Solvent-Dependent Electronic Dichotomy in Zinc Complexes with Non-Innocent Ligands: Divalent Zn(+II) *vs.* Monovalent Zn(+I) Forms.

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Table S1: Approximate spin-projection correction (AP) for the broken-symmetry (BS) solution calculated in the gas phase using the Yamaguchi procedure, as implemented in ORCA 6.0, and comparison between Gaussian and ORCA results.

Table S2: Structures and difference of energy between the singlet and triplet state ground state configurations $\Delta E_{S/T}$ ($\Delta E_{S/T} = E_S - E_T$, in kcal mol^{-1}) and $\Delta E_{BS/T}$ ($\Delta E_{BS/T} = E_{BS} - E_T$, in kcal mol^{-1}) for monomer (**ZnDAD**) in different ground state configurations (closed-shell singlet calculated by restricted DFT (R), open-shell triplet calculated by unrestricted DFT (U) and open-shell singlet calculated by broken symmetry formalism (BS)) calculated with implicit solvation (SMD) with different organic solvents defined by dielectric constants ε. The basis set used is def2-tzvp.

Table S3: Structures (distances in Å, angles in °) of **ZnDAD** monomers in different ground state configurations (singlet closed-shell calculated by restricted DFT (R), triplet open-shell calculated by unrestricted DFT (U) and singlet open-shell calculated by broken symmetry formalism (BS)) in the gas phase and in function of the solvent using SMD model.

Table S4: Energetics (in kcal mol^{-1}), structures (distances in Å, angles in °) and electronic structures (charges, spin densities) of the successive one-electron reductions intermediates of DAD ligand (i: experimental neutral DAD ligand; ii: experimental $[Na_2(LMes)(solv)_2]_2$ with dianonic ligand) with SMD solvation model.

Fig. S1: Visualization of the spin density for **ZnDAD$_U$** (isovalue for density is 0.004 a.u., H are omitted for clarity, with Gaussview software). One electron is delocalized on N–C–C–N backbone of the ligand and one electron is on zinc center.

Fig. S2: Logarithmic regression of the energy difference $\Delta E_{S/T}$ (= E_S(**ZnDAD$_R$**)–E_T(**ZnDAD$_U$**) in kcal mol^{-1}) between closed-shell singlet and open-shell triplet configurations for **ZnDAD** monomers as function of the dielectric constant ε of the solvent.

Fig. S3: Logarithmic regression of the dipole moment of **ZnDAD$_R$** as a function of the dielectric constant ε of the solvent.

Fig. S4: Structures of **ZnDAD$_R$** (left) and **ZnDAD$_U$** (right) with two explicit solvent molecules ($O(CH_3)_2$ as a model of THF).

Table S5: Energetics (in kcal mol^{-1}), structures (distances in Å, angles in °), and electronic structures (charges, spin densities) of **ZNDAD$_R$** and **ZNDAD$_U$** using explicit and hybrid solvation models.

Table S6: Structures (distances in Å, angles in °) of **ZnDAD$_R$**, **ZnDAD$_U$** and **ZnDAD$_{BS}$** using SMD solvation model in a function of DFT functionals.

Table S7: Difference of energy between the singlet and triplet state ground state configurations $\Delta E_{S/T}$ ($\Delta E_{S/T} = E_S - E_T$, in kcal mol^{-1}) and $\Delta E_{BS/T}$ ($\Delta E_{BS/T} = E_{BS} - E_T$, in kcal mol^{-1}) for monomer (**ZnDAD**) in different ground state configurations (closed-shell singlet calculated by restricted DFT (R), open-shell triplet calculated by unrestricted DFT (U) and open-shell singlet calculated by broken symmetry formalism (BS)) calculated with implicit solvation (SMD) in THF with different DFT functionals.

Cartesian coordinates

Table S1: Approximate spin-projection correction (AP) for the broken-symmetry (BS) solution calculated in the gas phase using the Yamaguchi procedure, as implemented in ORCA 6.0, and comparison between Gaussian and ORCA results.

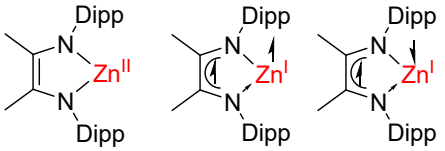
Gas phase	$\Delta E_{S/T}$	$\Delta E_{BS/T}$	$<S^2>$	C-C / C-N / Zn-N (Å) C-N-Zn-Zn dihedral angle (°)				Spin densities (ρ)	
				ZnDAD$_R$	**ZnDAD$_U$**	**ZnDAD$_{BS}$**	**ZnDAD$_{AP}$**	**ZnDAD$_U$**	**ZnDAD$_{BS}$**
Gaussian16	5.3	1.4	$<S^2>_U$ = 2.006 $<S^2>_{BS}$ = 1.005	1.45 1.32 2.16 33	1.43 1.34 2.03 0	1.43 1.34 2.03 0		ρ_{Zn} = 0.99 ρ_N = 0.40 ρ_C = 0.12	ρ_{Zn} = 0.98 ρ_N = 0.16 ρ_C = 0.24
Orca6	5.6	1.4 for BS 1.9 for AP	$<S^2>_U$ =2.006 $<S^2>_{BS}$ = 1.004 $<S^2>_{AP}$ = 0.91	1.45 1.31 2.20 33	1.43 1.34 2.03 0	1.42 1.34 2.03 2	1.42 1.33 2.02 2	ρ_{Zn} = 0.94 ρ_N = 0.28 ρ_C = 0.21	ρ_{Zn} = 0.84 ρ_N = 0.24 ρ_C = 0.20

Table S2: Structures and difference of energy between the singlet and triplet state ground state configurations $\Delta E_{S/T}$ ($\Delta E_{S/T} = E_S - E_T$, in kcal mol^{-1}) and $\Delta E_{BS/T}$ ($\Delta E_{BS/T} = E_{BS} - E_T$, in kcal mol^{-1}) for monomer (**ZnDAD**) in different ground state configurations (closed-shell singlet calculated by restricted DFT (R), open-shell triplet calculated by unrestricted DFT (U) and open-shell singlet calculated by broken symmetry formalism (BS)) calculated with implicit solvation (SMD) with different organic solvents defined by dielectric constants ε. The spin contamination $<S^2>$ is given for the singlet biradical (BS) and open-shell triplet configuration (U). Natural charges (q) for selected atoms, 4s electronic population for zinc and spin densities (ρ) for selected atoms are obtained from NBO analysis and Mulliken population analysis. **The basis set used is def2-tzvp.**

Def2-TZVP	**ZnDAD**	C–C	C–N	Zn–N	C–N–Zn–N
Gas phase	**ZnDAD$_R$**	1.45	1.32	2.16	32
	ZnDAD$_U$	1.43	1.34	2.03	0
	ZnDAD$_{BS}$	1.43	1.34	2.03	0
Toluene	**ZnDAD$_R$**	1.42	1.34	2.05	31
	ZnDAD$_U$	1.43	1.34	2.03	0
	ZnDAD$_{BS}$	1.43	1.34	2.03	0
THF	**ZnDAD$_R$**	1.37	1.41	1.92	8
	ZnDAD$_U$	1.43	1.33	2.10	1
	ZnDAD$_{BS}$	1.42	1.34	2.09	7
Water	**ZnDAD$_R$**	1.37	1.40	1.95	4
	ZnDAD$_U$	1.42	1.33	2.12	0
	ZnDAD$_{BS}$	1.37	1.41	1.92	3

Alhrich's basis set		$\Delta E_{S/T}$	$\Delta E_{BS/T}$	$<S^2>$	Natural charges (q)			4s Zn electronic population			Spin densities (ρ)	
					$ZnDAD_R$	**$ZnDAD_U$**	**$ZnDAD_{BS}$**	**$ZnDAD_R$**	**$ZnDAD_U$**	**$ZnDAD_{BS}$**	**$ZnDAD_U$**	**$ZnDAD_{BS}$**
Gas phase		5.9	1.4	$<S^2>_U$ = 2.006 $<S^2>_{BS}$ = 1,006	q_{Zn} = 0.46 q_N = -0.59 q_C = 0.20	q_{Zn} = 0.72 q_N = -0.70 q_C = 0.18	q_{Zn} = 0.68 q_N = -0.68 q_C = 0.18	$4s^{1.37}$	$4s^{1.02}$	$4s^{1.09}$	ρ_{Zn} = 0.94 ρ_N = 0.44 ρ_C = 0.12	ρ_{Zn} = 0.87 ρ_N = 0.25 ρ_C = 0.21
Solvent (SMD)	Dielectric constant ε											
Toluene	2.37	6.1	1.2	$<S^2>_U$ = 2.006 $<S^2>_{BS}$ = 1.00	q_{Zn} = 0.79 q_N = -0.68 q_C = 0.16	q_{Zn} = 0.75 q_N = -0.70 q_C = 0.18	q_{Zn} = 0.81 q_N = -0.70 q_C = 0.16	$4s^{1.01}$	$4s^{1.00}$	$4s^{0.97}$	ρ_{Zn} = 0.93 ρ_N = 0.46 ρ_C = 0.12	ρ_{Zn} = 0.88 ρ_N = 0.26 ρ_C = 0.20
THF	7.42	-1.0	1.0	$<S^2>_U$ = 2.0065 $<S^2>_{BS}$ = 0.98	q_{Zn} = 1.28 q_N = -0.84 q_C = 0.12	q_{Zn} = 0.85 q_N = -0.72 q_C = 0.18	q_{Zn} = 0.70 q_N = -0.67 q_C = 0.19	$4s^{0.67}$	$4s^{1.09}$	$4s^{1.26}$	ρ_{Zn} = 0.92 ρ_N = 0.28 ρ_C = 0.20	ρ_{Zn} = 0.87 ρ_N = 0.27 ρ_C = 0.19
Water	78.4	-11.2	-11.2	$<S^2>_U$ = 2.007 $<S^2>_{BS}$ = 0	q_{Zn} = 1.65 q_N = -0.88 q_C = 0.10	q_{Zn} = 0.80 q_N = -0.67 q_C = 0.17		$4s^{0.22}$	$4s^{1.00}$		ρ_{Zn} = 0.91 ρ_N = 0.28 ρ_C = 0.20	
Pople's basis set												
Gas phase		5.3	1.4	$<S^2>_U$ = 2.006 $<S^2>_{BS}$ = 1,005	q_{Zn} = 0.57 q_N = -0.63 q_C = 0.20	q_{Zn} = 0.85 q_N = -0.78 q_C = 0.19	q_{Zn} = 0.80 q_N = -0.78 q_C = 0.19	$4s^{1.4}$	$4s^{1.08}$	$4s^{1.15}$	ρ_{Zn} = 0.99 ρ_N = 0.40 ρ_C = 0.12	ρ_{Zn} = 0.98 ρ_N = 0.16 ρ_C = 0.24
Toluene	2.37	5.2	1.2	$<S^2>_U$ = 2.006 $<S^2>_{BS}$ = 0.994	q_{Zn} = 0.79 q_N = -0.71 q_C = 0.17	q_{Zn} = 0.85 q_N = -0.77 q_C = 0.19	q_{Zn} = 0.75 q_N = -0.73 q_C = 0.20	$4s^{1.18}$	$4s^{1.09}$	$4s^{1.21}$	ρ_{Zn} = 0.99 ρ_N = 0.38 ρ_C = 0.13	ρ_{Zn} = 0.99 ρ_N = 0.20 ρ_C = 0.23
THF	7.42	-1.2	1.0	$<S^2>_U$ = 2.006 $<S^2>_{BS}$ = 0.939	q_{Zn} = 1.29 q_N = -0.87 q_C = 0.12	q_{Zn} = 0.84 q_N = -0.76 q_C = 0.19	q_{Zn} = 0.72 q_N = -0.68 q_C = 0.19	$4s^{0.67}$	$4s^{1.09}$	$4s^{1.24}$	ρ_{Zn} = 0.99 ρ_N = 0.36 ρ_C = 0.25	ρ_{Zn} = 0.99 ρ_N = 0.22 ρ_C = 0.21
Water	78.4	-11.0	-11.0	$<S^2>_U$ = 2.006 $<S^2>_{BS}$ = 0	q_{Zn} = 1.34 q_N = -0.87 q_C = 0.12	q_{Zn} = 0.84 q_N = -0.75 q_C = 0.19		$4s^{0.62}$	$4s^{1.10}$		ρ_{Zn} = 0.97 ρ_N = 0.36 ρ_C = 0.36	

Table S3: Structures (distances in Å, angles in °) of **ZnDAD** monomers in different ground state configurations (singlet closed-shell calculated by restricted DFT (R), triplet open-shell calculated by unrestricted DFT (U) and singlet open-shell calculated by broken symmetry formalism (BS)) in the gas phase and in function of the solvent using SMD model.



ZnDAD$_R$ **ZnDAD$_U$** **ZnDAD$_{BS}$**

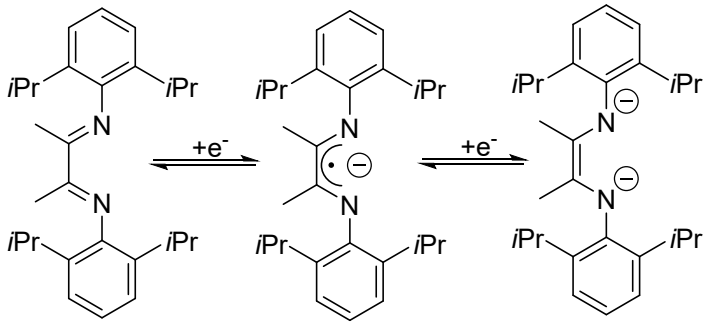
ZnDAD$_R$		C–C	C–N	Zn–N	C–N–Zn–N	
Gas phase		1.45	1.32	2.16	33	
Solvent (SMD)	Dielectric constant ε					
Hexane	1.88	1.43	1.34	2.07	32	
Toluene	2.37	1.42	1.35	2.05	31	
Chlorobenzene	5.79	1.38	1.41	1.91	10	
THF	7.42	1.38	1.42	1.91	8	
Dichloroethane	10.13	1.38	1.41	1.92	2	
1-pentanol	15.13	1.38	1.41	1.93	5	
Acetone	20.5	1.38	1.41	1.93	5	
Acetonitrile	35.7	1.38	1.41	1.94	5	
Water	78.4	1.38	1.41	1.95	4	

ZnDAD$_U$		C–C	C–N	Zn–N	C–N–Zn–N	
Gas phase		1.43	1.34	2.03	0	
Solvent (SMD)	Dielectric constant ε					
Hexane	1.88	1.43	1.34	2.05	1	
Toluene	2.37	1.43	1.34	2.05	1	
Chlorobenzene	5.79	1.43	1.34	2.07	1	
THF	7.42	1.43	1.34	2.08	0	
Dichloroethane	10.13	1.43	1.34	2.08	1	
1-pentanol	15.13	1.43	1.34	2.08	1	
Acetone	20.5	1.43	1.34	2.10	0	
Acetonitrile	35.7	1.43	1.34	2.11	0	
Water	78.4	1.43	1.34	2.11	0	

ZnDAD$_{BS}$		C–C	C–N	Zn–N	C–N–Zn–N	
Gas phase		1.43	1.34	2.03	0	
Solvent (SMD)	Dielectric constant ε					
Hexane	1.88	1.43	1.34	2.05	4	
Toluene	2.37	1.43	1.34	2.06	5	
Chlorobenzene	5.79	1.43	1.34	2.08	10	

THF	7.42	1.42	1.35	2.08	11	
Dichloroethane	10.13	1.43	1.34	2.08	12	
1-pentanol	15.13	1.43	1.35	2.08	16	
Acetone	20.5	1.42	1.35	2.09	15	
Acetonitrile	35.7	1.38	1.41	1.93	1	Singlet closed-shell
Water	78.4	1.38	1.41	1.95	1	Singlet closed-shell

Table S4: Energetics (in kcal mol^{-1}), structures (distances in Å, angles in °) and electronic structures (charges, spin densities) of the successive one-electron reductions intermediates of DAD ligand (i: experimental neutral DAD ligand; ii: experimental $[Na_2(LMes)(solv)_2]_2$ with dianonic ligand) with SMD solvation model.



	DAD	**DAD$^{\cdot-}$**	**DAD^{2-}**	**Exp[i]**	**Exp[ii]**
ΔE (kcal.mol^{-1})	0.0	- 50.8	- 79.9		
ΔG (kcal.mol^{-1})	0.0	- 53.9	- 78.4		
C–C (Å)	1.50	1.43	1.38	1.498(3)	1.356(4)
C–N (Å)	1.28	1.34	1.40	1.279(3) 1.280(3)	1.421(4)
N–C–C–N (°)	179.3	+ 7.9	170.0		
q_N	– 0.44	– 0.54	– 0.69		
q_C	+ 0.28	+ 0.16	+0.04		
Spin density C	--	0.15	--		
Spin density N	--	0.30	--		

[i] H. H. Haeri, R. Duraisamy, N. Harmgarth, P. Liebing, V. Lorenz, D. Hinderberger, F. T. Edelmann, F. T., *ChemistryOpen,* 2018, **7**, 701–708.

[ii] R. Duraisamy, P. Liebing, N. Harmgarth, V. Lorenz, L. Hilfert, S. Busse, F. C. Engelhardt, F. T. Edelmann, *Eur. J. Inorg. Chem.*, 2019, **2019** (28), 3343–3351.

Fig. S1: Visualization of the spin density for **ZnDAD$_U$** (isovalue for density is 0.004 a.u., H are omitted for clarity, with Gaussview software). One electron is delocalized on N–C–C–N backbone of the ligand and one electron is on zinc center

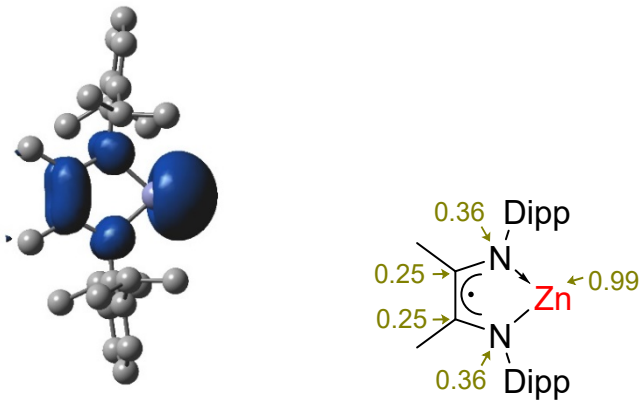


Fig. S2: Logarithmic regression of the energy difference $\Delta E_{S/T}$ (= E_S(**ZnDAD$_R$**)–E_T(**ZnDAD$_U$**) in kcal mol^{-1}) between closed-shell singlet and open-shell triplet configurations for **ZnDAD** monomers as function of the dielectric constant ε of the solvent

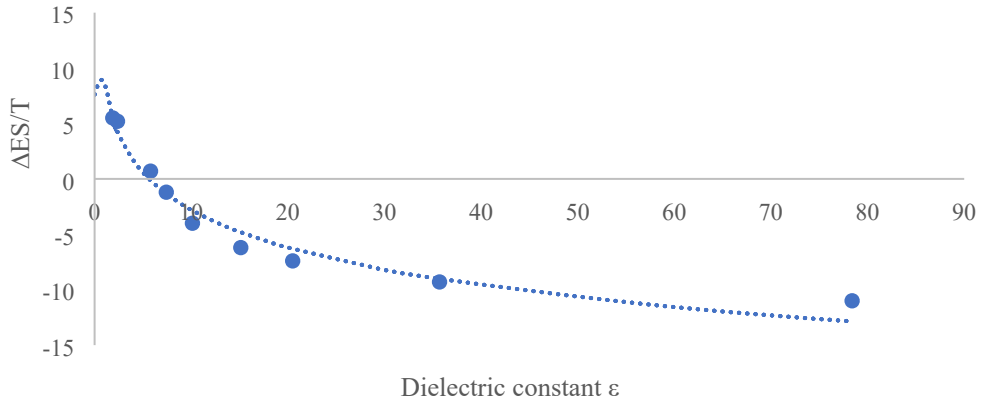


Fig. S3: Logarithmic regression of the dipole moment of **ZnDAD$_R$** as a function of the dielectric constant ε of the solvent.

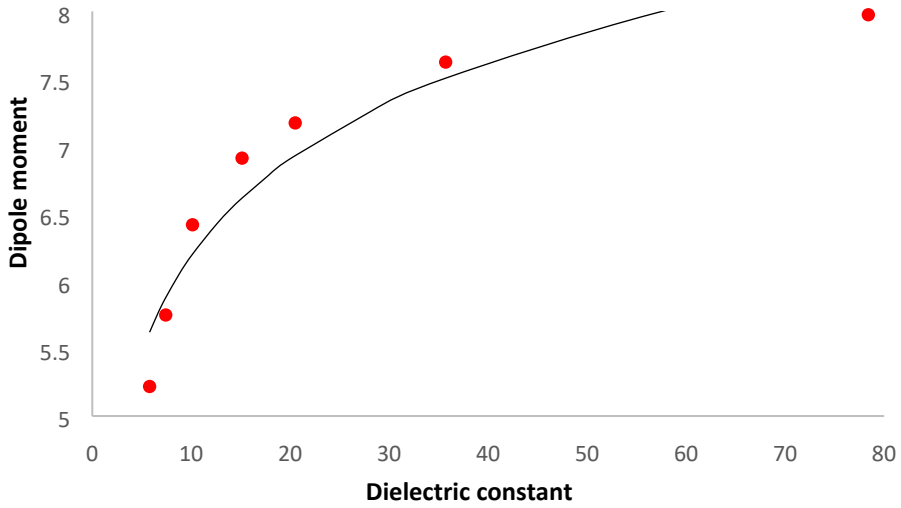


Fig. S4: Structures of **ZnDAD$_R$** (left) and **ZnDAD$_U$** (right) with two explicit solvent molecules ($O(CH_3)_2$ as a model of THF).

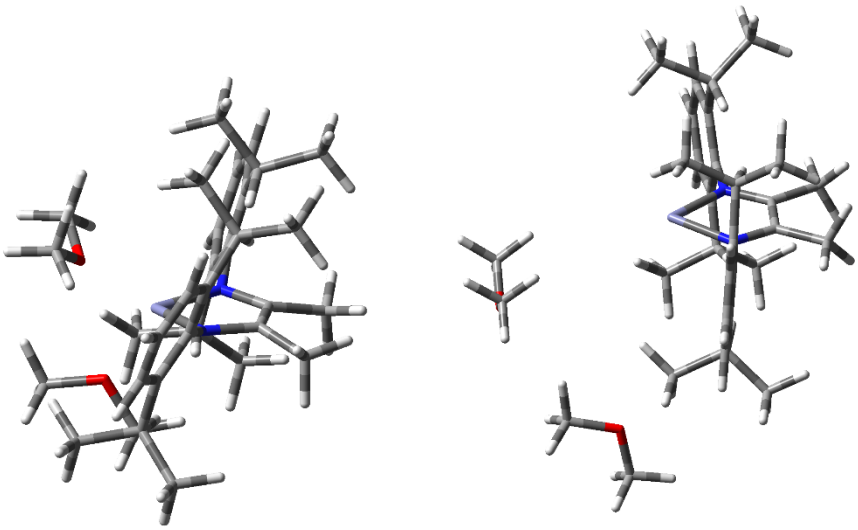


Table S5: Energetics (in kcal mol^{-1}), structures (distances in Å, angles in °), and electronic structures (charges, spin densities) of **ZnDAD$_R$** and **ZnDAD$_U$** using explicit and hybrid solvation models.

	Explicit solvation		**Hybrid solvation**	
	ZnDAD$_R$	**ZnDAD$_U$**	**ZnDAD$_R$**	**ZnDAD$_U$**
ΔE (kcal/mol)	0.0	7.2	0.0	1.5
ΔG (kcal/mol)	0.0	7.2	0.0	-12.5
C-C (Å)	1.37	1.43	1.38	1.43
C-N (Å)	1.42	1.34	1.42	1.34
Zn-N (Å)	1.91	2.02	1.94	2.09
Zn-O (Å)	2.15	5.29 / 6.55	2.10	4.50
N-Zn-N (°)	92	83	90	80
N-Zn-N-C (°)	5	0	2	0
q_{Zn}	1.60	0.85	1.59	0.84
q_N	-0.96	-0.78	-0.96	-0.76
q_C	0.05	0.19	0.10	0.20
Electronic configuration of Zn	$4s^{0.38}3d^{9.97}$	$4s^{1.08}3d^{9.9}$_	$4s^{0.38}3d^{9.97}$	$4s^{1.10}3d^{9.98}$
Spin density Zn	--	0.95	--	0.94
Spin density C	--	0.14	--	0.18
Spin density N	--	0.41	--	0.39

Table S6: Structures (distances in Å, angles in °) of **$ZnDAD_R$**, **$ZnDAD_U$** and **$ZnDAD_{BS}$** using SMD solvation model in a function of DFT functionals.

$ZnDAD_R$	C–C	C–N	Zn–N	C–N–Zn–N
BP86	1.40	1.41	1.94	12
PW91	1.40	1.41	1.94	11
PBE	1.38	1.41	1.91	5
M06L	1.38	1.41	1.93	8
B3LYP	1.38	1.42	1.93	11
B3PW91	1.38	1.42	1.91	8
M06-2X	1.37	1.42	1.95	7
TPSSh	1.38	1.42	1.92	7
CAM-B3LYP	1.37	1.42	1.90	7
LC-BLYP	1.36	1.42	1.87	5
B3PW91-D3	1.37	1.41	1.91	4

$ZnDAD_U$	C–C	C–N	Zn–N	C–N–Zn–N
BP86	1.42	1.35	2.10	0
PW91	1.44	1.35	2.1	0
PBE	1.43	1.34	2.08	1
M06L	1.43	1.34	2.1	1
B3LYP	1.43	1.34	2.11	1
B3PW91	1.43	1.34	2.08	0
M06-2X	1.43	1.34	2.11	1
TPSSh	1.43	1.35	2.08	1
CAM-B3LYP	1.42	1.34	2.08	1
LC-BLYP	1.42	1.33	2.02	1
B3PW91-D3	1.42	1.34	2.06	0

$ZnDAD_{BS}$	C–C	C–N	Zn–N	C–N–Zn–N
BP86	1.43	1.37	2.09	31
PW91	1.42	1.37	2.06	30
PBE	1.42	1.34	2.08	14
M06L	--	--	--	--
B3LYP	1.43	1.35	2.11	11
B3PW91	1.42	1.35	2.08	11
M06-2X	1.43	1.34	2.11	14
TPSSh	1.42	1.36	2.06	18
CAM-B3LYP	1.42	1.34	2.08	5
LC-BLYP	--	--	--	--
B3PW91-D3	1.37	1.41	1.91	4

Table S7: Difference of energy between the singlet and triplet state ground state configurations $\Delta E_{S/T}$ ($\Delta E_{S/T} = E_S - E_T$, in kcal mol^{-1}) and $\Delta E_{BS/T}$ ($\Delta E_{BS/T} = E_{BS} - E_T$, in kcal mol^{-1}) for monomer (**ZnDAD**) in different ground state configurations (closed-shell singlet calculated by restricted DFT (R), open-shell triplet calculated by unrestricted DFT (U) and open-shell singlet calculated by broken symmetry formalism (BS)) calculated with implicit solvation (SMD) in THF with different DFT functionals. The spin contamination $\langle S^2 \rangle$ is given for the singlet biradical (BS) and open-shell triplet configuration (U). Natural charges (q) for selected atoms, 4s electronic population for zinc and spin densities (ρ) for selected atoms are obtained from NBO analysis and Mulliken population analysis.

DFT functionals	$\Delta E_{S/T}$	$\Delta E_{BS/T}$	$<S^2>$	Natural charges (q)			4s Zn electronic population			Spin densities (ρ)	
				$ZnDAD_R$	**$ZnDAD_U$**	**$ZnDAD_{BS}$**	**$ZnDAD_R$**	**$ZnDAD_U$**	**$ZnDAD_{BS}$**	**$ZnDAD_U$**	**$ZnDAD_{BS}$**
BP86	-1.6	-1.6	$<S^2>_U$ = 2.003 $<S^2>_{BS}$ = 0	q_{Zn} = 0.99 q_N = -0.75 q_C = 0.12	q_{Zn} = 0.67 q_N = -0.69 q_C = 0.16		$4s^{0.80}$	$4s^{1.11}$		ρ_{Zn} = 1.05 ρ_N = 0.33 ρ_C = 0.21	
PW91	-2.2	-2.2	$<S^2>_U$ = 2.003 $<S^2>_{BS}$ = 0	q_{Zn} = 1.00 q_N = -0.76 q_C = 0.12	q_{Zn} = 0.68 q_N = -0.69 q_C = 0.16		$4s^{0.79}$	$4s^{1.10}$		ρ_{Zn} = 1.03 ρ_N = 0.35 ρ_C = 0.23	
PBE	-3.0	-3.8	$<S^2>_U$ = 2.007 $<S^2>_{BS}$ = 0.908	q_{Zn} = 1.27 q_N = -0.86 q_C = 0.10	q_{Zn} = 0.73 q_N = -0.74 q_C = 0.18	q_{Zn} = 0.61 q_N = - 0.69 q_C = 0.17	$4s^{0.53}$	$4s^{1.06}$	$4s^{1.18}$	ρ_{Zn} = 0.97 ρ_N = 0.37 ρ_C = 0.18	ρ_{Zn} = 0.98 ρ_N = 0.23 ρ_C = 0.25
M06L	-0.6	nc	$<S^2>_U$ = 2.009 $<S^2>_{BS}$ = nc	q_{Zn} = 1.08 q_N = -0.81 q_C = 0.13	q_{Zn} = 0.72 q_N = -0.71 q_C = 0.18		$4s^{0.72}$	$4s^{1.04}$		ρ_{Zn} = 1.00 ρ_N = 0.32 ρ_C = 0.33	
B3LYP	0.9	1.8	$<S^2>_U$ = 2.006 $<S^2>_{BS}$ = 0.927	q_{Zn} = 1.08 q_N = -0.82 q_C = 0.12	q_{Zn} = 0.72 q_N = -0.72 q_C = 0.18	q_{Zn} = 0.55 q_N = - 0.67 q_C = 0.19	$4s^{0.72}$	$4s^{1.09}$	$4s^{1.29}$	ρ_{Zn} = 0.97 ρ_N = 0.37 ρ_C = 0.13	ρ_{Zn} = 0.96 ρ_N = 0.21 ρ_C = 0.20
B3PW91	-1.2	-1.0	$<S^2>_U$ = 2.006 $<S^2>_{BS}$ = 0.939	q_{Zn} = 1.29 q_N = -0.87 q_C = 0.12	q_{Zn} = 0.84 q_N = -0.76 q_C = 0.19	q_{Zn} = 0.72 q_N = -0.68 q_C = 0.19	$4s^{0.67}$	$4s^{1.09}$	$4s^{1.24}$	ρ_{Zn} = 0.99 ρ_N = 0.36 ρ_C = 0.25	ρ_{Zn} = 0.99 ρ_N = 0.22 ρ_C = 0.21
M06-2X	-2.1	-2.6	$<S^2>_U$ = 2.010 $<S^2>_{BS}$ = 0.835	q_{Zn} = 1.35 q_N = -0.90 q_C = 0.10	q_{Zn} = 0.75 q_N = -0.75 q_C = 0.18	q_{Zn} = 0.65 q_N = -0.69 q_C = 0.17	$4s^{0.43}$	$4s^{1.02}$	$4s^{1.14}$	ρ_{Zn} = 0.86 ρ_N = 0.31 ρ_C = 0.22	ρ_{Zn} = 0.72 ρ_N = 0.36 ρ_C = 0.24
TPSSh	-2.2	-2.7	$<S^2>_U$= 2.006 $<S^2>_{BS}$ = 0.755	q_{Zn} = 1.14 q_N = -0.83 q_C = 0.11	q_{Zn} = 0.72 q_N = -0.73 q_C = 0.17	q_{Zn} = 0.64 q_N = - 0.69 q_C = 0.16	$4s^{0.66}$	$4s^{1.07}$	$4s^{1.15}$	ρ_{Zn} = 0.99 ρ_N = 0.37 ρ_C = 0.19	ρ_{Zn} = 0.89 ρ_N = 0.20 ρ_C = 0.19
CAM-B3LYP	-1.0	-1.9	$<S^2>_U$ = 2.005 $<S^2>_{BS}$ = 1.001	q_{Zn} = 1.32 q_N = -0.89 q_C = 0.10	q_{Zn} = 0.75 q_N = -0.75 q_C = 0.19	q_{Zn} = 0.56 q_N = - 0.68 q_C = 0.20	$4s^{0.49}$	$4s^{1.06}$	$4s^{1.27}$	ρ_{Zn} = 0.92 ρ_N = 0.39 ρ_C = 0.10	ρ_{Zn} = 0.95 ρ_N = 0.18 ρ_C = 0.22
LC-BLYP	-5.1	nc	$<S^2>_U$ = 2.013 $<S^2>_{BS}$ = nc	q_{Zn} = 1.43 q_N = -0.95 q_C = 0.10	q_{Zn} = 0.75 q_N = -0.77 q_C = 0.20		$4s^{0.38}$	$4s^{1.01}$		ρ_{Zn} = 0.96 ρ_N = 0.43 ρ_C = 0.17	
B3PW91-D3	-2.9	-2.9	$<S^2>_U$ = 2.006 $<S^2>_{BS}$ = 0	q_{Zn} = 1.24 q_N = -0.85 q_C = 0.10	q_{Zn} = 0.72 q_N = -0.72 q_C = 0.18		$4s^{0.55}$	$4s^{1.03}$		ρ_{Zn} = 1.02 ρ_N = 0.35 ρ_C = 0.26	

Cartesian coordinates:

DAD (THF)

70

scf done: -1200.245289

C	0.023678	-0.469693	-0.000094
C	0.199816	-0.319640	1.486563
N	1.092811	-0.408569	-0.704901
N	-0.867703	-0.395569	2.192209
C	1.091179	-0.479006	-2.114332
C	0.800196	0.689336	-2.865978
C	0.895700	0.625509	-4.260323
C	1.269237	-0.547006	-4.910776
C	1.574768	-1.675575	-4.155944
C	1.510431	-1.670405	-2.756829
C	0.471490	2.008374	-2.178201
H	0.673853	1.510644	-4.849480
H	1.330654	-0.577858	-5.995584
H	1.881567	-2.591075	-4.657801
C	1.914874	-2.947334	-2.027596
C	-0.872178	-0.258074	3.598144
C	-0.939077	1.033740	4.179682
C	-1.037386	1.124892	5.571493
C	-1.075712	-0.013142	6.376291
C	-1.031524	-1.271878	5.785733
C	-0.941752	-1.421580	4.396740
C	-0.970447	2.281631	3.307664
H	-1.083122	2.104336	6.038819
H	-1.144521	0.084295	7.456812
H	-1.067807	-2.159534	6.413029
C	-0.917679	-2.814009	3.783276
C	-0.501584	2.892924	-2.964397
H	-0.011608	1.782043	-1.222713
C	1.765106	2.777834	-1.862845
H	-0.796327	3.752316	-2.351567
H	-0.052640	3.291183	-3.881211
H	-1.411748	2.348968	-3.240603
H	1.542356	3.700789	-1.314073
H	2.450828	2.178541	-1.254519
H	2.287448	3.051588	-2.787439
C	0.759033	-3.644495	-1.296007
H	2.232442	-3.636043	-2.821193
C	3.128516	-2.755627	-1.107434
H	3.443872	-3.722151	-0.696403
H	3.976456	-2.330917	-1.656451
H	2.900936	-2.087937	-0.271536
H	1.078580	-4.637492	-0.957619
H	0.432556	-3.087779	-0.413335
H	-0.106803	-3.778170	-1.953951
H	-0.915112	-2.695426	2.695196
C	0.354649	-3.581967	4.168787
C	-2.172875	-3.618001	4.149639
H	-2.166306	-4.587929	3.638425
H	-2.228689	-3.811970	5.227004
H	-3.085321	-3.087541	3.855686
H	0.380073	-4.558314	3.670410
H	1.257945	-3.032581	3.881589
H	0.399971	-3.758507	5.249963
C	-0.372839	3.523512	3.975277
H	-0.368042	2.080490	2.415072
C	-2.406891	2.563857	2.836148
H	-2.428732	3.421263	2.152805
H	-2.835098	1.702230	2.313403
H	-3.054351	2.795386	3.690482
H	-0.309156	4.339630	3.246737
H	-0.988614	3.882503	4.807705
H	0.636779	3.334078	4.356646
C	-1.367564	-0.674749	-0.524244
C	1.587615	-0.095952	2.011107
H	1.586074	-0.009189	3.098811
H	2.242285	-0.921871	1.715714
H	2.018399	0.812204	1.577672
H	-1.356988	-0.859926	-1.599533
H	-1.847786	-1.514719	-0.014050
H	-1.984995	0.206563	-0.319902

Zero-point correction= 0.616471 (Hartree/Particle)

Thermal correction to Energy= 0.650286

Thermal correction to Enthalpy= 0.651230

Thermal correction to Gibbs Free Energy= 0.549043

Sum of electronic and zero-point Energies= -1199.628818

Sum of electronic and thermal Energies= -1199.595004

Sum of electronic and thermal Enthalpies= -1199.594059

Sum of electronic and thermal Free Energies= -1199.696246

$DAD^{\cdot-}$ (THF)

70

scf done: -1200.247948

H	0.297918	-0.687621	0.165181
H	0.699188	-0.576774	1.879002
H	1.992150	-0.529264	0.664411
C	0.969347	-0.202026	0.884432
C	0.843532	1.323786	0.850914
H	1.436332	1.713686	1.684384
C	1.347963	1.972241	-0.430460
C	-0.609541	1.755031	1.113173
H	2.434898	5.682893	-2.848784
H	-0.675469	2.845810	1.160517
H	-0.973844	1.346474	2.064566
H	-1.267460	1.397613	0.310795
C	1.979473	3.996473	-1.672863
C	1.963778	3.241736	-2.847424
C	1.666823	1.879409	-2.847056
C	1.347251	1.266690	-1.635583
H	1.078850	0.212682	-1.635563
H	1.668392	1.309224	-3.773172
H	2.192656	3.741287	-3.788856
C	2.278034	5.485313	-1.777026
H	3.802209	6.953107	-1.269656
H	3.463452	5.785269	0.023817
H	4.419015	5.291577	-1.389307
C	1.092190	6.352175	-1.324784
H	0.875478	6.172212	-0.267767
H	1.319583	7.416985	-1.468382
H	0.194288	6.114559	-1.907262
N	1.670120	4.119412	0.721754
C	2.444577	3.929792	1.789549
H	3.657566	2.237925	2.489829
C	3.673624	3.035942	1.733784
H	3.754653	2.561070	0.752713
H	4.597786	3.605918	1.904801

