Supporting Information

Density Functional Theory Investigations on the Coordination of Pa(V) with N, N-dialkylamide

Jun Ma[a], Chuting Yang[a], Jun Han[a], Sheng Hu[a], Haizhu Yu[b,*], Xinggui Long[a,*]

[a] *Institute of Nuclear Physics and Chemistry, China Academy of Engineering Physics, Mianyang 621900, Sichuan, China.*

[b] *Department of Chemistry and Center for Atomic Engineering of Advanced Materials, Anhui University, Hefei 230026, China.*

Emails: Xingguil@caep.cn

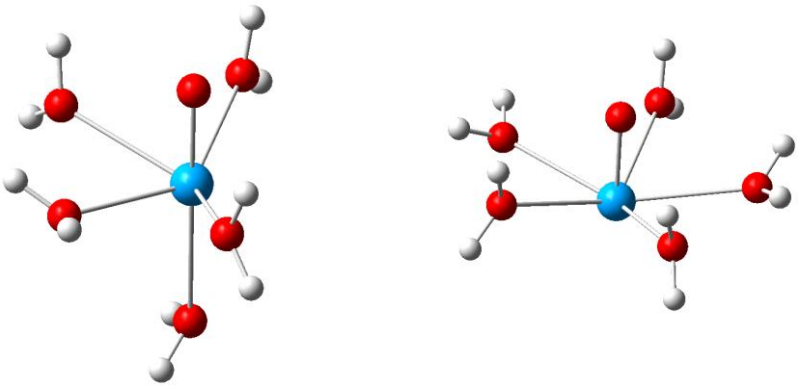
yuhaizhu@ahu.edu.cn

Table S1. The reaction Gibbs free energy of $[PaO(H_2O)_6]^{3+}$, **L1**, $[PaO(H_2O)_5(\mathbf{L1})]^{3+}$**-A** and H_2O in different solvents (in hartree), and the energy gap $\Delta\Delta G(X\text{-}H_2O)$ of certain species in different solvents and water (in kJ/mol).

solvent	**$[PaO(H_2O)_5(L1)]^{3+}$-A**	**H_2O**	**L1**	**$[PaO(H_2O)_6]^{3+}$**	**ΔG**
H_2O	-1540.228366	-76.451024	-641.508327	-975.161710	-24.7
methanol	-1540.21203	-76.450819	-641.508039	-975.147942	-18.1
toluene	-1539.976713	-76.447207	-641.503696	-974.877566	-112.4
n-dodecane	-1539.936998	-76.446644	-641.503304	-974.876268	-10.7
benzene	-1539.966510	-76.44706	-641.503564	-974.865072	-118.4
$\Delta\Delta G(X\text{-}H_2O)$	**$[PaO(H_2O)_5(L1)]^{3+}$-A**	**H_2O**	**L1**	**$[PaO(H_2O)_6]^{3+}$**	
X=methanol	42.9	0.5	0.8	36.2	
X=*n*-dodecane	765.5	11.5	13.2	750.0	
X=toluene	661.2	10.0	12.2	746.6	
X=benzene	688.0	10.4	12.5	779.4	

Table S2. Total electron energies and $<S^2>$ values of $[PaO(H_2O)_5(\mathbf{L1})]^{3+}$**-A** with different multiplicities.

Multiplicity	1	3	5	7
$<S^2>$	0	2.0062	6.0114	12.0143
E (A.U.)	-1540.67757094	-1540.54303499	-1540.45511146	-1540.16180911
Multiplicity	9	11	13	
$<S^2>$	20.0173	30.0187	42.0226	
E(A.U.)	-1540.10206110	-1539.88192949	-1539.77360611	



0.0 kJ/mol -22.3 kJ/mol

Figure S1. The relative Gibbs free energy of the two typical structure of $[PaO(H_2O)_5]^{3+}$.

