.131912		247.733637	74.150717
1194.777860		393.822200	117.941170
1195.978056		318.815757	95.574285
1198.902270		419.750868	126.140183
1200.552468		377.217620	113.514460
1204.353313		154.206197	46.551514
1207.396148		587.108291	177.683078
1209.564177		301.220875	91.325499
1214.643437		1178.878886	358.918685
1222.845928		5.726130	1.755137
1225.619886		0.284785	0.087488
1227.484475		31.374410	9.653163
1231.484219		21.877271	6.753052
1233.911734		50.348578	15.572179
1238.550541		256.151717	79.522326
1239.816293		265.694537	82.569192
1241.705906		487.986845	151.881519
1243.737898		132.922067	41.438500
1244.911094		160.700147	50.145583
1245.380664		262.112646	81.821637
1246.549693		1099.434459	343.523942
1246.905651		95.698508	29.910029
1247.889796		190.329200	59.533268
1249.984253		99.508794	31.177700
1250.614155	29.467075	9.237159	
1251.554352		208.944705	65.547956
1272.981990		93.347912	29.785503
1274.387120		17.222145	5.501317
1278.792788		27.087468	8.682537
1280.792415		180.760200	58.030943
1283.347279		1200.749718	386.255572
1285.834871		1045.514220	336.971533
1288.735421		432.146373	139.595914
1288.764677		1493.258380	482.377070
1293.070769		7.347862	2.381559
1294.693246		391.442972	127.032093
1296.485256		322.475075	104.795300
1296.859651		146.342667	47.570971
1299.292446		323.145556	105.240565
1299.566113		21.433470	6.981825
1300.297372		38.600041	12.580808
1300.601760		91.718051	29.900416
1319.639386		13.944585	4.612527
1328.049989		11.828912	3.937652
1331.460418		16.060321	5.359948
1339.228020		8.737118	2.932924
1340.447166		109.016579	36.628600
1343.407405		1420.267797	478.251178
1343.696905		1580.364123	532.275589
1348.807486		27.074525	9.153536
1353.223004		561.008453	190.290386
1355.823010		106.990101	36.360066
1358.571769		28.783069	9.801618
1359.002861		165.467258	56.365130
1361.242946		51.900145	17.708521
1365.771303		17.861827	6.114795
1367.105380		5.176366	1.773802
1370.618841		45.707197	15.702882
1373.304475		177.786036	61.198750
1374.246596		12.340855	4.250970
1375.069643		15.463061	5.329645