C	2.193381	4.651731	3.002185
N	1.097225	5.397870	3.128679
C	0.843750	6.263305	4.163352
C	3.171453	4.471981	4.152343
C	3.569967	5.900940	-1.057697
C	1.708374	3.360460	-0.421664
H	2.832722	5.026898	5.031010
H	3.270508	3.416499	4.440493
H	4.184505	4.822373	3.908592
C	1.632113	7.426123	4.432451
C	1.246360	8.297186	5.455334
C	0.103981	8.077488	6.221849
C	-0.690711	6.964968	5.936714
C	-0.352665	6.068188	4.925694
C	2.814562	7.791580	3.546859
H	1.849248	9.183451	5.649449
H	-0.171839	8.767335	7.016182
H	-1.595048	6.796958	6.518408
C	-1.205448	4.849672	4.621274
H	-1.021996	4.623537	3.563020
C	-0.733644	3.630471	5.429400
C	-2.707738	5.075875	4.816080
H	-1.304055	2.732719	5.157090
H	0.324852	3.428410	5.240795
H	-0.861763	3.803100	6.506175
H	-3.270490	4.207413	4.452375
H	-2.974202	5.213461	5.872189
H	-3.052078	5.958059	4.265268
C	4.084948	8.131492	4.337758
H	3.036290	6.924190	2.918838
C	2.441784	8.943086	2.598921
H	4.926686	8.307144	3.656032
H	3.958567	9.039235	4.940761
H	4.360359	7.317398	5.016335
H	3.269147	9.171628	1.914663
H	1.566425	8.678867	1.997948
H	2.203967	9.854518	3.162049

Zero-point correction= 0.612859 (Hartree/Particle)
Thermal correction to Energy= 0.647045
Thermal correction to Enthalpy= 0.647990
Thermal correction to Gibbs Free Energy= 0.544130
Sum of electronic and zero-point Energies= -1199.713415
Sum of electronic and thermal Energies= -1199.679228
Sum of electronic and thermal Enthalpies= -1199.678284
Sum of electronic and thermal Free Energies= -1199.782144

DAD^{2-} (THF)

70
scf done: -1200.372577

C	0.190327	-0.871153	0.137099
C	0.406167	-0.717672	1.490052
N	1.251204	-0.970878	-0.767404
N	-0.565093	-1.093491	2.426169
C	1.200510	-0.576716	-2.055498
C	0.419974	0.526575	-2.604931
C	0.405845	0.766543	-3.980871
C	1.165659	0.024844	-4.889630
C	2.005062	-0.969225	-4.365178
C	2.054460	-1.275657	-3.007541
C	-0.247699	1.553728	-1.694933
H	-0.196038	1.593798	-4.358795
H	1.132589	0.232071	-5.956904
H	2.638847	-1.540869	-5.045490
C	2.999454	-2.396826	-2.585326
C	-0.743977	-0.502797	3.624788
C	-0.496055	0.890470	3.969496
C	-0.676853	1.333157	5.282811
C	-1.138030	0.504170	6.308666
C	-1.472100	-0.818069	5.975086
C	-1.310739	-1.324730	4.691132
C	-0.238920	1.939585	2.890858
H	-0.482324	2.381991	5.509410
H	-1.259592	0.876129	7.323745
H	-1.864983	-1.469247	6.754607
C	-1.709926	-2.753392	4.361460
C	-1.670226	1.941691	-2.120373
H	-0.313594	1.121612	-0.691855
C	0.630045	2.811763	-1.573771
H	-2.130122	2.598354	-1.371230
H	-1.683266	2.483388	-3.074754
H	-2.311107	1.059627	-2.230515
H	0.199276	3.528459	-0.861581
H	1.637078	2.557044	-1.223834
H	0.731092	3.320037	-2.541802
C	2.281272	-3.644977	-2.047587
H	3.511652	-2.709569	-3.508319
C	4.096572	-1.942000	-1.612272
H	4.796619	-2.763420	-1.406038
H	4.674387	-1.107422	-2.029169
H	3.650989	-1.614160	-0.668909
H	2.999014	-4.461155	-1.885830
H	1.783558	-3.425603	-1.099432
H	1.524124	-4.001610	-2.756924
H	-0.972853	-3.107650	3.627896
C	-1.701729	-3.718380	5.550371
C	-3.075728	-2.794589	3.656428
H	-3.321899	-3.812256	3.323118
H	-3.874613	-2.457717	4.330621
H	-3.068983	-2.144447	2.776072
H	-1.879634	-4.743728	5.202195
H	-0.739600	-3.707597	6.076307
H	-2.486697	-3.488748	6.282637
C	0.869910	2.942304	3.235801
H	0.067451	1.415891	1.979810
C	-1.539943	2.687418	2.551700
H	-1.387863	3.392300	1.723177
H	-2.329739	1.987975	2.254509
H	-1.906965	3.257991	3.415186
H	1.064069	3.607306	2.384814
H	0.602700	3.579814	4.088231
H	1.808855	2.433878	3.482108
C	-1.200928	-1.254071	-0.335252
C	1.812852	-0.458729	1.990418
H	1.807288	-0.009106	2.989865
H	2.383754	-1.400058	2.067437
H	2.374862	0.196934	1.316307
H	-1.284023	-1.182444	-1.424793
H	-1.436668	-2.293525	-0.053242
H	-1.985815	-0.631703	0.111460

Zero-point correction= 0.612341 (Hartree/Particle)

Thermal correction to Energy= 0.645110
Thermal correction to Enthalpy= 0.646054
Thermal correction to Gibbs Free Energy= 0.551278
Sum of electronic and zero-point Energies= -1199.760236
Sum of electronic and thermal Energies= -1199.727467
Sum of electronic and thermal Enthalpies= -1199.726523
Sum of electronic and thermal Free Energies= -1199.821299

$ZnDAD_R$ (gas phase)

71
scf done: -2979.350428

Zn	-0.056868	0.494315	-0.009935
N	0.273013	0.070031	2.078362
N	2.068301	0.140022	0.150668
C	2.255492	-0.761132	1.100691
C	1.268771	-0.796270	2.166172
C	1.367627	-1.859737	3.225500
C	3.344107	-1.799041	1.073858
H	0.594577	-1.727408	3.983704
H	1.265896	-2.868216	2.802935
H	2.343021	-1.822047	3.722653
H	4.051656	-1.601628	0.267313
H	3.895717	-1.808252	2.019872
H	2.939344	-2.810374	0.933983
C	-0.762491	0.115516	3.053693
C	2.955883	0.252043	-0.956826
C	-1.863464	-0.768690	3.026394
C	-2.872508	-0.597312	3.983266
C	-2.800911	0.402252	4.944326
C	-1.708942	1.267372	4.956865
C	-0.682864	1.151003	4.017676
H	-3.730697	-1.264528	3.973577
H	-3.593052	0.511809	5.680064
H	-1.660077	2.049284	5.708625
C	2.881715	-0.612150	-2.074115
C	3.758364	-0.387991	-3.142109
C	4.687550	0.645648	-3.118640
C	4.738412	1.495514	-2.018197
C	3.874208	1.328495	-0.933272
H	3.711347	-1.039206	-4.011268
H	5.362951	0.793283	-3.956979
H	5.458561	2.309452	-2.005360
C	-2.008213	-1.875407	1.992451
H	-1.098674	-1.884968	1.380804
C	-2.147839	-3.261473	2.639365
H	-2.167776	-4.040381	1.868751
H	-1.318031	-3.477036	3.319999
H	-3.076928	-3.345398	3.213875
C	-3.182624	-1.598663	1.042255
H	-4.134096	-1.567042	1.585032
H	-3.052307	-0.641337	0.527302
H	-3.254758	-2.384816	0.281913
C	0.470919	2.142776	3.985328
H	1.350094	1.611339	3.604290
C	0.842635	2.710108	5.358814
H	1.020100	1.914996	6.090756
H	1.757494	3.307177	5.278970
H	0.064414	3.370254	5.758142
C	0.161048	3.277334	2.995100
H	-0.050377	2.884371	1.995156
H	-0.715273	3.847740	3.323715
H	1.007997	3.968557	2.916792
C	3.943603	2.276172	0.254366
H	3.052440	2.089077	0.862596
C	3.913493	3.750796	-0.168258
H	4.811720	4.036288	-0.727230
H	3.044397	3.966731	-0.797644
H	3.862044	4.396401	0.715576
C	5.173077	1.982760	1.128166
H	5.188536	2.636556	2.007877
H	5.177379	0.944890	1.476844
H	6.101489	2.149184	0.569335
C	1.873718	-1.747558	-2.174088
H	1.333478	-1.802738	-1.221929
C	0.829107	-1.466143	-3.264463
H	0.087666	-2.272429	-3.303168
H	0.299052	-0.528916	-3.066240
H	1.297065	-1.390915	-4.252523
C	2.547105	-3.108246	-2.406373
H	3.048161	-3.147934	-3.379851
H	3.297378	-3.326504	-1.639779
H	1.799840	-3.909640	-2.390149

Zero-point correction= 0.617502 (Hartree/Particle)
Thermal correction to Energy= 0.653291
Thermal correction to Enthalpy= 0.654235
Thermal correction to Gibbs Free Energy= 0.548060
Sum of electronic and zero-point Energies= -2978.732926
Sum of electronic and thermal Energies= -2978.697138
Sum of electronic and thermal Enthalpies= -2978.696193
Sum of electronic and thermal Free Energies= -2978.802368

$ZnDAD_U$ (gas phase)

71
scf done: -2979.358950

Zn	0.436392	1.233383	0.365526
N	0.145684	0.100506	2.019516
N	2.077393	0.059993	0.176484
C	2.155708	-0.831512	1.176468
C	1.120619	-0.810321	2.163152
C	1.154570	-1.783013	3.310192
C	3.274384	-1.831758	1.281071
H	0.238559	-1.721455	3.900193
H	1.267027	-2.814351	2.957349
H	1.999388	-1.582526	3.981660
H	4.044054	-1.634833	0.532854
H	3.743270	-1.806098	2.271108
H	2.912264	-2.856439	1.126906
C	-0.926126	0.226422	2.942484
C	3.038462	0.126219	-0.866777
C	-2.144133	-0.446868	2.691651
C	-3.211066	-0.249912	3.574129
C	-3.092858	0.589968	4.676550
C	-1.891595	1.252543	4.907357
C	-0.794650	1.088947	4.055604
H	-4.153370	-0.761113	3.392691
H	-3.933816	0.730802	5.350219
H	-1.805608	1.914815	5.765269
C	2.858031	-0.648306	-2.036390
C	3.778829	-0.507835	-3.079396
C	4.852471	0.371680	-2.984149
C	5.014396	1.132539	-1.831124

C	4.120905	1.029956	-0.760109
H	3.650619	-1.094734	-3.985533
H	5.556934	0.466446	-3.806111
H	5.850751	1.823856	-1.762365
C	4.317572	1.900755	0.471364
H	3.562355	1.603096	1.205900
C	4.081415	3.383285	0.145165
H	4.174661	3.997139	1.048445
H	4.811009	3.750149	-0.585815
H	3.082038	3.542653	-0.273102
C	5.694650	1.693748	1.117721
H	5.775314	2.279989	2.040142
H	5.865458	0.641534	1.367653
H	6.505655	2.013264	0.453694
C	1.675115	-1.591161	-2.196594
H	1.158995	-1.637356	-1.232373
C	0.673283	-1.045156	-3.225868
H	-0.200852	-1.702185	-3.301473
H	0.324689	-0.044970	-2.947886
H	1.127640	-0.974754	-4.220791
C	2.106353	-3.019661	-2.556643
H	2.579701	-3.064452	-3.543798
H	2.819892	-3.418436	-1.828233
H	1.236188	-3.685378	-2.580956
C	-2.323613	-1.350933	1.481727
H	-1.352088	-1.425432	0.982633
C	-3.310773	-0.740033	0.475521
H	-2.986233	0.256127	0.157010
H	-3.394678	-1.372302	-0.415897
H	-4.311537	-0.640969	0.911274
C	-2.749461	-2.772709	1.874221
H	-2.042999	-3.221736	2.579976
H	-3.739738	-2.783797	2.343204
H	-2.798991	-3.414747	0.987440
C	0.487944	1.862508	4.321078
H	1.240434	1.504126	3.611460
C	0.289277	3.363237	4.057796
H	-0.055128	3.543898	3.034134
H	-0.455499	3.789229	4.739765
H	1.228606	3.909232	4.202893
C	1.036781	1.622264	5.734369
H	0.361029	2.011649	6.503978
H	1.183714	0.555287	5.931021
H	2.000996	2.127809	5.859613

Zero-point correction= 0.617600 (Hartree/Particle)
Thermal correction to Energy= 0.653676
Thermal correction to Enthalpy= 0.654620
Thermal correction to Gibbs Free Energy= 0.544291
Sum of electronic and zero-point Energies= -2978.741350
Sum of electronic and thermal Energies= -2978.705275
Sum of electronic and thermal Enthalpies= -2978.704330
Sum of electronic and thermal Free Energies= -2978.814659

$ZnDAD_{BS}$ (gas phase)

71
scf done: -2979.356685

Zn	0.435169	1.224773	0.364749
N	0.145670	0.094913	2.020946
N	2.081841	0.058790	0.180120
C	2.158021	-0.835182	1.179152
C	1.121455	-0.816317	2.163847
C	1.152136	-1.790880	3.309365
C	3.276867	-1.835429	1.281579
H	0.222210	-1.750665	3.879230
H	1.295747	-2.818375	2.957373
H	1.976541	-1.572468	4.000630
H	4.061162	-1.617455	0.554568
H	3.724605	-1.834477	2.281412
H	2.921379	-2.856752	1.092302
C	-0.924646	0.222351	2.944684
C	3.041285	0.124170	-0.864016
C	-2.149069	-0.437001	2.687593
C	-3.214914	-0.237530	3.570849
C	-3.089590	0.591599	4.680551
C	-1.882095	1.240456	4.918121
C	-0.786086	1.073627	4.065867
H	-4.161850	-0.738296	3.384414
H	-3.929723	0.734756	5.354765
H	-1.790702	1.894555	5.781698
C	2.868376	-0.661628	-2.027484
C	3.787377	-0.520704	-3.071982
C	4.852543	0.369925	-2.984342
C	5.007513	1.141633	-1.837609
C	4.115273	1.039014	-0.765563
H	3.664513	-1.115857	-3.973448
H	5.555756	0.464757	-3.807370
H	5.837339	1.841344	-1.774650
C	4.303595	1.921149	0.459084
H	3.553334	1.619163	1.196987
C	4.048795	3.398259	0.122370
H	4.136001	4.020076	1.020800
H	4.772659	3.768382	-0.612667
H	3.046959	3.542547	-0.295650
C	5.684011	1.735733	1.104789
H	5.758880	2.329736	2.022721
H	5.867828	0.687534	1.362297
H	6.490183	2.060094	0.437232
C	1.692542	-1.614518	-2.180593
H	1.185037	-1.668510	-1.212213
C	0.677487	-1.072621	-3.199170
H	-0.192023	-1.736276	-3.270320
H	0.323290	-0.076162	-2.914665
H	1.123404	-0.994490	-4.197335
C	2.131408	-3.038269	-2.549726
H	2.593142	-3.076961	-3.542599
H	2.856788	-3.433067	-1.830909
H	1.266480	-3.711010	-2.565575
C	-2.335606	-1.329382	1.470121
H	-1.363452	-1.410457	0.973152
C	-3.313715	-0.699833	0.466544
H	-2.977980	0.295444	0.156786
H	-3.402474	-1.323920	-0.430160
H	-4.314309	-0.593419	0.900975
C	-2.777563	-2.749647	1.849973
H	-2.077478	-3.211987	2.553492
H	-3.768959	-2.754011	2.316704
H	-2.831949	-3.383837	0.957845
C	0.502687	1.835167	4.336261
H	1.257089	1.463433	3.635617
C	0.320961	3.335633	4.058863
H	-0.013736	3.511388	3.031052
H	-0.425618	3.773767	4.731123
H	1.264145	3.874087	4.207228
C	1.038581	1.601873	5.755539
H	0.363564	2.008152	6.516978
H	1.169989	0.535075	5.963868
H	2.008586	2.095848	5.882080

Zero-point correction= 0.617313 (Hartree/Particle)
Thermal correction to Energy= 0.653568
Thermal correction to Enthalpy= 0.654512
Thermal correction to Gibbs Free Energy= 0.543902
Sum of electronic and zero-point Energies= -2978.739373
Sum of electronic and thermal Energies= -2978.703117
Sum of electronic and thermal Enthalpies= -2978.702173
Sum of electronic and thermal Free Energies= -2978.812784

$ZnDAD_R$ (hexane)

71
scf done: -2979.377880

Zn	0.022520	0.359603	-0.047024
N	0.229384	0.115644	2.001563
N	2.072356	0.105495	0.118052
C	2.266714	-0.726397	1.154328
C	1.265684	-0.720325	2.178037
C	1.333461	-1.729845	3.291165
C	3.374730	-1.742581	1.202166
H	0.545581	-1.559577	4.026867
H	1.233492	-2.759783	2.920439
H	2.295842	-1.675928	3.812083
H	4.096021	-1.577697	0.399902
H	3.914349	-1.690681	2.154226
H	2.996097	-2.770434	1.110669
C	-0.832495	0.204614	2.942814
C	2.988847	0.183391	-0.966264
C	-1.937045	-0.682287	2.920228
C	-2.978073	-0.475773	3.833445
C	-2.941551	0.562117	4.758297
C	-1.851416	1.426621	4.771198
C	-0.792818	1.274899	3.870758
H	-3.834764	-1.145257	3.821462
H	-3.758838	0.698307	5.461848
H	-1.824481	2.241559	5.490697
C	2.936470	-0.710098	-2.064535
C	3.824722	-0.512955	-3.128720
C	4.753476	0.522053	-3.121148
C	4.795879	1.392980	-2.036901
C	3.921087	1.250613	-0.955695
H	3.789446	-1.187445	-3.980835
H	5.437157	0.651038	-3.956263
H	5.518285	2.205789	-2.032753
C	-2.042181	-1.835676	1.932902
H	-1.098164	-1.883661	1.378404
C	-2.236985	-3.188348	2.631977
H	-2.213714	-4.002698	1.898329
H	-1.453182	-3.378039	3.372685
H	-3.201681	-3.242740	3.149136
C	-3.157377	-1.592019	0.905981
H	-4.138380	-1.523814	1.390350
H	-2.989714	-0.660335	0.353462
H	-3.198598	-2.411301	0.178218
C	0.369851	2.256250	3.904394
H	1.035881	1.991725	3.078013
C	1.172995	2.140799	5.208044
H	1.542297	1.121526	5.363633
H	2.038876	2.813231	5.187935
H	0.564309	2.409901	6.079535
C	-0.095316	3.701554	3.678204
H	-0.653548	3.799609	2.740921
H	-0.743255	4.052733	4.489742
H	0.766662	4.377368	3.629876
C	3.985752	2.239343	0.199431
H	3.178084	1.978693	0.889449
C	3.745523	3.681298	-0.269159
H	4.538517	4.028252	-0.941866
H	2.793053	3.774920	-0.801869
H	3.720575	4.363096	0.589097
C	5.310862	2.130194	0.967461
H	5.313493	2.808173	1.829229
H	5.477352	1.113415	1.338918
H	6.165295	2.396141	0.333765
C	1.943040	-1.860645	-2.139083
H	1.409874	-1.900100	-1.182478
C	0.891876	-1.621559	-3.232466
H	0.159997	-2.438006	-3.250155
H	0.347222	-0.686161	-3.059895
H	1.353704	-1.563570	-4.224932
C	2.633201	-3.217011	-2.339981
H	3.128773	-3.279576	-3.315445
H	3.390475	-3.403894	-1.571507
H	1.897627	-4.028712	-2.294986

Zero-point correction= 0.616963 (Hartree/Particle)
Thermal correction to Energy= 0.652615
Thermal correction to Enthalpy= 0.653559
Thermal correction to Gibbs Free Energy= 0.548252
Sum of electronic and zero-point Energies= -2978.760917
Sum of electronic and thermal Energies= -2978.725265
Sum of electronic and thermal Enthalpies= -2978.724321
Sum of electronic and thermal Free Energies= -2978.829628

$ZnDAD_U$ (hexane)

71
scf done: -2979.386601

Zn	0.389651	1.171596	0.324574
N	0.151593	0.061280	2.027285
N	2.082178	0.019679	0.181410
C	2.178761	-0.848638	1.199694
C	1.145929	-0.825225	2.188990
C	1.204264	-1.775074	3.353709
C	3.314454	-1.826586	1.327859
H	0.327452	-1.666521	3.994357
H	1.249852	-2.818242	3.018043
H	2.094932	-1.602812	3.971119
H	4.022616	-1.717689	0.504676
H	3.864069	-1.685252	2.266688
H	2.953923	-2.862885	1.325730
C	-0.919215	0.198957	2.946162
C	3.042037	0.102396	-0.858460
C	-2.138542	-0.478485	2.704332
C	-3.210350	-0.263249	3.577288
C	-3.097706	0.599082	4.663406
C	-1.897243	1.266811	4.886182
C	-0.795788	1.085824	4.043122
H	-4.152139	-0.777529	3.401632
H	-3.942094	0.753503	5.330224
H	-1.815766	1.947220	5.730340
C	2.847147	-0.633813	-2.051948
C	3.762888	-0.471980	-3.097022

C	4.846799	0.393122	-2.982792
C	5.023696	1.118037	-1.808261
C	4.135991	0.992587	-0.734396
H	3.623077	-1.030644	-4.019273
H	5.547493	0.504954	-3.806210
H	5.866928	1.799484	-1.725451
C	4.340380	1.835709	0.515942
H	3.620248	1.490260	1.264022
C	4.036093	3.315441	0.236744
H	4.134081	3.910711	1.152446
H	4.726412	3.729901	-0.507333
H	3.017631	3.448037	-0.145171
C	5.743074	1.672366	1.116110
H	5.821032	2.227516	2.058256
H	5.972405	0.621712	1.323818
H	6.521020	2.056348	0.446351
C	1.652760	-1.559827	-2.230601
H	1.152788	-1.637402	-1.260034
C	0.640296	-0.966339	-3.221971
H	-0.240686	-1.613286	-3.310550
H	0.300527	0.024571	-2.899912
H	1.078542	-0.858540	-4.221114
C	2.060927	-2.977583	-2.652226
H	2.513511	-2.993335	-3.650314
H	2.782677	-3.413130	-1.952923
H	1.182585	-3.632939	-2.682644
C	-2.313778	-1.400948	1.506756
H	-1.331151	-1.515892	1.038386
C	-3.250501	-0.775686	0.462044
H	-2.882549	0.202044	0.130812
H	-3.333879	-1.421824	-0.420021
H	-4.258792	-0.631063	0.867523
C	-2.799806	-2.800586	1.905934
H	-2.137655	-3.259840	2.647746
H	-3.809828	-2.776675	2.330924
H	-2.830747	-3.457299	1.028611
C	0.483500	1.871010	4.294567
H	1.248338	1.476540	3.618603
C	0.291464	3.356028	3.950442
H	-0.032821	3.486245	2.911881
H	-0.465405	3.818275	4.594988
H	1.228699	3.909391	4.084032
C	1.006622	1.708323	5.727802
H	0.323291	2.145687	6.464613
H	1.145710	0.653814	5.988913
H	1.972758	2.214169	5.839788

Zero-point correction= 0.617364 (Hartree/Particle)
Thermal correction to Energy= 0.652360
Thermal correction to Enthalpy= 0.653304
Thermal correction to Gibbs Free Energy= 0.548055
Sum of electronic and zero-point Energies= -2978.769237
Sum of electronic and thermal Energies= -2978.734241
Sum of electronic and thermal Enthalpies= -2978.733296
Sum of electronic and thermal Free Energies= -2978.838546

$ZnDAD_{BS}$ (hexane)

71
scf done: -2979.384589

Zn	0.390183	1.165376	0.319248
N	0.164538	0.077808	2.038773
N	2.100864	0.036479	0.197914
C	2.166126	-0.867839	1.188127
C	1.131272	-0.843890	2.174901
C	1.151331	-1.835092	3.306057
C	3.265004	-1.890782	1.280578
H	0.281740	-1.710309	3.953563
H	1.152556	-2.868213	2.937352
H	2.049444	-1.719546	3.925743
H	4.009656	-1.740020	0.497057
H	3.778635	-1.841791	2.248189
H	2.875830	-2.912250	1.180755
C	-0.910963	0.212097	2.952040
C	3.055215	0.110137	-0.847199
C	-2.131616	-0.462744	2.708146
C	-3.204255	-0.245295	3.579642
C	-3.091479	0.615933	4.666676
C	-1.889803	1.280598	4.891991
C	-0.787837	1.097619	4.050128
H	-4.147110	-0.756991	3.402093
H	-3.936699	0.771693	5.332134
H	-1.807670	1.959869	5.737071
C	2.872298	-0.647862	-2.029292
C	3.785922	-0.487932	-3.076559
C	4.856925	0.394872	-2.975633
C	5.022601	1.140441	-1.812524
C	4.135795	1.018396	-0.737592
H	3.654728	-1.062024	-3.990499
H	5.556116	0.504096	-3.800683
H	5.856088	1.834931	-1.739417
C	4.326919	1.880875	0.501441
H	3.607755	1.536334	1.250918
C	4.007792	3.353372	0.201485
H	4.094712	3.961765	1.109648
H	4.696938	3.765950	-0.544758
H	2.989941	3.470215	-0.187351
C	5.729050	1.740055	1.108412
H	5.799054	2.310803	2.041829
H	5.966376	0.694780	1.333750
H	6.505787	2.119857	0.434815
C	1.688875	-1.590024	-2.196913
H	1.203586	-1.682517	-1.220204
C	0.654078	-1.001906	-3.168521
H	-0.219026	-1.660284	-3.251060
H	0.305115	-0.018628	-2.832926
H	1.077795	-0.879084	-4.172193
C	2.107851	-2.998947	-2.636912
H	2.535651	-3.002766	-3.645940
H	2.852714	-3.428367	-1.958452
H	1.238512	-3.666717	-2.650412
C	-2.308687	-1.383753	1.509630
H	-1.325694	-1.504470	1.043400
C	-3.239063	-0.752840	0.462564
H	-2.864231	0.222571	0.132102
H	-3.324325	-1.398566	-0.419637
H	-4.247314	-0.602130	0.865899
C	-2.804102	-2.780879	1.906276
H	-2.147994	-3.244463	2.650713
H	-3.815796	-2.751406	2.326866
H	-2.835157	-3.436984	1.028498
C	0.494505	1.876482	4.305069
H	1.253380	1.489245	3.618330
C	0.304731	3.366999	3.984681
H	-0.027829	3.513968	2.950978
H	-0.445139	3.822747	4.641913
H	1.244883	3.915255	4.118758
C	1.025522	1.689657	5.732456
H	0.344829	2.112157	6.480378

H 1.167764 0.630718 5.973319
H 1.991467 2.194978 5.848619
Zero-point correction= 0.617268 (Hartree/Particle)
Thermal correction to Energy= 0.653244
Thermal correction to Enthalpy= 0.654189
Thermal correction to Gibbs Free Energy= 0.545729
Sum of electronic and zero-point Energies= -2978.767321
Sum of electronic and thermal Energies= -2978.731345
Sum of electronic and thermal Enthalpies= -2978.730401
Sum of electronic and thermal Free Energies= -2978.838860

$ZnDAD_R$ (toluene)

71
scf done: -2979.380965
Zn 0.038920 0.346205 -0.031114
N 0.220651 0.116398 1.995601
N 2.067102 0.106924 0.110083
C 2.272417 -0.711152 1.165736
C 1.276833 -0.705305 2.183267
C 1.347524 -1.705352 3.305274
C 3.389167 -1.718144 1.216540
H 0.560622 -1.530389 4.041263
H 1.247493 -2.739410 2.945081
H 2.309858 -1.646537 3.825861
H 4.113251 -1.546291 0.417944
H 3.925543 -1.664308 2.170346
H 3.021181 -2.749867 1.120508
C -0.838585 0.204414 2.937762
C 2.984681 0.183218 -0.971586
C -1.945264 -0.680821 2.913024
C -2.989015 -0.474605 3.823429
C -2.952822 0.561041 4.751179
C -1.859253 1.421466 4.770824
C -0.798247 1.269286 3.872924
H -3.846784 -1.142818 3.808058
H -3.772015 0.697701 5.452601
H -1.831607 2.233547 5.493704
C 2.931606 -0.710629 -2.070379
C 3.816992 -0.514520 -3.137330
C 4.747218 0.519529 -3.131737
C 4.794919 1.388425 -2.045778
C 3.922607 1.246357 -0.962202
H 3.779424 -1.189250 -3.989295
H 5.428775 0.648415 -3.968754
H 5.519581 2.199394 -2.042262
C -2.045692 -1.835466 1.926847
H -1.095567 -1.887233 1.383298
C -2.251871 -3.186097 2.626194
H -2.223286 -4.001892 1.894197
H -1.475359 -3.376454 3.374499
H -3.221794 -3.237137 3.134001
C -3.149830 -1.590426 0.888500
H -4.135478 -1.518057 1.362935
H -2.975100 -0.659721 0.335806
H -3.186869 -2.410757 0.161513
C 0.367742 2.246243 3.915556
H 1.038226 1.979427 3.093628
C 1.161327 2.126838 5.224507
H 1.525786 1.105969 5.381427
H 2.030211 2.795674 5.210333
H 0.548134 2.398077 6.092284
C -0.090447 3.693530 3.687978
H -0.641080 3.795413 2.746380
H -0.743489 4.045672 4.495132
H 0.774307 4.366438 3.647143
C 3.994491 2.232929 0.194255
H 3.191468 1.970072 0.888715
C 3.751112 3.675693 -0.270100
H 4.539285 4.023468 -0.948191
H 2.794582 3.770817 -0.795643
H 3.732423 4.356193 0.589464
C 5.324455 2.123120 0.953450
H 5.331743 2.799251 1.816747
H 5.493349 1.105676 1.322165
H 6.175006 2.391079 0.315238
C 1.940632 -1.863526 -2.138553
H 1.418780 -1.906078 -1.175933
C 0.877821 -1.625295 -3.220702
H 0.147714 -2.443586 -3.233208
H 0.332137 -0.691234 -3.041951
H 1.329411 -1.563712 -4.217748
C 2.632051 -3.217523 -2.349327
H 3.117401 -3.277768 -3.330148
H 3.397582 -3.403220 -1.588665
H 1.899101 -4.031301 -2.297218
Zero-point correction= 0.616524 (Hartree/Particle)
Thermal correction to Energy= 0.652198
Thermal correction to Enthalpy= 0.653142
Thermal correction to Gibbs Free Energy= 0.547650
Sum of electronic and zero-point Energies= -2978.764441
Sum of electronic and thermal Energies= -2978.728767
Sum of electronic and thermal Enthalpies= -2978.727823
Sum of electronic and thermal Free Energies= -2978.833314

$ZnDAD_U$ (toluene)

71
scf done: -2979.389285
Zn 0.379776 1.172441 0.316940
N 0.150707 0.057969 2.026596
N 2.081816 0.018288 0.181325
C 2.180659 -0.847516 1.201401
C 1.147884 -0.824840 2.190521
C 1.209992 -1.771493 3.357670
C 3.318727 -1.822415 1.332418
H 0.330749 -1.668471 3.996027
H 1.264305 -2.815086 3.024537
H 2.097693 -1.591307 3.977236
H 4.025251 -1.717180 0.507266
H 3.870212 -1.674918 2.269308
H 2.960217 -2.859443 1.336978
C -0.919083 0.196599 2.945233
C 3.040859 0.101971 -0.858042
C -2.140015 -0.478526 2.702987
C -3.212750 -0.260337 3.574301
C -3.099829 0.602914 4.659916
C -1.897920 1.268109 4.883869
C -0.795629 1.083779 4.042408
H -4.155378 -0.772975 3.397959
H -3.944864 0.759806 5.325488
H -1.816070 1.948993 5.727686

C	2.845742	-0.632901	-2.052729
C	3.759660	-0.468518	-3.099188
C	4.842832	0.397922	-2.985449
C	5.020745	1.121210	-1.809812
C	4.134659	0.992999	-0.734753
H	3.619248	-1.026241	-4.021992
H	5.542239	0.511768	-3.809808
H	5.863494	1.803379	-1.727151
C	4.340490	1.833882	0.516855
H	3.621688	1.486567	1.265296
C	4.035209	3.313950	0.240971
H	4.134084	3.907402	1.157845
H	4.724422	3.730404	-0.503126
H	3.015937	3.446927	-0.139085
C	5.744160	1.670119	1.114350
H	5.823297	2.223611	2.057460
H	5.973953	0.619106	1.320236
H	6.520874	2.055568	0.443902
C	1.652817	-1.561023	-2.230248
H	1.155529	-1.641239	-1.258536
C	0.636877	-0.967951	-3.218167
H	-0.242802	-1.616888	-3.306137
H	0.295061	0.021453	-2.893023
H	1.072614	-0.856998	-4.218145
C	2.062779	-2.977106	-2.655336
H	2.512579	-2.990460	-3.654788
H	2.787118	-3.412286	-1.958322
H	1.185614	-3.634236	-2.684053
C	-2.315147	-1.402401	1.506477
H	-1.331702	-1.520616	1.040686
C	-3.247934	-0.776396	0.458799
H	-2.876295	0.199678	0.126184
H	-3.331329	-1.423958	-0.422318
H	-4.256731	-0.628150	0.861920
C	-2.805951	-2.799949	1.906709
H	-2.146636	-3.259721	2.650879
H	-3.817163	-2.772783	2.328841
H	-2.835929	-3.458075	1.030321
C	0.485211	1.866000	4.295264
H	1.250905	1.467168	3.622897
C	0.298452	3.350426	3.945993
H	-0.022188	3.478442	2.905856
H	-0.458936	3.816963	4.586963
H	1.236997	3.901476	4.080546
C	1.003481	1.706509	5.730491
H	0.319450	2.148513	6.463958
H	1.138843	0.652327	5.995269
H	1.971034	2.209580	5.843418

Zero-point correction= 0.617197 (Hartree/Particle)
Thermal correction to Energy= 0.652159
Thermal correction to Enthalpy= 0.653104
Thermal correction to Gibbs Free Energy= 0.547926
Sum of electronic and zero-point Energies= -2978.772088
Sum of electronic and thermal Energies= -2978.737126
Sum of electronic and thermal Enthalpies= -2978.736182
Sum of electronic and thermal Free Energies= -2978.841359

$ZnDAD_{BS}$ (toluene)

71
scf done: -2979.387345

Zn	0.387531	1.174753	0.315634
N	0.168758	0.083478	2.041638
N	2.104834	0.039622	0.201464
C	2.162585	-0.872280	1.185139
C	1.127653	-0.847155	2.171488
C	1.138326	-1.848137	3.294161
C	3.252493	-1.905423	1.270923
H	0.279573	-1.709669	3.953343
H	1.111487	-2.878252	2.917476
H	2.046190	-1.758166	3.903652
H	4.000072	-1.755231	0.489974
H	3.765276	-1.868001	2.239566
H	2.855115	-2.922985	1.163161
C	-0.908505	0.217343	2.951658
C	3.057588	0.111433	-0.844100
C	-2.127798	-0.461286	2.709227
C	-3.202840	-0.241491	3.577395
C	-3.094185	0.625756	4.660381
C	-1.894127	1.294047	4.884724
C	-0.790098	1.108762	4.045836
H	-4.144423	-0.755908	3.400567
H	-3.941209	0.783186	5.323298
H	-1.814832	1.977729	5.726643
C	2.874480	-0.646953	-2.026387
C	3.786412	-0.485947	-3.075161
C	4.856764	0.398193	-2.975858
C	5.023458	1.143732	-1.812630
C	4.138116	1.020486	-0.736456
H	3.654585	-1.060197	-3.988976
H	5.554726	0.508141	-3.801975
H	5.856653	1.838772	-1.740398
C	4.330858	1.881705	0.503177
H	3.612967	1.535699	1.253175
C	4.010898	3.354400	0.205536
H	4.098879	3.961648	1.114454
H	4.698898	3.768351	-0.541122
H	2.992215	3.471595	-0.181466
C	5.733976	1.740649	1.107507
H	5.805288	2.310328	2.041564
H	5.971529	0.695056	1.331661
H	6.509523	2.121318	0.432919
C	1.691942	-1.590568	-2.192302
H	1.210882	-1.687258	-1.213945
C	0.652361	-1.000614	-3.157571
H	-0.219958	-1.660284	-3.239171
H	0.302654	-0.019278	-2.816499
H	1.071959	-0.873228	-4.162493
C	2.110943	-2.997209	-2.639106
H	2.533210	-2.997312	-3.650532
H	2.859892	-3.427722	-1.965699
H	1.242504	-3.666313	-2.649796
C	-2.300791	-1.388722	1.515037
H	-1.316892	-1.509383	1.050822
C	-3.231040	-0.765406	0.463433
H	-2.857351	0.208908	0.127912
H	-3.313654	-1.416152	-0.415424
H	-4.240286	-0.614602	0.864422
C	-2.793584	-2.784880	1.917944
H	-2.137646	-3.242937	2.666083
H	-3.806381	-2.755794	2.336077
H	-2.820796	-3.445704	1.043491
C	0.491263	1.888930	4.301493
H	1.247672	1.508758	3.608150
C	0.297511	3.381751	3.995358
H	-0.040223	3.537349	2.964456
H	-0.449338	3.831248	4.660398
H	1.237728	3.930040	4.129350

C	1.028119	1.690030	5.725019
H	0.347164	2.100673	6.479421
H	1.177215	0.629228	5.953713
H	1.991894	2.199164	5.843398

Zero-point correction= 0.617070 (Hartree/Particle)
Thermal correction to Energy= 0.653030
Thermal correction to Enthalpy= 0.653974
Thermal correction to Gibbs Free Energy= 0.545690
Sum of electronic and zero-point Energies= -2978.770275
Sum of electronic and thermal Energies= -2978.734315
Sum of electronic and thermal Enthalpies= -2978.733371
Sum of electronic and thermal Free Energies= -2978.841655

$ZnDAD_R$ (chlorobenzene)