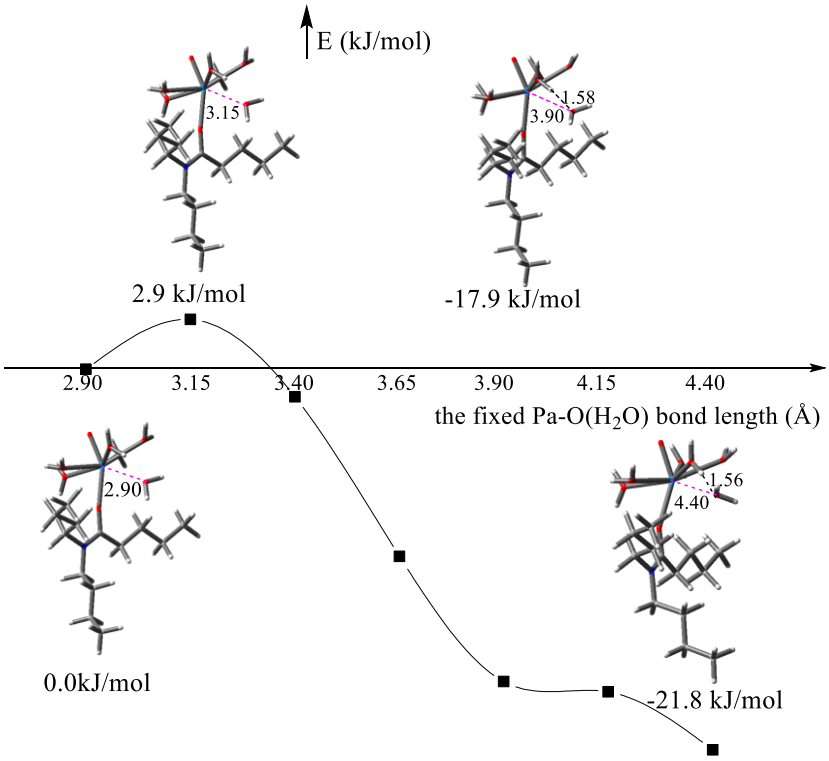


Figure S2. Electronic energy profile for the water dissociation process starting from $[PaO(H_2O)_6(\mathbf{L1})]^{3+}$ calculated via the partial optimization by fixing the red Pa-O(H_2O) bond at different distances.

Table S3. WBI analysis of $[PaO(H_2O)_5(\mathbf{Ln})]^{3+}$**-A**.

	n=	1	2	3	4	5	6	7
WBI	Pa-O(amide)	0.634	0.656	0.657	0.664	0.661	0.686	0.667
	Pa=O	1.963	1.971	1.971	1.971	1.971	1.964	1.965
	C=O	1.189	1.165	1.164	1.160	1.161	1.151	1.163
	C=N	1.447	1.460	1.460	1.462	1.462	1.469	1.465
	Pa-O(H_2O)$^{eq}_{av}$	0.361	0.364	0.364	0.365	0.364	0.362	0.370
	n=	8	9	10	11	12	13	14
WBI	Pa-O(amide)	0.654	0.663	0.668	0.648	0.661	0.661	0.650
	Pa=O	1.968	1.973	1.972	1.967	1.963	1.973	1.971
	C=O	1.164	1.161	1.153	1.180	1.177	1.161	1.177
	C=N	1.460	1.467	1.478	1.450	1.458	1.468	1.447
	Pa-O(H_2O)$^{eq}_{av}$	0.361	0.367	0.367	0.366	0.357	0.363	0.364
	n=	15	16	17	18	19	20	
WBI	Pa-O(amide)	0.653	0.650	0.648	0.650	0.650	0.649	
	Pa=O	1.971	1.965	1.970	1.967	1.971	1.966	
	C=O	1.175	1.176	1.179	1.174	1.177	1.177	
	C=N	1.447	1.451	1.444	1.454	1.452	1.452	
	Pa-O(H_2O)$^{eq}_{av}$	0.365	0.365	0.364	0.364	0.367	0.365	

Table S4. The reaction Gibbs free energy for the ligand exchange reactions of $[Pa(OH)_2(NO_3)_3(H_2O)_2]+Ln\rightarrow[Pa(OH)_2(NO_3)_3(H_2O)(Ln)]+H_2O$ (n=1-20) (in kJ/mol).

Ln	**L1**	**L2**	**L3**	**L4**	**L5**	**L6**	**L7**
ΔG	7.6	7.3	3.8	9.3	2.6	6.7	3.3
Ln	**L8**	**L9**	**L10**	**L11**	**L12**	**L13**	**L14**
ΔG	5.1	14.4	14.9	17.6	30.1	10.5	13.8
Ln	**L15**	**L16**	**L17**	**L18**	**L19**	**L20**	
ΔG	7.5	19.1	30.7	22.0	20.5	17.7	

Cartesian coordinates and thermal energies of all species in this study:

L1

Sum of electronic and thermal Free Energies=

-641.508327

C	-0.70617700	-0.84110000	-0.52274400
O	-0.68928000	-2.06403000	-0.36483900
N	0.42686700	-0.15861300	-0.86003800
C	-2.00222100	-0.04744900	-0.35574000
H	-1.83155000	0.79743400	0.31918500
H	-2.27108800	0.39170400	-1.32403000
C	-3.16288900	-0.89945200	0.16087300
H	-3.32297100	-1.74225800	-0.51831500
H	-2.88984600	-1.33653500	1.12725400
C	-4.46226400	-0.10006300	0.30784100
H	-4.29767500	0.73995300	0.99349500
H	-4.72727100	0.34326700	-0.65977400
C	-5.63062300	-0.95049400	0.81494900
H	-5.84037300	-1.77851300	0.13057000
H	-5.40836700	-1.38038700	1.79676600
C	1.66309400	-0.93353000	-1.04637600
H	1.40925200	-1.84556500	-1.59168400
H	2.32540700	-0.33921600	-1.68066500
C	0.47665600	1.28922500	-1.09573600
H	1.11949500	1.45889100	-1.96511000
H	-0.51555200	1.63944600	-1.37868300
C	0.99390700	2.11298300	0.09183100
H	0.37122400	1.90822500	0.97033300
H	2.00921100	1.79076900	0.34590600
C	0.99587900	3.61760700	-0.20109800
H	1.60910100	3.81251800	-1.08900100
H	-0.02157500	3.93821500	-0.45504500
C	1.51654500	4.45431700	0.97108100
H	0.90288000	4.30552500	1.86495900
H	2.54511500	4.18006600	1.22520800
C	2.38393100	-1.31302800	0.25388600
H	1.69547100	-1.88766500	0.88052900
H	2.64314900	-0.40576400	0.80996900
C	3.65095300	-2.13489300	-0.00762700
H	3.38501300	-3.04050600	-0.56623600
H	4.32771800	-1.56416800	-0.65523700
C	4.38681500	-2.52771700	1.27671000
H	3.74415900	-3.12401300	1.93193900
H	4.70206900	-1.64240200	1.83766800
H	1.50539700	5.52139000	0.73303200
H	-6.54424200	-0.35726400	0.91040200
H	5.28037700	-3.11905800	1.05844100

L2

Sum of electronic and thermal Free Energies=

-759.404046

C	0.05466800	2.06273400	-0.32912200
N	0.09187700	0.71037800	-0.15335000
C	-1.10142700	2.83197800	0.31011100
H	-2.05154800	2.35491300	0.04991400
C	-1.13513300	4.30847200	-0.08849800
H	-0.18080800	4.77320200	0.17277700
C	1.19667600	-0.04462900	-0.75831900
H	0.82670600	-1.04546800	-0.99628300
H	1.46424500	0.44244300	-1.69671500
C	-0.90504900	-0.05663000	0.60201900
H	-0.37420500	-0.85408900	1.13090800
H	-1.34493700	0.57624200	1.37274700
C	-2.01011900	-0.66589900	-0.27230900
H	-2.53747900	0.13788200	-0.79822700
C	-3.00991100	-1.49399800	0.54249600
H	-2.47299500	-2.28866400	1.07607100
C	-4.11867800	-2.11988900	-0.31105600

H	-3.66608300	-2.76042100	-1.07884500
C	-5.12616500	-2.94146000	0.50140700
H	-5.57836800	-2.30022800	1.26760200
C	-6.22978300	-3.56536000	-0.35785300
H	-5.80914800	-4.23612400	-1.11376400
H	-6.92932100	-4.14599400	0.24994700
H	-6.80444400	-2.79517000	-0.88219000
C	2.43257100	-0.14086400	0.14482700
H	2.78704900	0.87279000	0.35829600
C	3.55949000	-0.96118100	-0.49216900
H	3.82971400	-0.51584500	-1.45822200
C	4.81256800	-1.05890600	0.38537400
H	4.54475400	-1.50856100	1.35026400
C	5.94521100	-1.87186300	-0.25194200
H	6.21239500	-1.42214800	-1.21587300
C	7.19326400	-1.96489600	0.63084600
H	6.96393900	-2.44248600	1.58877900
H	7.98166400	-2.54935000	0.14831700
H	7.59937300	-0.97124200	0.84549600
H	3.19382200	-1.97235500	-0.71277600
H	-3.46329500	-0.85900300	1.31423400
H	5.17614700	-0.04779300	0.60970800
H	-4.65207300	-1.32642500	-0.85025200
H	-4.59266200	-3.73289000	1.04163600
H	5.58110100	-2.88173300	-0.47665100
C	-2.28574600	5.06444600	0.58153800
H	-2.20281800	5.02748700	1.67242400
H	-3.25599000	4.63741400	0.30879400
H	-1.01302500	2.74832800	1.40029600
H	-1.22268900	4.38629400	-1.17645100
H	-1.55438900	-1.29618800	-1.04409100
H	2.14946500	-0.58841100	1.10484400
O	0.92607900	2.65026500	-0.97468300
H	-2.29049900	6.11649900	0.28410600