1375.415804	14.496049	4.997603
1376.974818	83.833369	28.934833
1378.019021	13.335426	4.606172
1378.735223	12.568108	4.343390
1380.635801	78.946809	27.320698
1381.496773	4.481148	1.551734
1382.530464	23.074037	7.996066
1384.079798	46.453014	16.115845
1385.748204	100.057491	34.754577
1388.980160	239.393418	83.346299
1390.127040	18.975377	6.611850
1390.938198	185.564717	64.696578
1392.876072	20.883822	7.291226
1394.757723	32.777515	11.459162
1396.284460	2.509782	0.878391
1397.201716	24.432367	8.556629
1397.840353	3.356646	1.176092
1399.019131	2.447500	0.858271
1402.764151	40.880148	14.373919
1404.653762	1.992691	0.701596
1405.697837	131.535134	46.345953
1407.508914	159.358489	56.221759
1408.335288	109.552359	38.672822
1409.356916	248.954933	87.946750
1410.058240	501.104351	177.110086
1411.356191	388.196937	137.330439
1412.390880	213.902639	75.726715
1415.484849	111.746236	39.647536
1416.937106	173.926645	61.772441
1419.323998	7.087867	2.521594
1429.423158	338.684955	121.348605
1430.412855	316.289221	113.402823
1431.108448	166.787554	59.829346
1431.335962	40.587242	14.561603
1431.660831	122.514776	43.964960
1431.962141	169.618507	60.881149
1432.381324	56.038065	20.119623
1432.822769	63.101622	22.662669
1433.411630	50.899040	18.287679
1433.427817	42.261436	15.184418
1434.870291	27.780469	9.991491
1436.069566	18.726490	6.740776
1439.686577	20.656839	7.454352
1442.193937	36.557629	13.215383
1451.866587	5.348366	1.946372
1457.579563	6.746407	2.464807
1465.556938	18.724469	6.878445
1473.389629	1.074703	0.396903
1603.209318	146.553037	58.892925
1609.113867	84.578743	34.113484
1624.690039	253.917611	103.404969
1633.326376	2369.096459	969.915253
1698.017428	21.758836	9.260957
1700.407086	60.672247	25.859556
1704.886769	16.254930	6.946383
1706.824195	7.125807	3.048603
1708.370650	28.475646	12.193651
1712.341220	89.619024	38.465253
1718.170831	7.191080	3.096981
1718.369614	200.408759	86.319985
1724.574522	571.461413	247.028435
1727.119390	54.876610	23.756787
1736.044785	1176.872042	512.115877
1737.971134	986.920991	429.935212
1740.650811	6402.043044	2793.240412
1748.313946	23.763710	10.413860
2868.758705	80.272171	57.721433
2869.390345	67.096031	48.257468
2876.457550	77.654579	55.989051
2887.739288	28.298309	20.483140
2889.426790	80.672322	58.427099
2892.365097	26.164848	18.969216
2896.834280	14.133939	10.262778
2897.631194	18.684469	13.570690
2901.652646	9.887263	7.191171
2902.045689	7.999954	5.819288
2906.104951	2.671831	1.946249
2908.131381	112.507978	82.011624
2908.691897	9.031243	6.584508
2911.585295	48.525961	35.414550
2912.130318	29.544444	21.565756
2915.531946	67.528769	49.349722
2916.476118	157.790138	115.349668
2916.784691	100.663804	73.596266
2918.861950	17.646235	12.910518
2920.378154	66.693735	48.820498
2922.947558	64.188532	47.028003
2923.092730	74.098207	54.291065
2926.017277	108.020776	79.225001
2929.336041	14.318369	10.513343
2930.014981	213.454436	156.766440

2935.607555	52.143031	38.368280
2935.795772	10.074176	7.413332
2936.438601	118.498691	87.219290
2936.865469	14.035538	10.332162
2941.409313	108.340882	79.877764
2946.310695	53.136606	39.241936
2947.441328	114.389855	84.510515
2965.012516	6.156605	4.575577
2980.131513	22.007129	16.439056
2985.385216	6.669238	4.990622
2986.641751	10.922473	8.176778
2990.175227	15.537519	11.645453
3001.733823	15.564691	11.710913
3038.254336	22.167799	16.882034
3039.315182	7.786759	5.932129
3041.428208	6.777470	5.166819
3041.697490	12.787948	9.749783
3042.504415	12.916842	9.850667
3045.219523	5.055221	3.858663
3046.038217	7.187483	5.487698
3047.065570	14.896518	11.377442
3048.322151	3.714778	2.838388
3048.374016	7.239937	5.531987
3048.853479	10.779572	8.237893
3049.083886	12.365036	9.450240
3051.836195	7.873539	6.022950
3051.988949	8.444915	6.460354
3305.161985	149.692349	124.013916
3315.895586	60.723430	50.470222
3381.366914	63.397038	53.732783
3385.182006	99.044081	84.040498

Zero-Point Energy :	1.160976	a.u.
==========	31.591769	eV

(imaginary frequencies were excluded from the summation)

Statistical Thermal Analysis *** ideal gas assumed ***

Temp		Transl	Rotat	Vibrat	Total
298.15	Entropy (cal/mole-K):	47.731	42.155	284.867	374.753
	Internal Energy (Kcal/mole):	0.889	0.889	772.951	774.728
	Constant Volume Heat Capacity (cal/mole-K):	2.981	2.981	298.505	304.467

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