71
scf done: -2979.396749

Zn	0.177101	0.067642	0.108497
N	0.157773	-0.202845	1.997792
N	2.063464	-0.208985	0.048983
C	2.414836	-0.678921	1.334280
C	1.449706	-0.675183	2.321929
C	1.609022	-1.346215	3.659754
C	3.754807	-1.351473	1.466342
H	1.291283	-0.695872	4.482797
H	0.989665	-2.253278	3.727247
H	2.640558	-1.636760	3.861941
H	4.570694	-0.704661	1.123898
H	3.981364	-1.634071	2.494996
H	3.806368	-2.263457	0.852770
C	-0.841506	0.031019	2.956314
C	2.998434	0.013602	-0.975345
C	-2.041753	-0.737067	2.935731
C	-3.066834	-0.436677	3.840453
C	-2.930881	0.578375	4.783424
C	-1.751307	1.319526	4.815148
C	-0.707900	1.076430	3.915871
H	-3.984309	-1.020489	3.818331
H	-3.734051	0.790564	5.485030
H	-1.649570	2.121909	5.542417
C	2.950253	-0.767538	-2.166045
C	3.827137	-0.474828	-3.217273
C	4.769534	0.544718	-3.116110
C	4.829845	1.297376	-1.944969
C	3.958592	1.061978	-0.876317
H	3.782648	-1.067698	-4.128167
H	5.449092	0.751371	-3.939436
H	5.557346	2.102454	-1.869605
C	-2.233236	-1.875092	1.944442
H	-1.244142	-2.091446	1.526515
C	-2.748001	-3.163589	2.598288
H	-2.760197	-3.980470	1.866764
H	-2.108132	-3.469394	3.433242
H	-3.769476	-3.054200	2.980679
C	-3.150612	-1.461312	0.783716
H	-4.162007	-1.235015	1.142460
H	-2.783375	-0.562338	0.272130
H	-3.230673	-2.263762	0.039830
C	0.504161	1.999195	3.916630
H	1.287914	1.517223	3.324943
C	1.076020	2.256700	5.316450
H	1.302949	1.320703	5.838525
H	2.005278	2.833929	5.243703
H	0.385579	2.831514	5.944805
C	0.161243	3.330321	3.228215
H	-0.203692	3.171933	2.206992
H	-0.617551	3.870056	3.780824
H	1.044257	3.978287	3.172838
C	3.989987	1.994691	0.327566
H	3.416252	1.520180	1.129006
C	3.296599	3.324682	-0.009550
H	3.831414	3.856610	-0.805924
H	2.266454	3.165813	-0.348314
H	3.264094	3.980036	0.869131
C	5.403971	2.253040	0.863066
H	5.355650	2.839924	1.787859
H	5.928150	1.317459	1.086828
H	6.017304	2.818388	0.151608
C	1.959538	-1.911626	-2.320199
H	1.558370	-2.110890	-1.320645
C	0.782669	-1.518668	-3.226065
H	0.040952	-2.325301	-3.279596
H	0.273394	-0.615424	-2.866254
H	1.123733	-1.309301	-4.247172
C	2.610612	-3.206891	-2.821472
H	2.980876	-3.113128	-3.848941
H	3.454041	-3.499875	-2.186746
H	1.881410	-4.025889	-2.811480

Zero-point correction= 0.615572 (Hartree/Particle)
Thermal correction to Energy= 0.651127
Thermal correction to Enthalpy= 0.652071
Thermal correction to Gibbs Free Energy= 0.546583
Sum of electronic and zero-point Energies= -2978.781177
Sum of electronic and thermal Energies= -2978.745622
Sum of electronic and thermal Enthalpies= -2978.744678
Sum of electronic and thermal Free Energies= -2978.850166

$ZnDAD_U$ (chlorobenzene)

71
scf done: -2979.397855

Zn	0.237209	0.891568	0.172209
N	0.228125	-0.010656	2.032660
N	2.095093	0.004502	0.124902
C	2.353473	-0.697872	1.238847
C	1.354325	-0.704277	2.261901
C	1.591691	-1.475247	3.531810
C	3.630454	-1.468417	1.435711
H	0.695773	-1.492858	4.155422
H	1.878044	-2.512386	3.321466
H	2.403922	-1.037099	4.126427
H	4.320784	-1.306021	0.605917
H	4.139143	-1.176303	2.362192
H	3.440666	-2.547421	1.505365
C	-0.819766	0.097724	2.976078
C	2.999857	0.098446	-0.958890
C	-1.986824	-0.688455	2.811671
C	-3.054406	-0.505846	3.698792
C	-2.987465	0.427209	4.729328
C	-1.838719	1.201324	4.879012
C	-0.746083	1.058887	4.016727
H	-3.953966	-1.105503	3.579661

H	-3.825641	0.554016	5.410107
H	-1.794252	1.936108	5.679005
C	2.905126	-0.817185	-2.036376
C	3.746417	-0.645988	-3.141719
C	4.663964	0.400138	-3.199005
C	4.745430	1.298124	-2.137922
C	3.925519	1.170086	-1.010778
H	3.679594	-1.341797	-3.974860
H	5.308973	0.516495	-4.066471
H	5.457481	2.118759	-2.187528
C	-2.108303	-1.708122	1.688488
H	-1.139675	-1.745339	1.179822
C	-2.409928	-3.119526	2.210340
H	-2.415134	-3.838173	1.382230
H	-1.657924	-3.447541	2.936486
H	-3.390627	-3.171827	2.697371
C	-3.156338	-1.273259	0.653564
H	-4.156097	-1.212095	1.099775
H	-2.915731	-0.289337	0.233704
H	-3.202692	-1.991179	-0.174213
C	0.463092	1.971744	4.165744
H	1.285743	1.524730	3.599695
C	0.935098	2.121757	5.616964
H	1.121078	1.147882	6.083178
H	1.868571	2.695511	5.650740
H	0.204133	2.655687	6.234803
C	0.177014	3.347678	3.543092
H	-0.105573	3.257020	2.487653
H	-0.643327	3.852773	4.067124
H	1.062630	3.991941	3.601774
C	4.023039	2.193970	0.110997
H	3.372567	1.851686	0.921602
C	3.503939	3.565609	-0.345993
H	4.115866	3.971899	-1.160078
H	2.470131	3.500623	-0.704706
H	3.529714	4.283603	0.482526
C	5.444650	2.310894	0.677087
H	5.458236	2.998583	1.530970
H	5.821553	1.341030	1.019830
H	6.148677	2.699003	-0.068167
C	1.888019	-1.949294	-2.029661
H	1.449949	-1.987425	-1.027525
C	0.747224	-1.667789	-3.019431
H	-0.007151	-2.462704	-2.976782
H	0.249468	-0.717272	-2.793603
H	1.120431	-1.613905	-4.049154
C	2.523778	-3.317737	-2.307272
H	2.930920	-3.380068	-3.323054
H	3.338081	-3.531707	-1.606290
H	1.774146	-4.111358	-2.205918

Zero-point correction= 0.616310 (Hartree/Particle)
Thermal correction to Energy= 0.652125
Thermal correction to Enthalpy= 0.653069
Thermal correction to Gibbs Free Energy= 0.545005
Sum of electronic and zero-point Energies= -2978.781544
Sum of electronic and thermal Energies= -2978.745729
Sum of electronic and thermal Enthalpies= -2978.744785
Sum of electronic and thermal Free Energies= -2978.852849

$ZnDAD_{BS}$ (chlorobenzene)

71
scf done: -2979.396480

Zn	0.390657	1.203109	0.355159
N	0.209690	0.094796	2.097815
N	2.129625	0.064122	0.242358
C	2.144167	-0.910624	1.166873
C	1.116987	-0.894082	2.159585
C	1.073865	-1.969010	3.214240
C	3.169762	-2.012205	1.170954
H	0.199389	-1.853789	3.856736
H	1.044125	-2.973347	2.771840
H	1.965783	-1.932216	3.854376
H	3.992141	-1.787108	0.483161
H	3.593566	-2.160429	2.174760
H	2.730127	-2.978690	0.865964
C	-0.877342	0.205137	2.993928
C	3.060900	0.136426	-0.817490
C	-2.092963	-0.482439	2.743147
C	-3.179179	-0.265280	3.597708
C	-3.086774	0.606251	4.681248
C	-1.890487	1.277693	4.918599
C	-0.776801	1.094161	4.094194
H	-4.116227	-0.785036	3.411855
H	-3.941909	0.761874	5.334430
H	-1.823364	1.961393	5.763260
C	2.870024	-0.617071	-2.004588
C	3.766910	-0.442982	-3.065053
C	4.834108	0.447292	-2.974963
C	5.009385	1.188573	-1.810507
C	4.138424	1.054353	-0.723586
H	3.624869	-1.013384	-3.979112
H	5.520360	0.566486	-3.809807
H	5.839154	1.890663	-1.743338
C	4.344527	1.907107	0.518715
H	3.621849	1.568366	1.267396
C	4.052043	3.385783	0.229100
H	4.147401	3.985376	1.141406
H	4.749024	3.793985	-0.511756
H	3.034262	3.523420	-0.158922
C	5.745444	1.738440	1.120294
H	5.831191	2.308644	2.054205
H	5.960323	0.687331	1.346683
H	6.526619	2.101080	0.442013
C	1.689615	-1.564552	-2.165862
H	1.224954	-1.680349	-1.181911
C	0.631215	-0.963763	-3.103994
H	-0.237891	-1.628119	-3.182697
H	0.280869	0.008721	-2.735865
H	1.035088	-0.815207	-4.112924
C	2.107278	-2.961118	-2.646852
H	2.506940	-2.938249	-3.666448
H	2.873292	-3.397020	-1.997362
H	1.241572	-3.633857	-2.647135
C	-2.249663	-1.414015	1.549944
H	-1.262269	-1.534720	1.095854
C	-3.170435	-0.794837	0.484540
H	-2.790573	0.176868	0.148261
H	-3.244828	-1.450876	-0.391204
H	-4.183774	-0.642982	0.876784
C	-2.747974	-2.808316	1.949853
H	-2.102549	-3.263667	2.708700
H	-3.767094	-2.778133	2.352850
H	-2.761796	-3.472338	1.077450
C	0.502180	1.879409	4.346488
H	1.304409	1.381142	3.792302

C	0.379404	3.306796	3.790418
H	0.142702	3.299898	2.717852
H	-0.415002	3.860624	4.303190
H	1.317265	3.859579	3.923305
C	0.915751	1.907617	5.822561
H	0.206043	2.472514	6.439788
H	0.991890	0.898618	6.239521
H	1.893358	2.391992	5.931518

Zero-point correction= 0.615742 (Hartree/Particle)
Thermal correction to Energy= 0.650983
Thermal correction to Enthalpy= 0.651927
Thermal correction to Gibbs Free Energy= 0.545112
Sum of electronic and zero-point Energies= -2978.780738
Sum of electronic and thermal Energies= -2978.745497
Sum of electronic and thermal Enthalpies= -2978.744553
Sum of electronic and thermal Free Energies= -2978.851368

$ZnDAD_R$ (THF)

71
scf done: -2979.391195

C	3.705861	-1.153248	-0.936563
C	2.847444	-0.015950	-1.030053
C	2.898429	0.785367	-2.208671
C	3.798356	0.441078	-3.227491
C	4.655019	-0.651061	-3.121837
C	4.598405	-1.438504	-1.975174
N	1.937434	0.285324	-0.002970
C	2.359414	0.622942	1.306243
C	3.770342	1.127845	1.449971
Zn	0.049974	0.016254	0.131513
N	0.087823	0.285338	2.019401
C	-0.884095	0.039034	3.002581
C	-2.039441	0.870715	3.073930
C	-3.045007	0.577823	4.002441
C	-2.932182	-0.494843	4.882854
C	-1.798221	-1.302716	4.823198
C	-0.778045	-1.067685	3.895133
C	1.426598	0.633092	2.323221
C	1.676634	1.186377	3.700849
H	1.395831	0.476925	4.488286
H	2.722482	1.447717	3.865720
H	1.077513	2.092288	3.876459
H	4.509687	0.375611	1.149295
H	3.945767	2.002643	0.808091
H	4.009448	1.417002	2.473895
C	-2.204686	2.070115	2.153216
H	-3.928135	1.211548	4.048372
H	-3.718452	-0.701031	5.605257
H	-1.716581	-2.150796	5.499623
C	0.370121	-2.062924	3.789290
C	2.033003	2.017770	-2.469546
H	3.836706	1.063628	-4.120058
H	5.353193	-0.885513	-3.921788
H	5.248500	-2.306888	-1.895362
C	3.593589	-2.132317	0.225420
H	2.455470	2.468242	-3.378020
C	0.582372	1.669373	-2.831416
C	2.101129	3.107547	-1.392357
H	1.560679	3.999726	-1.733111
H	1.662513	2.777915	-0.447818
H	3.138092	3.403467	-1.198446
H	0.045994	2.564244	-3.170339
H	0.538086	0.924769	-3.634051
H	0.029105	1.270918	-1.971769
C	4.947678	-2.587280	0.783770
H	3.057094	-1.628979	1.035166
C	2.757173	-3.352079	-0.195148
H	4.798378	-3.191500	1.686349
H	5.503034	-3.205720	0.068897
H	5.581953	-1.735355	1.052427
H	2.621306	-4.041014	0.647137
H	1.763320	-3.055273	-0.549954
H	3.249026	-3.904679	-1.005114
C	-3.222125	1.784874	1.038323
C	-2.578869	3.354049	2.904579
H	-1.229514	2.235149	1.682900
H	-3.293226	2.632057	0.344887
H	-2.947556	0.895916	0.456149
H	-4.221957	1.605866	1.452103
H	-2.583214	4.208247	2.216770
H	-3.576400	3.292919	3.355130
H	-1.862250	3.570266	3.704656
C	0.980714	-2.441560	5.144337
C	-0.089724	-3.325979	3.043039
H	1.159123	-1.597007	3.191244
H	0.743276	-4.027571	2.914852
H	-0.881844	-3.843632	3.597891
H	-0.482307	-3.085065	2.048402
H	1.869098	-3.066722	4.995847
H	1.285512	-1.555884	5.712616
H	0.282037	-3.013768	5.765837

Zero-point correction= 0.616275 (Hartree/Particle)
Thermal correction to Energy= 0.651485
Thermal correction to Enthalpy= 0.652429
Thermal correction to Gibbs Free Energy= 0.547756
Sum of electronic and zero-point Energies= -2978.774920
Sum of electronic and thermal Energies= -2978.739710
Sum of electronic and thermal Enthalpies= -2978.738766
Sum of electronic and thermal Free Energies= -2978.843439

$ZnDAD_U$ (THF)

71
scf done: -2979.388806

C	3.725574	-1.139153	-1.034893
C	2.843516	-0.025236	-1.040699
C	2.821515	0.854725	-2.155028
C	3.697614	0.604078	-3.220331
C	4.570038	-0.480591	-3.219093
C	4.573615	-1.344889	-2.129067
N	1.927958	0.137618	0.025794
C	2.287308	0.644815	1.216494
C	3.641984	1.250669	1.466360
Zn	0.030483	-0.704148	0.076070
N	0.149443	0.017510	2.030701
C	-0.880978	-0.085128	2.993054

C	-1.958127	0.835516	2.964214
C	-3.017783	0.664739	3.862742
C	-3.032060	-0.387429	4.774428
C	-1.972151	-1.291030	4.792240
C	-0.889724	-1.163058	3.914339
C	1.326699	0.612677	2.274930
C	1.661944	1.237119	3.602620
H	0.820825	1.167896	4.294927
H	2.525422	0.748811	4.071757
H	1.920624	2.297541	3.492801
H	4.254600	1.236935	0.563245
H	3.557730	2.292257	1.799931
H	4.187145	0.711940	2.251681
C	-1.993057	1.990196	1.974167
H	-3.847517	1.368021	3.846258
H	-3.863824	-0.504247	5.464938
H	-1.988802	-2.116646	5.500001
C	0.223378	-2.200478	3.938372
C	1.888852	2.054501	-2.303018
H	3.688190	1.281676	-4.072135
H	5.237038	-0.651214	-4.060545
H	5.244250	-2.200798	-2.129182
C	3.727904	-2.150120	0.104016
H	2.227117	2.561454	-3.216475
C	0.434525	1.637718	-2.561244
C	1.983022	3.097249	-1.182152
H	1.427307	3.997823	-1.470611
H	1.561072	2.732062	-0.242744
H	3.021852	3.393426	-0.999004
H	-0.187159	2.520490	-2.755533
H	0.360949	0.974550	-3.430528
H	0.006162	1.106077	-1.702102
C	5.137600	-2.476784	0.613021
H	3.174711	-1.712746	0.939630
C	2.989105	-3.432063	-0.311369
H	5.078587	-3.124529	1.495574
H	5.734324	-3.005438	-0.139050
H	5.683267	-1.570105	0.896747
H	2.950892	-4.144450	0.521622
H	1.958495	-3.216031	-0.618152
H	3.493479	-3.923359	-1.152206
C	-3.132815	1.821276	0.959071
C	-2.083583	3.352423	2.675088
H	-1.050986	1.967961	1.417552
H	-3.114474	2.631753	0.220504
H	-3.046362	0.870765	0.419451
H	-4.112413	1.840113	1.451456
H	-2.035434	4.163904	1.939196
H	-3.024855	3.462094	3.226440
H	-1.261125	3.492347	3.385392
C	0.815065	-2.402000	5.339560
C	-0.262307	-3.536577	3.356054
H	1.026740	-1.835438	3.291723
H	0.555627	-4.266637	3.328582
H	-1.071217	-3.961697	3.962247
H	-0.639162	-3.412403	2.334218
H	1.669674	-3.087438	5.294941
H	1.164038	-1.456398	5.768842
H	0.084557	-2.835035	6.032687

Zero-point correction= 0.616621
(Hartree/Particle)
Thermal correction to Energy= 0.652216
Thermal correction to Enthalpy= 0.653160
Thermal correction to Gibbs Free Energy= 0.545940
Sum of electronic and zero-point Energies= -2978.772185
Sum of electronic and thermal Energies= -2978.736590
Sum of electronic and thermal Enthalpies= -2978.735646
Sum of electronic and thermal Free Energies= -2978.842866

$ZnDAD_{BS}$ (THF)

71
scf done: -2979.391195

C	3.705861	-1.153248	-0.936563
C	2.847444	-0.015950	-1.030053
C	2.898429	0.785367	-2.208671
C	3.798356	0.441078	-3.227491
C	4.655019	-0.651061	-3.121837
C	4.598405	-1.438504	-1.975174
N	1.937434	0.285324	-0.002970
C	2.359414	0.622942	1.306243
C	3.770342	1.127845	1.449971
Zn	0.049974	0.016254	0.131513
N	0.087823	0.285338	2.019401
C	-0.884095	0.039034	3.002581
C	-2.039441	0.870715	3.073930
C	-3.045007	0.577823	4.002441
C	-2.932182	-0.494843	4.882854
C	-1.798221	-1.302716	4.823198
C	-0.778045	-1.067685	3.895133
C	1.426598	0.633092	2.323221
C	1.676634	1.186377	3.700849
H	1.395831	0.476925	4.488286
H	2.722482	1.447717	3.865720
H	1.077513	2.092288	3.876459
H	4.509687	0.375611	1.149295
H	3.945767	2.002643	0.808091
H	4.009448	1.417002	2.473895
C	-2.204686	2.070115	2.153216
H	-3.928135	1.211548	4.048372
H	-3.718452	-0.701031	5.605257
H	-1.716581	-2.150796	5.499623
C	0.370121	-2.062924	3.789290
C	2.033003	2.017770	-2.469546
H	3.836706	1.063628	-4.120058
H	5.353193	-0.885513	-3.921788
H	5.248500	-2.306888	-1.895362
C	3.593589	-2.132317	0.225420
H	2.455470	2.468242	-3.378020
C	0.582372	1.669373	-2.831416
C	2.101129	3.107547	-1.392357
H	1.560679	3.999726	-1.733111
H	1.662513	2.777915	-0.447818
H	3.138092	3.403467	-1.198446
H	0.045994	2.564244	-3.170339
H	0.538086	0.924769	-3.634051
H	0.029105	1.270918	-1.971769
C	4.947678	-2.587280	0.783770
H	3.057094	-1.628979	1.035166
C	2.757173	-3.352079	-0.195148
H	4.798378	-3.191500	1.686349
H	5.503034	-3.205720	0.068897

H	5.581953	-1.735355	1.052427
H	2.621306	-4.041014	0.647137
H	1.763320	-3.055273	-0.549954
H	3.249026	-3.904679	-1.005114
C	-3.222125	1.784874	1.038323
C	-2.578869	3.354049	2.904579
H	-1.229514	2.235149	1.682900
H	-3.293226	2.632057	0.344887
H	-2.947556	0.895916	0.456149
H	-4.221957	1.605866	1.452103
H	-2.583214	4.208247	2.216770
H	-3.576400	3.292919	3.355130
H	-1.862250	3.570266	3.704656
C	0.980714	-2.441560	5.144337
C	-0.089724	-3.325979	3.043039
H	1.159123	-1.597007	3.191244
H	0.743276	-4.027571	2.914852
H	-0.881844	-3.843632	3.597891
H	-0.482307	-3.085065	2.048402
H	1.869098	-3.066722	4.995847
H	1.285512	-1.555884	5.712616
H	0.282037	-3.013768	5.765837

Zero-point correction= 0.616275 (Hartree/Particle)
Thermal correction to Energy= 0.651485
Thermal correction to Enthalpy= 0.652429
Thermal correction to Gibbs Free Energy= 0.547757
Sum of electronic and zero-point Energies= -2978.774920
Sum of electronic and thermal Energies= -2978.739710
Sum of electronic and thermal Enthalpies= -2978.738766
Sum of electronic and thermal Free Energies= -2978.843438

$ZnDAD_R$ (dichloroethane)

71
scf done: -2979.404284

Zn	0.188410	-0.041580	0.122611
N	0.187824	-0.300400	2.025459
N	2.089556	-0.305478	0.078362
C	2.468366	-0.678385	1.387427
C	1.505019	-0.673722	2.375104
C	1.694515	-1.278485	3.741029
C	3.834902	-1.290557	1.545878
H	1.332611	-0.616860	4.536270
H	1.127261	-2.216864	3.840666
H	2.739542	-1.500177	3.961596
H	4.626494	-0.631712	1.171042
H	4.075031	-1.519357	2.584998
H	3.917455	-2.226663	0.972275
C	-0.812457	-0.019688	2.964709
C	3.006468	-0.039583	-0.946611
C	-2.020927	-0.780621	2.942848
C	-3.054412	-0.461001	3.829833
C	-2.924843	0.570855	4.757685
C	-1.744064	1.309836	4.786241
C	-0.690431	1.047552	3.903155
H	-3.974095	-1.040778	3.810142
H	-3.734556	0.797418	5.447324
H	-1.649558	2.128687	5.496185
C	2.952903	-0.811394	-2.146955
C	3.814502	-0.502538	-3.205079
C	4.747743	0.527916	-3.107359
C	4.808833	1.275782	-1.933438
C	3.951813	1.024476	-0.855931
H	3.770851	-1.090042	-4.119033
H	5.417396	0.746000	-3.935965
H	5.523991	2.092519	-1.862782
C	-2.193058	-1.924037	1.954803
H	-1.182188	-2.258355	1.694030
C	-2.950044	-3.129833	2.522272
H	-2.911817	-3.963215	1.810772
H	-2.509486	-3.473058	3.464950
H	-4.008485	-2.910437	2.704681
C	-2.862396	-1.441111	0.659209
H	-3.875213	-1.067870	0.854218
H	-2.297820	-0.620751	0.194999
H	-2.936027	-2.253338	-0.074548
C	0.510875	1.984658	3.888513
H	1.307060	1.497146	3.317858
C	1.067368	2.293196	5.284265
H	1.303181	1.377199	5.837229
H	1.988958	2.881307	5.201126
H	0.363309	2.877216	5.888573
C	0.155292	3.290050	3.157972
H	-0.198536	3.096632	2.138803
H	-0.635398	3.834270	3.689005
H	1.029500	3.948850	3.091147
C	3.972619	1.968967	0.339486
H	3.416177	1.491040	1.151360
C	3.245777	3.278775	-0.007074
H	3.763478	3.813731	-0.812772
H	2.217123	3.092450	-0.336432
H	3.204784	3.943069	0.864569
C	5.383635	2.268228	0.861659
H	5.327276	2.864263	1.780198
H	5.933120	1.348786	1.092100
H	5.977092	2.840705	0.139124
C	1.961216	-1.956824	-2.283436
H	1.722683	-2.278333	-1.262944
C	0.650455	-1.484855	-2.930904
H	-0.079543	-2.301966	-2.985332
H	0.191408	-0.664303	-2.362169
H	0.823701	-1.117067	-3.949635
C	2.514486	-3.171996	-3.036171
H	2.673580	-2.966879	-4.101213
H	3.467223	-3.507443	-2.611537
H	1.805683	-4.006008	-2.971064

Zero-point correction= 0.617618 (Hartree/Particle)
Thermal correction to Energy= 0.652094
Thermal correction to Enthalpy= 0.653038
Thermal correction to Gibbs Free Energy= 0.552337
Sum of electronic and zero-point Energies= -2978.786666
Sum of electronic and thermal Energies= -2978.752190
Sum of electronic and thermal Enthalpies= -2978.751246
Sum of electronic and thermal Free Energies= -2978.851946

$ZnDAD_U$ (dichloroethane)

71
scf done: -2979.397913

Zn	0.227175	0.893195	0.163886
N	0.226885	-0.012652	2.032804

N	2.093600	0.004881	0.123463
C	2.353502	-0.695507	1.238224
C	1.354902	-0.703525	2.261445
C	1.594817	-1.474818	3.530897
C	3.632278	-1.463141	1.436074
H	0.697243	-1.500603	4.152068
H	1.889795	-2.509273	3.319301
H	2.402066	-1.031390	4.128463
H	4.325382	-1.294464	0.609706
H	4.136314	-1.174025	2.366000
H	3.445490	-2.543119	1.499625
C	-0.818406	0.095193	2.977376
C	2.997751	0.098810	-0.959422
C	-1.988600	-0.686627	2.811143
C	-3.056379	-0.502641	3.698111
C	-2.986666	0.427663	4.731395
C	-1.834696	1.197109	4.883918
C	-0.742082	1.053004	4.021536
H	-3.958029	-1.098847	3.576711
H	-3.824792	0.555756	5.412153
H	-1.788063	1.929695	5.685905
C	2.903950	-0.817539	-2.036832
C	3.741913	-0.644136	-3.144642
C	4.656634	0.404813	-3.204336
C	4.738849	1.302687	-2.142766
C	3.921808	1.172150	-1.013523
H	3.674728	-1.340191	-3.977660
H	5.299059	0.523076	-4.073587
H	5.449027	2.125000	-2.193538
C	-2.111986	-1.703790	1.686050
H	-1.141757	-1.745677	1.180841
C	-2.424333	-3.114030	2.204584
H	-2.430316	-3.831023	1.375024
H	-1.676709	-3.447744	2.932847
H	-3.407387	-3.160902	2.687497
C	-3.153412	-1.260563	0.648081
H	-4.153913	-1.191881	1.091773
H	-2.902385	-0.278710	0.228997
H	-3.202569	-1.978116	-0.179897
C	0.470132	1.961321	4.172851
H	1.293111	1.510093	3.610661
C	0.938032	2.112876	5.625116
H	1.120641	1.139105	6.093142
H	1.873031	2.684093	5.659951
H	0.206480	2.649799	6.239696
C	0.190716	3.336697	3.545909
H	-0.088389	3.243895	2.489575
H	-0.629283	3.845746	4.066858
H	1.078621	3.977715	3.605835
C	4.021173	2.194473	0.109335
H	3.373132	1.850479	0.921135
C	3.500057	3.566311	-0.344514
H	4.109818	3.973419	-1.159928
H	2.464808	3.500813	-0.699364
H	3.528245	4.283134	0.484966
C	5.444304	2.311244	0.671488
H	5.459742	2.998295	1.525878
H	5.821650	1.340959	1.012929
H	6.145794	2.699947	-0.075915
C	1.890811	-1.953027	-2.026510
H	1.458946	-1.994958	-1.021849
C	0.743264	-1.672404	-3.008617
H	-0.007669	-2.470507	-2.964144
H	0.243175	-0.724745	-2.775247
H	1.110850	-1.613711	-4.040198
C	2.529494	-3.318522	-2.311360
H	2.931518	-3.376408	-3.329477
H	3.347697	-3.531720	-1.614498
H	1.782608	-4.114492	-2.208027

Zero-point correction= 0.615837 (Hartree/Particle)
Thermal correction to Energy= 0.651732
Thermal correction to Enthalpy= 0.652676
Thermal correction to Gibbs Free Energy= 0.543905
Sum of electronic and zero-point Energies= -2978.782076
Sum of electronic and thermal Energies= -2978.746181
Sum of electronic and thermal Enthalpies= -2978.745237
Sum of electronic and thermal Free Energies= -2978.854008

$ZnDAD_{BS}$ (dichloroethane)

71
scf done: -2979.396777

Zn	0.390785	1.216841	0.375390
N	0.227167	0.100825	2.125848
N	2.138964	0.079186	0.261927
C	2.132565	-0.924187	1.157171
C	1.110301	-0.913145	2.152666
C	1.044092	-2.023358	3.166818
C	3.132896	-2.048387	1.128935
H	0.226370	-1.865190	3.872547
H	0.897048	-3.002268	2.692778
H	1.974863	-2.089228	3.743789
H	3.894828	-1.880150	0.365401
H	3.642681	-2.150242	2.094512
H	2.655734	-3.015094	0.921302
C	-0.865652	0.196271	3.017131
C	3.062630	0.155391	-0.805236
C	-2.068033	-0.514160	2.774437
C	-3.157721	-0.306639	3.629903
C	-3.078991	0.575494	4.703856
C	-1.893762	1.272025	4.934135
C	-0.778814	1.100993	4.106736
H	-4.086541	-0.842706	3.448871
H	-3.935869	0.721708	5.357104
H	-1.838013	1.962734	5.771620
C	2.855590	-0.578943	-2.001397
C	3.746217	-0.398321	-3.066423
C	4.821493	0.482327	-2.973286
C	5.013550	1.204766	-1.798204
C	4.149288	1.060891	-0.706686
H	3.592287	-0.953463	-3.988871
H	5.502443	0.606774	-3.811828
H	5.849258	1.897503	-1.727809
C	4.376607	1.890810	0.548197
H	3.643032	1.559604	1.289547
C	4.123404	3.381831	0.280050
H	4.234153	3.964043	1.202767
H	4.833955	3.780397	-0.454063
H	3.111848	3.551538	-0.106843
C	5.772770	1.675072	1.147128
H	5.873430	2.230626	2.087131
H	5.957728	0.616295	1.360250
H	6.562393	2.024521	0.471558
C	1.668328	-1.516849	-2.168309
H	1.199258	-1.632024	-1.186462
C	0.617099	-0.906754	-3.108327
H	-0.255534	-1.565966	-3.191428
H	0.271215	0.066176	-2.738837

H	1.025153	-0.760203	-4.115623
C	2.078697	-2.914832	-2.649685
H	2.485800	-2.892404	-3.667194
H	2.836101	-3.360231	-1.995405
H	1.208310	-3.581479	-2.660472
C	-2.215334	-1.456569	1.588242
H	-1.223332	-1.583751	1.144218
C	-3.123712	-0.844363	0.510823
H	-2.736918	0.123054	0.168468
H	-3.191444	-1.508138	-0.359664
H	-4.139410	-0.686204	0.892883
C	-2.720020	-2.847348	1.995362
H	-2.086927	-3.295248	2.769108
H	-3.745792	-2.811849	2.380260
H	-2.718954	-3.518743	1.128555
C	0.487790	1.911620	4.339764
H	1.307728	1.374766	3.851689
C	0.374502	3.287415	3.663605
H	0.167990	3.190908	2.590263
H	-0.437465	3.875639	4.108507
H	1.305824	3.855249	3.777975
C	0.854357	2.067630	5.819563
H	0.130189	2.685770	6.362552
H	0.915195	1.096884	6.324397
H	1.830997	2.556675	5.912562

Zero-point correction= 0.615399 (Hartree/Particle)
Thermal correction to Energy= 0.651456
Thermal correction to Enthalpy= 0.652400
Thermal correction to Gibbs Free Energy= 0.543292
Sum of electronic and zero-point Energies= -2978.781378
Sum of electronic and thermal Energies= -2978.745321
Sum of electronic and thermal Enthalpies= -2978.744377
Sum of electronic and thermal Free Energies= -2978.853486

$ZnDAD_R$ (1-pentanol)

71
scf done: -2979.403994

Zn	0.181670	-0.047397	0.120057
N	0.196199	-0.305892	2.029906
N	2.089703	-0.309379	0.080054
C	2.477480	-0.666085	1.390084
C	1.516899	-0.663123	2.380356
C	1.714443	-1.262020	3.747723
C	3.849218	-1.266384	1.548895
H	1.355381	-0.599919	4.544211
H	1.149410	-2.201545	3.852716
H	2.760738	-1.482066	3.964794
H	4.635417	-0.606669	1.163752
H	4.096934	-1.482768	2.589097
H	3.936169	-2.208247	0.984732
C	-0.801911	-0.031233	2.971462
C	3.002042	-0.040247	-0.946681
C	-2.009137	-0.795091	2.948404
C	-3.039262	-0.487330	3.843290
C	-2.909053	0.536653	4.779929
C	-1.731842	1.281587	4.807273
C	-0.681917	1.031402	3.916342
H	-3.957405	-1.069852	3.822973
H	-3.716064	0.753694	5.476060
H	-1.638782	2.096172	5.522470
C	2.947316	-0.813301	-2.146718
C	3.806535	-0.505121	-3.206884
C	4.739082	0.526436	-3.112659
C	4.800373	1.277188	-1.940443
C	3.945342	1.026794	-0.861170
H	3.761719	-1.093526	-4.120416
H	5.407186	0.743915	-3.942914
H	5.513809	2.095943	-1.873826
C	-2.183636	-1.928158	1.949449
H	-1.173476	-2.255764	1.677283
C	-2.931636	-3.142962	2.508910
H	-2.894684	-3.968860	1.788409
H	-2.483239	-3.495261	3.444850
H	-3.989973	-2.930875	2.701015
C	-2.863629	-1.432063	0.664670
H	-3.879514	-1.072440	0.870567
H	-2.309887	-0.599670	0.209718
H	-2.933697	-2.234006	-0.080880
C	0.510404	1.979635	3.896432
H	1.312810	1.496262	3.330579
C	1.062575	2.306536	5.289323
H	1.303739	1.398225	5.853002
H	1.980949	2.899218	5.201234
H	0.355056	2.893268	5.887056
C	0.141382	3.274240	3.153717
H	-0.209857	3.067641	2.136059
H	-0.655356	3.815267	3.679287
H	1.008350	3.942167	3.080555
C	3.962114	1.977907	0.328894
H	3.415446	1.498992	1.147088
C	3.217407	3.276164	-0.022486
H	3.724741	3.812995	-0.833726
H	2.189583	3.074885	-0.346172
H	3.171226	3.945770	0.845039
C	5.371569	2.297458	0.842266
H	5.312437	2.895655	1.759412
H	5.934847	1.386289	1.073304
H	5.954333	2.875669	0.115489
C	1.956018	-1.958994	-2.280702
H	1.714869	-2.276665	-1.259546
C	0.647007	-1.488721	-2.932459
H	-0.084068	-2.305320	-2.983127
H	0.187832	-0.664706	-2.369443
H	0.822269	-1.128316	-3.953763
C	2.511481	-3.176854	-3.027094
H	2.672544	-2.977186	-4.092990
H	3.463758	-3.510483	-2.599270
H	1.803407	-4.011506	-2.959442

Zero-point correction= 0.617360 (Hartree/Particle)
Thermal correction to Energy= 0.651881
Thermal correction to Enthalpy= 0.652825
Thermal correction to Gibbs Free Energy= 0.551950
Sum of electronic and zero-point Energies= -2978.786634
Sum of electronic and thermal Energies= -2978.752113
Sum of electronic and thermal Enthalpies= -2978.751168
Sum of electronic and thermal Free Energies= -2978.852044

$ZnDAD_U$ (1-pentanol)

71

scf done: -2979.394090

Zn	0.233603	0.903849	0.161877
N	0.236160	0.011125	2.038753
N	2.098295	-0.005600	0.123698
C	2.352833	-0.700807	1.243525
C	1.357184	-0.689571	2.269051
C	1.587414	-1.457105	3.542252
C	3.622680	-1.481981	1.444992
H	0.808333	-1.245056	4.277475
H	1.589249	-2.540702	3.363347
H	2.555138	-1.208657	3.993427
H	4.210202	-1.523854	0.525348
H	4.254568	-1.037027	2.224959
H	3.412090	-2.511406	1.757910
C	-0.821142	0.101192	2.972107
C	3.012875	0.091880	-0.948572
C	-1.896653	-0.819465	2.909563
C	-2.985166	-0.644802	3.772551
C	-3.025772	0.408688	4.682750
C	-1.963243	1.308050	4.738567
C	-0.852992	1.175671	3.896486
H	-3.818138	-1.342922	3.729323
H	-3.880402	0.528617	5.344503
H	-2.000221	2.131495	5.448056
C	2.803294	-0.689358	-2.112726
C	3.655396	-0.511413	-3.209238
C	4.697199	0.411673	-3.173789
C	4.894392	1.178040	-2.026945
C	4.067589	1.039553	-0.906226
H	3.500151	-1.105528	-4.107166
H	5.350007	0.535772	-4.034666
H	5.703164	1.904752	-2.006658
C	-1.905108	-1.960373	1.902937
H	-0.905104	-2.013226	1.461180
C	-2.194452	-3.320150	2.550853
H	-2.098976	-4.120989	1.807951
H	-1.493931	-3.533023	3.366303
H	-3.210660	-3.371685	2.958710
C	-2.895794	-1.676595	0.763890
H	-3.923360	-1.606494	1.141144
H	-2.658335	-0.733498	0.256579
H	-2.866214	-2.478403	0.015960
C	0.271236	2.199356	3.955813
H	1.115067	1.790184	3.391524
C	0.761054	2.468190	5.383961
H	1.058572	1.541672	5.888107
H	1.631805	3.134284	5.364507
H	-0.006659	2.953120	5.997957
C	-0.148812	3.507648	3.268671
H	-0.442742	3.332912	2.226356
H	-0.999136	3.969468	3.785362
H	0.677744	4.228742	3.269424
C	4.275655	1.942504	0.301151
H	3.688757	1.530769	1.127627
C	3.737027	3.353448	0.018015
H	4.287182	3.827785	-0.803839
H	2.676374	3.326853	-0.258859
H	3.838523	3.992060	0.904011
C	5.737216	2.001656	0.761600
H	5.816230	2.577341	1.691394
H	6.140619	1.000516	0.950862
H	6.382069	2.488902	0.021089
C	1.668200	-1.698989	-2.198129
H	1.205352	-1.750043	-1.207290
C	0.588807	-1.236853	-3.187663
H	-0.245103	-1.949071	-3.210592
H	0.186106	-0.256347	-2.905095
H	0.989278	-1.156742	-4.205607
C	2.163436	-3.108210	-2.548939
H	2.597215	-3.149546	-3.554971
H	2.925277	-3.453103	-1.840553
H	1.330683	-3.821157	-2.520557

Zero-point correction= 0.615587 (Hartree/Particle)
Thermal correction to Energy= 0.651541
Thermal correction to Enthalpy= 0.652485
Thermal correction to Gibbs Free Energy= 0.543240
Sum of electronic and zero-point Energies= -2978.778503
Sum of electronic and thermal Energies= -2978.742549
Sum of electronic and thermal Enthalpies= -2978.741605
Sum of electronic and thermal Free Energies= -2978.850850

$ZnDAD_{BS}$ (1-pentanol)