L3

Sum of electronic and thermal Free Energies=

-798.700557

C	-0.10652200	1.75162100	-0.34056300
O	0.65184100	2.48913600	-0.97457500
N	0.15987600	0.42253600	-0.18645200
C	-1.37688300	2.30166000	0.30780000
H	-2.22521700	1.65227200	0.07197700
C	-1.69187100	3.73892200	-0.11096600
H	-0.83746300	4.38068800	0.12368100
C	1.37650900	-0.12628300	-0.79856900
H	1.17201600	-1.16440600	-1.07445100
H	1.57225300	0.42960600	-1.71588700
C	-0.67877300	-0.51065500	0.57416600
H	-0.00967700	-1.21515400	1.07723900
H	-1.19944200	0.02848500	1.36560000
C	-1.68556200	-1.28560900	-0.28762000
H	-2.36599400	-0.57688300	-0.77289600
C	-2.49122200	-2.30118200	0.52985300
H	-1.80179100	-3.00668000	1.01079400
C	-3.51161500	-3.08277400	-0.30538100
H	-2.99104200	-3.60067200	-1.12126500
C	-4.31397200	-4.10428700	0.50853200
H	-4.83248900	-3.58710500	1.32497500
C	-5.33299600	-4.87972000	-0.33148600
H	-4.84055300	-5.43464000	-1.13639800
H	-5.88737100	-5.59927800	0.27747000
H	-6.06024900	-4.20372700	-0.79240600
C	2.60146900	-0.05722100	0.12191200
H	2.79318900	0.99220700	0.36874900
C	3.85018100	-0.67766100	-0.51404800
H	4.07240800	-0.16085100	-1.45636400
C	5.08418200	-0.62522200	0.39388700
H	4.86227000	-1.14442800	1.33520400
C	6.33773900	-1.24190100	-0.23710700
H	6.56279500	-0.72005300	-1.17511500
C	7.56306500	-1.19234600	0.68041400
H	7.37988600	-1.73607100	1.61263500
H	8.43895800	-1.63902500	0.20156900
H	7.81765300	-0.16072600	0.94349500
H	3.64191200	-1.72224300	-0.77920700
H	-3.01347200	-1.78063900	1.34279300
H	5.29187200	0.41865800	0.66221800
H	-4.20437400	-2.37801800	-0.78304600
H	-3.62144100	-4.80900800	0.98458800
H	6.12836900	-2.28343400	-0.50980400
C	-2.95194200	4.28775900	0.56711200
H	-2.82605800	4.24476800	1.65581900
H	-3.80415400	3.63845400	0.33267900
H	-1.25584300	2.25333900	1.39714000
H	-1.81386300	3.78087200	-1.19886700
C	-3.27661500	5.72462500	0.14849800
H	-3.44138000	5.79263800	-0.93148500

H	-4.17822000	6.09137400	0.64677200
H	-2.45617800	6.40356300	0.40158500
H	-1.14988900	-1.80315400	-1.09146600
H	2.37767300	-0.56991700	1.06483600

L4

Sum of electronic and thermal Free Energies=

-837.999756

C	0.21499600	-1.37092400	-0.43193100
O	-0.35070200	-2.24533000	-1.09278500
N	-0.36998200	-0.15863600	-0.21055000
C	1.59521000	-1.61570200	0.17697300
H	2.25745400	-0.77637900	-0.05646000
C	2.23534600	-2.92628700	-0.28462900
H	1.56543800	-3.75862300	-0.04904800
C	-1.69915700	0.09340200	-0.78217800
H	-1.77640800	1.16440700	-0.98790300
H	-1.76263100	-0.43371100	-1.73478800
C	0.23801000	0.92761700	0.56689400
H	-0.56592100	1.42900500	1.11408000
H	0.90201500	0.50880300	1.32329500
C	0.99465500	1.95206400	-0.28973200
H	1.79792200	1.44248000	-0.83358600
C	1.57990000	3.09623200	0.54542800
H	0.77050400	3.59901300	1.08993400
C	2.34335400	4.12932100	-0.29082600
H	1.67163100	4.54677900	-1.05190800
C	2.93557900	5.27329600	0.54014500
H	3.60733000	4.85585600	1.29993200
C	3.69531700	6.30199700	-0.30251800
H	3.03989200	6.76146900	-1.04921900
H	4.10433300	7.10338800	0.31910400
H	4.52966800	5.83602600	-0.83631700
C	-2.84626000	-0.35141200	0.13335700
H	-2.75329800	-1.42802500	0.30948700
C	-4.22450300	-0.03936400	-0.45964500
H	-4.31455400	-0.52202600	-1.44128400
C	-5.38683900	-0.49072500	0.43191800
H	-5.29749000	-0.00914000	1.41432800
C	-6.76782900	-0.18080400	-0.15689200
H	-6.85660700	-0.66127400	-1.13882700
C	-7.92346800	-0.63566100	0.73928700
H	-7.88047000	-0.14604600	1.71743700
H	-8.89294100	-0.39952200	0.29168300
H	-7.88956000	-1.71661800	0.90859600
H	-4.30656300	1.04012500	-0.64068300
H	2.25118600	2.68193600	1.30847600
H	-5.30553200	-1.57036500	0.61236700
H	3.15059300	3.62606000	-0.83841400
H	2.12896600	5.77494300	1.08853400
H	-6.84851600	0.89811800	-0.33670700
C	3.60594400	-3.16577300	0.35676000
H	3.50064400	-3.16983400	1.44956400
H	4.27303300	-2.32720300	0.11795800
H	1.49327200	-1.62157300	1.26921800
H	2.33593200	-2.91622300	-1.37522600
C	4.26654700	-4.47559500	-0.08889200
H	4.37242400	-4.47187700	-1.18051600
H	3.60070300	-5.31358200	0.15036200
H	0.31656500	2.36011800	-1.04757300
H	-2.74561300	0.14048300	1.10807000
C	5.63551500	-4.71179900	0.55535100
H	6.33337200	-3.90631900	0.30542500
H	5.55604200	-4.75427200	1.64629500
H	6.07876500	-5.65261100	0.21723700

L5

Sum of electronic and thermal Free Energies=

-877.297059

C	0.28087300	-1.05413200	-0.43147000
O	0.02660900	-2.06717500	-1.08753500
N	-0.66240800	-0.09239300	-0.21728100
C	1.66633600	-0.83998300	0.17787800
H	2.02302000	0.16723500	-0.05774000
C	2.69236800	-1.87618900	-0.28415500
H	2.32222200	-2.87913200	-0.05233800
C	-2.00090300	-0.28259900	-0.79076900
H	-2.41391500	0.70568700	-1.01026500
H	-1.89058300	-0.81419700	-1.73657400
C	-0.44053800	1.13097300	0.56228700
H	-1.36422700	1.34311000	1.10922600
H	0.32293300	0.94922800	1.31884000
C	-0.05844500	2.34835400	-0.29118800
H	0.87685400	2.13778100	-0.82197900
C	0.09572000	3.62358600	0.54494100
H	-0.84263900	3.82232400	1.07826200
C	0.47224700	4.85392000	-0.28818200
H	-0.29027700	5.01390700	-1.06132400

C	0.62343100	6.13330900	0.54258400	**-916.596827**
H	1.38662900	5.97383300	1.31394600	
C	0.99570100	7.35843300	-0.29765500	
H	0.23241200	7.56371100	-1.05492800	
H	1.09716500	8.25281500	0.32339600	
H	1.94617900	7.20539900	-0.81865500	
C	-2.94998200	-1.05775800	0.13144700	
H	-2.51980700	-2.04645800	0.32177800	
C	-4.35388600	-1.20806400	-0.46440000	
H	-4.28243100	-1.70771000	-1.43904000	
C	-5.31553400	-1.99312600	0.43473300	
H	-5.38799700	-1.49413700	1.40981600	
C	-6.72106500	-2.14749800	-0.15729100	
H	-6.64854700	-2.64603700	-1.13152800	
C	-7.67527100	-2.93295100	0.74717300	
H	-7.79505100	-2.43979900	1.71712100	
H	-8.66741900	-3.02549500	0.29653300	
H	-7.29905800	-3.94379700	0.93421500	
H	-4.77397700	-0.21313700	-0.66053500	
H	0.85884800	3.46260200	1.31708100	
H	-4.89570100	-2.98811700	0.63113900	
H	1.41139900	4.65689700	-0.82104600	
H	-0.31430400	6.32848700	1.07687100	
H	-7.14014500	-1.15318000	-0.35376100	
C	4.06856600	-1.67001900	0.35807500	
H	3.97056600	-1.71413900	1.45054900	
H	4.43362800	-0.66153900	0.12468100	
H	1.57217400	-0.87649500	1.27026700	
H	2.78563100	-1.83130900	-1.37454000	
C	5.10880900	-2.69986800	-0.09649000	
H	5.20729900	-2.65611100	-1.18899400	
H	4.74447700	-3.70869700	0.13698800	
H	-0.82389900	2.50454000	-1.05956800	
H	-3.01477000	-0.54736000	1.09967000	
C	6.48867300	-2.50261800	0.54148500	
H	6.85173000	-1.49409500	0.30916300	
H	6.39032500	-2.54765400	1.63294100	
C	7.52175800	-3.53482300	0.07999900	
H	7.66706500	-3.48968400	-1.00406800	
H	8.49344500	-3.36714900	0.55301800	
H	7.20157700	-4.55167600	0.32862200	