71

scf done: -2979.393122

Zn	0.398134	1.223391	0.383876
N	0.236491	0.107410	2.137217
N	2.149551	0.085293	0.273971
C	2.132493	-0.926898	1.160503
C	1.110881	-0.915422	2.154891
C	1.031848	-2.036259	3.156114
C	3.122997	-2.059478	1.123153
H	0.247216	-1.853806	3.893290
H	0.825273	-3.001988	2.676238
H	1.978534	-2.150761	3.698113
H	3.859825	-1.914954	0.330497
H	3.667328	-2.141441	2.072264
H	2.633345	-3.027716	0.956450
C	-0.860792	0.195537	3.022894
C	3.071036	0.153606	-0.795200
C	-2.059312	-0.519857	2.776448
C	-3.152686	-0.317079	3.628663
C	-3.080587	0.564385	4.703449
C	-1.898637	1.265373	4.938552
C	-0.781008	1.099487	4.114066
H	-4.079291	-0.856259	3.444876
H	-3.940155	0.706588	5.354346
H	-1.848985	1.954934	5.777386
C	2.849374	-0.568609	-1.995973
C	3.737120	-0.390686	-3.064080
C	4.823994	0.475092	-2.968697
C	5.033148	1.183075	-1.787453
C	4.172998	1.040256	-0.692693
H	3.572090	-0.935914	-3.990686
H	5.502081	0.598560	-3.809934
H	5.879413	1.862783	-1.716473
C	4.411930	1.857439	0.568124
H	3.726124	1.478412	1.332137
C	4.070747	3.336716	0.333804
H	4.190474	3.913476	1.259015
H	4.727747	3.779500	-0.424814
H	3.035849	3.458588	-0.007603
C	5.838785	1.707374	1.110089
H	5.940913	2.243222	2.061384
H	6.091147	0.655838	1.288314
H	6.584291	2.119775	0.420123
C	1.652384	-1.493528	-2.163948
H	1.181417	-1.605320	-1.182453

C	0.607995	-0.872221	-3.103645
H	-0.271521	-1.522332	-3.187735
H	0.271277	0.103474	-2.732307
H	1.017019	-0.728248	-4.111080
C	2.049732	-2.894750	-2.646331
H	2.457386	-2.875876	-3.663826
H	2.802617	-3.348241	-1.992090
H	1.173315	-3.553697	-2.657500
C	-2.199997	-1.462145	1.589616
H	-1.206269	-1.588527	1.148980
C	-3.104288	-0.850233	0.508985
H	-2.716021	0.117459	0.168361
H	-3.167923	-1.513327	-0.362516
H	-4.122004	-0.692674	0.886328
C	-2.705243	-2.853167	1.994349
H	-2.078211	-3.299305	2.774256
H	-3.734603	-2.820008	2.370094
H	-2.694932	-3.526163	1.128679
C	0.483679	1.912454	4.347274
H	1.313147	1.350966	3.904150
C	0.395213	3.257376	3.608808
H	0.212462	3.114269	2.535951
H	-0.423004	3.869256	4.008575
H	1.327307	3.825092	3.718659
C	0.813971	2.131746	5.826902
H	0.084465	2.781884	6.323555
H	0.851754	1.184535	6.377167
H	1.793816	2.614085	5.922349

Zero-point correction= 0.615327 (Hartree/Particle)
Thermal correction to Energy= 0.651315
Thermal correction to Enthalpy= 0.652260
Thermal correction to Gibbs Free Energy= 0.544033
Sum of electronic and zero-point Energies= -2978.777796
Sum of electronic and thermal Energies= -2978.741807
Sum of electronic and thermal Enthalpies= -2978.740863
Sum of electronic and thermal Free Energies= -2978.849089

$ZnDAD_R$ (acetone)

71
scf done: -2979.411490

Zn	0.186589	-0.053230	0.119212
N	0.201148	-0.310995	2.033280
N	2.097456	-0.320242	0.089460
C	2.483491	-0.671669	1.400803
C	1.520367	-0.665172	2.389216
C	1.715603	-1.258409	3.759945
C	3.854315	-1.274058	1.564214
H	1.349525	-0.594657	4.551761
H	1.154982	-2.200432	3.866384
H	2.762218	-1.471711	3.982089
H	4.642752	-0.615221	1.182188
H	4.097686	-1.492181	2.605060
H	3.941357	-2.215467	0.999306
C	-0.802190	-0.029491	2.965890
C	3.006667	-0.047845	-0.937734
C	-2.014374	-0.786491	2.931672
C	-3.051910	-0.471538	3.815587
C	-2.925634	0.552528	4.753145
C	-1.744138	1.290638	4.791566
C	-0.686442	1.033744	3.911521
H	-3.973146	-1.048777	3.785545
H	-3.738570	0.775159	5.440485
H	-1.653506	2.106156	5.506010
C	2.940275	-0.810890	-2.144592
C	3.795881	-0.500243	-3.207037
C	4.736965	0.523745	-3.110134
C	4.809148	1.265199	-1.932314
C	3.957789	1.013070	-0.850321
H	3.741064	-1.081261	-4.124775
H	5.402062	0.743012	-3.942265
H	5.527478	2.079453	-1.863270
C	-2.185985	-1.920308	1.932565
H	-1.174924	-2.246300	1.662193
C	-2.933306	-3.135773	2.492530
H	-2.896753	-3.961163	1.771525
H	-2.484186	-3.488002	3.428131
H	-3.991339	-2.923084	2.685447
C	-2.864122	-1.427032	0.645367
H	-3.880382	-1.067430	0.849435
H	-2.309057	-0.596964	0.188628
H	-2.933140	-2.231732	-0.097186
C	0.509505	1.977883	3.900957
H	1.314571	1.490777	3.342346
C	1.051294	2.304467	5.298252
H	1.288049	1.395717	5.863044
H	1.970033	2.897430	5.217000
H	0.338540	2.890692	5.890140
C	0.152003	3.273165	3.153266
H	-0.190900	3.066260	2.132922
H	-0.646998	3.817473	3.671854
H	1.022383	3.937300	3.087452
C	3.983434	1.959746	0.343425
H	3.439491	1.479076	1.162255
C	3.239668	3.261299	0.001106
H	3.744797	3.799843	-0.810312
H	2.209870	3.063298	-0.317977
H	3.199935	3.927102	0.871799
C	5.396182	2.274346	0.851410
H	5.342362	2.871660	1.769375
H	5.957276	1.360917	1.078702
H	5.977004	2.851631	0.122434
C	1.940838	-1.949372	-2.282900
H	1.694462	-2.266066	-1.262786
C	0.636004	-1.470719	-2.937620
H	-0.097805	-2.284503	-2.992376
H	0.178126	-0.646570	-2.374432
H	0.816847	-1.109846	-3.957796
C	2.490972	-3.170227	-3.029088
H	2.659766	-2.968376	-4.093339
H	3.438151	-3.512284	-2.596667
H	1.775612	-3.999039	-2.967598

Zero-point correction= 0.616981 (Hartree/Particle)
Thermal correction to Energy= 0.651551
Thermal correction to Enthalpy= 0.652496
Thermal correction to Gibbs Free Energy= 0.551366
Sum of electronic and zero-point Energies= -2978.794510
Sum of electronic and thermal Energies= -2978.759939
Sum of electronic and thermal Enthalpies= -2978.758995
Sum of electronic and thermal Free Energies= -2978.860124

$ZnDAD_U$ (acetone)

71
scf done: -2979.399772

Zn	0.344140	1.191996	0.294207
N	0.153429	0.046384	2.033471
N	2.077198	0.005466	0.179023
C	2.186859	-0.848813	1.207371
C	1.158309	-0.826464	2.199718
C	1.235140	-1.764246	3.374210
C	3.333683	-1.813452	1.347730
H	0.361803	-1.659202	4.021014
H	1.289125	-2.810605	3.048996
H	2.128984	-1.575996	3.982691
H	4.027067	-1.728461	0.508714
H	3.898941	-1.635831	2.271473
H	2.981110	-2.851737	1.388391
C	-0.912662	0.184338	2.949603
C	3.034405	0.094562	-0.855399
C	-2.130809	-0.503278	2.716837
C	-3.213302	-0.268600	3.573084
C	-3.112986	0.620643	4.640875
C	-1.912846	1.292784	4.861870
C	-0.802467	1.092618	4.032891
H	-4.152928	-0.788176	3.399640
H	-3.965053	0.790640	5.294838
H	-1.838881	1.991744	5.692005
C	2.831249	-0.620107	-2.063140
C	3.736257	-0.439232	-3.115910
C	4.823134	0.424153	-2.996847
C	5.014328	1.124132	-1.807486
C	4.136477	0.977702	-0.726688
H	3.585982	-0.981092	-4.046972
H	5.515579	0.551843	-3.825590
H	5.859972	1.802491	-1.718937
C	4.357276	1.792436	0.539595
H	3.656715	1.420868	1.293480
C	4.030541	3.274629	0.301232
H	4.142863	3.848778	1.228938
H	4.701445	3.712107	-0.448046
H	3.000580	3.402731	-0.052559
C	5.773739	1.632118	1.106788
H	5.862129	2.166452	2.060184
H	6.016912	0.579082	1.287684
H	6.532584	2.041271	0.429725
C	1.638229	-1.547436	-2.242893
H	1.161952	-1.656631	-1.263588
C	0.600609	-0.929050	-3.192075
H	-0.276934	-1.580744	-3.282833
H	0.259584	0.046916	-2.825706
H	1.018491	-0.785903	-4.196016
C	2.043689	-2.948765	-2.717953
H	2.473345	-2.929880	-3.726334
H	2.781486	-3.401937	-2.046217
H	1.166729	-3.606310	-2.747326
C	-2.288862	-1.454452	1.539546
H	-1.291042	-1.622872	1.122557
C	-3.146933	-0.819347	0.434608
H	-2.714318	0.128567	0.091617
H	-3.220943	-1.489164	-0.430800
H	-4.164103	-0.616839	0.791644
C	-2.854240	-2.820141	1.949975
H	-2.249908	-3.284179	2.737657
H	-3.884274	-2.743281	2.317144
H	-2.863328	-3.498933	1.088952
C	0.475854	1.879821	4.282079
H	1.248176	1.465359	3.627122
C	0.293062	3.356092	3.897625
H	-0.012235	3.458914	2.849412
H	-0.472194	3.835147	4.520375
H	1.230603	3.909132	4.032069
C	0.977659	1.751700	5.726147
H	0.280936	2.203402	6.441785
H	1.118539	0.702829	6.010389
H	1.941013	2.263119	5.838583

Zero-point correction= 0.615346 (Hartree/Particle)
Thermal correction to Energy= 0.651402
Thermal correction to Enthalpy= 0.652346
Thermal correction to Gibbs Free Energy= 0.541860
Sum of electronic and zero-point Energies= -2978.784426
Sum of electronic and thermal Energies= -2978.748370
Sum of electronic and thermal Enthalpies= -2978.747425
Sum of electronic and thermal Free Energies= -2978.857912

$ZnDAD_{BS}$ (acetone)

71
scf done: -2979.398552

Zn	0.395136	1.221292	0.414774
N	0.244088	0.094106	2.162175
N	2.152764	0.101151	0.297290
C	2.121499	-0.940159	1.152464
C	1.104157	-0.943155	2.148826
C	1.007661	-2.094448	3.114160
C	3.089768	-2.090473	1.071889
H	0.258053	-1.902265	3.884664
H	0.739108	-3.033094	2.611219
H	1.966038	-2.270229	3.616930
H	3.815658	-1.941259	0.270176
H	3.648788	-2.203444	2.009245
H	2.579790	-3.045764	0.892519
C	-0.853809	0.174220	3.046225
C	3.063961	0.184347	-0.779556
C	-2.044967	-0.558857	2.816515
C	-3.133001	-0.364596	3.678435
C	-3.062719	0.525418	4.746080
C	-1.889560	1.248569	4.962045
C	-0.779371	1.094203	4.125842
H	-4.053704	-0.917695	3.506870
H	-3.916839	0.658585	5.405943
H	-1.842141	1.945129	5.794842
C	2.837066	-0.522967	-1.989274
C	3.721029	-0.333569	-3.058645
C	4.809659	0.530055	-2.958194
C	5.021728	1.226578	-1.770709
C	4.164529	1.073057	-0.674720
H	3.550883	-0.867941	-3.990659
H	5.485145	0.661346	-3.800285
H	5.867554	1.906480	-1.693840
C	4.416321	1.873876	0.594162
H	3.669121	1.555065	1.327369
C	4.216861	3.377259	0.351773
H	4.342581	3.938191	1.285721
H	4.945144	3.764586	-0.371006
H	3.213772	3.589198	-0.036392
C	5.802676	1.598146	1.191485
H	5.922371	2.135424	2.139960
H	5.948086	0.530092	1.389205

H	6.605224	1.928334	0.521238
C	1.637549	-1.443242	-2.166666
H	1.163022	-1.559334	-1.187547
C	0.597419	-0.813321	-3.105808
H	-0.283053	-1.461221	-3.195849
H	0.262106	0.160618	-2.728859
H	1.010055	-0.664997	-4.111077
C	2.032136	-2.842602	-2.657633
H	2.444220	-2.816098	-3.673143
H	2.780692	-3.303318	-2.003682
H	1.153336	-3.498034	-2.677595
C	-2.188250	-1.505981	1.633675
H	-1.197946	-1.624718	1.183746
C	-3.107433	-0.903375	0.559853
H	-2.729509	0.066333	0.213663
H	-3.173411	-1.569421	-0.309136
H	-4.122651	-0.753707	0.946859
C	-2.679601	-2.900231	2.045062
H	-2.043548	-3.339766	2.821236
H	-3.706385	-2.873076	2.428126
H	-2.670644	-3.574463	1.180456
C	0.476635	1.929839	4.324787
H	1.322233	1.325004	3.978236
C	0.422397	3.185150	3.439341
H	0.280437	2.921767	2.381983
H	-0.408317	3.836639	3.737903
H	1.352122	3.761243	3.521354
C	0.749505	2.313278	5.781827
H	0.005202	3.017328	6.171743
H	0.760610	1.434870	6.437341
H	1.727628	2.801857	5.859291

Zero-point correction= 0.615189 (Hartree/Particle)
Thermal correction to Energy= 0.650972
Thermal correction to Enthalpy= 0.651917
Thermal correction to Gibbs Free Energy= 0.545830
Sum of electronic and zero-point Energies= -2978.783363
Sum of electronic and thermal Energies= -2978.747579
Sum of electronic and thermal Enthalpies= -2978.746635
Sum of electronic and thermal Free Energies= -2978.852722

$ZnDAD_R$ (acetonitrile)

71
scf done: -2979.414215

Zn	0.192361	-0.088563	0.131759
N	0.221986	-0.329808	2.054822
N	2.110196	-0.339370	0.104375
C	2.507062	-0.662087	1.417655
C	1.547444	-0.661573	2.410462
C	1.751732	-1.265165	3.775898
C	3.896214	-1.219462	1.588814
H	1.406245	-0.605639	4.580531
H	1.177274	-2.199334	3.878893
H	2.797096	-1.499706	3.981750
H	4.658995	-0.547792	1.177994
H	4.155739	-1.392511	2.634206
H	4.009671	-2.175776	1.054446
C	-0.779807	-0.049191	2.984309
C	3.008617	-0.068219	-0.932224
C	-2.015878	-0.766605	2.907460
C	-3.042793	-0.477330	3.811473
C	-2.890728	0.489570	4.805103
C	-1.696109	1.204941	4.871055
C	-0.647061	0.974455	3.973381
H	-3.977757	-1.029755	3.750787
H	-3.695005	0.690255	5.509116
H	-1.589579	1.985779	5.621076
C	2.959007	-0.863215	-2.118968
C	3.805214	-0.559524	-3.190969
C	4.718840	0.491620	-3.123555
C	4.771047	1.268267	-1.967182
C	3.928945	1.021380	-0.876554
H	3.762854	-1.165357	-4.093262
H	5.376481	0.706216	-3.962781
H	5.465101	2.104980	-1.922845
C	-2.224418	-1.823282	1.834180
H	-1.224169	-2.155525	1.532405
C	-2.999894	-3.055786	2.311979
H	-3.001481	-3.823573	1.529049
H	-2.546076	-3.492941	3.208828
H	-4.047030	-2.826470	2.541598
C	-2.898186	-1.217163	0.592679
H	-3.918182	-0.886321	0.826041
H	-2.351842	-0.341218	0.217366
H	-2.959850	-1.950722	-0.220713
C	0.549138	1.919175	3.978919
H	1.361855	1.435714	3.428187
C	1.077376	2.251390	5.379703
H	1.307707	1.345175	5.951342
H	1.997563	2.842687	5.303646
H	0.360659	2.842410	5.961894
C	0.195544	3.212269	3.224755
H	-0.139204	3.001820	2.202516
H	-0.608132	3.756299	3.736470
H	1.065608	3.877415	3.163687
C	3.924694	2.000643	0.290608
H	3.403582	1.522035	1.125394
C	3.128219	3.261795	-0.083715
H	3.608741	3.796523	-0.912400
H	2.105933	3.013791	-0.391765
H	3.065475	3.949658	0.768229
C	5.326295	2.383440	0.781439
H	5.253326	3.006941	1.680395
H	5.921462	1.498696	1.034333
H	5.882115	2.958804	0.031859
C	1.979367	-2.021438	-2.227825
H	1.733821	-2.312654	-1.200082
C	0.670376	-1.576366	-2.898445
H	-0.058596	-2.395958	-2.920119
H	0.211252	-0.733231	-2.365258
H	0.848660	-1.255075	-3.932277
C	2.550218	-3.253669	-2.938560
H	2.725295	-3.076176	-4.006092
H	3.498021	-3.573142	-2.490286
H	1.844545	-4.089432	-2.861614

Zero-point correction= 0.616816 (Hartree/Particle)
Thermal correction to Energy= 0.651243
Thermal correction to Enthalpy= 0.652187
Thermal correction to Gibbs Free Energy= 0.552053
Sum of electronic and zero-point Energies= -2978.797400
Sum of electronic and thermal Energies= -2978.762973
Sum of electronic and thermal Enthalpies= -2978.762028

Sum of electronic and thermal Free Energies= -2978.862163

$ZnDAD_U$ (acetonitrile)

71
scf done: -2979.399423

Zn	0.342194	1.190662	0.295660
N	0.155344	0.041387	2.037570
N	2.077252	0.000937	0.180768
C	2.189664	-0.851036	1.210725
C	1.162184	-0.829008	2.204094
C	1.241998	-1.765397	3.379635
C	3.339252	-1.812232	1.352878
H	0.376614	-1.650119	4.035317
H	1.281772	-2.812930	3.055848
H	2.144292	-1.585185	3.977778
H	4.024255	-1.737489	0.506014
H	3.913289	-1.620853	2.268505
H	2.988612	-2.850169	1.411571
C	-0.910360	0.178773	2.953501
C	3.033528	0.091156	-0.853832
C	-2.125873	-0.515274	2.724435
C	-3.210385	-0.278252	3.577520
C	-3.114158	0.618373	4.639907
C	-1.916190	1.295247	4.858513
C	-0.804200	1.093509	4.031728
H	-4.148282	-0.801420	3.406032
H	-3.967703	0.789991	5.291483
H	-1.844889	1.999420	5.684489
C	2.828655	-0.621433	-2.062727
C	3.731385	-0.437966	-3.117123
C	4.818264	0.425780	-2.998524
C	5.011753	1.123152	-1.807831
C	4.135985	0.974081	-0.725524
H	3.579069	-0.977868	-4.048969
H	5.508856	0.555607	-3.828452
H	5.857154	1.801824	-1.719307
C	4.358512	1.786536	0.541915
H	3.662369	1.410380	1.297554
C	4.024703	3.267896	0.308007
H	4.139103	3.840431	1.236402
H	4.690795	3.708985	-0.443456
H	2.992498	3.392207	-0.040583
C	5.777805	1.630919	1.103211
H	5.867399	2.163952	2.057156
H	6.025655	0.578498	1.281332
H	6.532082	2.044481	0.423777
C	1.634885	-1.547976	-2.241360
H	1.168805	-1.669140	-1.258601
C	0.587328	-0.918011	-3.171920
H	-0.290528	-1.569252	-3.262415
H	0.249526	0.052669	-2.788733
H	0.995824	-0.761705	-4.177791
C	2.035398	-2.943112	-2.738077
H	2.453591	-2.911691	-3.750905
H	2.780521	-3.404337	-2.080023
H	1.158029	-3.600085	-2.765574
C	-2.277425	-1.471797	1.550613
H	-1.273800	-1.666926	1.159995
C	-3.090583	-0.821887	0.420446
H	-2.623349	0.111563	0.082556
H	-3.161227	-1.495564	-0.442215
H	-4.110160	-0.589906	0.751894
C	-2.886245	-2.821000	1.952494
H	-2.316126	-3.293833	2.760236
H	-3.924805	-2.719043	2.287890
H	-2.885019	-3.504353	1.095148
C	0.471687	1.885533	4.277857
H	1.244710	1.471616	3.623453
C	0.283919	3.360168	3.889606
H	-0.021434	3.458804	2.841001
H	-0.482850	3.837942	4.511474
H	1.219706	3.916394	4.022727
C	0.974521	1.762692	5.722032
H	0.275047	2.211700	6.436656
H	1.121509	0.715028	6.007660
H	1.934957	2.279765	5.833132

Zero-point correction= 0.615077 (Hartree/Particle)
Thermal correction to Energy= 0.651205
Thermal correction to Enthalpy= 0.652149
Thermal correction to Gibbs Free Energy= 0.540916
Sum of electronic and zero-point Energies= -2978.784347
Sum of electronic and thermal Energies= -2978.748219
Sum of electronic and thermal Enthalpies= -2978.747274
Sum of electronic and thermal Free Energies= -2978.858507

$ZnDAD_R$ (water)

71
scf done: -2979.392475

Zn	0.179397	-0.208104	0.106906
N	0.209322	-0.436305	2.038502
N	2.110092	-0.443931	0.100943
C	2.502849	-0.739740	1.423828
C	1.536869	-0.729686	2.408298
C	1.747861	-1.255617	3.803864
C	3.882793	-1.316233	1.604376
H	1.367446	-0.562542	4.563499
H	1.206612	-2.202572	3.954407
H	2.798936	-1.434489	4.034466
H	4.666685	-0.645371	1.233544
H	4.116501	-1.535506	2.647102
H	3.989388	-2.253808	1.036754
C	-0.782149	-0.080606	2.956047
C	3.011176	-0.091881	-0.903643
C	-2.004035	-0.822516	2.974699
C	-3.032738	-0.441857	3.842346
C	-2.890211	0.637509	4.713737
C	-1.700924	1.364401	4.698009
C	-0.651034	1.040503	3.830644
H	-3.960859	-1.008504	3.850399
H	-3.696751	0.912332	5.389150
H	-1.598608	2.224304	5.356483
C	2.943727	-0.773478	-2.160429
C	3.815233	-0.414550	-3.192916
C	4.770139	0.588752	-3.028155
C	4.826739	1.269080	-1.812992
C	3.959100	0.968494	-0.756415
H	3.759226	-0.939776	-4.143540
H	5.449350	0.844553	-3.837719
H	5.543548	2.078750	-1.694634
C	-2.195861	-2.006920	2.041498
H	-1.191139	-2.357914	1.781109
C	-2.952586	-3.179972	2.673327
H	-2.936976	-4.042060	1.996328
H	-2.496692	-3.489124	3.620680

H	-4.004552	-2.940992	2.867583
C	-2.878774	-1.573774	0.735633
H	-3.893449	-1.204632	0.930040
H	-2.323473	-0.768563	0.238130
H	-2.953106	-2.413435	0.033888
C	0.548905	1.975463	3.745719
H	1.350516	1.446232	3.221017
C	1.097615	2.402384	5.112147
H	1.338745	1.536417	5.738717
H	2.014348	2.989242	4.982782
H	0.386849	3.028696	5.663509
C	0.192046	3.212672	2.905480
H	-0.157851	2.931872	1.905748
H	-0.601959	3.795677	3.388232
H	1.063923	3.866621	2.786123
C	3.948363	1.881508	0.464109
H	3.422213	1.361419	1.270746
C	3.152241	3.159806	0.152971
H	3.637481	3.736872	-0.643916
H	2.131861	2.928833	-0.172722
H	3.085653	3.801533	1.039588
C	5.344678	2.242744	0.984264
H	5.262257	2.810846	1.918091
H	5.944765	1.348694	1.187235
H	5.900411	2.866275	0.274404
C	1.910234	-1.864654	-2.387092
H	1.634210	-2.238766	-1.394878
C	0.638670	-1.286818	-3.027446
H	-0.144358	-2.050634	-3.107265
H	0.234736	-0.448758	-2.444688
H	0.848708	-0.911741	-4.036945
C	2.426228	-3.051931	-3.206639
H	2.632155	-2.780601	-4.248461
H	3.345874	-3.466289	-2.778250
H	1.674604	-3.849816	-3.222983

Zero-point correction= 0.616412 (Hartree/Particle)
Thermal correction to Energy= 0.651022
Thermal correction to Enthalpy= 0.651966
Thermal correction to Gibbs Free Energy= 0.551302
Sum of electronic and zero-point Energies= -2978.776063
Sum of electronic and thermal Energies= -2978.741453
Sum of electronic and thermal Enthalpies= -2978.740509
Sum of electronic and thermal Free Energies= -2978.841173

$ZnDAD_U$ (water)

71
scf done: -2979.374913

Zn	0.292605	1.231949	0.286247
N	0.128806	0.062898	2.030058
N	2.037576	0.051781	0.155608
C	2.165058	-0.804484	1.180193
C	1.146421	-0.798286	2.181155
C	1.247143	-1.739221	3.351008
C	3.323982	-1.756299	1.306823
H	0.340568	-1.711198	3.958954
H	1.401542	-2.772972	3.020602
H	2.094462	-1.484720	4.001020
H	4.051013	-1.602978	0.507072
H	3.842718	-1.630714	2.264808
H	2.991320	-2.801192	1.262306
C	-0.918500	0.180006	2.969464
C	2.987435	0.138227	-0.885699
C	-2.145558	-0.491335	2.733701
C	-3.214502	-0.273854	3.610595
C	-3.091515	0.581559	4.704176
C	-1.880799	1.231037	4.932934
C	-0.782918	1.045463	4.083529
H	-4.160714	-0.779702	3.435289
H	-3.933505	0.739524	5.373542
H	-1.787048	1.899993	5.785341
C	2.808917	-0.621206	-2.069047
C	3.706125	-0.444289	-3.129247
C	4.763037	0.459093	-3.040879
C	4.932255	1.201383	-1.873927
C	4.060608	1.059399	-0.787621
H	3.572907	-1.023437	-4.040399
H	5.449698	0.583531	-3.874527
H	5.756309	1.908153	-1.805265
C	4.275480	1.900272	0.461553
H	3.531901	1.584448	1.199258
C	4.040985	3.390537	0.177737
H	4.152275	3.978637	1.096310
H	4.761718	3.773339	-0.554550
H	3.033059	3.565507	-0.215697
C	5.662360	1.674415	1.077732
H	5.759687	2.239682	2.011944
H	5.830628	0.615917	1.304957
H	6.461560	2.006444	0.404935
C	1.664490	-1.612616	-2.212920
H	1.123281	-1.625858	-1.262119
C	0.676642	-1.172419	-3.302058
H	-0.166317	-1.870938	-3.361104
H	0.274778	-0.174353	-3.093155
H	1.157634	-1.144233	-4.286937
C	2.168881	-3.037379	-2.477997
H	2.694702	-3.106082	-3.437419
H	2.856102	-3.369924	-1.692190
H	1.327407	-3.739295	-2.509789
C	-2.317697	-1.403120	1.528319
H	-1.314964	-1.666389	1.176373
C	-3.026386	-0.659509	0.386006
H	-2.471561	0.241984	0.095572
H	-3.114491	-1.301535	-0.498638
H	-4.036627	-0.355313	0.686045
C	-3.047558	-2.710154	1.857351
H	-2.563421	-3.244140	2.682608
H	-4.094108	-2.538857	2.133494
H	-3.045304	-3.369630	0.982010
C	0.510500	1.799560	4.352955
H	1.266322	1.413600	3.662572
C	0.342700	3.297924	4.061457
H	0.021599	3.467209	3.027147
H	-0.404832	3.747440	4.725952
H	1.290046	3.828682	4.212914
C	1.032212	1.577179	5.778113
H	0.350471	1.991704	6.529528
H	1.164133	0.511119	5.993569
H	2.002933	2.069841	5.906598

Zero-point correction= 0.615680 (Hartree/Particle)
Thermal correction to Energy= 0.651542
Thermal correction to Enthalpy= 0.652486
Thermal correction to Gibbs Free Energy= 0.544327
Sum of electronic and zero-point Energies= -2978.759233

Sum of electronic and thermal Energies= -2978.723371
Sum of electronic and thermal Enthalpies= -2978.722427
Sum of electronic and thermal Free Energies= -2978.830586

$ZnDAD_R$ ($O(CH_3)_2$)

89
scf done: -3289.332214

Zn	0.112219	0.020359	0.075377
N	0.107588	-0.357881	1.948352
N	1.971080	-0.382332	-0.073311
C	2.345153	-0.851598	1.214297
C	1.415153	-0.839574	2.224012
C	1.612552	-1.555989	3.534493
C	3.660367	-1.579089	1.315899
H	1.067040	-1.060146	4.343277
H	1.231818	-2.588295	3.490389
H	2.662489	-1.606261	3.830295
H	4.432713	-1.089026	0.714545
H	4.029277	-1.635015	2.342095
H	3.580369	-2.610367	0.938160
C	-0.746989	0.111044	2.965372
C	2.936902	0.059656	-1.002100
C	-2.035567	-0.477997	3.123225
C	-2.920229	0.021388	4.083726
C	-2.566603	1.071286	4.923955
C	-1.301352	1.633643	4.791527
C	-0.389375	1.187479	3.829644
H	-3.899233	-0.440763	4.195190
H	-3.261436	1.440440	5.673686
H	-1.018348	2.456305	5.445000
C	3.082916	-0.618254	-2.245389
C	4.010350	-0.159277	-3.185985
C	4.824445	0.938054	-2.928791
C	4.693617	1.597775	-1.711139
C	3.761519	1.193947	-0.749897
H	4.115371	-0.688416	-4.131190
H	5.551618	1.272847	-3.663939
H	5.325067	2.460123	-1.507051
C	-2.452377	-1.693794	2.312009
H	-1.640326	-1.876548	1.603409
C	-2.580483	-2.938816	3.202763
H	-2.818514	-3.826356	2.603174
H	-1.647704	-3.131951	3.741567
H	-3.375607	-2.817568	3.947692
C	-3.745090	-1.461493	1.518992
H	-4.599417	-1.277454	2.180486
H	-3.656293	-0.597361	0.851256
H	-3.992845	-2.339688	0.909452
C	0.940844	1.918798	3.709092
H	1.533823	1.403813	2.947820
C	1.748846	1.895703	5.015358
H	1.922506	0.872928	5.361610
H	2.725135	2.371937	4.868966
H	1.235473	2.437434	5.818452
C	0.731543	3.368797	3.246527
H	0.214504	3.407097	2.282086
H	0.132386	3.936834	3.967716
H	1.692497	3.883163	3.134117
C	3.632857	2.016572	0.523938
H	2.815520	1.583723	1.108151
C	3.275441	3.478089	0.212163
H	4.074170	3.979470	-0.346113
H	2.362834	3.546589	-0.389302
H	3.114707	4.043145	1.136707
C	4.901498	1.959919	1.387965
H	4.764429	2.535911	2.310507
H	5.149359	0.932417	1.667105
H	5.763721	2.381831	0.857818
C	2.283189	-1.871369	-2.558865
H	1.624887	-2.028436	-1.699944
C	1.414442	-1.709089	-3.813463
H	0.813735	-2.609568	-3.993779
H	0.732568	-0.856613	-3.719577
H	2.024743	-1.543060	-4.708714
C	3.190844	-3.103798	-2.684714
H	3.882102	-3.009040	-3.530306
H	3.790599	-3.243113	-1.780005
H	2.595912	-4.011932	-2.842706
O	-0.888116	1.625784	-0.806785
O	-1.159578	-1.352616	-1.122796
C	-2.179550	-1.106044	-2.081155
H	-2.284355	-0.024854	-2.170697
H	-1.902364	-1.531990	-3.053621
H	-3.130607	-1.540395	-1.748733
C	-0.933720	-2.743884	-0.902302
H	-1.847520	-3.221001	-0.528464
H	-0.617088	-3.228483	-1.833392
H	-0.142740	-2.827674	-0.155797
C	-0.276964	2.370105	-1.865779
H	0.233281	3.251620	-1.463762
H	0.452765	1.718504	-2.347672
H	-1.041548	2.680856	-2.587505
C	-1.818126	2.396624	-0.036067
H	-1.324952	3.283817	0.374929
H	-2.659311	2.699359	-0.670487
H	-2.169409	1.766732	0.782079

Zero-point correction= 0.780540 (Hartree/Particle)
Thermal correction to Energy= 0.827902
Thermal correction to Enthalpy= 0.828846
Thermal correction to Gibbs Free Energy= 0.695792
Sum of electronic and zero-point Energies= -3288.551675
Sum of electronic and thermal Energies= -3288.504313
Sum of electronic and thermal Enthalpies= -3288.503368
Sum of electronic and thermal Free Energies= -3288.636422

$ZnDAD_U$ ($O(CH_3)_2$)

89
scf done: -3289.320750

Zn	0.891232	1.159448	0.883625
N	0.781969	0.036755	2.563286
N	2.606702	0.121193	0.614705
C	2.808664	-0.748600	1.616597
C	1.831397	-0.794144	2.659732
C	2.004725	-1.746128	3.811410
C	4.005415	-1.658507	1.666662
H	1.120414	-1.749187	4.450859
H	2.178746	-2.769784	3.461319
H	2.866624	-1.471326	4.433070
H	4.717365	-1.409327	0.877990
H	4.521672	-1.588490	2.630611
H	3.715966	-2.709213	1.535893

C	-0.242789	0.090681	3.545327
C	3.500371	0.243613	-0.482344
C	-1.414152	-0.682681	3.373298
C	-2.439483	-0.559983	4.316615
C	-2.325767	0.302267	5.402134
C	-1.171565	1.063914	5.554362
C	-0.117048	0.977384	4.640006
H	-3.345743	-1.148443	4.196134
H	-3.134182	0.383526	6.123844
H	-1.089633	1.743158	6.399341
C	3.323473	-0.569956	-1.625768
C	4.173460	-0.377140	-2.719450
C	5.173242	0.590094	-2.698868
C	5.331279	1.388378	-1.570782
C	4.507012	1.236290	-0.451205
H	4.046923	-0.993034	-3.606366
H	5.823410	0.723518	-3.559385
H	6.109590	2.147576	-1.560160
C	-1.591907	-1.612877	2.183207
H	-0.650227	-1.614149	1.625027
C	-1.873837	-3.060269	2.610365
H	-1.926614	-3.712042	1.731166
H	-1.090070	-3.443305	3.272274
H	-2.828658	-3.146712	3.141188
C	-2.685839	-1.097585	1.235744
H	-3.664181	-1.087230	1.730384
H	-2.470447	-0.076541	0.903864
H	-2.762441	-1.733044	0.346973
C	1.111506	1.856082	4.820505
H	1.848722	1.547501	4.072493
C	1.758537	1.685182	6.201951
H	2.003547	0.637081	6.402349
H	2.683656	2.269376	6.264401
H	1.098402	2.031131	7.005162
C	0.776472	3.331258	4.550941
H	0.360003	3.465828	3.547092
H	0.039883	3.707202	5.270253
H	1.674898	3.953823	4.633672
C	4.694177	2.147380	0.752328
H	4.009399	1.801232	1.533230
C	4.311247	3.596441	0.415177
H	4.963620	4.008615	-0.363162
H	3.279679	3.659287	0.052948
H	4.400809	4.236058	1.300826
C	6.117281	2.074717	1.323568
H	6.196258	2.685149	2.230338
H	6.393119	1.046818	1.580689
H	6.859750	2.449240	0.609987
C	2.213690	-1.607089	-1.706489
H	1.755500	-1.677305	-0.714919
C	1.116867	-1.160777	-2.685471
H	0.287398	-1.875992	-2.696319
H	0.713927	-0.181663	-2.406456
H	1.509452	-1.080657	-3.705938
C	2.737305	-3.003364	-2.070253
H	3.158297	-3.028486	-3.081603
H	3.518508	-3.332669	-1.377188
H	1.921621	-3.734242	-2.037785
O	-2.686589	2.404975	-2.809922
O	-3.080810	-2.447273	-2.874139
C	-3.621519	-1.291010	-3.476577
H	-3.113938	-0.423510	-3.051570
H	-3.466245	-1.298344	-4.567104
H	-4.702068	-1.205719	-3.280338
C	-3.672298	-3.628311	-3.357982
H	-4.755471	-3.651394	-3.156599
H	-3.518990	-3.743411	-4.443163
H	-3.198522	-4.467433	-2.842643
C	-3.060082	3.005944	-1.590330
H	-3.255071	4.082883	-1.716303
H	-3.977135	2.516934	-1.253731
H	-2.281518	2.877724	-0.822713
C	-1.502067	2.959513	-3.335533
H	-1.620969	4.033908	-3.548211
H	-0.655188	2.831197	-2.644147
H	-1.283062	2.435716	-4.268879

Zero-point correction= 0.778075 (Hartree/Particle)
Thermal correction to Energy= 0.827840
Thermal correction to Enthalpy= 0.828784
Thermal correction to Gibbs Free Energy= 0.672837
Sum of electronic and zero-point Energies= -3288.542675
Sum of electronic and thermal Energies= -3288.492910
Sum of electronic and thermal Enthalpies= -3288.491966
Sum of electronic and thermal Free Energies= -3288.647914

$ZnDAD_R$ ($O(CH_3)_2$ + SMD)

89
scf done: -3289.364319

Zn	0.122601	0.051735	0.088164
N	0.161546	-0.354694	1.980215
N	1.984191	-0.446705	-0.070406
C	2.379479	-0.886638	1.219165
C	1.464761	-0.848916	2.244861
C	1.672352	-1.538741	3.567653
C	3.709164	-1.591782	1.315402
H	1.343355	-0.920125	4.409760
H	1.086226	-2.469693	3.625220
H	2.716960	-1.799064	3.746496
H	4.479649	-1.067424	0.739837
H	4.074714	-1.668564	2.341524
H	3.658874	-2.613182	0.905554
C	-0.686110	0.070447	3.019464
C	2.950223	-0.006931	-1.000768
C	-1.977658	-0.521488	3.162812
C	-2.845970	-0.074464	4.165078
C	-2.479160	0.929737	5.056206
C	-1.217206	1.505262	4.929427
C	-0.319989	1.108529	3.931393
H	-3.824856	-0.540310	4.262922
H	-3.162853	1.258451	5.835455
H	-0.928728	2.300938	5.613309
C	3.147922	-0.725455	-2.215525
C	4.093054	-0.276793	-3.145934
C	4.868915	0.854361	-2.909602
C	4.679539	1.561962	-1.725158
C	3.731264	1.165276	-0.775305
H	4.238739	-0.838478	-4.066749
H	5.608620	1.180938	-3.636949
H	5.275157	2.453801	-1.539070

C	-2.433781	-1.667677	2.273533
H	-1.619710	-1.854655	1.568397
C	-2.659139	-2.955449	3.079196
H	-2.918498	-3.787656	2.412796
H	-1.760132	-3.239336	3.637248
H	-3.477611	-2.841402	3.800396
C	-3.692128	-1.311577	1.470609
H	-4.547449	-1.118365	2.129646
H	-3.537884	-0.417328	0.856808
H	-3.974566	-2.135462	0.803996
C	0.993376	1.870149	3.803264
H	1.624723	1.326296	3.094484
C	1.767219	1.973404	5.125029
H	1.936673	0.989152	5.574546
H	2.746421	2.436290	4.954380
H	1.240164	2.591054	5.862039
C	0.745924	3.273201	3.227912
H	0.264062	3.222723	2.245660
H	0.099435	3.862870	3.889860
H	1.690261	3.818203	3.113422
C	3.537848	2.034463	0.459022
H	2.725394	1.591290	1.042478
C	3.121224	3.462314	0.075862
H	3.906004	3.971733	-0.495998
H	2.210797	3.462429	-0.533502
H	2.926738	4.061645	0.972565
C	4.788626	2.068730	1.348935
H	4.602075	2.662169	2.252026
H	5.086843	1.063791	1.664412
H	5.638782	2.522437	0.824549
C	2.380786	-2.002812	-2.517001
H	1.696333	-2.152578	-1.677384
C	1.551472	-1.889743	-3.803169
H	0.969872	-2.804118	-3.972754
H	0.852934	-1.046648	-3.758746
H	2.190824	-1.743608	-4.682354
C	3.313239	-3.220802	-2.586891
H	4.019819	-3.138594	-3.421883
H	3.896585	-3.330080	-1.666132
H	2.735319	-4.142256	-2.730932
O	-0.803934	1.767217	-0.653553
O	-1.204598	-1.186834	-1.118845
C	-2.202188	-0.809918	-2.065638
H	-2.349137	0.266285	-1.986894
H	-1.880885	-1.064991	-3.082929
H	-3.146337	-1.321672	-1.845102
C	-1.034326	-2.604058	-1.055071
H	-1.970020	-3.082466	-0.742663
H	-0.736616	-2.996488	-2.034042
H	-0.253806	-2.813629	-0.322961
C	-0.442882	2.385290	-1.894418
H	-0.121599	3.417315	-1.717512
H	0.379011	1.812362	-2.324973
H	-1.297336	2.382114	-2.581439
C	-1.874470	2.444690	0.015012
H	-1.598565	3.489284	0.195918
H	-2.783879	2.406850	-0.596451
H	-2.045036	1.940113	0.965916

Zero-point correction= 0.779683 (Hartree/Particle)
Thermal correction to Energy= 0.826656
Thermal correction to Enthalpy= 0.827600
Thermal correction to Gibbs Free Energy= 0.698031
Sum of electronic and zero-point Energies= -3288.584636
Sum of electronic and thermal Energies= -3288.537663
Sum of electronic and thermal Enthalpies= -3288.536719
Sum of electronic and thermal Free Energies= -3288.666288

$ZnDAD_U$ ($O(CH_3)_2$ + SMD)

89
scf done: -3289.361912

Zn	0.475832	0.231302	0.397497
N	0.641031	-0.352504	2.396385
N	2.449482	-0.458862	0.425910
C	2.814514	-0.917389	1.632600
C	1.851345	-0.853659	2.686888
C	2.217997	-1.350972	4.059158
C	4.182627	-1.480330	1.908851
H	1.356486	-1.332128	4.729339
H	2.594639	-2.380247	4.022246
H	3.009826	-0.741568	4.513520
H	4.833468	-1.381975	1.038035
H	4.663855	-0.966892	2.749988
H	4.135839	-2.544441	2.174002
C	-0.375410	-0.182596	3.363265
C	3.300716	-0.496019	-0.701964
C	-1.455267	-1.099980	3.403340
C	-2.501862	-0.874418	4.304926
C	-2.502485	0.230005	5.152637
C	-1.441343	1.131074	5.101545
C	-0.370316	0.948882	4.219250
H	-3.330767	-1.577848	4.343908
H	-3.324397	0.389457	5.846470
H	-1.448213	1.998547	5.757621
C	3.375268	-1.663904	-1.502952
C	4.155270	-1.635466	-2.664751
C	4.853872	-0.491250	-3.042811
C	4.771978	0.651846	-2.251994
C	4.002830	0.674818	-1.082863
H	4.214302	-2.525023	-3.287794
H	5.455481	-0.490290	-3.948601
H	5.315857	1.546187	-2.548247
C	-1.497026	-2.320997	2.496539
H	-0.594246	-2.294235	1.877856
C	-1.470649	-3.629338	3.299291
H	-1.438641	-4.492598	2.623721
H	-0.593027	-3.680344	3.953310
H	-2.363222	-3.732784	3.927881
C	-2.705745	-2.285809	1.551364
H	-3.651324	-2.326146	2.105238
H	-2.709506	-1.372918	0.944967
H	-2.683630	-3.143454	0.868264
C	0.741984	1.986842	4.167345
H	1.539132	1.586298	3.534248
C	1.349104	2.273147	5.547115
H	1.699555	1.355518	6.032051
H	2.204937	2.951687	5.450612
H	0.626913	2.751553	6.218823
C	0.248746	3.285810	3.512283
H	-0.138992	3.101608	2.504155
H	-0.553336	3.746747	4.101292
H	1.066253	4.012511	3.431719
C	3.932337	1.949983	-0.255872
H	3.306964	1.735443	0.616423
C	3.261042	3.089495	-1.035390
H	3.842110	3.364032	-1.923958
H	2.255158	2.805985	-1.365520
H	3.169673	3.983653	-0.407043

C	5.313231	2.380414	0.257803
H	5.222775	3.261652	0.904149
H	5.790900	1.583856	0.839045
H	5.986373	2.642831	-0.567021
C	2.602949	-2.926863	-1.149032
H	2.162051	-2.775943	-0.159113
C	1.448010	-3.161739	-2.133881
H	0.866429	-4.045018	-1.843244
H	0.767072	-2.303692	-2.161497
H	1.821871	-3.326524	-3.151632
C	3.506094	-4.165021	-1.068619
H	3.932241	-4.421530	-2.045604
H	4.336882	-4.013363	-0.370876
H	2.930663	-5.032533	-0.724252
O	-1.709957	4.000651	-0.725726
O	-2.306443	-0.394300	-3.071914
C	-1.535454	0.436181	-3.914619
H	-0.753797	0.890813	-3.300210
H	-1.062989	-0.139520	-4.725923
H	-2.146712	1.235164	-4.362876
C	-3.351348	-1.032903	-3.773633
H	-4.049189	-0.302887	-4.213360
H	-2.964230	-1.674397	-4.580975
H	-3.896347	-1.655306	-3.058547
C	-1.934159	5.295812	-1.239819
H	-2.323813	5.976859	-0.466776
H	-0.974354	5.679263	-1.596858
H	-2.645606	5.280097	-2.080571
C	-2.897583	3.413945	-0.236058
H	-3.331229	4.005568	0.585424
H	-3.653731	3.310370	-1.030008
H	-2.640575	2.419661	0.139238

Zero-point correction= 0.775756 (Hartree/Particle)
Thermal correction to Energy= 0.825278
Thermal correction to Enthalpy= 0.826222
Thermal correction to Gibbs Free Energy= 0.675734
Sum of electronic and zero-point Energies= -3288.586156
Sum of electronic and thermal Energies= -3288.536634
Sum of electronic and thermal Enthalpies= -3288.535690
Sum of electronic and thermal Free Energies= -3288.686178

$ZnDAD_R$ (H)

9
scf done: -1967.100590

Zn	0.157072	-0.117189	0.091133
N	0.226472	-0.021783	2.023940
N	2.091325	-0.029569	0.115225
C	2.391048	-0.612383	1.299759
C	1.415267	-0.608312	2.298486
H	3.305951	-1.185794	1.434735
H	1.569140	-1.178555	3.212386
H	-0.488960	-0.216316	2.714627
H	2.764393	-0.229898	-0.615244

Zero-point correction= 0.065000 (Hartree/Particle)
Thermal correction to Energy= 0.070008
Thermal correction to Enthalpy= 0.070952
Thermal correction to Gibbs Free Energy= 0.036203
Sum of electronic and zero-point Energies= -1967.035590
Sum of electronic and thermal Energies= -1967.030582
Sum of electronic and thermal Enthalpies= -1967.029638
Sum of electronic and thermal Free Energies= -1967.064387

$ZnDAD_U$ (H)

9
scf done: -1967.106564

Zn	0.138157	0.297164	0.070900
N	0.186981	-0.246401	1.965097
N	2.030675	-0.254128	0.078057
C	2.385242	-0.693648	1.282219
C	1.397252	-0.689496	2.293439
H	3.392580	-1.046242	1.497272
H	1.634234	-1.038831	3.296987
H	-0.494859	-0.257259	2.712006
H	2.761447	-0.270958	-0.620930

Zero-point correction= 0.065249 (Hartree/Particle)
Thermal correction to Energy= 0.070371
Thermal correction to Enthalpy= 0.071315
Thermal correction to Gibbs Free Energy= 0.035282
Sum of electronic and zero-point Energies= -1967.041315
Sum of electronic and thermal Energies= -1967.036193
Sum of electronic and thermal Enthalpies= -1967.035249
Sum of electronic and thermal Free Energies= -1967.071283

$ZnDAD_R$ (H + SMD)

9
scf done: -1967.137103

Zn	0.278229	0.360680	0.208368
N	0.077600	-0.398992	1.930181
N	1.992871	-0.406404	-0.030210
C	2.350546	-0.739615	1.282890
C	1.397330	-0.735506	2.258960
H	3.386744	-0.986903	1.507709
H	1.644583	-0.979931	3.290668
H	-0.482320	-0.150509	2.735166
H	2.786124	-0.162620	-0.608685

Zero-point correction= 0.063157 (Hartree/Particle)
Thermal correction to Energy= 0.068537
Thermal correction to Enthalpy= 0.069481
Thermal correction to Gibbs Free Energy= 0.034082
Sum of electronic and zero-point Energies= -1967.073947
Sum of electronic and thermal Energies= -1967.068566
Sum of electronic and thermal Enthalpies= -1967.067622
Sum of electronic and thermal Free Energies= -1967.103022

$ZnDAD_U$ (H + SMD)

9
scf done: -1967.123200

Zn	0.098487	0.286375	0.030916
N	0.184577	-0.237433	1.973051
N	2.038561	-0.244170	0.075874
C	2.383788	-0.691461	1.281318
C	1.396226	-0.687246	2.292270
H	3.388769	-1.052516	1.498256
H	1.635625	-1.044320	3.293582
H	-0.481009	-0.257659	2.737439
H	2.786685	-0.271371	-0.607658

Zero-point correction= 0.064571 (Hartree/Particle)
Thermal correction to Energy= 0.069845
Thermal correction to Enthalpy= 0.070789
Thermal correction to Gibbs Free Energy= 0.034439
Sum of electronic and zero-point Energies= -1967.058630
Sum of electronic and thermal Energies= -1967.053356
Sum of electronic and thermal Enthalpies= -1967.052411
Sum of electronic and thermal Free Energies= -1967.088761

$ZnDAD_R$ (BP86)

71
scf done: -2980.049126

Zn	0.170206	-0.010869	0.115636
N	0.203058	-0.204370	2.047388
N	2.104222	-0.203783	0.090933
C	2.477246	-0.644937	1.379766
C	1.502189	-0.642282	2.385119
C	1.676060	-1.320977	3.726820
C	3.818439	-1.333400	1.513311
H	1.285809	-0.699186	4.552712
H	1.120529	-2.280835	3.772286
H	2.730036	-1.535499	3.955342
H	4.642963	-0.706112	1.128716
H	4.060733	-1.582344	2.556484
H	3.848263	-2.276501	0.929020
C	-0.824205	0.002378	2.991269
C	3.022455	-0.001746	-0.960478
C	-2.019406	-0.793330	2.937676
C	-3.072164	-0.516238	3.833373
C	-2.968469	0.499828	4.795656
C	-1.794467	1.268005	4.856164
C	-0.722741	1.051919	3.967713
H	-3.985383	-1.121084	3.793116
H	-3.793620	0.692052	5.490784
H	-1.720652	2.072488	5.597265
C	2.933097	-0.795840	-2.154810
C	3.799669	-0.520254	-3.231979
C	4.768463	0.492071	-3.154052
C	4.866666	1.255790	-1.979922
C	4.008752	1.040451	-0.883367
H	3.731642	-1.123749	-4.144439
H	5.440217	0.683676	-3.998479
H	5.613340	2.056830	-1.924330
C	-2.157422	-1.927152	1.920728
H	-1.128531	-2.218807	1.637585
C	-2.862531	-3.181488	2.477844
H	-2.801988	-4.005840	1.744448
H	-2.391460	-3.526338	3.415138
H	-3.934231	-3.005600	2.681664
C	-2.863321	-1.443581	0.632823
H	-3.883218	-1.075924	0.849001
H	-2.306258	-0.609282	0.157506
H	-2.941226	-2.259629	-0.109485
C	0.471919	2.010878	3.975127
H	1.310675	1.509459	3.461649
C	0.956349	2.392695	5.389379
H	1.178579	1.498967	5.998996
H	1.879742	2.995820	5.323290
H	0.210677	2.997960	5.936219
C	0.132433	3.283876	3.161429
H	-0.169123	3.034402	2.128509
H	-0.698986	3.841485	3.631010
H	1.006159	3.958706	3.105345
C	4.066138	1.993057	0.315161
H	3.529156	1.514365	1.152176
C	3.321070	3.309320	-0.015652
H	3.818091	3.846984	-0.844214
H	2.276012	3.117011	-0.317429
H	3.302143	3.980708	0.862351
C	5.500784	2.294978	0.797589
H	5.471437	2.904800	1.718591
H	6.057346	1.368041	1.022931
H	6.080969	2.863080	0.047907
C	1.911749	-1.928949	-2.264003
H	1.658064	-2.219737	-1.227105
C	0.604152	-1.445986	-2.932553
H	-0.139301	-2.262704	-2.989867
H	0.144041	-0.612469	-2.361986
H	0.790954	-1.077808	-3.958076
C	2.449049	-3.183873	-2.983309
H	2.624253	-3.008813	-4.060187
H	3.398578	-3.528770	-2.537382
H	1.717317	-4.007974	-2.902470

Zero-point correction= 0.598059 (Hartree/Particle)
Thermal correction to Energy= 0.633702
Thermal correction to Enthalpy= 0.634647
Thermal correction to Gibbs Free Energy= 0.530250
Sum of electronic and zero-point Energies= -2979.451067
Sum of electronic and thermal Energies= -2979.415424
Sum of electronic and thermal Enthalpies= -2979.414479
Sum of electronic and thermal Free Energies= -2979.518876

$ZnDAD_U$ (BP86)

71
scf done: -2980.046651

Zn	0.394630	1.142678	0.324580
N	0.160662	-0.009272	2.052523
N	2.133790	-0.025336	0.211429
C	2.229121	-0.897579	1.243316
C	1.178201	-0.886439	2.228374
C	1.233060	-1.840714	3.400962
C	3.382768	-1.866311	1.382608
H	0.280558	-1.842877	3.952907
H	1.439821	-2.874607	3.070828
H	2.033229	-1.569717	4.116715
H	4.183353	-1.633163	0.663979
H	3.816114	-1.838982	2.398458
H	3.064556	-2.911175	1.200180
C	-0.907051	0.144855	2.978029

C	3.092786	0.050285	-0.835399
C	-2.177026	-0.439329	2.682884
C	-3.258853	-0.185127	3.550616
C	-3.107339	0.621840	4.687916
C	-1.856269	1.192732	4.969093
C	-0.743112	0.971646	4.132937
H	-4.237384	-0.628060	3.332429
H	-3.959636	0.807233	5.351272
H	-1.745139	1.829035	5.854277
C	2.940584	-0.762747	-2.000581
C	3.846471	-0.591239	-3.067171
C	4.882202	0.353469	-3.001076
C	5.021208	1.149173	-1.853894
C	4.141497	1.017526	-0.759973
H	3.739927	-1.206660	-3.967410
H	5.577011	0.469545	-3.840494
H	5.829739	1.887520	-1.807529
C	4.281745	1.930725	0.459860
H	3.722463	1.459478	1.287059
C	3.624777	3.304778	0.184474
H	3.685982	3.954752	1.076572
H	4.129187	3.822956	-0.651801
H	2.556262	3.191795	-0.081420
C	5.741449	2.108555	0.927638
H	5.769272	2.686760	1.868692
H	6.229967	1.135345	1.112170
H	6.350585	2.658574	0.187936
C	1.781013	-1.754602	-2.120372
H	1.431120	-1.977434	-1.097135
C	0.596604	-1.108995	-2.879760
H	-0.260923	-1.804643	-2.932505
H	0.254427	-0.183844	-2.377951
H	0.888002	-0.845665	-3.913167
C	2.180363	-3.093647	-2.774824
H	2.444453	-2.973245	-3.840951
H	3.042359	-3.555894	-2.261937
H	1.335461	-3.803841	-2.726765
C	-2.381163	-1.293952	1.430092
H	-1.378829	-1.563735	1.053292
C	-3.086182	-0.477012	0.321208
H	-2.504483	0.428044	0.060469
H	-3.203027	-1.081605	-0.596936
H	-4.091576	-0.151957	0.646557
C	-3.143199	-2.606967	1.709645
H	-2.655453	-3.196525	2.506075
H	-4.188223	-2.421983	2.017129
H	-3.174941	-3.229114	0.797052
C	0.587549	1.671397	4.421075
H	1.374850	1.130723	3.867931
C	0.559747	3.120465	3.877332
H	0.343350	3.137861	2.792897
H	-0.218151	3.717746	4.387465
H	1.533533	3.618153	4.038501
C	0.979592	1.656828	5.913501
H	0.293972	2.265988	6.529590
H	0.981735	0.631040	6.322728
H	1.993520	2.076310	6.042048

Zero-point correction= 0.596369 (Hartree/Particle)
Thermal correction to Energy= 0.633188
Thermal correction to Enthalpy= 0.634132
Thermal correction to Gibbs Free Energy= 0.523312
Sum of electronic and zero-point Energies= -2979.450282
Sum of electronic and thermal Energies= -2979.413464
Sum of electronic and thermal Enthalpies= -2979.412519
Sum of electronic and thermal Free Energies= -2979.523339

$ZnDAD_{BS}$ (BP86)

71
scf done: -2980.049769

Zn	0.085013	0.726975	0.093992
N	0.201771	0.154880	2.101438
N	2.095993	0.162578	0.231431
C	2.165723	-0.824245	1.173764
C	1.148465	-0.827569	2.179989
C	1.051400	-1.985334	3.150037
C	3.137343	-1.981723	1.080513
H	0.307729	-1.785733	3.936780
H	0.766041	-2.932510	2.648208
H	2.020958	-2.172015	3.644580
H	3.890861	-1.807957	0.297351
H	3.673425	-2.131256	2.034789
H	2.627933	-2.939982	0.852707
C	-0.893864	0.214154	3.012766
C	3.023741	0.234311	-0.849578
C	-2.101213	-0.519223	2.799327
C	-3.183787	-0.313250	3.682253
C	-3.087458	0.570498	4.765403
C	-1.890515	1.273758	4.978580
C	-0.786312	1.116452	4.118448
H	-4.119010	-0.861912	3.519361
H	-3.938405	0.711390	5.441418
H	-1.818491	1.964828	5.825748
C	2.825823	-0.487934	-2.068170
C	3.731855	-0.285239	-3.130883
C	4.823527	0.586488	-3.009029
C	5.015947	1.283789	-1.806727
C	4.129880	1.131985	-0.721425
H	3.581990	-0.826948	-4.072277
H	5.518573	0.722348	-3.845312
H	5.867374	1.967988	-1.710938
C	4.363826	1.925798	0.565879
H	3.497029	1.734669	1.221729
C	4.430448	3.447418	0.305378
H	4.522273	3.996867	1.259819
H	5.301945	3.717538	-0.318432
H	3.522462	3.809383	-0.208810
C	5.632233	1.444085	1.307293
H	5.755332	1.989750	2.260674
H	5.581046	0.365419	1.537567
H	6.540315	1.616956	0.700698
C	1.662715	-1.464254	-2.257884
H	1.144963	-1.551734	-1.285225
C	0.632795	-0.924484	-3.276257
H	-0.212311	-1.628778	-3.386618
H	0.222413	0.048511	-2.946745
H	1.088947	-0.783034	-4.272949
C	2.140782	-2.876800	-2.662950
H	2.612024	-2.877702	-3.662437
H	2.876253	-3.278258	-1.943929
H	1.284669	-3.574726	-2.700001
C	-2.261427	-1.508388	1.642788
H	-1.280518	-1.587939	1.139642
C	-3.272042	-0.992311	0.593364
H	-2.950383	-0.018253	0.179339
H	-3.359943	-1.705487	-0.246896
H	-4.277341	-0.861239	1.033393
C	-2.654960	-2.921205	2.129775

H	-1.940893	-3.306154	2.878773
H	-3.660391	-2.929542	2.588084
H	-2.672124	-3.628233	1.280519
C	0.483859	1.946504	4.322219
H	1.310758	1.405923	3.830079
C	0.346269	3.315724	3.613331
H	0.126199	3.192088	2.538111
H	-0.472014	3.909339	4.061177
H	1.280451	3.899519	3.703926
C	0.867878	2.139715	5.803292
H	0.136792	2.765265	6.346660
H	0.947254	1.173430	6.332357
H	1.846772	2.646844	5.874971

Zero-point correction= 0.595777 (Hartree/Particle)
Thermal correction to Energy= 0.632586
Thermal correction to Enthalpy= 0.633530
Thermal correction to Gibbs Free Energy= 0.524090
Sum of electronic and zero-point Energies= -2979.453992
Sum of electronic and thermal Energies= -2979.417184
Sum of electronic and thermal Enthalpies= -2979.416239
Sum of electronic and thermal Free Energies= -2979.525679

$ZnDAD_R$ (PW91)

71
scf done: -2979.468748

Zn	0.165727	-0.052121	0.119892
N	0.201423	-0.252647	2.046848
N	2.096916	-0.243991	0.094004
C	2.473101	-0.675885	1.380764
C	1.500721	-0.677454	2.384702
C	1.675526	-1.353662	3.723569
C	3.816532	-1.352138	1.512574
H	1.289567	-0.731943	4.548789
H	1.116604	-2.309042	3.769266
H	2.726705	-1.572131	3.949870
H	4.635343	-0.716154	1.136420
H	4.057698	-1.608355	2.551739
H	3.854758	-2.287221	0.920078
C	-0.814539	-0.012366	2.987802
C	3.010951	-0.005690	-0.947448
C	-2.022721	-0.783263	2.947086
C	-3.065003	-0.475166	3.840274
C	-2.937642	0.548175	4.788151
C	-1.750190	1.291959	4.836695
C	-0.688396	1.044954	3.949118
H	-3.988130	-1.061300	3.810584
H	-3.754665	0.764733	5.481989
H	-1.658934	2.101347	5.566849
C	2.938039	-0.778918	-2.152948
C	3.798196	-0.468861	-3.221955
C	4.745641	0.558476	-3.124771
C	4.828948	1.301055	-1.938990
C	3.976219	1.050215	-0.849673
H	3.742946	-1.056231	-4.143118
H	5.412563	0.777712	-3.963210
H	5.558786	2.113311	-1.868486
C	-2.180692	-1.925170	1.948054
H	-1.158582	-2.237883	1.670753
C	-2.906142	-3.155836	2.520398
H	-2.860997	-3.988873	1.799544
H	-2.441521	-3.495579	3.459982
H	-3.972006	-2.958301	2.721874
C	-2.875397	-1.449311	0.655859
H	-3.889213	-1.068402	0.865368
H	-2.310332	-0.629140	0.172085
H	-2.961124	-2.271714	-0.075039
C	0.523137	1.976225	3.931979
H	1.365584	1.426638	3.481710
C	0.972997	2.445668	5.326252
H	1.149280	1.594944	6.004376
H	1.913859	3.014542	5.246010
H	0.232556	3.109763	5.802562
C	0.239126	3.192004	3.022291
H	-0.034412	2.876423	2.002262
H	-0.591633	3.796912	3.423928
H	1.127866	3.841030	2.947215
C	4.011622	1.978936	0.363632
H	3.487898	1.473233	1.190280
C	3.235839	3.279026	0.058837
H	3.718099	3.842587	-0.757977
H	2.197824	3.067144	-0.245513
H	3.201400	3.931726	0.947435
C	5.435039	2.305302	0.850634
H	5.391021	2.894934	1.781236
H	6.012047	1.389485	1.057687
H	6.000221	2.900364	0.114059
C	1.941552	-1.927143	-2.278192
H	1.696241	-2.237661	-1.247209
C	0.626492	-1.462197	-2.935966
H	-0.099705	-2.290677	-3.000524
H	0.152507	-0.646016	-2.357087
H	0.803829	-1.080270	-3.955523
C	2.501263	-3.156845	-3.015094
H	2.671753	-2.962183	-4.086864
H	3.455729	-3.488692	-2.575717
H	1.787477	-3.994371	-2.946687

Zero-point correction= 0.600990 (Hartree/Particle)
Thermal correction to Energy= 0.636542
Thermal correction to Enthalpy= 0.637486
Thermal correction to Gibbs Free Energy= 0.532894
Sum of electronic and zero-point Energies= -2978.867758
Sum of electronic and thermal Energies= -2978.832207
Sum of electronic and thermal Enthalpies= -2978.831262
Sum of electronic and thermal Free Energies= -2978.935854

$ZnDAD_U$ (PW91)

71
scf done: -2979.465282

Zn	0.387363	1.128820	0.324825
N	0.168558	-0.009880	2.057556
N	2.121893	-0.041623	0.208342
C	2.228205	-0.899906	1.246618
C	1.185468	-0.882318	2.235164
C	1.251074	-1.818393	3.416512
C	3.380924	-1.863369	1.387155
H	0.315779	-1.793939	3.992373
H	1.429475	-2.859110	3.098131
H	2.074270	-1.553038	4.104322
H	4.142022	-1.685247	0.615392
H	3.867343	-1.774542	2.373304

H	3.046982	-2.912305	1.292645
C	-0.900193	0.140503	2.975843
C	3.081018	0.046067	-0.830970
C	-2.140523	-0.512726	2.718276
C	-3.227886	-0.258968	3.574462
C	-3.107008	0.612398	4.664120
C	-1.881986	1.245648	4.911756
C	-0.764932	1.025916	4.085367
H	-4.185807	-0.752109	3.386564
H	-3.963331	0.797184	5.318524
H	-1.794208	1.926127	5.763168
C	2.884950	-0.694640	-2.032690
C	3.787828	-0.507161	-3.095467
C	4.864279	0.382258	-2.986700
C	5.051286	1.101635	-1.799195
C	4.175326	0.951869	-0.708531
H	3.647549	-1.066526	-4.024596
H	5.556284	0.513064	-3.823191
H	5.894081	1.793855	-1.720436
C	4.358697	1.783188	0.558903
H	3.845201	1.251865	1.376791
C	3.672033	3.157522	0.404628
H	3.755663	3.742951	1.335972
H	4.137896	3.739272	-0.408685
H	2.598655	3.046036	0.169386
C	5.829781	1.956192	0.975121
H	5.886875	2.465457	1.951040
H	6.341459	0.984574	1.069165
H	6.396311	2.569147	0.254940
C	1.690824	-1.634071	-2.182424
H	1.348481	-1.891208	-1.166631
C	0.522525	-0.914555	-2.890177
H	-0.359057	-1.574399	-2.958442
H	0.222343	-0.003015	-2.342767
H	0.806764	-0.616045	-3.913458
C	2.033104	-2.950643	-2.901879
H	2.294082	-2.789237	-3.960761
H	2.878767	-3.467347	-2.419687
H	1.164168	-3.628580	-2.880275
C	-2.300477	-1.434293	1.511851
H	-1.287941	-1.735203	1.196448
C	-2.941225	-0.674646	0.330582
H	-2.342866	0.211850	0.052910
H	-3.015923	-1.324559	-0.557829
H	-3.956778	-0.329608	0.588748
C	-3.089240	-2.718346	1.824606
H	-2.652411	-3.263622	2.676941
H	-4.145253	-2.508960	2.062117
H	-3.078476	-3.389987	0.950534
C	0.543839	1.772185	4.333574
H	1.347409	1.202401	3.839739
C	0.501817	3.166661	3.671804
H	0.301118	3.091066	2.588669
H	-0.290474	3.789904	4.119828
H	1.464033	3.690183	3.802691
C	0.911590	1.888856	5.823164
H	0.209371	2.535079	6.375165
H	0.923157	0.903034	6.315769
H	1.914736	2.333171	5.929533

Zero-point correction= 0.599339 (Hartree/Particle)
Thermal correction to Energy= 0.635985
Thermal correction to Enthalpy= 0.636930
Thermal correction to Gibbs Free Energy= 0.526843
Sum of electronic and zero-point Energies= -2978.865943
Sum of electronic and thermal Energies= -2978.829296
Sum of electronic and thermal Enthalpies= -2978.828352
Sum of electronic and thermal Free Energies= -2978.938439

$ZnDAD_{BS}$ (PW91)

71
scf done: -2979.465711

Zn	0.220261	0.876787	-0.031711
N	0.109596	0.396259	1.959458
N	2.154749	0.188393	0.263816
C	2.071610	-0.752385	1.255607
C	0.986669	-0.633900	2.168746
C	0.721433	-1.727072	3.176670
C	2.984659	-1.953103	1.324563
H	-0.101563	-1.454406	3.851551
H	0.453988	-2.686054	2.691801
H	1.610136	-1.927761	3.797169
H	3.840018	-1.844129	0.643901
H	3.383519	-2.085058	2.343618
H	2.467161	-2.896360	1.065088
C	-1.007931	0.620162	2.805108
C	3.113276	0.086805	-0.782979
C	-2.295687	0.079778	2.508402
C	-3.387337	0.443953	3.320515
C	-3.230691	1.295914	4.419741
C	-1.959238	1.802049	4.719401
C	-0.839920	1.484186	3.929909
H	-4.379494	0.042698	3.092369
H	-4.091703	1.561792	5.039203
H	-1.833170	2.467104	5.579515
C	2.937474	-0.818198	-1.873949
C	3.877821	-0.816661	-2.922202
C	4.982190	0.041090	-2.909048
C	5.144136	0.930179	-1.838991
C	4.226481	0.982354	-0.772306
H	3.740977	-1.501201	-3.764835
H	5.706182	0.024058	-3.728288
H	5.999627	1.613398	-1.828201
C	4.471715	2.023788	0.321555
H	5.391865	2.552997	0.013642
C	4.762498	1.417294	1.708726
H	5.081948	2.210577	2.405642
H	3.872979	0.930419	2.134787
H	5.571299	0.670192	1.656582
C	3.359301	3.089021	0.397402
H	3.636412	3.877323	1.117492
H	3.199370	3.568567	-0.582157
H	2.406939	2.645052	0.727343
C	1.737083	-1.758154	-1.960893
H	1.184570	-1.680589	-1.010157
C	0.772976	-1.322596	-3.083649
H	-0.108929	-1.984546	-3.116562
H	0.415172	-0.291162	-2.921354
H	1.263600	-1.362334	-4.070491
C	2.150287	-3.231694	-2.142683
H	2.643741	-3.399435	-3.114274
H	2.844502	-3.559287	-1.352717
H	1.261869	-3.883931	-2.106948
C	-2.521411	-0.884372	1.346923
H	-1.530384	-1.125766	0.926265
C	-3.348658	-0.234243	0.220513
H	-2.842607	0.663988	-0.174199
H	-3.487818	-0.938972	-0.616995

H	-4.346932	0.068005	0.578894
C	-3.168357	-2.206835	1.803478
H	-2.581521	-2.688623	2.602102
H	-4.191204	-2.051157	2.184660
H	-3.234377	-2.911479	0.957777
C	0.520902	2.083899	4.275897
H	1.237693	1.717729	3.525423
C	0.503040	3.623220	4.188159
H	0.183509	3.965053	3.190162
H	-0.183977	4.062840	4.930552
H	1.509443	4.031577	4.379863
C	1.015068	1.622079	5.661141
H	0.349090	1.976718	6.465770
H	1.064725	0.523090	5.724745
H	2.023920	2.019557	5.862404

Zero-point correction= 0.598592 (Hartree/Particle)
Thermal correction to Energy= 0.635188
Thermal correction to Enthalpy= 0.636132
Thermal correction to Gibbs Free Energy= 0.528444
Sum of electronic and zero-point Energies= -2978.867119
Sum of electronic and thermal Energies= -2978.830523
Sum of electronic and thermal Enthalpies= -2978.829579
Sum of electronic and thermal Free Energies= -2978.937267

$ZnDAD_R$ (PBE)

71
scf done: -2978.147737

Zn	0.175793	-0.103947	0.108036
N	0.161475	-0.371054	1.999988
N	2.065869	-0.374314	0.056685
C	2.440383	-0.746022	1.366014
C	1.477794	-0.742414	2.349558
C	1.665304	-1.322938	3.722821
C	3.815220	-1.330772	1.526643
H	1.361697	-0.622483	4.509896
H	1.044995	-2.221974	3.856532
H	2.700320	-1.601420	3.924340
H	4.600318	-0.626809	1.225548
H	4.028129	-1.628433	2.553967
H	3.939153	-2.219209	0.889499
C	-0.810235	-0.037016	2.949486
C	2.999985	-0.057521	-0.936203
C	-2.031487	-0.769524	2.979004
C	-3.032689	-0.404697	3.882536
C	-2.854998	0.648114	4.776098
C	-1.659827	1.360924	4.753160
C	-0.638343	1.050516	3.850849
H	-3.964026	-0.965381	3.903959
H	-3.640016	0.910739	5.481052
H	-1.527787	2.195343	5.438583
C	3.007919	-0.806662	-2.147472
C	3.895412	-0.457221	-3.168418
C	4.793210	0.596427	-3.019927
C	4.792053	1.324904	-1.834064
C	3.906979	1.029196	-0.793306
H	3.900765	-1.030504	-4.092275
H	5.485140	0.847313	-3.820232
H	5.481357	2.159354	-1.724477
C	-2.246400	-1.929459	2.024903
H	-1.248257	-2.311164	1.779095
C	-3.056783	-3.081924	2.617651
H	-3.054631	-3.933746	1.927620
H	-2.635582	-3.420263	3.570718
H	-4.104556	-2.809315	2.789526
C	-2.889266	-1.452018	0.718445
H	-3.891045	-1.043997	0.900051
H	-2.297248	-0.655700	0.246391
H	-2.982418	-2.273776	-0.002236
C	0.582599	1.953346	3.773738
H	1.357323	1.421400	3.212415
C	1.168097	2.310998	5.141286
H	1.388260	1.415776	5.733369
H	2.103341	2.869050	5.016131
H	0.490142	2.942181	5.727694
C	0.243600	3.228786	2.992163
H	-0.131758	2.997457	1.988670
H	-0.527230	3.812027	3.511010
H	1.129670	3.865358	2.882014
C	3.854942	1.945181	0.419058
H	3.306987	1.422810	1.209686
C	3.070452	3.219077	0.081129
H	3.575905	3.792107	-0.706075
H	2.059275	2.986405	-0.272148
H	2.979238	3.865824	0.961949
C	5.234291	2.304899	0.974883
H	5.128359	2.873060	1.906399
H	5.827865	1.410206	1.193217
H	5.809670	2.927122	0.279436
C	2.048020	-1.967107	-2.330977
H	1.819505	-2.336441	-1.324155
C	0.731614	-1.493419	-2.955572
H	0.005795	-2.313127	-3.023285
H	0.275185	-0.686517	-2.366046
H	0.895915	-1.100545	-3.966360
C	2.622949	-3.130719	-3.138222
H	2.774770	-2.871428	-4.192446
H	3.583350	-3.466011	-2.731492
H	1.931381	-3.980888	-3.112134

Zero-point correction= 0.620497 (Hartree/Particle)
Thermal correction to Energy= 0.654791
Thermal correction to Enthalpy= 0.655735
Thermal correction to Gibbs Free Energy= 0.555745
Sum of electronic and zero-point Energies= -2977.527240
Sum of electronic and thermal Energies= -2977.492946
Sum of electronic and thermal Enthalpies= -2977.492002
Sum of electronic and thermal Free Energies= -2977.591993

$ZnDAD_U$ (PBE)

71
scf done: -2978.142891

Zn	0.361872	1.155267	0.313013
N	0.150240	0.008289	2.024552
N	2.084149	-0.008483	0.194572
C	2.181408	-0.883405	1.203563
C	1.142869	-0.877440	2.182112
C	1.189479	-1.837654	3.336291
C	3.324623	-1.850214	1.325838
H	0.217127	-1.902598	3.830143
H	1.472612	-2.843375	3.008596
H	1.923459	-1.528487	4.093033

H	4.147560	-1.569381	0.664771
H	3.709310	-1.890553	2.350347
H	3.020026	-2.871108	1.057524
C	-0.896168	0.153896	2.959238
C	3.047436	0.080970	-0.832086
C	-2.158441	-0.420512	2.684923
C	-3.213744	-0.184728	3.571911
C	-3.038154	0.594509	4.710208
C	-1.790965	1.155391	4.972813
C	-0.707882	0.952215	4.113537
H	-4.189289	-0.619953	3.367849
H	-3.868701	0.766006	5.390480
H	-1.660948	1.767811	5.861357
C	2.941030	-0.745897	-1.975968
C	3.855486	-0.570877	-3.018123
C	4.856498	0.394537	-2.947350
C	4.950613	1.204000	-1.820424
C	4.059782	1.064451	-0.751325
H	3.784497	-1.197678	-3.903347
H	5.558440	0.515287	-3.768757
H	5.731381	1.959736	-1.769352
C	4.174782	1.979448	0.455040
H	3.488602	1.597528	1.217954
C	3.728564	3.403146	0.105392
H	3.770517	4.050069	0.989995
H	4.375313	3.842368	-0.663748
H	2.699507	3.415189	-0.273622
C	5.581423	1.983443	1.058165
H	5.600414	2.591014	1.970488
H	5.908388	0.971062	1.320378
H	6.320000	2.406116	0.367258
C	1.818444	-1.761807	-2.097649
H	1.473187	-1.990872	-1.084054
C	0.632469	-1.156315	-2.858154
H	-0.201913	-1.866556	-2.906218
H	0.270534	-0.241584	-2.372218
H	0.918817	-0.899493	-3.885326
C	2.254330	-3.078591	-2.741142
H	2.512842	-2.955455	-3.799107
H	3.122146	-3.509517	-2.229350
H	1.437017	-3.807054	-2.691045
C	-2.387155	-1.256801	1.438401
H	-1.402990	-1.473324	1.009625
C	-3.182898	-0.468052	0.392766
H	-2.670530	0.463906	0.123150
H	-3.312923	-1.058564	-0.522272
H	-4.178997	-0.207208	0.770577
C	-3.064569	-2.595418	1.739626
H	-2.505201	-3.168414	2.487605
H	-4.086294	-2.462185	2.113578
H	-3.126519	-3.200640	0.827734
C	0.623218	1.634563	4.379423
H	1.396309	1.067469	3.850838
C	0.618927	3.052339	3.794728
H	0.399237	3.041535	2.720006
H	-0.139796	3.673667	4.285975
H	1.594398	3.533596	3.935534
C	1.010384	1.664018	5.858254
H	0.347830	2.309165	6.446428
H	0.986252	0.662113	6.301362
H	2.026989	2.057886	5.969926