L6

Sum of electronic and thermal Free Energies=

C	-0.03804900	-0.88063500	-0.51325500
O	-0.16733000	-1.90892600	-1.18197000
N	-1.09776400	-0.05892800	-0.26265600
C	1.31830300	-0.49181900	0.07497500
H	1.53462500	0.55684300	-0.15057300
C	2.46302200	-1.37856100	-0.41786800
H	2.22366000	-2.42513200	-0.20769400
C	-2.41315800	-0.42717000	-0.80228800
H	-2.96812200	0.49616900	-0.98878400
H	-2.25824600	-0.92240400	-1.76132900
C	-1.02418700	1.17246900	0.53169700
H	-1.95868900	1.25531600	1.09461300
H	-0.23144600	1.08106900	1.27447700
C	-0.81552600	2.44026200	-0.30827300
H	0.12673800	2.35457100	-0.86098500
C	-0.79973600	3.71154200	0.54772400
H	-1.74930400	3.79408600	1.09160100
C	-0.57072200	4.99016800	-0.26597900
H	-1.35275600	5.07820600	-1.03113600
C	-0.55515700	6.26360900	0.58732100
H	0.22234300	6.17217800	1.35543500
C	-0.31640900	7.53626100	-0.23042800
H	-1.09661300	7.67216600	-0.98619300
H	-0.31212000	8.42521500	0.40650800
H	0.64539000	7.49563000	-0.75156100
C	-3.21290700	-1.34467300	0.13093800
H	-2.63988800	-2.26426500	0.28823900
C	-4.59936900	-1.68636300	-0.42525400
H	-4.48944400	-2.15264800	-1.41272200
C	-5.40517600	-2.61931600	0.48588200
H	-5.51333300	-2.15488300	1.47461100
C	-6.79433000	-2.96465800	-0.06241600
H	-6.68654600	-3.42685600	-1.05115700
C	-7.59015200	-3.89951300	0.85323200
H	-7.74187200	-3.45022400	1.83987900
H	-8.57537300	-4.12473500	0.43539900
H	-7.06558100	-4.84914600	0.99933900
H	-5.16582200	-0.75988400	-0.58537200
H	-0.01588100	3.62497800	1.31105800
H	-4.83920400	-3.54641400	0.64421700
H	0.38002500	4.90801700	-0.80824900
H	-1.50723200	6.34839900	1.12505200
H	-7.36021700	-2.03818900	-0.21861200

C	3.80703200	-1.01583200	0.22313700
H	3.72110900	-1.09563300	1.31461200
H	4.04223100	0.03531700	0.01174600
H	1.24891400	-0.55494600	1.16796000
H	2.54077800	-1.29806400	-1.50750200
C	4.96499300	-1.89818100	-0.25669800
H	5.05824600	-1.81066000	-1.34687800
H	4.72403400	-2.94979900	-0.05432700
H	-1.61107800	2.51197600	-1.05848400
H	-3.31897100	-0.86440200	1.11078100
C	6.30926000	-1.55450800	0.39452000
H	6.55128900	-0.50273800	0.19309000
H	6.21548500	-1.64232200	1.48486600
C	7.46790800	-2.43752100	-0.08279700
H	7.56512400	-2.34687100	-1.17151800
H	7.22418300	-3.48847300	0.11505200
C	8.80530200	-2.09161200	0.57852900
H	8.74867800	-2.20547900	1.66582000
H	9.60920300	-2.73943300	0.21778100
H	9.09301800	-1.05633000	0.36910100

L7

Sum of electronic and thermal Free Energies= -955.893547

C	-0.37987900	-0.79444900	-0.47929600
O	-0.40347400	-1.82840700	-1.15141200
N	-1.52012200	-0.09373000	-0.21615600
C	0.93227900	-0.25889300	0.09377900
H	1.04805800	0.79526400	-0.17842600
C	2.15655900	-1.05288300	-0.36446200
H	2.03543400	-2.10115500	-0.07482400
C	-2.78977200	-0.58963000	-0.76267500
H	-3.44210800	0.27273600	-0.92313900
H	-2.58778200	-1.03887700	-1.73581900
C	-1.57307500	1.14309800	0.57139700
H	-2.49727500	1.12046700	1.15683900
H	-0.75694900	1.15040500	1.29356700
C	-1.53381400	2.41936100	-0.28092200
H	-0.60457100	2.43536700	-0.86143300
C	-1.63754500	3.69361600	0.56444900
H	-2.56092600	3.66240400	1.15671100
C	-1.61812100	4.97806000	-0.27204000
H	-2.44926600	4.95484500	-0.98853400
C	-1.71227400	6.25792800	0.56643500
H	-0.87905100	6.28371800	1.27904800
C	-1.70015800	7.53506300	-0.27882300
H	-2.54165400	7.55242200	-0.97870400
H	-1.76965900	8.42907800	0.34712800
H	-0.77952900	7.61063400	-0.86618200
C	-3.48458300	-1.61243300	0.14490900
H	-2.82388000	-2.47714500	0.26458300
C	-4.83753200	-2.06564900	-0.41428100
H	-4.69423300	-2.47734800	-1.42159000
C	-5.53928700	-3.11038700	0.46092100
H	-5.67715000	-2.70314800	1.47094200
C	-6.89739000	-3.55900800	-0.09054800
H	-6.76018000	-3.96160900	-1.10148500
C	-7.58967600	-4.60710900	0.78577200
H	-7.76945400	-4.22152800	1.79442100
H	-8.55508000	-4.90396200	0.36641900
H	-6.97652700	-5.50894100	0.88080500
H	-5.49319500	-1.19309300	-0.53052000
H	-0.81097500	3.71917400	1.28587000
H	-4.88700700	-3.98628600	0.57082700
H	-0.69870400	5.00620600	-0.87089800
H	-2.62842300	6.22735000	1.16860600
H	-7.54958800	-2.68362300	-0.19647700
C	3.46500700	-0.50361500	0.21438000
H	3.40475700	-0.49831500	1.31042600
H	3.58692100	0.54406000	-0.08964700
H	0.86921900	-0.27983500	1.18833300
H	2.20553700	-1.04424800	-1.45828000
C	4.70064200	-1.30127600	-0.21784000
H	4.75649300	-1.31465700	-1.31397100
H	4.58153300	-2.34671000	0.09472200
H	-2.35421200	2.39384400	-1.00681300
H	-3.62564700	-1.17786600	1.14162800
C	6.01488600	-0.75123300	0.34780300
H	6.13675700	0.29196500	0.02852800
H	5.95555400	-0.73009900	1.44374200
C	7.24981400	-1.55520600	-0.07425500
H	7.30870900	-1.57992500	-1.17027200
H	7.13025400	-2.59782300	0.24824800
C	8.56513700	-1.00325100	0.48726800
H	8.50575400	-0.97606900	1.58216100
H	8.68672900	0.03733800	0.16254600
C	9.79265900	-1.81549000	0.06396400
H	10.71263900	-1.39702500	0.48186200

H	9.71500700	-2.85338400	0.40328400
H	9.89906700	-1.83089600	-1.02545300

L8

Sum of electronic and thermal Free Energies=

-995.192550

C	-0.83335500	-0.77260300	-0.48741700
O	-0.83301200	-1.80656700	-1.15998600
N	-1.99115400	-0.10575900	-0.21311200
C	0.46805300	-0.19948400	0.07391000
H	0.54543700	0.86081200	-0.18725600
C	1.71122300	-0.94752300	-0.41032600
H	1.62755200	-2.00280700	-0.13339600
C	-3.25022100	-0.63723300	-0.75032900
H	-3.92678000	0.20653100	-0.90982700
H	-3.04153700	-1.08403100	-1.72314700
C	-2.07321900	1.12818100	0.57664500
H	-2.99457300	1.08039000	1.16497900
H	-1.25523000	1.15547600	1.29634800
C	-2.07067800	2.40613100	-0.27396100
H	-1.14039700	2.45191400	-0.85120800
C	-2.21794100	3.67577700	0.57180400
H	-3.14591300	3.61774500	1.15479300
C	-2.22633900	4.96129100	-0.26318500
H	-3.04582600	4.91318200	-0.99181300
C	-2.37245400	6.23667800	0.57458600
H	-1.55217000	6.28671400	1.30083700
C	-2.38496400	7.51469800	-0.26932000
H	-3.21517300	7.50778000	-0.98273300
H	-2.49141500	8.40537000	0.35620700
H	-1.45761400	7.61870500	-0.84156800
C	-3.91162600	-1.67599300	0.16416000
H	-3.22404500	-2.51893600	0.28769800
C	-5.25014800	-2.17446000	-0.39109400
H	-5.09417500	-2.58845500	-1.39557600
C	-5.91919700	-3.23469600	0.49122000
H	-6.07342500	-2.82379100	1.49737700
C	-7.25987300	-3.73313200	-0.06004100
H	-7.10596400	-4.14040000	-1.06669500
C	-7.91963300	-4.79563400	0.82405800
H	-8.11701800	-4.40641000	1.82800200
H	-8.87237200	-5.12994600	0.40390000
H	-7.27608400	-5.67469700	0.93070300
H	-5.93260200	-1.32352900	-0.51318100
H	-1.39961300	3.72375300	1.30147100
H	-5.23833500	-4.08734000	0.61017100
H	-1.29958000	5.01864300	-0.84848200
H	-3.29700700	6.17799100	1.16163000
H	-7.94048400	-2.88101100	-0.17619600
C	3.00951800	-0.36456300	0.15826200
H	2.96439500	-0.37536700	1.25498900
H	3.09452200	0.69025300	-0.13338200
H	0.42035900	-0.23504500	1.16897000
H	1.74527700	-0.92299000	-1.50449900
C	4.26295200	-1.11793700	-0.30145400
H	4.30329800	-1.11605800	-1.39834800
H	4.18036200	-2.17038100	-0.00078500
H	-2.88717800	2.35541500	-1.00293100
H	-4.06497200	-1.24058500	1.15870500
C	5.56801800	-0.53518000	0.25242900
H	5.65508700	0.51432200	-0.05739800
H	5.52314300	-0.52695200	1.34920300
C	6.81981900	-1.29890500	-0.19483500
H	6.86229900	-1.31217900	-1.29167500
H	6.73409700	-2.34710500	0.11986000
C	8.12614400	-0.71339900	0.35290000
H	8.08271100	-0.69467700	1.44977500
C	9.37746300	-1.48211300	-0.08713300
H	9.28899400	-2.52725200	0.23369700
H	9.42082600	-1.50224600	-1.18292100
C	10.67780800	-0.88869600	0.46294800
H	11.54955400	-1.46062300	0.13269800
H	10.81209100	0.14502600	0.12859700
H	10.67758500	-0.88476100	1.55763300
H	8.21597600	0.33317700	0.03348900