Zero-point correction= 0.618423 (Hartree/Particle)
Thermal correction to Energy= 0.653367
Thermal correction to Enthalpy= 0.654311
Thermal correction to Gibbs Free Energy= 0.547450
Sum of electronic and zero-point Energies= -2977.524468
Sum of electronic and thermal Energies= -2977.489523
Sum of electronic and thermal Enthalpies= -2977.488579
Sum of electronic and thermal Free Energies= -2977.595441

$ZnDAD_{BS}$ (PBE)

71
scf done: -2978.141730

Zn	0.432334	1.202090	0.378283
N	0.250742	0.108428	2.123209
N	2.168980	0.064746	0.280234
C	2.136637	-0.946049	1.163129
C	1.108927	-0.923276	2.149541
C	1.003333	-2.042832	3.145645
C	3.103317	-2.094727	1.118960
H	0.163542	-1.887670	3.825861
H	0.867006	-3.014359	2.653691
H	1.913990	-2.120978	3.752359
H	3.923581	-1.893679	0.426537
H	3.535038	-2.288180	2.107245
H	2.615778	-3.025720	0.799044
C	-0.844204	0.214249	3.007185
C	3.097577	0.116612	-0.780862
C	-2.053846	-0.471391	2.750823
C	-3.142556	-0.255806	3.602965
C	-3.051733	0.610083	4.686884
C	-1.855884	1.280730	4.932282
C	-0.743199	1.100003	4.107417
H	-4.079680	-0.773757	3.411664
H	-3.908315	0.763454	5.338623
H	-1.790451	1.957341	5.780340
C	2.877898	-0.606363	-1.975886
C	3.778154	-0.445076	-3.034795
C	4.875018	0.402674	-2.928370
C	5.085207	1.108992	-1.746515
C	4.211382	0.983447	-0.663935
H	3.614431	-0.991439	-3.960944
H	5.564653	0.513291	-3.761562
H	5.944284	1.770193	-1.668162
C	4.417268	1.796094	0.602152
H	3.933294	1.248210	1.418125
C	3.713828	3.153134	0.481287
H	3.801157	3.722450	1.414602
H	4.158406	3.750718	-0.323968
H	2.646249	3.033378	0.257331
C	5.885986	1.986383	0.979501
H	5.958906	2.474862	1.957859
H	6.414461	1.028474	1.041298
H	6.418824	2.620522	0.261675
C	1.671996	-1.513467	-2.148034
H	1.192769	-1.614474	-1.169027
C	0.646591	-0.882658	-3.096457
H	-0.239920	-1.521890	-3.187736
H	0.319768	0.098474	-2.731302
H	1.068407	-0.746548	-4.099525
C	2.055445	-2.917735	-2.621388
H	2.473930	-2.905082	-3.634428
H	2.796733	-3.377446	-1.958519
H	1.171191	-3.565450	-2.640791
C	-2.207313	-1.397463	1.556830
H	-1.214824	-1.533535	1.115490
C	-3.101836	-0.763277	0.486033

H	-2.700816	0.202283	0.155033
H	-3.176912	-1.416970	-0.391395
H	-4.115901	-0.594776	0.868053
C	-2.731257	-2.780958	1.949897
H	-2.104304	-3.244940	2.719238
H	-3.755969	-2.732740	2.336222
H	-2.741465	-3.444103	1.077003
C	0.539945	1.875604	4.347315
H	1.357180	1.286468	3.916749
C	0.497475	3.214147	3.600462
H	0.312337	3.070488	2.528344
H	-0.302820	3.852972	3.993716
H	1.446593	3.752597	3.710173
C	0.858059	2.098441	5.825368
H	0.141167	2.774607	6.305123
H	0.860467	1.156262	6.384788
H	1.849625	2.553730	5.928259

Zero-point correction= 0.618549 (Hartree/Particle)
Thermal correction to Energy= 0.654180
Thermal correction to Enthalpy= 0.655124
Thermal correction to Gibbs Free Energy= 0.548763
Sum of electronic and zero-point Energies= -2977.523181
Sum of electronic and thermal Energies= -2977.487550
Sum of electronic and thermal Enthalpies= -2977.486606
Sum of electronic and thermal Free Energies= -2977.592967

$ZnDAD_R$ (M06L)

71
scf done: -2979.616254

Zn	0.119957	-0.025792	0.105463
N	0.155402	-0.306387	2.013776
N	2.036731	-0.257934	0.065766
C	2.421277	-0.686116	1.351731
C	1.463150	-0.713437	2.343967
C	1.642239	-1.371011	3.678108
C	3.795103	-1.265777	1.482607
H	1.405237	-0.700514	4.515854
H	0.963147	-2.231066	3.785800
H	2.658603	-1.731877	3.840212
H	4.581651	-0.523758	1.285845
H	3.989071	-1.676421	2.473997
H	3.957032	-2.071071	0.749825
C	-0.806101	-0.052123	2.994549
C	2.983193	-0.006259	-0.933820
C	-2.017348	-0.798925	3.003268
C	-3.000956	-0.503080	3.950959
C	-2.808627	0.488165	4.908928
C	-1.616099	1.209530	4.911203
C	-0.614517	0.973313	3.966141
H	-3.925481	-1.077436	3.956706
H	-3.577552	0.695761	5.648947
H	-1.473190	1.990878	5.654310
C	2.976708	-0.784615	-2.125498
C	3.887660	-0.491190	-3.143544
C	4.822925	0.531502	-3.007447
C	4.838679	1.284004	-1.835827
C	3.933137	1.043527	-0.799116
H	3.881395	-1.088629	-4.053189
H	5.531675	0.739473	-3.805178
H	5.556619	2.096317	-1.733605
C	-2.234998	-1.907518	1.993813
H	-1.238355	-2.280878	1.722583
C	-3.044470	-3.081163	2.533277
H	-3.060744	-3.898931	1.804715
H	-2.620967	-3.470553	3.465001
H	-4.087532	-2.808243	2.730280
C	-2.883481	-1.370580	0.717918
H	-3.895418	-0.998202	0.919377
H	-2.316756	-0.528908	0.296360
H	-2.957304	-2.145291	-0.054683
C	0.605986	1.874993	3.901692
H	1.469972	1.267171	3.608066
C	0.954078	2.547293	5.223809
H	1.046173	1.821836	6.039797
H	1.909517	3.075248	5.137254
H	0.204651	3.290027	5.521615
C	0.424331	2.927851	2.806010
H	0.249000	2.459284	1.830563
H	-0.428737	3.581093	3.028209
H	1.315600	3.559490	2.717584
C	3.900313	1.985429	0.391696
H	3.349682	1.495311	1.203119
C	3.133356	3.256750	0.021177
H	3.637692	3.790968	-0.793731
H	2.113910	3.031337	-0.313191
H	3.063304	3.941278	0.874172
C	5.285439	2.339971	0.923846
H	5.202558	2.933810	1.840595
H	5.872088	1.444495	1.157144
H	5.861952	2.935838	0.206627
C	1.984714	-1.917873	-2.287881
H	1.752610	-2.276423	-1.276082
C	0.679355	-1.415977	-2.905246
H	-0.083876	-2.202856	-2.933050
H	0.266729	-0.565410	-2.345841
H	0.841262	-1.067400	-3.932678
C	2.520831	-3.096439	-3.092070
H	2.676437	-2.840685	-4.146436
H	3.474301	-3.458397	-2.693327
H	1.809270	-3.928779	-3.067445

Zero-point correction= 0.617846 (Hartree/Particle)
Thermal correction to Energy= 0.651807
Thermal correction to Enthalpy= 0.652752
Thermal correction to Gibbs Free Energy= 0.554193
Sum of electronic and zero-point Energies= -2978.998408
Sum of electronic and thermal Energies= -2978.964447
Sum of electronic and thermal Enthalpies= -2978.963502
Sum of electronic and thermal Free Energies= -2979.062061

$ZnDAD_U$ (M06L)

71
scf done: -2979.615251

Zn	0.335256	1.011144	0.259859
N	0.251644	-0.142734	2.016708
N	2.204608	0.073660	0.253836
C	2.421252	-0.736927	1.303766
C	1.373245	-0.838619	2.266433
C	1.490614	-1.681442	3.499775
C	3.716965	-1.476538	1.441055
H	1.762702	-1.086171	4.383390

H	0.530342	-2.155238	3.730948
H	2.235189	-2.472583	3.398395
H	4.551782	-0.846810	1.113865
H	3.916786	-1.785346	2.468201
H	3.747636	-2.379477	0.814351
C	-0.772028	-0.028166	2.974192
C	3.095670	0.115895	-0.833885
C	-1.966016	-0.764459	2.803382
C	-3.007181	-0.577351	3.717311
C	-2.880892	0.314547	4.778483
C	-1.701623	1.039786	4.934620
C	-0.634618	0.888489	4.044745
H	-3.929462	-1.142106	3.599630
H	-3.698763	0.445286	5.482573
H	-1.612852	1.740004	5.762038
C	3.051308	-0.903239	-1.815818
C	3.896929	-0.799586	-2.923522
C	4.763063	0.281690	-3.071443
C	4.789699	1.282915	-2.104766
C	3.964878	1.220685	-0.977537
H	3.877424	-1.574563	-3.686233
H	5.415006	0.343102	-3.939179
H	5.468059	2.124858	-2.225157
C	-2.113364	-1.703996	1.622699
H	-1.105129	-2.046849	1.352218
C	-2.957876	-2.935814	1.926442
H	-2.935057	-3.630300	1.080160
H	-2.593223	-3.470925	2.810020
H	-4.009051	-2.680010	2.101960
C	-2.678256	-0.950680	0.416514
H	-3.688824	-0.580878	0.629500
H	-2.054567	-0.081184	0.155603
H	-2.735781	-1.599289	-0.465412
C	0.616214	1.740243	4.163880
H	1.465698	1.140707	3.812688
C	0.926074	2.176223	5.590346
H	0.967533	1.323838	6.277382
H	1.894317	2.685812	5.628377
H	0.179234	2.879455	5.975939
C	0.519946	2.960031	3.243906
H	0.335214	2.668624	2.198401
H	-0.301825	3.617238	3.553513
H	1.446987	3.544942	3.267882
C	3.963336	2.325768	0.060800
H	3.656196	1.875285	1.014945
C	2.921797	3.388137	-0.297121
H	3.172076	3.871464	-1.249559
H	1.916766	2.949469	-0.400505
H	2.869138	4.166973	0.472629
C	5.329383	2.968905	0.267886
H	5.293914	3.674050	1.104835
H	6.101156	2.223468	0.488575
H	5.654042	3.534478	-0.612919
C	2.046444	-2.034150	-1.692776
H	1.938247	-2.273162	-0.627099
C	0.671375	-1.579608	-2.189148
H	-0.080151	-2.363158	-2.036746
H	0.326284	-0.676779	-1.661584
H	0.702224	-1.345663	-3.260298
C	2.471898	-3.312490	-2.403658
H	2.487234	-3.191157	-3.492748
H	3.469152	-3.640729	-2.090285
H	1.767798	-4.120978	-2.181881

Zero-point correction= 0.618184 (Hartree/Particle)
Thermal correction to Energy= 0.652280
Thermal correction to Enthalpy= 0.653225
Thermal correction to Gibbs Free Energy= 0.553572
Sum of electronic and zero-point Energies= -2978.997068
Sum of electronic and thermal Energies= -2978.962971
Sum of electronic and thermal Enthalpies= -2978.962027
Sum of electronic and thermal Free Energies= -2979.061679

$ZnDAD_R$ (B3LYP)

71
scf done: -2979.879742

Zn	0.151873	0.048434	0.091300
N	0.154690	-0.216753	2.000735
N	2.060044	-0.213655	0.046657
C	2.409747	-0.708270	1.326403
C	1.444793	-0.709500	2.317220
C	1.598810	-1.403369	3.650710
C	3.752881	-1.389495	1.448917
H	1.327863	-0.749105	4.487353
H	0.938311	-2.281140	3.720246
H	2.618332	-1.745666	3.829931
H	4.572641	-0.732219	1.136918
H	3.969738	-1.707067	2.469095
H	3.810072	-2.280290	0.804915
C	-0.841082	0.027814	2.967296
C	2.998485	0.017878	-0.980290
C	-2.050235	-0.732648	2.956670
C	-3.070024	-0.417271	3.865980
C	-2.921018	0.604034	4.803645
C	-1.733639	1.336884	4.826237
C	-0.694295	1.079689	3.922488
H	-3.992592	-0.991600	3.853298
H	-3.719266	0.826750	5.507083
H	-1.623456	2.141475	5.548759
C	2.974591	-0.776537	-2.166185
C	3.848829	-0.468641	-3.218632
C	4.764461	0.578487	-3.122937
C	4.802633	1.343071	-1.956063
C	3.934182	1.092045	-0.885574
H	3.824435	-1.068346	-4.124788
H	5.440017	0.796444	-3.946210
H	5.509697	2.165710	-1.886056
C	-2.256860	-1.876842	1.967072
H	-1.266849	-2.143202	1.584899
C	-2.854232	-3.141866	2.609816
H	-2.861561	-3.964100	1.884143
H	-2.266125	-3.463672	3.476613
H	-3.887920	-2.991996	2.941904
C	-3.112010	-1.433143	0.762682
H	-4.117153	-1.130990	1.080690
H	-2.661340	-0.575934	0.244805
H	-3.217995	-2.247298	0.034737
C	0.529591	1.996111	3.917127
H	1.304788	1.514351	3.317365
C	1.120450	2.239733	5.318072
H	1.350255	1.297103	5.827139
H	2.051079	2.814277	5.239175
H	0.439029	2.810149	5.959965
C	0.194590	3.340496	3.237253
H	-0.180871	3.191317	2.218294
H	-0.572268	3.887209	3.799568
H	1.085759	3.977185	3.177152
C	3.947362	2.031967	0.319945

H	3.371475	1.557639	1.117568
C	3.245706	3.362934	-0.023082
H	3.782940	3.900374	-0.814061
H	2.219253	3.196554	-0.369928
H	3.201312	4.015988	0.857057
C	5.360061	2.299567	0.871148
H	5.299281	2.894308	1.790384
H	5.881967	1.366068	1.109391
H	5.980500	2.858934	0.161253
C	2.009296	-1.949837	-2.315693
H	1.630651	-2.174260	-1.314245
C	0.799043	-1.577934	-3.195958
H	0.083667	-2.408168	-3.249842
H	0.267606	-0.700828	-2.804894
H	1.113516	-1.337974	-4.218928
C	2.684445	-3.227695	-2.846709
H	3.027149	-3.116827	-3.881917
H	3.550064	-3.504184	-2.234310
H	1.976018	-4.064639	-2.825394

Zero-point correction= 0.613863 (Hartree/Particle)
Thermal correction to Energy= 0.649541
Thermal correction to Enthalpy= 0.650485
Thermal correction to Gibbs Free Energy= 0.544164
Sum of electronic and zero-point Energies= -2979.265879
Sum of electronic and thermal Energies= -2979.230201
Sum of electronic and thermal Enthalpies= -2979.229257
Sum of electronic and thermal Free Energies= -2979.335578

$ZnDAD_U$ (B3LYP)

71
scf done: -2979.881246

Zn	0.322418	1.217088	0.282955
N	0.134882	0.061800	2.031170
N	2.066788	0.034204	0.161228
C	2.171594	-0.830249	1.185737
C	1.143109	-0.814969	2.182250
C	1.224608	-1.767901	3.352262
C	3.318823	-1.805658	1.316313
H	0.336443	-1.698368	3.982187
H	1.318489	-2.807654	3.016004
H	2.099498	-1.560073	3.982181
H	4.040694	-1.679753	0.508171
H	3.850852	-1.676740	2.267106
H	2.966019	-2.844812	1.291512
C	-0.930473	0.195919	2.959251
C	3.024791	0.126059	-0.881793
C	-2.156758	-0.480679	2.722827
C	-3.232247	-0.253694	3.593093
C	-3.118556	0.618335	4.675704
C	-1.911754	1.281293	4.898315
C	-0.806764	1.088374	4.057209
H	-4.175503	-0.764975	3.419879
H	-3.964055	0.781976	5.338814
H	-1.828613	1.965389	5.738769
C	2.832673	-0.607682	-2.082355
C	3.739535	-0.428610	-3.136505
C	4.815808	0.451718	-3.026871
C	4.993878	1.172450	-1.846023
C	4.114353	1.029502	-0.763612
H	3.599441	-0.985102	-4.059681
H	5.508451	0.576792	-3.855104
H	5.829868	1.862450	-1.765026
C	4.335219	1.859119	0.499625
H	3.585506	1.547967	1.231481
C	4.116733	3.361571	0.231524
H	4.225805	3.937075	1.158830
H	4.845385	3.748843	-0.490524
H	3.113908	3.551805	-0.168163
C	5.720842	1.613541	1.127102
H	5.815113	2.166977	2.069164
H	5.879698	0.551134	1.343207
H	6.530054	1.945651	0.466322
C	1.656371	-1.566131	-2.256076
H	1.124716	-1.607982	-1.301869
C	0.660778	-1.048458	-3.313369
H	-0.202005	-1.721229	-3.391135
H	0.288592	-0.050733	-3.052835
H	1.126645	-0.985315	-4.303953
C	2.112429	-2.999040	-2.591455
H	2.618764	-3.047135	-3.562553
H	2.803298	-3.386130	-1.834053
H	1.248183	-3.672657	-2.635386
C	-2.334200	-1.418244	1.530172
H	-1.348443	-1.565647	1.081026
C	-3.238545	-0.783306	0.454138
H	-2.835410	0.177608	0.112855
H	-3.322322	-1.443233	-0.418058
H	-4.249558	-0.605795	0.840126
C	-2.865258	-2.805559	1.936954
H	-2.227082	-3.271586	2.696214
H	-3.882900	-2.751708	2.340671
H	-2.892376	-3.470225	1.065231
C	0.482340	1.865328	4.317466
H	1.242891	1.480324	3.633506
C	0.301877	3.364258	4.002474
H	-0.021990	3.516200	2.966222
H	-0.447973	3.821091	4.659315
H	1.246166	3.904048	4.144027
C	1.012287	1.670299	5.750633
H	0.328995	2.088827	6.498551
H	1.155070	0.609205	5.983800
H	1.978766	2.174627	5.869073

Zero-point correction= 0.614902 (Hartree/Particle)
Thermal correction to Energy= 0.650722
Thermal correction to Enthalpy= 0.651667
Thermal correction to Gibbs Free Energy= 0.542831
Sum of electronic and zero-point Energies= -2979.266343
Sum of electronic and thermal Energies= -2979.230523
Sum of electronic and thermal Enthalpies= -2979.229579
Sum of electronic and thermal Free Energies= -2979.338415

$ZnDAD_{BS}$ (B3LYP)

71
scf done: -2979.879848

Zn	0.374380	1.242976	0.350376
N	0.210913	0.108864	2.114082
N	2.133712	0.083073	0.240172
C	2.131915	-0.909123	1.150512
C	1.106118	-0.896233	2.148290
C	1.049585	-2.002905	3.176156

C	3.141511	-2.033648	1.134369
H	0.221293	-1.855699	3.870736
H	0.927776	-2.988658	2.709043
H	1.974338	-2.045300	3.765048
H	3.929675	-1.847878	0.403019
H	3.615904	-2.155671	2.114966
H	2.675681	-2.997251	0.887621
C	-0.884051	0.210804	3.011813
C	3.066014	0.157529	-0.827694
C	-2.093043	-0.493552	2.768466
C	-3.184486	-0.274927	3.622156
C	-3.102392	0.612586	4.694066
C	-1.910981	1.301351	4.925508
C	-0.792333	1.118155	4.101766
H	-4.116194	-0.804878	3.442294
H	-3.959984	0.768360	5.343421
H	-1.852981	1.994803	5.759751
C	2.864602	-0.582437	-2.024168
C	3.761394	-0.403640	-3.087162
C	4.836256	0.480198	-2.992001
C	5.022417	1.208003	-1.817051
C	4.152597	1.066876	-0.726849
H	3.614231	-0.961990	-4.007867
H	5.520563	0.602673	-3.827529
H	5.856903	1.900977	-1.746371
C	4.379255	1.902742	0.530941
H	3.636868	1.586808	1.268415
C	4.148449	3.402491	0.257843
H	4.257781	3.983172	1.181863
H	4.870596	3.792037	-0.469623
H	3.142721	3.584715	-0.138456
C	5.771372	1.668937	1.147770
H	5.870671	2.228539	2.085667
H	5.937027	0.608471	1.369005
H	6.573352	2.000932	0.478063
C	1.679095	-1.530777	-2.195183
H	1.190123	-1.628417	-1.222646
C	0.637828	-0.947464	-3.172086
H	-0.229469	-1.614105	-3.253709
H	0.280251	0.031665	-2.832223
H	1.061447	-0.822383	-4.175693
C	2.105630	-2.943568	-2.637212
H	2.537624	-2.942667	-3.644572
H	2.848300	-3.371156	-1.954621
H	1.237206	-3.612926	-2.653271
C	-2.246190	-1.449252	1.586513
H	-1.263381	-1.560552	1.121500
C	-3.193214	-0.867381	0.517436
H	-2.836634	0.105675	0.159585
H	-3.259555	-1.541134	-0.345628
H	-4.205768	-0.730298	0.915169
C	-2.711073	-2.853694	2.016876
H	-2.045349	-3.282578	2.773963
H	-3.725099	-2.837287	2.432738
H	-2.720641	-3.530209	1.153889
C	0.483199	1.920766	4.350236
H	1.292112	1.420118	3.811008
C	0.355329	3.343201	3.766204
H	0.127295	3.315970	2.693744
H	-0.446270	3.901921	4.264616
H	1.289861	3.902178	3.898206
C	0.888712	1.979111	5.833648
H	0.170315	2.545639	6.437151
H	0.973750	0.975502	6.265679
H	1.861801	2.473639	5.936507

Zero-point correction= 0.614649 (Hartree/Particle)
Thermal correction to Energy= 0.650554
Thermal correction to Enthalpy= 0.651498
Thermal correction to Gibbs Free Energy= 0.543394
Sum of electronic and zero-point Energies= -2979.265199
Sum of electronic and thermal Energies= -2979.229294
Sum of electronic and thermal Enthalpies= -2979.228350
Sum of electronic and thermal Free Energies= -2979.336454

$ZnDAD_R$ (M06-2X)

71
scf done: -2979.263130

Zn	0.112194	-0.115513	0.053493
N	0.134357	-0.396753	1.978948
N	2.035506	-0.392831	0.029050
C	2.407382	-0.790207	1.336045
C	1.450727	-0.794737	2.316743
C	1.642491	-1.350972	3.704738
C	3.806746	-1.325954	1.496797
H	1.532382	-0.580572	4.478953
H	0.879218	-2.112396	3.916092
H	2.620422	-1.811324	3.842143
H	4.563925	-0.545782	1.347690
H	3.980034	-1.760378	2.480761
H	4.008596	-2.100329	0.743903
C	-0.802220	-0.064336	2.967245
C	3.001470	-0.069247	-0.934897
C	-2.028580	-0.780677	3.038159
C	-2.983367	-0.420513	3.993429
C	-2.749709	0.614307	4.895550
C	-1.547441	1.314663	4.829678
C	-0.574691	1.006081	3.874755
H	-3.918983	-0.970379	4.049445
H	-3.496432	0.873068	5.640772
H	-1.374408	2.133353	5.523679
C	3.057053	-0.810481	-2.146825
C	3.993174	-0.463234	-3.124966
C	4.889611	0.584564	-2.928572
C	4.835071	1.312471	-1.742521
C	3.899252	1.015712	-0.747642
H	4.038161	-1.031970	-4.049900
H	5.620153	0.833126	-3.693073
H	5.521202	2.143826	-1.599333
C	-2.299145	-1.920781	2.070778
H	-1.324925	-2.352428	1.816423
C	-3.173162	-3.034022	2.653921
H	-3.204917	-3.881785	1.961391
H	-2.780319	-3.391468	3.611247
H	-4.205956	-2.704277	2.811486
C	-2.933356	-1.395194	0.775484
H	-3.916029	-0.954733	0.981504
H	-2.320101	-0.611837	0.310489
H	-3.065494	-2.201022	0.044473
C	0.652208	1.897465	3.737242
H	1.438519	1.329170	3.233316
C	1.216964	2.380404	5.076251
H	1.387672	1.545697	5.764705
H	2.173969	2.887775	4.914453
H	0.549394	3.095430	5.569491
C	0.314971	3.097286	2.840128
H	-0.025704	2.768948	1.851177
H	-0.481293	3.702454	3.289995

H	1.193276	3.737477	2.702264
C	3.771831	1.937309	0.457760
H	3.225581	1.405981	1.242491
C	2.938858	3.167745	0.068461
H	3.436687	3.730356	-0.730382
H	1.945529	2.876474	-0.292358
H	2.807613	3.837692	0.925159
C	5.118445	2.374950	1.041998
H	4.959021	2.919442	1.978909
H	5.763112	1.515492	1.254679
H	5.659563	3.044196	0.364157
C	2.090005	-1.959318	-2.377167
H	1.853885	-2.371859	-1.390289
C	0.782557	-1.448535	-2.998920
H	0.048507	-2.256617	-3.095785
H	0.330641	-0.647731	-2.398576
H	0.970088	-1.035081	-3.996987
C	2.661814	-3.088048	-3.238330
H	2.803715	-2.777654	-4.279274
H	3.625423	-3.436588	-2.852834
H	1.970447	-3.937335	-3.243894

Zero-point correction= 0.622310 (Hartree/Particle)
Thermal correction to Energy= 0.656183
Thermal correction to Enthalpy= 0.657127
Thermal correction to Gibbs Free Energy= 0.558257
Sum of electronic and zero-point Energies= -2978.640820
Sum of electronic and thermal Energies= -2978.606947
Sum of electronic and thermal Enthalpies= -2978.606003
Sum of electronic and thermal Free Energies= -2978.704873

$ZnDAD_U$ (M06-2X)

71
scf done: -2979.259733

Zn	0.311480	1.145848	0.280791
N	0.175424	-0.010358	2.040760
N	2.061840	-0.034731	0.189437
C	2.201585	-0.879114	1.219904
C	1.175688	-0.878625	2.213942
C	1.225340	-1.830679	3.384818
C	3.403773	-1.779282	1.319122
H	0.312154	-1.757438	3.978939
H	1.325198	-2.867446	3.047373
H	2.073783	-1.617914	4.045691
H	4.327640	-1.189831	1.276095
H	3.411418	-2.355587	2.244108
H	3.438118	-2.482367	0.476838
C	-0.884160	0.154878	2.957775
C	3.049139	0.042538	-0.820493
C	-2.166555	-0.321308	2.615576
C	-3.234763	-0.066024	3.483818
C	-3.046156	0.640801	4.665563
C	-1.773974	1.111089	4.993316
C	-0.681296	0.886853	4.153530
H	-4.227295	-0.430444	3.228222
H	-3.883748	0.828427	5.331123
H	-1.637344	1.665825	5.916852
C	2.972661	-0.812409	-1.942593
C	3.913531	-0.661826	-2.965092
C	4.911694	0.307412	-2.886759
C	4.981040	1.139852	-1.773145
C	4.061871	1.021205	-0.725672
H	3.869401	-1.310046	-3.835691
H	5.634568	0.410927	-3.690878
H	5.764634	1.890877	-1.717029
C	4.124014	1.954710	0.473348
H	3.589781	1.469208	1.297688
C	3.401534	3.272268	0.157687
H	3.390073	3.929343	1.034723
H	3.909787	3.799067	-0.658778
H	2.363476	3.096701	-0.151399
C	5.553811	2.233208	0.945668
H	5.532416	2.804491	1.879597
H	6.104713	1.304235	1.126490
H	6.114980	2.824365	0.214145
C	1.851862	-1.835208	-2.045981
H	1.583367	-2.134698	-1.026851
C	0.609964	-1.194862	-2.682953
H	-0.223665	-1.905906	-2.708124
H	0.285457	-0.308066	-2.124123
H	0.827340	-0.884202	-3.711745
C	2.248668	-3.099861	-2.810699
H	2.406786	-2.899291	-3.875783
H	3.166060	-3.542376	-2.407987
H	1.449578	-3.844324	-2.734582
C	-2.407520	-1.102131	1.333121
H	-1.440621	-1.228566	0.834792
C	-3.329821	-0.331762	0.380334
H	-2.919802	0.658350	0.147830
H	-3.453028	-0.879440	-0.560748
H	-4.322920	-0.191887	0.822810
C	-2.968572	-2.499395	1.621565
H	-2.305659	-3.060796	2.288528
H	-3.955121	-2.441392	2.094908
H	-3.077068	-3.065823	0.690365
C	0.689697	1.468800	4.467985
H	1.445188	0.750132	4.133423
C	0.907378	2.766741	3.675479
H	0.791366	2.602861	2.597369
H	0.179372	3.526476	3.983373
H	1.913325	3.163875	3.853025
C	0.925343	1.717429	5.958634
H	0.297247	2.530089	6.339343
H	0.723168	0.821075	6.554491
H	1.968015	2.007270	6.123038

Zero-point correction= 0.620938 (Hartree/Particle)
Thermal correction to Energy= 0.655860
Thermal correction to Enthalpy= 0.656805
Thermal correction to Gibbs Free Energy= 0.552454
Sum of electronic and zero-point Energies= -2978.638795
Sum of electronic and thermal Energies= -2978.603873
Sum of electronic and thermal Enthalpies= -2978.602929
Sum of electronic and thermal Free Energies= -2978.707279

$ZnDAD_{BS}$ (M06-2X)

71
scf done: -2979.259055

Zn	0.471044	1.239514	0.424070
N	0.327821	0.105362	2.194076
N	2.225727	0.064166	0.349416
C	2.118350	-1.013232	1.140516

C	1.093177	-0.992914	2.132171
C	0.877191	-2.196980	3.013500
C	2.976866	-2.240902	0.976667
H	0.070622	-2.022092	3.727772
H	0.622076	-3.086459	2.423160
H	1.782567	-2.437315	3.581344
H	3.841805	-2.035468	0.342415
H	3.341422	-2.598998	1.943983
H	2.413616	-3.065799	0.519273
C	-0.789167	0.212448	3.053128
C	3.133701	0.118797	-0.731834
C	-1.994231	-0.469737	2.779612
C	-3.094359	-0.251289	3.617455
C	-3.015056	0.616748	4.700992
C	-1.822013	1.291375	4.958659
C	-0.701700	1.107179	4.146076
H	-4.030313	-0.765895	3.412845
H	-3.878365	0.771621	5.341686
H	-1.767659	1.969697	5.805257
C	2.899246	-0.594452	-1.926700
C	3.795709	-0.434905	-2.990273
C	4.898921	0.404956	-2.884245
C	5.117868	1.110973	-1.701521
C	4.246129	0.986300	-0.618217
H	3.621902	-0.974132	-3.918573
H	5.586122	0.512483	-3.718497
H	5.980830	1.766192	-1.626211
C	4.436547	1.793445	0.656292
H	4.089156	1.172360	1.489521
C	3.557273	3.052402	0.615223
H	3.631546	3.608959	1.556048
H	3.879501	3.712017	-0.199346
H	2.500242	2.805905	0.446685
C	5.890975	2.179751	0.930178
H	5.969898	2.643077	1.918908
H	6.551042	1.306241	0.910652
H	6.263661	2.905786	0.199417
C	1.677852	-1.483813	-2.103806
H	1.184074	-1.582914	-1.131845
C	0.674129	-0.833929	-3.066346
H	-0.225320	-1.453030	-3.159349
H	0.370903	0.157830	-2.711287
H	1.112545	-0.718758	-4.064389
C	2.049586	-2.890729	-2.586091
H	2.453471	-2.868879	-3.604251
H	2.800143	-3.351922	-1.935940
H	1.162948	-3.533723	-2.596173
C	-2.140459	-1.388930	1.576217
H	-1.151712	-1.520810	1.125243
C	-3.049697	-0.749822	0.517225
H	-2.666944	0.228777	0.205262
H	-3.114736	-1.389766	-0.369998
H	-4.063400	-0.609040	0.909900
C	-2.664500	-2.775857	1.966045
H	-2.046329	-3.233211	2.745402
H	-3.693251	-2.722218	2.339050
H	-2.663184	-3.439224	1.094514
C	0.584818	1.884251	4.376307
H	1.415613	1.233847	4.080801
C	0.617155	3.123444	3.469176
H	0.488201	2.856782	2.411777
H	-0.192356	3.811714	3.740077
H	1.568813	3.656365	3.572850
C	0.803133	2.297852	5.832664
H	0.077906	3.053670	6.153388
H	0.727093	1.442037	6.511467
H	1.800481	2.734636	5.946778

Zero-point correction= 0.621877 (Hartree/Particle)
Thermal correction to Energy= 0.656242
Thermal correction to Enthalpy= 0.657186
Thermal correction to Gibbs Free Energy= 0.556689
Sum of electronic and zero-point Energies= -2978.637178
Sum of electronic and thermal Energies= -2978.602813
Sum of electronic and thermal Enthalpies= -2978.601869
Sum of electronic and thermal Free Energies= -2978.702366

$ZnDAD_R$ (TPSSh)

71
scf done: -2979.915244

Zn	0.171699	-0.015436	0.104565
N	0.160611	-0.274492	2.005230
N	2.069549	-0.278335	0.052422
C	2.440931	-0.688602	1.358368
C	1.474614	-0.685547	2.347886
C	1.651096	-1.315395	3.708729
C	3.804894	-1.319178	1.505272
H	1.325508	-0.644758	4.513028
H	1.044686	-2.229454	3.801282
H	2.689632	-1.582352	3.910647
H	4.601977	-0.649229	1.160946
H	4.029588	-1.584794	2.539429
H	3.883618	-2.234122	0.898318
C	-0.833949	-0.003008	2.964265
C	3.005217	-0.019275	-0.967848
C	-2.048829	-0.755462	2.951788
C	-3.072008	-0.429073	3.854421
C	-2.920326	0.597512	4.789012
C	-1.727368	1.324688	4.811121
C	-0.685393	1.056249	3.911649
H	-3.997689	-0.999794	3.839631
H	-3.719833	0.828899	5.488314
H	-1.614739	2.136455	5.526351
C	2.964892	-0.785637	-2.173011
C	3.840466	-0.467936	-3.222244
C	4.774848	0.563285	-3.105553
C	4.825651	1.302826	-1.921080
C	3.953989	1.042604	-0.853713
H	3.804299	-1.049293	-4.140733
H	5.452695	0.788346	-3.925102
H	5.541540	2.117234	-1.834804
C	-2.248712	-1.901296	1.965783
H	-1.251823	-2.181555	1.607537
C	-2.884796	-3.149755	2.602421
H	-2.890800	-3.975456	1.880702
H	-2.322429	-3.474755	3.484828
H	-3.923019	-2.974459	2.907567
C	-3.072841	-1.448161	0.743488
H	-4.079363	-1.132859	1.043665
H	-2.599228	-0.595448	0.237616
H	-3.173147	-2.261552	0.013911
C	0.534515	1.974842	3.887974
H	1.320838	1.474109	3.314921
C	1.099789	2.280653	5.286611
H	1.324071	1.361066	5.838610
H	2.028373	2.856889	5.197007
H	0.402591	2.874810	5.889243
C	0.192254	3.289365	3.155332

H	-0.165387	3.096837	2.137110
H	-0.591393	3.840580	3.689631
H	1.075828	3.935779	3.087678
C	3.961423	1.970851	0.358962
H	3.406816	1.477122	1.162729
C	3.223278	3.284235	0.024465
H	3.739148	3.827983	-0.776542
H	2.196118	3.091034	-0.306288
H	3.178841	3.937821	0.904214
C	5.374291	2.277586	0.887200
H	5.309151	2.863243	1.811922
H	5.928603	1.358329	1.107080
H	5.961612	2.862632	0.169528
C	1.980061	-1.938450	-2.335450
H	1.637995	-2.200845	-1.328154
C	0.743687	-1.507684	-3.150576
H	0.019313	-2.328232	-3.227440
H	0.237050	-0.651380	-2.684459
H	1.027862	-1.207430	-4.166290
C	2.614118	-3.195931	-2.956462
H	2.905164	-3.038033	-4.001530
H	3.505213	-3.506571	-2.399703
H	1.896261	-4.024820	-2.938056

Zero-point correction= 0.613816 (Hartree/Particle)
Thermal correction to Energy= 0.649559
Thermal correction to Enthalpy= 0.650504
Thermal correction to Gibbs Free Energy= 0.544913
Sum of electronic and zero-point Energies= -2979.301428
Sum of electronic and thermal Energies= -2979.265685
Sum of electronic and thermal Enthalpies= -2979.264741
Sum of electronic and thermal Free Energies= -2979.370331

$ZnDAD_U$ (TPPSh)

71
scf done: -2979.911806

Zn	0.377308	1.160809	0.317202
N	0.153447	0.009715	2.028796
N	2.104293	-0.002677	0.201109
C	2.197043	-0.886445	1.214292
C	1.153696	-0.878923	2.193710
C	1.197307	-1.846987	3.351848
C	3.343618	-1.860968	1.340037
H	0.242445	-1.861438	3.882306
H	1.413890	-2.865022	3.008499
H	1.978765	-1.578624	4.075627
H	4.155898	-1.595678	0.659540
H	3.742540	-1.877087	2.360479
H	3.028819	-2.886046	1.101080
C	-0.906373	0.160875	2.960690
C	3.066680	0.079955	-0.839150
C	-2.184375	-0.371718	2.649458
C	-3.251376	-0.127038	3.528041
C	-3.074011	0.623693	4.690980
C	-1.812750	1.148117	4.986526
C	-0.716213	0.933777	4.138588
H	-4.234188	-0.531478	3.296973
H	-3.910888	0.802552	5.361134
H	-1.682429	1.740473	5.888452
C	2.970151	-0.778343	-1.967665
C	3.877878	-0.605814	-3.022942
C	4.859768	0.387955	-2.981397
C	4.941008	1.229784	-1.871302
C	4.057276	1.094550	-0.789094
H	3.815561	-1.253797	-3.893155
H	5.553597	0.505255	-3.809850
H	5.703302	2.005123	-1.842808
C	4.161320	2.043553	0.400515
H	3.467762	1.682538	1.166423
C	3.721868	3.468773	0.009816
H	3.762007	4.135084	0.880234
H	4.376327	3.884794	-0.765631
H	2.694765	3.472751	-0.374832
C	5.572639	2.059742	1.016716
H	5.587043	2.696867	1.909097
H	5.889566	1.053320	1.312524
H	6.315681	2.455434	0.314433
C	1.859805	-1.820893	-2.061349
H	1.535351	-2.049948	-1.041341
C	0.642658	-1.238345	-2.810167
H	-0.178842	-1.964906	-2.835651
H	0.275962	-0.326457	-2.321947
H	0.907812	-0.985478	-3.843908
C	2.309150	-3.140982	-2.710363
H	2.545556	-3.016697	-3.773474
H	3.193587	-3.552541	-2.210974
H	1.503812	-3.881328	-2.639763
C	-2.418495	-1.182663	1.379018
H	-1.441801	-1.343138	0.911172
C	-3.292287	-0.401760	0.377414
H	-2.831366	0.559351	0.118469
H	-3.423112	-0.976498	-0.547666
H	-4.286354	-0.200258	0.794547
C	-3.030791	-2.565120	1.671892
H	-2.408306	-3.136126	2.370000
H	-4.033754	-2.478407	2.106092
H	-3.119220	-3.142746	0.744003
C	0.630271	1.585835	4.440391
H	1.398193	1.034299	3.889522
C	0.646701	3.038118	3.918781
H	0.430217	3.075169	2.844038
H	-0.105483	3.645342	4.436809
H	1.629422	3.496545	4.084538
C	1.011556	1.543350	5.930136
H	0.347804	2.164939	6.542054
H	0.977293	0.521048	6.323374
H	2.030657	1.924701	6.063303

Zero-point correction= 0.614049 (Hartree/Particle)
Thermal correction to Energy= 0.650336
Thermal correction to Enthalpy= 0.651281
Thermal correction to Gibbs Free Energy= 0.541281
Sum of electronic and zero-point Energies= -2979.297757
Sum of electronic and thermal Energies= -2979.261469
Sum of electronic and thermal Enthalpies= -2979.260525
Sum of electronic and thermal Free Energies= -2979.370525

$ZnDAD_{BS}$ (TPPSh)

71
scf done: -2979.911015

Zn	0.394858	1.173917	0.418581
N	0.251776	0.101286	2.173925

N	2.161500	0.111648	0.314560
C	2.115284	-0.953971	1.151978
C	1.095593	-0.959176	2.146463
C	0.963498	-2.134291	3.085627
C	3.062233	-2.125102	1.038593
H	0.221262	-1.933800	3.861433
H	0.664161	-3.050664	2.558774
H	1.918577	-2.349229	3.579414
H	3.803108	-1.956029	0.254459
H	3.600972	-2.284639	1.980989
H	2.533241	-3.060385	0.812238
C	-0.857692	0.179411	3.056666
C	3.075390	0.192100	-0.771214
C	-2.048692	-0.556381	2.823965
C	-3.141219	-0.358633	3.684798
C	-3.071583	0.536334	4.752563
C	-1.896002	1.261613	4.970585
C	-0.782169	1.104158	4.134710
H	-4.061642	-0.911608	3.512518
H	-3.926579	0.671491	5.410043
H	-1.849194	1.959053	5.802273
C	2.851744	-0.523786	-1.978717
C	3.737932	-0.333188	-3.050347
C	4.824158	0.538827	-2.950741
C	5.031944	1.243064	-1.763170
C	4.171807	1.088664	-0.665608
H	3.571592	-0.872013	-3.980256
H	5.499745	0.670352	-3.792051
H	5.874286	1.927083	-1.686855
C	4.416317	1.893115	0.606941
H	3.661934	1.580632	1.335336
C	4.232042	3.402858	0.356159
H	4.356206	3.964155	1.290212
H	4.970185	3.778371	-0.362776
H	3.234082	3.620753	-0.041565
C	5.803459	1.610275	1.213700
H	5.923157	2.156783	2.156941
H	5.936182	0.542364	1.420379
H	6.608566	1.927166	0.540020
C	1.652509	-1.451364	-2.152104
H	1.176138	-1.565959	-1.173572
C	0.609778	-0.826943	-3.101432
H	-0.265712	-1.481540	-3.193054
H	0.269464	0.145969	-2.726507
H	1.029534	-0.679173	-4.103706
C	2.056215	-2.854285	-2.643117
H	2.471266	-2.822556	-3.657291
H	2.805485	-3.308891	-1.985920
H	1.178993	-3.511841	-2.665541
C	-2.187293	-1.506390	1.638130
H	-1.196397	-1.625386	1.189272
C	-3.110933	-0.902579	0.560520
H	-2.730445	0.065978	0.214108
H	-3.177794	-1.571953	-0.305989
H	-4.124164	-0.751360	0.951785
C	-2.685005	-2.903657	2.052552
H	-2.049473	-3.341848	2.829748
H	-3.711532	-2.868799	2.435771
H	-2.678548	-3.577149	1.187277
C	0.482636	1.934698	4.330721
H	1.329275	1.310237	4.023733
C	0.460193	3.164258	3.399205
H	0.332189	2.863608	2.349715
H	-0.367598	3.834435	3.660964
H	1.397464	3.728651	3.477833
C	0.725024	2.372512	5.783275
H	-0.025050	3.094972	6.125928
H	0.713792	1.517916	6.469372
H	1.704633	2.857676	5.863028

Zero-point correction= 0.614395 (Hartree/Particle)
Thermal correction to Energy= 0.650259
Thermal correction to Enthalpy= 0.651203
Thermal correction to Gibbs Free Energy= 0.545133
Sum of electronic and zero-point Energies= -2979.296620
Sum of electronic and thermal Energies= -2979.260756
Sum of electronic and thermal Enthalpies= -2979.259812
Sum of electronic and thermal Free Energies= -2979.365882

$ZnDAD_R$ (CAM-B3LYP)

71
scf done: -2979.230768

Zn	0.193240	-0.036234	0.079589
N	0.133722	-0.327397	1.956988
N	2.067632	-0.341945	0.040819
C	2.406857	-0.779871	1.346759
C	1.434340	-0.771061	2.310354
C	1.585109	-1.366552	3.685432
C	3.769369	-1.400921	1.510257
H	1.346924	-0.643346	4.472314
H	0.897830	-2.211963	3.824297
H	2.594935	-1.726329	3.877453
H	4.575119	-0.688389	1.305137
H	3.934185	-1.791511	2.513460
H	3.904512	-2.231663	0.804805
C	-0.842508	-0.003951	2.918147
C	3.032867	-0.045487	-0.937467
C	-2.043474	-0.757748	2.978759
C	-3.041951	-0.387844	3.881703
C	-2.875469	0.689340	4.743135
C	-1.694644	1.420583	4.692922
C	-0.678457	1.102827	3.790746
H	-3.963762	-0.960345	3.923573
H	-3.658892	0.957398	5.446161
H	-1.569954	2.270189	5.358189
C	3.047276	-0.789868	-2.146997
C	3.958453	-0.455073	-3.149476
C	4.869723	0.580959	-2.981404
C	4.860414	1.305795	-1.796073
C	3.952955	1.022003	-0.773946
H	3.969382	-1.022294	-4.075032
H	5.579029	0.821899	-3.767957
H	5.562832	2.124968	-1.672085
C	-2.261974	-1.946977	2.056650
H	-1.271941	-2.260824	1.716579
C	-2.916857	-3.147145	2.747319
H	-2.927722	-4.008200	2.070481
H	-2.369208	-3.435948	3.649931
H	-3.954580	-2.946603	3.032931
C	-3.071644	-1.541392	0.817188
H	-4.077294	-1.209302	1.098149
H	-2.594914	-0.714617	0.277000
H	-3.175738	-2.382230	0.122306
C	0.543575	2.007367	3.699888
H	1.306539	1.479905	3.125297
C	1.150987	2.348989	5.064869
H	1.380427	1.446832	5.640490
H	2.083130	2.908359	4.932108

H	0.481625	2.970589	5.668624
C	0.199506	3.293729	2.935126
H	-0.189727	3.073668	1.935619
H	-0.560439	3.875456	3.468831
H	1.086560	3.925736	2.819054
C	3.905736	1.928027	0.449665
H	3.333059	1.415242	1.223924
C	3.163010	3.230727	0.118624
H	3.693981	3.798925	-0.653408
H	2.150934	3.032348	-0.248947
H	3.079878	3.866561	1.006709
C	5.288247	2.240478	1.032507
H	5.183540	2.797243	1.969741
H	5.851100	1.326478	1.246334
H	5.891029	2.854542	0.355404
C	2.061552	-1.928089	-2.357249
H	1.813098	-2.309310	-1.362961
C	0.761722	-1.415110	-2.991327
H	0.021604	-2.218090	-3.081284
H	0.314990	-0.609679	-2.394796
H	0.947667	-1.011741	-3.992953
C	2.619548	-3.094714	-3.176413
H	2.789485	-2.824003	-4.223543
H	3.566330	-3.457558	-2.764200
H	1.908768	-3.927816	-3.169455

Zero-point correction= 0.622930 (Hartree/Particle)
Thermal correction to Energy= 0.657422
Thermal correction to Enthalpy= 0.658366
Thermal correction to Gibbs Free Energy= 0.555934
Sum of electronic and zero-point Energies= -2978.607838
Sum of electronic and thermal Energies= -2978.573346
Sum of electronic and thermal Enthalpies= -2978.572401
Sum of electronic and thermal Free Energies= -2978.674833

$ZnDAD_U$ (CAM-B3LYP)

71
scf done: -2979.229178

Zn	0.328729	1.207571	0.300434
N	0.137300	0.068706	2.018900
N	2.049665	0.050963	0.166011
C	2.164878	-0.812156	1.181930
C	1.141722	-0.802639	2.173520
C	1.226420	-1.746550	3.343323
C	3.315204	-1.775991	1.306728
H	0.317804	-1.714639	3.944799
H	1.376019	-2.779138	3.011768
H	2.070064	-1.497775	3.998222
H	4.049721	-1.621636	0.516463
H	3.825762	-1.665927	2.269459
H	2.972159	-2.815374	1.246939
C	-0.923100	0.191732	2.951006
C	3.004175	0.141230	-0.877379
C	-2.139882	-0.483435	2.714667
C	-3.205828	-0.275853	3.591868
C	-3.086900	0.576933	4.682142
C	-1.884826	1.236873	4.905991
C	-0.791639	1.060085	4.056142
H	-4.147580	-0.787872	3.417132
H	-3.927239	0.727813	5.353425
H	-1.796272	1.906975	5.756092
C	2.817484	-0.601047	-2.063155
C	3.723133	-0.433192	-3.112162
C	4.793883	0.445916	-3.007263
C	4.966416	1.175222	-1.837329
C	4.085269	1.041502	-0.762923
H	3.585746	-0.998535	-4.029605
H	5.488798	0.563778	-3.833554
H	5.800819	1.866406	-1.758151
C	4.301514	1.874308	0.491827
H	3.533581	1.586435	1.212664
C	4.125987	3.371176	0.206273
H	4.231923	3.952748	1.128471
H	4.877379	3.731921	-0.504306
H	3.137483	3.581716	-0.214691
C	5.665912	1.601173	1.136168
H	5.764368	2.161764	2.071956
H	5.794640	0.538423	1.364455
H	6.488696	1.904829	0.480352
C	1.648401	-1.560596	-2.227685
H	1.109232	-1.585673	-1.278420
C	0.669499	-1.066399	-3.300393
H	-0.191405	-1.739666	-3.374772
H	0.295913	-0.064374	-3.065306
H	1.147294	-1.024266	-4.285120
C	2.112190	-2.989820	-2.532918
H	2.626937	-3.049566	-3.497587
H	2.797946	-3.360092	-1.764259
H	1.253147	-3.668006	-2.574045
C	-2.318329	-1.400889	1.514080
H	-1.333058	-1.548522	1.066641
C	-3.213622	-0.746852	0.453090
H	-2.805516	0.215802	0.127282
H	-3.302829	-1.391834	-0.427960
H	-4.221695	-0.569730	0.843806
C	-2.859211	-2.781706	1.901532
H	-2.229065	-3.260612	2.657772
H	-3.877088	-2.723373	2.300654
H	-2.888183	-3.435588	1.023491
C	0.494871	1.830752	4.313893
H	1.260097	1.427527	3.647566
C	0.321522	3.315654	3.967295
H	0.009456	3.446861	2.925923
H	-0.435620	3.783306	4.606146
H	1.262871	3.857664	4.109379
C	1.003196	1.665574	5.750413
H	0.317729	2.111142	6.478548
H	1.129578	0.610017	6.011266
H	1.973019	2.160641	5.867328

Zero-point correction= 0.622118 (Hartree/Particle)
Thermal correction to Energy= 0.657553
Thermal correction to Enthalpy= 0.658497
Thermal correction to Gibbs Free Energy= 0.550293
Sum of electronic and zero-point Energies= -2978.607060
Sum of electronic and thermal Energies= -2978.571625
Sum of electronic and thermal Enthalpies= -2978.570681
Sum of electronic and thermal Free Energies= -2978.678885

$ZnDAD_{BS}$ (CAM-B3LYP)

71
scf done: -2979.227687

Zn	0.340152	1.215469	0.320729
N	0.161406	0.089803	2.050240
N	2.065966	0.065866	0.190869
C	2.148334	-0.841016	1.171904
C	1.127418	-0.830028	2.165512
C	1.168633	-1.829702	3.290489
C	3.252746	-1.861623	1.248311
H	0.275018	-1.764842	3.911265
H	1.245780	-2.854742	2.913052
H	2.037359	-1.663312	3.938527
H	4.000787	-1.695638	0.473158
H	3.758790	-1.830019	2.218938
H	2.864348	-2.879671	1.126159
C	-0.909844	0.195660	2.971621
C	3.018518	0.152914	-0.854352
C	-2.119423	-0.486613	2.726367
C	-3.190861	-0.292261	3.601442
C	-3.081892	0.553978	4.696501
C	-1.884442	1.221486	4.930467
C	-0.787741	1.058412	4.083832
H	-4.127748	-0.811254	3.419811
H	-3.925198	0.694139	5.366407
H	-1.805620	1.882871	5.787471
C	2.828049	-0.580230	-2.045756
C	3.735811	-0.410222	-3.092420
C	4.813047	0.460426	-2.979678
C	4.990136	1.179178	-1.804193
C	4.106125	1.043893	-0.732153
H	3.596465	-0.966880	-4.014584
H	5.509610	0.579015	-3.804488
H	5.830488	1.862376	-1.717996
C	4.328241	1.862097	0.530985
H	3.545310	1.586356	1.240407
C	4.192984	3.365157	0.256721
H	4.300794	3.935727	1.185525
H	4.961937	3.714563	-0.440586
H	3.215634	3.603739	-0.175193
C	5.678347	1.548884	1.187088
H	5.783883	2.102702	2.126163
H	5.774849	0.481945	1.412056
H	6.515112	1.831740	0.539595
C	1.645144	-1.521218	-2.220107
H	1.155909	-1.616774	-1.248473
C	0.616916	-0.935649	-3.197104
H	-0.251716	-1.597354	-3.285531
H	0.262555	0.044239	-2.860203
H	1.048386	-0.812053	-4.196405
C	2.071071	-2.926589	-2.659718
H	2.511968	-2.923152	-3.661932
H	2.806039	-3.355614	-1.971229
H	1.203011	-3.593840	-2.685478
C	-2.286875	-1.410080	1.528957
H	-1.318918	-1.475361	1.027677
C	-3.289933	-0.836348	0.519951
H	-2.982326	0.157005	0.176816
H	-3.368284	-1.487743	-0.357315
H	-4.288826	-0.746008	0.960222
C	-2.686229	-2.830877	1.944617
H	-1.967202	-3.257066	2.651497
H	-3.673683	-2.851272	2.417477
H	-2.726374	-3.486108	1.067904
C	0.497500	1.835399	4.329414
H	1.304465	1.300638	3.822804
C	0.408897	3.233679	3.701628
H	0.195227	3.178196	2.628773
H	-0.387745	3.820839	4.172029
H	1.351272	3.777292	3.830994
C	0.876426	1.936135	5.809839
H	0.171690	2.554664	6.374695
H	0.914320	0.949899	6.283441
H	1.864671	2.396595	5.910799

Zero-point correction= 0.621913 (Hartree/Particle)
Thermal correction to Energy= 0.657461
Thermal correction to Enthalpy= 0.658405
Thermal correction to Gibbs Free Energy= 0.550711
Sum of electronic and zero-point Energies= -2978.605774
Sum of electronic and thermal Energies= -2978.570226
Sum of electronic and thermal Enthalpies= -2978.569282
Sum of electronic and thermal Free Energies= -2978.676975

$ZnDAD_R$ (LC-BLYP)

71
scf done: -2975.827055

Zn	0.147628	0.042437	0.144321
N	0.131673	-0.309608	1.976679
N	1.967742	-0.359366	-0.010090
C	2.343829	-0.825530	1.272378
C	1.423362	-0.805351	2.267894
C	1.609511	-1.412767	3.624539
C	3.712549	-1.423926	1.379102
H	1.519324	-0.671744	4.424453
H	0.839628	-2.169531	3.814161
H	2.578864	-1.893904	3.737946
H	4.494002	-0.685601	1.175450
H	3.912188	-1.839544	2.364633
H	3.844400	-2.226606	0.644178
C	-0.797326	0.000606	2.978251
C	2.933698	-0.033971	-0.976877
C	-2.016167	-0.702456	3.029059
C	-2.965048	-0.354114	3.978568
C	-2.730226	0.659229	4.888200
C	-1.531756	1.344640	4.840930
C	-0.563455	1.041384	3.895146
H	-3.905020	-0.895111	4.019739
H	-3.479888	0.914237	5.631344
H	-1.353107	2.148889	5.548344
C	3.049427	-0.816730	-2.139193
C	3.963184	-0.452769	-3.117688
C	4.777375	0.652486	-2.961978
C	4.672559	1.412634	-1.813166
C	3.759828	1.092504	-0.819325
H	4.050570	-1.052116	-4.018689
H	5.492788	0.919928	-3.734029
H	5.308025	2.285438	-1.692811
C	-2.292901	-1.814688	2.043521
H	-1.320791	-2.230404	1.767578
C	-3.141134	-2.941810	2.611129
H	-3.183884	-3.770795	1.898906
H	-2.727257	-3.324522	3.548017
H	-4.171239	-2.627184	2.801913
C	-2.939923	-1.270419	0.775425
H	-3.911506	-0.818330	0.998951
H	-2.322718	-0.498974	0.301613
H	-3.099458	-2.067595	0.042754
C	0.683857	1.894608	3.805052
H	1.429396	1.339023	3.235183
C	1.292276	2.223314	5.160243

H	1.471078	1.320660	5.751151
H	2.250904	2.733045	5.027416
H	0.651376	2.886772	5.747848
C	0.386228	3.176227	3.035348
H	0.001625	2.961523	2.034069
H	-0.362001	3.779802	3.559279
H	1.290436	3.782546	2.925617
C	3.621087	2.001979	0.382221
H	3.010998	1.481190	1.121544
C	2.889583	3.281260	-0.006587
H	3.460842	3.845826	-0.750390
H	1.906422	3.066857	-0.436110
H	2.743103	3.926720	0.864430
C	4.954448	2.334837	1.036045
H	4.791991	2.910193	1.952230
H	5.508669	1.430683	1.302127
H	5.590354	2.937526	0.381077
C	2.171779	-2.031375	-2.332728
H	1.850493	-2.340225	-1.335729
C	0.925156	-1.673750	-3.132561
H	0.258527	-2.536433	-3.228332
H	0.361343	-0.863017	-2.660495
H	1.193599	-1.342511	-4.140942
C	2.890910	-3.205688	-2.978403
H	3.149577	-3.008409	-4.022646
H	3.812508	-3.453993	-2.444740
H	2.247277	-4.090116	-2.967116

Zero-point correction= 0.632858 (Hartree/Particle)
Thermal correction to Energy= 0.666518
Thermal correction to Enthalpy= 0.667463
Thermal correction to Gibbs Free Energy= 0.568053
Sum of electronic and zero-point Energies= -2975.194197
Sum of electronic and thermal Energies= -2975.160537
Sum of electronic and thermal Enthalpies= -2975.159592
Sum of electronic and thermal Free Energies= -2975.259002

$ZnDAD_U$ (LC-BLYP)

71
scf done: -2975.818919

Zn	0.405267	1.211443	0.380749
N	0.178224	0.058898	2.014575
N	2.060704	0.065388	0.180448
C	2.171547	-0.834055	1.153843
C	1.152318	-0.842260	2.136357
C	1.157822	-1.812412	3.273251
C	3.311852	-1.804413	1.218008
H	0.178204	-2.285482	3.380523
H	1.898541	-2.598495	3.139360
H	1.370903	-1.305951	4.220979
H	4.073354	-1.560350	0.478329
H	3.786363	-1.799951	2.201948
H	2.976292	-2.828064	1.023388
C	-0.860580	0.149740	2.967057
C	2.987705	0.170470	-0.877307
C	-2.071663	-0.511257	2.733232
C	-3.108490	-0.343866	3.639678
C	-2.955866	0.451361	4.758377
C	-1.751482	1.090467	4.984424
C	-0.690835	0.953198	4.101742
H	-4.055322	-0.846147	3.468215
H	-3.777041	0.572248	5.458546
H	-1.637366	1.710778	5.867414
C	2.906885	-0.703391	-1.970334
C	3.801688	-0.541578	-3.016600
C	4.749838	0.464413	-2.997248
C	4.806298	1.331052	-1.924073
C	3.929886	1.205121	-0.855341
H	3.757248	-1.211442	-3.868695
H	5.443522	0.575176	-3.825299
H	5.548123	2.123100	-1.918312
C	4.013818	2.141043	0.329023
H	3.018143	2.172472	0.780165
C	4.392514	3.563880	-0.049035
H	4.307645	4.215732	0.824915
H	5.424554	3.632588	-0.403905
H	3.739499	3.961627	-0.830658
C	4.976196	1.597686	1.378088
H	5.002272	2.252081	2.254742
H	4.687598	0.597992	1.711441
H	5.991875	1.535808	0.973919
C	1.828532	-1.763332	-2.027499
H	1.618740	-2.078148	-1.003175
C	0.543170	-1.173259	-2.596487
H	-0.261220	-1.915215	-2.589293
H	0.209171	-0.306317	-2.018678
H	0.694120	-0.848509	-3.630927
C	2.229844	-3.004962	-2.806945
H	2.337127	-2.801749	-3.876015
H	3.174114	-3.422303	-2.446034
H	1.459481	-3.773654	-2.700591
C	-2.262254	-1.362907	1.498399
H	-1.269096	-1.646345	1.142768
C	-2.935049	-0.556083	0.394487
H	-2.362887	0.344427	0.150558
H	-3.032236	-1.151812	-0.518394
H	-3.937950	-0.242665	0.701814
C	-3.035773	-2.644664	1.767491
H	-2.588926	-3.222454	2.581456
H	-4.078570	-2.446127	2.029952
H	-3.041277	-3.272511	0.872033
C	0.606857	1.695255	4.332544
H	1.397676	1.138043	3.825588
C	0.544155	3.080336	3.699712
H	0.320331	3.023102	2.630075
H	-0.235622	3.685434	4.173179
H	1.497283	3.604856	3.818527
C	0.992680	1.799979	5.799676
H	0.314898	2.452886	6.356539
H	0.994801	0.821702	6.288634
H	1.996486	2.224157	5.890921

Zero-point correction= 0.631845 (Hartree/Particle)
Thermal correction to Energy= 0.666454
Thermal correction to Enthalpy= 0.667398
Thermal correction to Gibbs Free Energy= 0.562210
Sum of electronic and zero-point Energies= -2975.187074
Sum of electronic and thermal Energies= -2975.152465
Sum of electronic and thermal Enthalpies= -2975.151520
Sum of electronic and thermal Free Energies= -2975.256708

$ZnDAD_R$ (B3PW91-D3)

71
scf done: -2979.574752

Zn	0.168821	-0.119459	0.099200
N	0.164703	-0.399489	1.989341
N	2.054171	-0.419040	0.052091
C	2.438424	-0.783414	1.360976
C	1.478699	-0.773208	2.345318
C	1.660823	-1.333286	3.726493
C	3.819540	-1.352009	1.514891
H	1.400797	-0.604372	4.502957
H	1.000777	-2.198618	3.884883
H	2.685859	-1.654022	3.915077
H	4.596260	-0.624447	1.250661
H	4.022224	-1.686097	2.532943
H	3.962177	-2.210606	0.842792
C	-0.789564	-0.046868	2.945955
C	2.993024	-0.076605	-0.923781
C	-2.016974	-0.762201	2.998332
C	-2.993156	-0.384393	3.923972
C	-2.776083	0.664126	4.816562
C	-1.571188	1.362912	4.766896
C	-0.578662	1.038557	3.837895
H	-3.931859	-0.930527	3.965070
H	-3.539653	0.935924	5.540991
H	-1.411600	2.194903	5.448407
C	3.019376	-0.800131	-2.147093
C	3.929478	-0.434021	-3.142200
C	4.830967	0.611411	-2.948423
C	4.805647	1.319593	-1.748216
C	3.892829	1.006780	-0.737161
H	3.951064	-0.986746	-4.077694
H	5.543148	0.873969	-3.726618
H	5.493565	2.149609	-1.607218
C	-2.253712	-1.915373	2.043813
H	-1.261707	-2.307824	1.791380
C	-3.078641	-3.055517	2.641263
H	-3.097728	-3.906442	1.950762
H	-2.653724	-3.399413	3.590411
H	-4.118965	-2.762684	2.823323
C	-2.895978	-1.420642	0.742327
H	-3.888237	-0.995186	0.933419
H	-2.292148	-0.632781	0.272282
H	-3.006209	-2.236222	0.017646
C	0.646325	1.925243	3.699486
H	1.406959	1.365603	3.146897
C	1.260066	2.342640	5.036773
H	1.477952	1.472694	5.665767
H	2.199922	2.880286	4.867577
H	0.600328	3.010138	5.602894
C	0.287146	3.158510	2.860858
H	-0.095011	2.868719	1.875679
H	-0.486293	3.755293	3.359257
H	1.163874	3.797687	2.709385
C	3.776349	1.903679	0.482498
H	3.248420	1.346046	1.261909
C	2.915354	3.124019	0.131862
H	3.388425	3.718731	-0.658892
H	1.924848	2.819145	-0.223985
H	2.776735	3.769896	1.005671
C	5.123351	2.341011	1.059523
H	4.971091	2.882773	1.999892
H	5.767851	1.479904	1.267119
H	5.664897	3.011042	0.381965
C	2.052170	-1.947128	-2.359521
H	1.817603	-2.334311	-1.361124
C	0.742086	-1.442409	-2.975712
H	0.004069	-2.249106	-3.059633
H	0.298264	-0.640884	-2.370484
H	0.915135	-1.030586	-3.977030
C	2.622335	-3.094766	-3.193082
H	2.784856	-2.806563	-4.237896
H	3.577206	-3.445706	-2.787152
H	1.924289	-3.939726	-3.195054

Zero-point correction= 0.619508 (Hartree/Particle)
Thermal correction to Energy= 0.653616
Thermal correction to Enthalpy= 0.654560
Thermal correction to Gibbs Free Energy= 0.554687
Sum of electronic and zero-point Energies= -2978.955244
Sum of electronic and thermal Energies= -2978.921136
Sum of electronic and thermal Enthalpies= -2978.920192
Sum of electronic and thermal Free Energies= -2979.020065

$ZnDAD_U$ (B3PW91-D3)

71
scf done: -2979.570132

Zn	0.342881	0.953164	0.247248
N	0.309747	0.014416	2.070709
N	2.098549	-0.116023	0.137290
C	2.344434	-0.841135	1.236515
C	1.371854	-0.778791	2.275777
C	1.512735	-1.563845	3.545294
C	3.587791	-1.673230	1.374680
H	1.262386	-0.943161	4.412012
H	0.824397	-2.419504	3.560364
H	2.525142	-1.947153	3.680316
H	4.265824	-1.265093	2.134812
H	3.352588	-2.702195	1.666282
H	4.133489	-1.706484	0.429575
C	-0.727500	0.106961	3.018002
C	3.026861	0.006709	-0.912908
C	-1.804275	-0.804618	2.963628
C	-2.859748	-0.646754	3.866714
C	-2.854943	0.385803	4.802919
C	-1.785663	1.278537	4.846715
C	-0.709725	1.155964	3.962311
H	-3.697690	-1.337389	3.839560
H	-3.682837	0.493247	5.499053
H	-1.788993	2.078346	5.581842
C	2.925995	-0.843790	-2.034908
C	3.800449	-0.643687	-3.107113
C	4.754374	0.372063	-3.074717
C	4.846221	1.202763	-1.959610
C	3.992654	1.035629	-0.864871
H	3.738481	-1.289004	-3.978611
H	5.427070	0.514428	-3.916579
H	5.593205	1.991427	-1.942401
C	-1.824142	-1.882643	1.896317
H	-0.782922	-2.139477	1.673677
C	-2.534070	-3.165006	2.328972
H	-2.404929	-3.938860	1.564219
H	-2.130090	-3.549784	3.271896
H	-3.611600	-3.014097	2.458949
C	-2.441161	-1.326954	0.606059
H	-3.489210	-1.048337	0.768020
H	-1.903693	-0.431848	0.264268
H	-2.404013	-2.071732	-0.197478
C	0.442801	2.142131	3.965720

H	1.325444	1.606756	3.598446
C	0.776489	2.692050	5.352029
H	0.941267	1.885650	6.075187
H	1.689291	3.296097	5.304345
H	-0.019752	3.337339	5.739648
C	0.158299	3.283810	2.981140
H	-0.028292	2.897271	1.969873
H	-0.727806	3.849607	3.292788
H	1.006410	3.976184	2.928963
C	4.046388	1.967814	0.331010
H	3.651411	1.417032	1.190959
C	3.125988	3.173231	0.098351
H	3.475357	3.766730	-0.755004
H	2.096843	2.852839	-0.116152
H	3.102040	3.822653	0.980996
C	5.460755	2.425559	0.687166
H	5.444617	2.993491	1.624038
H	6.136246	1.573173	0.818910
H	5.886890	3.079860	-0.081532
C	1.851256	-1.913204	-2.067467
H	1.678384	-2.226084	-1.031610
C	0.537406	-1.318809	-2.591473
H	-0.269463	-2.060075	-2.555630
H	0.228750	-0.450993	-1.993205
H	0.652142	-0.986358	-3.630094
C	2.242033	-3.154675	-2.868174
H	2.327255	-2.942088	-3.939771
H	3.197939	-3.567809	-2.527675
H	1.476879	-3.930028	-2.751206

Zero-point correction= 0.618364 (Hartree/Particle)
Thermal correction to Energy= 0.653244
Thermal correction to Enthalpy= 0.654188
Thermal correction to Gibbs Free Energy= 0.551459
Sum of electronic and zero-point Energies= -2978.951768
Sum of electronic and thermal Energies= -2978.916888
Sum of electronic and thermal Enthalpies= -2978.915944
Sum of electronic and thermal Free Energies= -2979.018673

$ZnDAD_{BS}$ (B3PW91-D3)

71
scf done: -2979.574752

Zn	0.168821	-0.119459	0.099200
N	0.164703	-0.399489	1.989341
N	2.054171	-0.419040	0.052091
C	2.438424	-0.783414	1.360976
C	1.478699	-0.773209	2.345318
C	1.660823	-1.333286	3.726493
C	3.819540	-1.352009	1.514891
H	1.400797	-0.604372	4.502957
H	1.000777	-2.198618	3.884883
H	2.685859	-1.654022	3.915077
H	4.596260	-0.624447	1.250661
H	4.022224	-1.686097	2.532943
H	3.962177	-2.210606	0.842792
C	-0.789564	-0.046868	2.945955
C	2.993024	-0.076605	-0.923781
C	-2.016974	-0.762201	2.998332
C	-2.993156	-0.384393	3.923972
C	-2.776083	0.664126	4.816562
C	-1.571188	1.362912	4.766896
C	-0.578662	1.038557	3.837895
H	-3.931859	-0.930527	3.965069
H	-3.539653	0.935925	5.540991
H	-1.411600	2.194903	5.448407
C	3.019376	-0.800131	-2.147093
C	3.929478	-0.434021	-3.142200
C	4.830967	0.611411	-2.948423
C	4.805647	1.319593	-1.748216
C	3.892829	1.006780	-0.737161
H	3.951065	-0.986746	-4.077694
H	5.543148	0.873969	-3.726617
H	5.493565	2.149610	-1.607218
C	-2.253712	-1.915373	2.043813
H	-1.261707	-2.307824	1.791379
C	-3.078641	-3.055517	2.641263
H	-3.097728	-3.906442	1.950762
H	-2.653724	-3.399413	3.590411
H	-4.118965	-2.762684	2.823323
C	-2.895979	-1.420642	0.742327
H	-3.888237	-0.995186	0.933419
H	-2.292148	-0.632781	0.272282
H	-3.006209	-2.236222	0.017646
C	0.646325	1.925242	3.699486
H	1.406959	1.365603	3.146898
C	1.260066	2.342640	5.036773
H	1.477952	1.472694	5.665767
H	2.199922	2.880286	4.867577
H	0.600328	3.010138	5.602894
C	0.287146	3.158510	2.860858
H	-0.095011	2.868719	1.875679
H	-0.486293	3.755293	3.359257
H	1.163874	3.797687	2.709385
C	3.776349	1.903679	0.482498
H	3.248420	1.346046	1.261909
C	2.915354	3.124019	0.131862
H	3.388425	3.718731	-0.658892
H	1.924849	2.819145	-0.223985
H	2.776735	3.769896	1.005670
C	5.123351	2.341011	1.059524
H	4.971091	2.882773	1.999892
H	5.767850	1.479904	1.267119
H	5.664897	3.011042	0.381965
C	2.052170	-1.947128	-2.359521
H	1.817603	-2.334311	-1.361124
C	0.742086	-1.442409	-2.975712
H	0.004070	-2.249106	-3.059633
H	0.298264	-0.640884	-2.370485
H	0.915135	-1.030586	-3.977030
C	2.622335	-3.094765	-3.193082
H	2.784856	-2.806562	-4.237896
H	3.577206	-3.445706	-2.787152
H	1.924289	-3.939726	-3.195054

Zero-point correction= 0.619508 (Hartree/Particle)
Thermal correction to Energy= 0.653616
Thermal correction to Enthalpy= 0.654560
Thermal correction to Gibbs Free Energy= 0.554687
Sum of electronic and zero-point Energies= -2978.955244
Sum of electronic and thermal Energies= -2978.921136
Sum of electronic and thermal Enthalpies= -2978.920192
Sum of electronic and thermal Free Energies= -2979.020065

SET_R def2-tzvp THF

71

scf done: -2979.992315

Zn	0.167237	0.041854	0.101620
N	0.161374	-0.230505	2.000928
N	2.062868	-0.240131	0.046229
C	2.418370	-0.671546	1.338140
C	1.460957	-0.665800	2.323092
C	1.639779	-1.305407	3.668465
C	3.764398	-1.318415	1.481700
H	1.302327	-0.651737	4.477575
H	1.047061	-2.226169	3.752100
H	2.676152	-1.561630	3.876555
H	4.570021	-0.665186	1.134726
H	3.992240	-1.588709	2.510254
H	3.830328	-2.232547	0.876780
C	-0.826922	0.012442	2.958642
C	2.994157	-0.004349	-0.968907
C	-2.026944	-0.746970	2.945255
C	-3.040237	-0.447757	3.852906
C	-2.897207	0.560108	4.792781
C	-1.722107	1.295975	4.816509
C	-0.690286	1.054341	3.913943
H	-3.956617	-1.028644	3.835794
H	-3.692895	0.771135	5.499335
H	-1.614936	2.096099	5.541556
C	2.945453	-0.768093	-2.165254
C	3.826345	-0.475786	-3.203855
C	4.772732	0.529786	-3.090326
C	4.831140	1.269494	-1.918969
C	3.956600	1.034157	-0.861823
H	3.782730	-1.059953	-4.117230
H	5.457883	0.735715	-3.905829
H	5.561543	2.067423	-1.834183
C	-2.230135	-1.878591	1.955872
H	-1.245531	-2.108146	1.542567
C	-2.763762	-3.155770	2.604462
H	-2.788235	-3.968908	1.872929
H	-2.130691	-3.473033	3.436969
H	-3.781062	-3.031398	2.985348
C	-3.133611	-1.451803	0.795742
H	-4.141045	-1.213611	1.149835
H	-2.752840	-0.559362	0.288756
H	-3.221027	-2.249661	0.051679
C	0.512776	1.981237	3.903599
H	1.301223	1.494045	3.327812
C	1.074023	2.271119	5.295397
H	1.305761	1.349990	5.836070
H	1.996961	2.852564	5.215249
H	0.378460	2.851881	5.907490
C	0.164762	3.290573	3.187798
H	-0.189098	3.108848	2.169468
H	-0.621886	3.831968	3.722013
H	1.039509	3.944723	3.127001
C	3.983955	1.964066	0.338602
H	3.427153	1.481887	1.143610
C	3.266284	3.276571	0.006864
H	3.781750	3.812936	-0.795572
H	2.237576	3.099714	-0.318332
H	3.233215	3.933231	0.881219
C	5.392300	2.247415	0.860645
H	5.341026	2.832869	1.783106
H	5.933454	1.323804	1.081080
H	5.988638	2.821565	0.146140
C	1.946847	-1.896771	-2.336613
H	1.561794	-2.122867	-1.339755
C	0.761906	-1.467152	-3.206257
H	0.014617	-2.263890	-3.273851
H	0.267271	-0.575361	-2.807670
H	1.087127	-1.226493	-4.222756
C	2.573850	-3.177509	-2.887133
H	2.922008	-3.057771	-3.916631
H	3.425252	-3.496011	-2.280370
H	1.839076	-3.988072	-2.885523

Zero-point correction= 0.613545 (Hartree/Particle)

Thermal correction to Energy= 0.649157

Thermal correction to Enthalpy= 0.650101

Thermal correction to Gibbs Free Energy= 0.544525

Sum of electronic and zero-point Energies= -2979.378771

Sum of electronic and thermal Energies= -2979.343158

Sum of electronic and thermal Enthalpies= -2979.342214

Sum of electronic and thermal Free Energies= -2979.447791

SET_U def2-tzvp THF

71

scf done: -2979.990657

Zn	0.342107	1.192923	0.288577
N	0.146828	0.053927	2.026407
N	2.073557	0.013819	0.173370
C	2.174942	-0.834556	1.198133
C	1.148976	-0.812269	2.186380
C	1.226461	-1.750124	3.354513
C	3.314603	-1.799857	1.339759
H	0.356900	-1.646651	4.001842
H	1.279295	-2.792792	3.026422
H	2.119928	-1.565716	3.959702
H	4.013269	-1.711106	0.509266
H	3.870784	-1.631903	2.267478
H	2.959279	-2.834735	1.370306
C	-0.914748	0.190882	2.942746
C	3.030713	0.100543	-0.856749
C	-2.129743	-0.489411	2.712558
C	-3.201898	-0.261201	3.572140
C	-3.096232	0.615698	4.639872
C	-1.900412	1.281060	4.858682
C	-0.799653	1.086618	4.027513
H	-4.139880	-0.778635	3.400511
H	-3.942562	0.781085	5.297951
H	-1.821233	1.971486	5.691802
C	2.834493	-0.615014	-2.057307
C	3.739999	-0.439257	-3.101168
C	4.820731	0.419780	-2.981489
C	5.006304	1.119749	-1.799897
C	4.128427	0.978464	-0.727624
H	3.594479	-0.984349	-4.027866
H	5.515205	0.543671	-3.805544
H	5.850443	1.795266	-1.709515
C	4.349371	1.793342	0.533190
H	3.646349	1.428684	1.283942
C	4.034651	3.272154	0.291358
H	4.147565	3.847009	1.215341
H	4.708642	3.702541	-0.455025
H	3.010078	3.407304	-0.066369
C	5.758424	1.624912	1.102736
H	5.850153	2.161948	2.051229
H	5.992402	0.573597	1.288449
H	6.520178	2.022894	0.426883
C	1.648956	-1.543863	-2.241468

H	1.160334	-1.641596	-1.270330
C	0.627062	-0.944236	-3.211081
H	-0.245380	-1.597658	-3.305624
H	0.279169	0.033915	-2.866499
H	1.057385	-0.813953	-4.208309
C	2.064884	-2.945566	-2.689244
H	2.514072	-2.937887	-3.686106
H	2.788575	-3.387379	-1.999513
H	1.192828	-3.604682	-2.728671
C	-2.298421	-1.433573	1.536813
H	-1.310571	-1.582528	1.096998
C	-3.191851	-0.812722	0.459451
H	-2.789607	0.143405	0.112039
H	-3.273540	-1.477843	-0.405423
H	-4.201530	-0.632178	0.839810
C	-2.827106	-2.806043	1.954843
H	-2.193821	-3.262766	2.719715
H	-3.843626	-2.746851	2.353247
H	-2.852587	-3.479911	1.093638
C	0.476542	1.867647	4.280206
H	1.246039	1.456083	3.624952
C	0.297823	3.341686	3.906036
H	-0.007886	3.452621	2.861839
H	-0.464591	3.817539	4.529663
H	1.233826	3.891254	4.043259
C	0.976274	1.730099	5.718671
H	0.281390	2.176066	6.435321
H	1.115393	0.682088	5.995849
H	1.937450	2.238868	5.835658

Zero-point correction= 0.614359 (Hartree/Particle)
Thermal correction to Energy= 0.650303
Thermal correction to Enthalpy= 0.651247
Thermal correction to Gibbs Free Energy= 0.541753
Sum of electronic and zero-point Energies= -2979.376298
Sum of electronic and thermal Energies= -2979.340354
Sum of electronic and thermal Enthalpies= -2979.339410
Sum of electronic and thermal Free Energies= -2979.448905

SET_{BS} def2-tzvp THF

71
scf done: -2979.988985

Zn	0.370489	1.220248	0.317141
N	0.185985	0.095355	2.064766
N	2.111203	0.054163	0.211949
C	2.142292	-0.880244	1.165709
C	1.116116	-0.858802	2.152492
C	1.103774	-1.900165	3.232078
C	3.201225	-1.941358	1.224089
H	0.295116	-1.724312	3.939994
H	0.977727	-2.907144	2.820686
H	2.044024	-1.905404	3.791500
H	3.932580	-1.813271	0.427503
H	3.737383	-1.915840	2.177774
H	2.774062	-2.945191	1.131371
C	-0.890454	0.216606	2.965505
C	3.054061	0.124923	-0.832151
C	-2.094393	-0.485178	2.739087
C	-3.173996	-0.259886	3.590276
C	-3.086757	0.632737	4.646724
C	-1.901944	1.318223	4.862545
C	-0.795149	1.128541	4.038553
H	-4.104308	-0.791447	3.420408
H	-3.939026	0.794350	5.298046
H	-1.835767	2.019688	5.687649
C	2.865365	-0.618044	-2.017833
C	3.765059	-0.448524	-3.067811
C	4.833193	0.428971	-2.969143
C	5.011156	1.155971	-1.802965
C	4.137856	1.022799	-0.726061
H	3.624568	-1.012610	-3.983774
H	5.523202	0.546154	-3.797921
H	5.845773	1.845179	-1.727854
C	4.351623	1.860539	0.520626
H	3.639848	1.510635	1.270281
C	4.046635	3.336288	0.250355
H	4.152302	3.926310	1.165582
H	4.730377	3.751606	-0.495723
H	3.026798	3.470638	-0.120975
C	5.755164	1.694128	1.104174
H	5.845239	2.251878	2.040825
H	5.978168	0.645145	1.315350
H	6.524622	2.069511	0.424001
C	1.688062	-1.560712	-2.185427
H	1.219916	-1.675064	-1.206154
C	0.639309	-0.961622	-3.126725
H	-0.227623	-1.623764	-3.210996
H	0.287940	0.008589	-2.763462
H	1.048487	-0.815413	-4.130647
C	2.107438	-2.953037	-2.658164
H	2.524787	-2.932008	-3.668494
H	2.857265	-3.392760	-1.995701
H	1.242272	-3.622011	-2.676868
C	-2.248353	-1.441800	1.571178
H	-1.254925	-1.603083	1.148825
C	-3.118184	-0.825490	0.471828
H	-2.701271	0.123062	0.120669
H	-3.191198	-1.499662	-0.386814
H	-4.132253	-0.632143	0.833741
C	-2.794816	-2.806344	1.992145
H	-2.184015	-3.258137	2.777812
H	-3.820719	-2.737639	2.363882
H	-2.802807	-3.489747	1.138186
C	0.471888	1.924298	4.289968
H	1.240644	1.526261	3.625447
C	0.273628	3.399511	3.931319
H	-0.042460	3.517451	2.890986
H	-0.488543	3.861730	4.565428
H	1.204542	3.958284	4.065831
C	0.981215	1.777808	5.724184
H	0.280678	2.200492	6.449524
H	1.141277	0.728737	5.985960
H	1.933288	2.302859	5.843950

Zero-point correction= 0.614114 (Hartree/Particle)
Thermal correction to Energy= 0.650157
Thermal correction to Enthalpy= 0.651102
Thermal correction to Gibbs Free Energy= 0.541608
Sum of electronic and zero-point Energies= -2979.374871
Sum of electronic and thermal Energies= -2979.338828
Sum of electronic and thermal Enthalpies= -2979.337883
Sum of electronic and thermal Free Energies= -2979.447377

SET_{R} def2-tzvp Water

71
scf done: -2979.989253

Zn	0.169245	-0.190929	0.094887
N	0.201054	-0.406984	2.037232
N	2.105831	-0.426571	0.105933
C	2.486595	-0.716100	1.425139
C	1.523725	-0.707204	2.403638
C	1.727802	-1.261025	3.784055
C	3.875180	-1.251942	1.619869
H	1.367648	-0.579684	4.560290
H	1.165158	-2.195579	3.914913
H	2.771843	-1.472795	4.004400
H	4.636104	-0.563059	1.241272
H	4.111104	-1.445103	2.664047
H	4.013210	-2.191652	1.068028
C	-0.784261	-0.058310	2.951189
C	3.015476	-0.108936	-0.897512
C	-2.034781	-0.741673	2.913396
C	-3.044284	-0.386460	3.802183
C	-2.864883	0.616503	4.744804
C	-1.658097	1.299570	4.772651
C	-0.624224	1.002145	3.887898
H	-3.990317	-0.916432	3.769629
H	-3.658611	0.869476	5.439400
H	-1.528057	2.109680	5.482793
C	3.006939	-0.863080	-2.105280
C	3.873975	-0.521370	-3.138958
C	4.768985	0.532105	-3.018392
C	4.778780	1.272922	-1.845829
C	3.914499	0.987976	-0.791394
H	3.862550	-1.100949	-4.055885
H	5.445423	0.776300	-3.830393
H	5.458156	2.114653	-1.759619
C	-2.278927	-1.837413	1.895196
H	-1.294316	-2.212228	1.605326
C	-3.085263	-3.016975	2.434047
H	-3.120441	-3.816622	1.688759
H	-2.637382	-3.426689	3.343194
H	-4.118808	-2.743139	2.662202
C	-2.940846	-1.273804	0.634361
H	-3.945484	-0.901566	0.858111
H	-2.370550	-0.438560	0.214402
H	-3.031238	-2.042287	-0.139030
C	0.589254	1.916030	3.848521
H	1.390493	1.388909	3.327318
C	1.118889	2.305343	5.227715
H	1.332042	1.425883	5.840834
H	2.046614	2.875217	5.125980
H	0.412971	2.934054	5.777024
C	0.268281	3.172706	3.031828
H	-0.063794	2.920911	2.021475
H	-0.525198	3.754810	3.510408
H	1.149445	3.815065	2.945724
C	3.861886	1.939699	0.391405
H	3.355069	1.426840	1.210883
C	3.021296	3.170707	0.035492
H	3.486256	3.736177	-0.777822
H	2.014605	2.890224	-0.284568
H	2.926700	3.838608	0.896446
C	5.237298	2.368081	0.900305
H	5.131428	2.968536	1.808051
H	5.863964	1.505359	1.140725
H	5.773684	2.979246	0.169500
C	2.047656	-2.023825	-2.277607
H	1.788275	-2.358919	-1.270515
C	0.750892	-1.569126	-2.952466
H	0.031054	-2.390872	-3.012139
H	0.277786	-0.748199	-2.404382
H	0.945061	-1.216564	-3.970133
C	2.644013	-3.214328	-3.025426
H	2.839064	-2.988526	-4.077191
H	3.582740	-3.543563	-2.572289
H	1.946957	-4.056670	-3.000680

Zero-point correction= 0.614700 (Hartree/Particle)
Thermal correction to Energy= 0.649403
Thermal correction to Enthalpy= 0.650348
Thermal correction to Gibbs Free Energy= 0.549008
Sum of electronic and zero-point Energies= -2979.374553
Sum of electronic and thermal Energies= -2979.339850
Sum of electronic and thermal Enthalpies= -2979.338906
Sum of electronic and thermal Free Energies= -2979.440245

SET_U def2-tzvp Water

71
scf done: -2979.971444

Zn	0.289866	1.239416	0.284578
N	0.128919	0.063601	2.033367
N	2.038781	0.050366	0.157212
C	2.157770	-0.799263	1.178888
C	1.143100	-0.791468	2.176877
C	1.245990	-1.732762	3.340429
C	3.309495	-1.752225	1.308500
H	0.350243	-1.694415	3.958877
H	1.382592	-2.765248	3.006665
H	2.103731	-1.491839	3.977151
H	4.030609	-1.612540	0.504585
H	3.833329	-1.618802	2.259704
H	2.971632	-2.793115	1.279497
C	-0.915188	0.179189	2.969004
C	2.986364	0.135336	-0.879577
C	-2.132512	-0.500973	2.742877
C	-3.196741	-0.285690	3.615097
C	-3.080705	0.576881	4.695173
C	-1.880822	1.233870	4.916294
C	-0.787421	1.050181	4.071649
H	-4.135994	-0.800931	3.446794
H	-3.921335	0.733340	5.362427
H	-1.790557	1.908424	5.761245
C	2.803499	-0.610691	-2.063596
C	3.695590	-0.432416	-3.119016
C	4.753598	0.458422	-3.026482
C	4.930209	1.185287	-1.859119
C	4.064130	1.041462	-0.777334
H	3.556543	-1.002505	-4.031825
H	5.437558	0.584754	-3.858712
H	5.757724	1.883341	-1.785980
C	4.289244	1.869810	0.473068
H	3.563248	1.539487	1.217521
C	4.033579	3.354708	0.206812
H	4.154892	3.936077	1.125238
H	4.734698	3.749270	-0.534160
H	3.019337	3.520976	-0.166226
C	5.683427	1.655707	1.063431
H	5.788673	2.212724	1.998618
H	5.866977	0.599977	1.278460
H	6.466301	2.001891	0.383229
C	1.657761	-1.592660	-2.215093
H	1.120079	-1.613929	-1.265841

C	0.673014	-1.138211	-3.293973
H	-0.169695	-1.832105	-3.361193
H	0.274755	-0.144309	-3.072763
H	1.152390	-1.098582	-4.276181
C	2.154529	-3.011779	-2.495148
H	2.680252	-3.071313	-3.452071
H	2.837636	-3.355498	-1.714290
H	1.312349	-3.708229	-2.536127
C	-2.298027	-1.423989	1.550721
H	-1.296119	-1.708371	1.222338
C	-2.970049	-0.687092	0.388749
H	-2.397235	0.199687	0.097660
H	-3.051884	-1.337983	-0.486642
H	-3.978175	-0.363657	0.664884
C	-3.053493	-2.709643	1.881402
H	-2.595353	-3.239744	2.720327
H	-4.099396	-2.517805	2.134229
H	-3.045923	-3.378825	1.016837
C	0.496678	1.812432	4.337215
H	1.254424	1.425461	3.654151
C	0.321468	3.302253	4.033503
H	0.003896	3.460726	2.999252
H	-0.429709	3.751286	4.689650
H	1.262430	3.839155	4.183819
C	1.013283	1.605579	5.761072
H	0.325109	2.015940	6.504826
H	1.155659	0.544963	5.983064
H	1.975634	2.108436	5.890632

Zero-point correction= 0.613984 (Hartree/Particle)
Thermal correction to Energy= 0.649874
Thermal correction to Enthalpy= 0.650818
Thermal correction to Gibbs Free Energy= 0.542202
Sum of electronic and zero-point Energies= -2979.357461
Sum of electronic and thermal Energies= -2979.321570
Sum of electronic and thermal Enthalpies= -2979.320626
Sum of electronic and thermal Free Energies= -2979.429242

SET_{BS} def2-tzvp Water

71
scf done: -2979.992478

Zn	0.757791	1.213003	0.618035
N	0.096825	-0.004664	1.947386
N	2.334914	0.146647	0.377903
C	2.228115	-0.903056	1.315927
C	1.127625	-0.948896	2.132909
C	0.913740	-1.983521	3.198081
C	3.424965	-1.796820	1.459085
H	-0.064734	-2.461585	3.078661
H	1.662136	-2.772113	3.162760
H	0.927341	-1.562776	4.209446
H	4.327737	-1.199276	1.637126
H	3.328831	-2.491168	2.291090
H	3.625684	-2.390097	0.560826
C	-0.941360	0.167387	2.877404
C	3.206124	0.107696	-0.711794
C	-2.264009	-0.193422	2.518791
C	-3.307469	0.047144	3.410419
C	-3.078446	0.617200	4.652049
C	-1.784326	0.965329	5.008956
C	-0.711643	0.759160	4.145278
H	-4.319842	-0.226546	3.130922
H	-3.901493	0.789708	5.337576
H	-1.608123	1.422911	5.976856
C	3.156903	-0.924425	-1.686598
C	4.046710	-0.895469	-2.757657
C	4.959454	0.135484	-2.919115
C	4.984018	1.165544	-1.990606
C	4.133663	1.170648	-0.889124
H	4.008724	-1.686188	-3.499634
H	5.640575	0.139856	-3.763490
H	5.695332	1.974251	-2.119001
C	4.182251	2.312848	0.106457
H	3.826184	1.904622	1.056139
C	3.215905	3.429616	-0.299313
H	3.192661	4.226113	0.450731
H	3.507209	3.873735	-1.255835
H	2.193938	3.049993	-0.416663
C	5.579524	2.882788	0.338169
H	5.556677	3.605035	1.159354
H	6.292846	2.098190	0.603154
H	5.966619	3.406972	-0.539902
C	2.069555	-1.985192	-1.656767
H	1.686284	-2.042152	-0.636513
C	0.901534	-1.564054	-2.555914
H	0.079879	-2.283612	-2.488175
H	0.509908	-0.583364	-2.272167
H	1.213599	-1.507408	-3.603212
C	2.554505	-3.381611	-2.043328
H	2.847229	-3.440065	-3.095313
H	3.411624	-3.692414	-1.440504
H	1.755309	-4.112405	-1.890207
C	-2.566407	-0.824148	1.173025
H	-1.602983	-1.088309	0.733053
C	-3.250256	0.172963	0.233739
H	-2.651307	1.078763	0.100983
H	-3.411703	-0.269471	-0.754001
H	-4.224996	0.479730	0.624932
C	-3.394030	-2.104485	1.288608
H	-2.915138	-2.831046	1.949820
H	-4.398058	-1.911068	1.676520
H	-3.508638	-2.571131	0.305738
C	0.668079	1.251934	4.544132
H	1.388825	0.785582	3.870446
C	0.770786	2.768554	4.350742
H	0.530180	3.061262	3.324647
H	0.079664	3.295966	5.014934
H	1.782898	3.121161	4.570801
C	1.060326	0.874535	5.972341
H	0.440428	1.382823	6.716003
H	0.971642	-0.201188	6.143291
H	2.098346	1.159802	6.165836

Zero-point correction= 0.615247 (Hartree/Particle)
Thermal correction to Energy= 0.650116
Thermal correction to Enthalpy= 0.651060
Thermal correction to Gibbs Free Energy= 0.548300
Sum of electronic and zero-point Energies= -2979.377231
Sum of electronic and thermal Energies= -2979.342362
Sum of electronic and thermal Enthalpies= -2979.341418
Sum of electronic and thermal Free Energies= -2979.444178

SET_{R} def2-tzvp Toluene

71

scf done: -2979.975991

Zn	0.012304	0.302106	0.006817
N	0.225694	0.047897	2.031411
N	2.046218	0.091156	0.114875
C	2.278376	-0.720467	1.160171
C	1.303151	-0.741050	2.189909
C	1.419435	-1.740924	3.301900
C	3.412917	-1.701149	1.189909
H	0.653728	-1.580549	4.059343
H	1.324915	-2.772274	2.940383
H	2.392880	-1.670705	3.793860
H	4.113354	-1.518565	0.376426
H	3.968170	-1.633000	2.128849
H	3.064166	-2.737747	1.107792
C	-0.799100	0.118942	3.003568
C	2.948536	0.209816	-0.969026
C	-1.933682	-0.716443	2.962806
C	-2.946628	-0.513768	3.900358
C	-2.849224	0.465681	4.870853
C	-1.720360	1.269626	4.916153
C	-0.688748	1.119855	3.996256
H	-3.827941	-1.145542	3.871362
H	-3.646758	0.602371	5.592914
H	-1.645376	2.034093	5.680803
C	2.900434	-0.651811	-2.085791
C	3.768315	-0.415609	-3.150423
C	4.677392	0.627521	-3.127607
C	4.720485	1.465651	-2.026127
C	3.865125	1.283624	-0.943714
H	3.732462	-1.067684	-4.016498
H	5.347109	0.788323	-3.965284
H	5.429070	2.286963	-2.008882
C	-2.096532	-1.827055	1.942047
H	-1.169016	-1.881524	1.366348
C	-2.309978	-3.191390	2.600817
H	-2.334638	-3.979846	1.843115
H	-1.509795	-3.427480	3.306043
H	-3.255932	-3.233968	3.147173
C	-3.224527	-1.522247	0.954705
H	-4.188744	-1.439732	1.463840
H	-3.045268	-0.581532	0.426382
H	-3.308678	-2.315969	0.206441
C	0.508896	2.052131	4.026270
H	1.344127	1.523816	3.562805
C	0.946361	2.445710	5.435469
H	1.113147	1.568670	6.065870
H	1.882791	3.008418	5.390964
H	0.213529	3.084349	5.935634
C	0.235077	3.298634	3.179300
H	-0.018150	3.032667	2.150517
H	-0.598898	3.874591	3.590955
H	1.113125	3.950323	3.151138
C	3.932045	2.245068	0.228454
H	3.138608	1.961249	0.921232
C	3.670302	3.688789	-0.205242
H	4.445803	4.055723	-0.883216
H	2.709796	3.783724	-0.717726
H	3.653670	4.351842	0.664417
C	5.263973	2.136686	0.974027
H	5.271061	2.796475	1.846506
H	5.446415	1.117623	1.323084
H	6.104411	2.423677	0.335485
C	1.930553	-1.815059	-2.178007
H	1.421305	-1.894851	-1.214461
C	0.856502	-1.562504	-3.238345
H	0.142323	-2.390663	-3.270371
H	0.297718	-0.646588	-3.025903
H	1.296307	-1.461496	-4.234398
C	2.639266	-3.145940	-2.436071
H	3.117263	-3.166358	-3.419022
H	3.410989	-3.343571	-1.688683
H	1.921568	-3.970716	-2.405589

Zero-point correction= 0.614539 (Hartree/Particle)
Thermal correction to Energy= 0.650318
Thermal correction to Enthalpy= 0.651262
Thermal correction to Gibbs Free Energy= 0.545149
Sum of electronic and zero-point Energies= -2979.361452
Sum of electronic and thermal Energies= -2979.325673
Sum of electronic and thermal Enthalpies= -2979.324729
Sum of electronic and thermal Free Energies= -2979.430842

SET_U def2-tzvp Toluene

71

scf done: -2979.985642

Zn	0.436392	1.233383	0.365526
N	0.145684	0.100506	2.019516
N	2.077393	0.059993	0.176484
C	2.155708	-0.831512	1.176468
C	1.120619	-0.810321	2.163152
C	1.154570	-1.783013	3.310192
C	3.274384	-1.831758	1.281071
H	0.238559	-1.721455	3.900193
H	1.267027	-2.814351	2.957349
H	1.999388	-1.582526	3.981660
H	4.044054	-1.634833	0.532854
H	3.743270	-1.806098	2.271108
H	2.912264	-2.856439	1.126906
C	-0.926126	0.226422	2.942484
C	3.038462	0.126219	-0.866777
C	-2.144133	-0.446868	2.691651
C	-3.211066	-0.249912	3.574129
C	-3.092858	0.589968	4.676550
C	-1.891595	1.252543	4.907357
C	-0.794650	1.088947	4.055604
H	-4.153370	-0.761113	3.392691
H	-3.933816	0.730802	5.350219
H	-1.805608	1.914815	5.765269
C	2.858031	-0.648306	-2.036390
C	3.778829	-0.507835	-3.079396
C	4.852471	0.371680	-2.984149
C	5.014396	1.132539	-1.831124
C	4.120905	1.029956	-0.760109
H	3.650619	-1.094734	-3.985533
H	5.556934	0.466446	-3.806111
H	5.850751	1.823856	-1.762365
C	4.317572	1.900755	0.471364
H	3.562355	1.603096	1.205900
C	4.081415	3.383285	0.145165
H	4.174661	3.997139	1.048445
H	4.811009	3.750149	-0.585815
H	3.082038	3.542653	-0.273102
C	5.694650	1.693748	1.117721
H	5.775314	2.279989	2.040142
H	5.865458	0.641534	1.367653
H	6.505655	2.013264	0.453694
C	1.675115	-1.591161	-2.196594
H	1.158995	-1.637356	-1.232373
C	0.673283	-1.045156	-3.225868

H	-0.200852	-1.702185	-3.301473
H	0.324689	-0.044970	-2.947886
H	1.127640	-0.974754	-4.220791
C	2.106353	-3.019661	-2.556643
H	2.579701	-3.064452	-3.543798
H	2.819892	-3.418436	-1.828233
H	1.236188	-3.685378	-2.580956
C	-2.323613	-1.350933	1.481727
H	-1.352088	-1.425432	0.982633
C	-3.310773	-0.740033	0.475521
H	-2.986233	0.256127	0.157010
H	-3.394678	-1.372302	-0.415897
H	-4.311537	-0.640969	0.911274
C	-2.749461	-2.772709	1.874221
H	-2.042999	-3.221736	2.579976
H	-3.739738	-2.783797	2.343204
H	-2.798991	-3.414747	0.987440
C	0.487944	1.862508	4.321078
H	1.240434	1.504126	3.611460
C	0.289277	3.363237	4.057796
H	-0.055128	3.543898	3.034134
H	-0.455499	3.789229	4.739765
H	1.228606	3.909232	4.202893
C	1.036781	1.622264	5.734369
H	0.361029	2.011649	6.503978
H	1.183714	0.555287	5.931021
H	2.000996	2.127809	5.859613

Zero-point correction= 0.615558 (Hartree/Particle)
Thermal correction to Energy= 0.651365
Thermal correction to Enthalpy= 0.652309
Thermal correction to Gibbs Free Energy= 0.543858
Sum of electronic and zero-point Energies= -2979.370084
Sum of electronic and thermal Energies= -2979.334277
Sum of electronic and thermal Enthalpies= -2979.333333
Sum of electronic and thermal Free Energies= -2979.441784

SET_{BS} def2-tzvp Toluene

71
scf done: -2979.983713

Zn	0.375400	1.181297	0.309245
N	0.157745	0.075151	2.034786
N	2.093633	0.035409	0.189962
C	2.159835	-0.853493	1.184083
C	1.130172	-0.830016	2.169033
C	1.166417	-1.810308	3.303168
C	3.261266	-1.865787	1.288473
H	0.295264	-1.700430	3.946789
H	1.190870	-2.842515	2.941016
H	2.058883	-1.673750	3.922198
H	3.998135	-1.729270	0.498756
H	3.780029	-1.795344	2.249123
H	2.876013	-2.887968	1.214124
C	-0.910508	0.208254	2.948420
C	3.047295	0.110319	-0.848375
C	-2.127858	-0.462545	2.709437
C	-3.195014	-0.243906	3.576980
C	-3.082005	0.614702	4.657421
C	-1.884539	1.273499	4.881195
C	-0.788039	1.088916	4.043338
H	-4.135692	-0.754481	3.400794
H	-3.924895	0.771993	5.321381
H	-1.800582	1.950964	5.724126
C	2.866639	-0.639295	-2.029387
C	3.776104	-0.477361	-3.071301
C	4.842822	0.399757	-2.968175
C	5.009417	1.135511	-1.806937
C	4.127029	1.010736	-0.737105
H	3.644467	-1.047480	-3.984559
H	5.540446	0.511156	-3.790956
H	5.842373	1.826158	-1.730473
C	4.326034	1.863598	0.502082
H	3.610808	1.519140	1.250993
C	4.013941	3.334288	0.212589
H	4.108452	3.936124	1.121180
H	4.699836	3.746072	-0.533092
H	2.997134	3.458735	-0.169286
C	5.725538	1.713322	1.099800
H	5.803862	2.280227	2.031853
H	5.956804	0.668746	1.321877
H	6.498952	2.088526	0.424347
C	1.689689	-1.581729	-2.201423
H	1.203533	-1.676593	-1.228730
C	0.659554	-0.998730	-3.172833
H	-0.208615	-1.658768	-3.259074
H	0.305866	-0.019502	-2.838758
H	1.085196	-0.873756	-4.172464
C	2.114379	-2.983829	-2.639628
H	2.551207	-2.983486	-3.641766
H	2.851258	-3.412523	-1.956204
H	1.248972	-3.652181	-2.663157
C	-2.308301	-1.386008	1.518816
H	-1.328210	-1.514128	1.055522
C	-3.232185	-0.758467	0.471515
H	-2.853507	0.210610	0.135278
H	-3.321289	-1.407367	-0.404690
H	-4.236919	-0.600240	0.873421
C	-2.809570	-2.773472	1.921824
H	-2.155551	-3.236744	2.664455
H	-3.817342	-2.735586	2.343936
H	-2.846773	-3.432110	1.049446
C	0.491263	1.863179	4.301699
H	1.253130	1.467276	3.628049
C	0.310505	3.346232	3.966326
H	-0.009783	3.484987	2.930312
H	-0.443098	3.808744	4.609925
H	1.248509	3.891791	4.104871
C	1.006458	1.689265	5.730872
H	0.321045	2.118627	6.466366
H	1.144891	0.634923	5.982019
H	1.969869	2.192745	5.851400

Zero-point correction= 0.615190 (Hartree/Particle)
Thermal correction to Energy= 0.651186
Thermal correction to Enthalpy= 0.652130
Thermal correction to Gibbs Free Energy= 0.543801
Sum of electronic and zero-point Energies= -2979.368522
Sum of electronic and thermal Energies= -2979.332527
Sum of electronic and thermal Enthalpies= -2979.331582
Sum of electronic and thermal Free Energies= -2979.439912

SET_{R} def2-tzvp Gas

71
scf done: -2979.946010

Zn	-0.056868	0.494315	-0.009935
N	0.273013	0.070031	2.078362
N	2.068301	0.140022	0.150668
C	2.255492	-0.761132	1.100691
C	1.268771	-0.796270	2.166172
C	1.367627	-1.859737	3.225500
C	3.344107	-1.799041	1.073858
H	0.594577	-1.727408	3.983704
H	1.265896	-2.868216	2.802935
H	2.343021	-1.822047	3.722653
H	4.051656	-1.601628	0.267313
H	3.895717	-1.808252	2.019872
H	2.939344	-2.810374	0.933983
C	-0.762491	0.115516	3.053693
C	2.955883	0.252043	-0.956826
C	-1.863464	-0.768690	3.026394
C	-2.872508	-0.597312	3.983266
C	-2.800911	0.402252	4.944326
C	-1.708942	1.267372	4.956865
C	-0.682864	1.151003	4.017676
H	-3.730697	-1.264528	3.973577
H	-3.593052	0.511809	5.680064
H	-1.660077	2.049284	5.708625
C	2.881715	-0.612150	-2.074115
C	3.758364	-0.387991	-3.142109
C	4.687550	0.645648	-3.118640
C	4.738412	1.495514	-2.018197
C	3.874208	1.328495	-0.933272
H	3.711347	-1.039206	-4.011268
H	5.362951	0.793283	-3.956979
H	5.458561	2.309452	-2.005360
C	-2.008213	-1.875407	1.992451
H	-1.098674	-1.884968	1.380804
C	-2.147839	-3.261473	2.639365
H	-2.167776	-4.040381	1.868751
H	-1.318031	-3.477036	3.319999
H	-3.076928	-3.345398	3.213875
C	-3.182624	-1.598663	1.042255
H	-4.134096	-1.567042	1.585032
H	-3.052307	-0.641337	0.527302
H	-3.254758	-2.384816	0.281913
C	0.470919	2.142776	3.985328
H	1.350094	1.611339	3.604290
C	0.842635	2.710108	5.358814
H	1.020100	1.914996	6.090756
H	1.757494	3.307177	5.278970
H	0.064414	3.370254	5.758142
C	0.161048	3.277334	2.995100
H	-0.050377	2.884371	1.995156
H	-0.715273	3.847740	3.323715
H	1.007997	3.968557	2.916792
C	3.943603	2.276172	0.254366
H	3.052440	2.089077	0.862596
C	3.913493	3.750796	-0.168258
H	4.811720	4.036288	-0.727230
H	3.044397	3.966731	-0.797644
H	3.862044	4.396401	0.715576
C	5.173077	1.982760	1.128166
H	5.188536	2.636556	2.007877
H	5.177379	0.944890	1.476844
H	6.101489	2.149184	0.569335
C	1.873718	-1.747558	-2.174088
H	1.333478	-1.802738	-1.221929
C	0.829107	-1.466143	-3.264463
H	0.087666	-2.272429	-3.303168
H	0.299052	-0.528916	-3.066240
H	1.297065	-1.390915	-4.252523
C	2.547105	-3.108246	-2.406373
H	3.048161	-3.147934	-3.379851
H	3.297378	-3.326504	-1.639779
H	1.799840	-3.909640	-2.390149

Zero-point correction= 0.615525 (Hartree/Particle)
Thermal correction to Energy= 0.651403
Thermal correction to Enthalpy= 0.652347
Thermal correction to Gibbs Free Energy= 0.545835
Sum of electronic and zero-point Energies= -2979.330486
Sum of electronic and thermal Energies= -2979.294607
Sum of electronic and thermal Enthalpies= -2979.293663
Sum of electronic and thermal Free Energies= -2979.400176

SET_U def2-tzvp Gas

71
scf done: -2979.955382

Zn	0.431146	1.243573	0.358345
N	0.144871	0.109469	2.020164
N	2.073332	0.060623	0.169508
C	2.145193	-0.821393	1.168835
C	1.116850	-0.795282	2.155718
C	1.157141	-1.766613	3.297562
C	3.256798	-1.821765	1.279853
H	0.290535	-1.643769	3.944543
H	1.172695	-2.800720	2.941526
H	2.056042	-1.629899	3.906460
H	3.977695	-1.694606	0.474349
H	3.787932	-1.724249	2.231041
H	2.876963	-2.847051	1.235184
C	-0.925408	0.229895	2.939116
C	3.035580	0.127144	-0.866863
C	-2.124718	-0.471341	2.708273
C	-3.189675	-0.277317	3.583330
C	-3.089136	0.585389	4.660983
C	-1.907073	1.272997	4.874887
C	-0.812821	1.114153	4.029441
H	-4.118937	-0.810443	3.414454
H	-3.930378	0.723486	5.330634
H	-1.833048	1.953061	5.716453
C	2.842011	-0.615312	-2.047882
C	3.761259	-0.472778	-3.083249
C	4.847168	0.378174	-2.971188
C	5.024792	1.105832	-1.807334
C	4.134151	0.999535	-0.742915
H	3.621098	-1.037306	-3.998569
H	5.551513	0.475740	-3.789459
H	5.873340	1.776093	-1.724084
C	4.353055	1.838762	0.501400
H	3.604840	1.535352	1.236214
C	4.131239	3.325455	0.209376
H	4.244026	3.918826	1.120765
H	4.853716	3.696090	-0.522545
H	3.131091	3.505407	-0.191248
C	5.730140	1.604031	1.125662
H	5.827605	2.168728	2.056633
H	5.891675	0.547801	1.351513
H	6.534937	1.927530	0.460811
C	1.648978	-1.534446	-2.227992
H	1.126214	-1.583485	-1.270842
C	0.667487	-0.965303	-3.256561
H	-0.212560	-1.607749	-3.347418

H	0.330369	0.033937	-2.971791
H	1.130733	-0.890417	-4.243933
C	2.061981	-2.960352	-2.598212
H	2.550992	-2.998671	-3.574782
H	2.754158	-3.379244	-1.864630
H	1.184303	-3.610276	-2.646453
C	-2.290881	-1.403773	1.523582
H	-1.320286	-1.481376	1.029838
C	-3.278160	-0.828646	0.504132
H	-2.962374	0.159060	0.160791
H	-3.356685	-1.482636	-0.368545
H	-4.277056	-0.726215	0.936279
C	-2.703434	-2.814764	1.947906
H	-1.996525	-3.239438	2.663911
H	-3.692043	-2.823108	2.413669
H	-2.745232	-3.476858	1.079018
C	0.451213	1.912716	4.284649
H	1.205785	1.566409	3.575778
C	0.223431	3.403349	4.018091
H	-0.126423	3.574246	2.997517
H	-0.525473	3.815961	4.699223
H	1.149954	3.966643	4.158475
C	1.007249	1.688290	5.692297
H	0.322699	2.057006	6.460249
H	1.184216	0.628505	5.887816
H	1.954795	2.219143	5.816490

Zero-point correction= 0.615678 (Hartree/Particle)
Thermal correction to Energy= 0.651790
Thermal correction to Enthalpy= 0.652734
Thermal correction to Gibbs Free Energy= 0.542144
Sum of electronic and zero-point Energies= -2979.339704
Sum of electronic and thermal Energies= -2979.303592
Sum of electronic and thermal Enthalpies= -2979.302647
Sum of electronic and thermal Free Energies= -2979.413237

SET$_{BS}$ def2-tzvp Gas

71
scf done: -2979.953143

Zn	0.430994	1.236390	0.358258
N	0.145188	0.105022	2.021853
N	2.077761	0.059605	0.172811
C	2.147563	-0.824443	1.171627
C	1.118107	-0.800043	2.156832
C	1.156260	-1.772302	3.297950
C	3.258252	-1.826091	1.280119
H	0.266317	-1.680274	3.917903
H	1.219702	-2.804055	2.941438
H	2.029674	-1.605064	3.936197
H	4.005536	-1.664542	0.505320
H	3.755048	-1.767449	2.252360
H	2.884291	-2.849864	1.178435
C	-0.924081	0.226926	2.941029
C	3.038301	0.125044	-0.864545
C	-2.129838	-0.460955	2.703064
C	-3.194238	-0.264484	3.578287
C	-3.087144	0.588121	4.663283
C	-1.898841	1.262609	4.884708
C	-0.804972	1.100496	4.039473
H	-4.128129	-0.787671	3.403824
H	-3.927997	0.728528	5.332946
H	-1.819801	1.934879	5.732044
C	2.851419	-0.628945	-2.039526
C	3.768482	-0.486137	-3.076748
C	4.846428	0.375946	-2.972444
C	5.018034	1.114632	-1.814671
C	4.128974	1.008614	-0.748899
H	3.633057	-1.059153	-3.987481
H	5.549255	0.473433	-3.792032
H	5.860487	1.793263	-1.737372
C	4.340646	1.859275	0.488856
H	3.596791	1.552651	1.226785
C	4.102316	3.341324	0.186339
H	4.209863	3.942673	1.093130
H	4.819717	3.714316	-0.549384
H	3.099814	3.507719	-0.214434
C	5.720870	1.643988	1.113123
H	5.813537	2.217039	2.039473
H	5.893579	0.591319	1.347261
H	6.521492	1.970536	0.444722
C	1.665092	-1.558196	-2.211923
H	1.151696	-1.615342	-1.250147
C	0.669386	-0.992752	-3.228955
H	-0.206304	-1.641840	-3.314799
H	0.326898	0.002727	-2.937223
H	1.123465	-0.909797	-4.219944
C	2.085493	-2.979269	-2.591840
H	2.561993	-3.011011	-3.574785
H	2.790565	-3.394400	-1.868473
H	1.212729	-3.636383	-2.630835
C	-2.302361	-1.382618	1.510907
H	-1.331448	-1.464748	1.018424
C	-3.283128	-0.791306	0.494437
H	-2.958881	0.196610	0.159498
H	-3.365646	-1.437596	-0.383601
H	-4.281874	-0.684022	0.925773
C	-2.727333	-2.793338	1.923658
H	-2.024343	-3.229830	2.636425
H	-3.716170	-2.796843	2.389017
H	-2.774431	-3.448091	1.049483
C	0.465356	1.887073	4.300617
H	1.222049	1.528502	3.600159
C	0.254398	3.378120	4.022129
H	-0.085650	3.545791	2.997635
H	-0.496519	3.801883	4.694169
H	1.184937	3.933749	4.166601
C	1.008323	1.667138	5.713937
H	0.323855	2.051366	6.474288
H	1.169925	0.606776	5.919398
H	1.961878	2.186581	5.840307

Zero-point correction= 0.615372 (Hartree/Particle)
Thermal correction to Energy= 0.651676
Thermal correction to Enthalpy= 0.652621
Thermal correction to Gibbs Free Energy= 0.541616
Sum of electronic and zero-point Energies= -2979.337771
Sum of electronic and thermal Energies= -2979.301467
Sum of electronic and thermal Enthalpies= -2979.300522
Sum of electronic and thermal Free Energies= -2979.411527