L9

Sum of electronic and thermal Free Energies=

-759.402386

C	0.08681300	2.17011000	-0.35969100
O	0.99613400	2.72210300	-0.98640800
N	0.06277500	0.81764900	-0.19176200
C	-1.02468800	3.01974000	0.27119400
H	-1.90478400	2.40618800	0.46756900
C	-1.43683500	4.14139500	-0.69089800
H	-0.57814700	4.76650300	-0.94114700
H	-1.84397800	3.73695400	-1.62159100
C	1.13287500	0.02023200	-0.80758100

H	0.71323100	-0.95617500	-1.06454500
H	1.42667600	0.51140200	-1.73557000
C	-0.94999400	0.07818200	0.57352400
H	-0.44442000	-0.77279900	1.03886000
H	-1.31448900	0.69389300	1.39569400
C	-2.12292300	-0.42308100	-0.27893400
H	-2.62402800	0.43570100	-0.73994300
C	-3.13458800	-1.23681400	0.53565300
H	-2.62425800	-2.08890100	1.00245700
H	-3.51722500	-0.62010400	1.35883100
C	-4.31294900	-1.75029500	-0.29956800
H	-4.81715200	-0.89917400	-0.77517600
H	-3.93155000	-2.37557900	-1.11698800
C	-5.33631600	-2.55162300	0.51317400
H	-4.83205600	-3.40027100	0.99104700
H	-5.71830400	-1.92500400	1.32818000
C	-6.50879600	-3.06369600	-0.32860300
H	-6.16077800	-3.72306500	-1.13003900
H	-7.22114300	-3.62754700	0.28012600
H	-7.05166600	-2.23490600	-0.79420300
C	2.35921400	-0.15441600	0.09633000
H	2.76921600	0.83529500	0.32221300
C	3.43923100	-1.02989800	-0.54847900
H	3.01622900	-2.01560700	-0.78150600
H	3.73686400	-0.58986200	-1.50889800
C	4.68240100	-1.21012600	0.32993600
H	4.38581600	-1.64900600	1.29141000
H	5.10728100	-0.22496600	0.56184300
C	5.76372400	-2.08705000	-0.31154300
H	6.05896000	-1.64892500	-1.27266600
H	5.33838400	-3.07121000	-0.54275100
C	7.00290400	-2.26228700	0.57117300
H	6.74342900	-2.72856400	1.52701900
H	7.75305900	-2.89323500	0.08624500
H	7.47100700	-1.29728900	0.79023600
C	-0.51960900	3.58998300	1.61069500
H	-1.28936000	4.21398300	2.07187100
H	-0.25859000	2.79735500	2.31724700
H	-2.20428800	4.76825700	-0.22944400
H	0.36934500	4.20561500	1.44926500
H	-1.73446600	-1.03473200	-1.10105500
H	2.04990200	-0.59672200	1.05071400

L10

Sum of electronic and thermal Free Energies= -916.573361

C	0.01278500	2.09889500	-0.61683600
O	0.91136500	2.56605300	-1.32673600
N	0.01407800	0.78566200	-0.23031600
C	-1.12819100	3.04222800	-0.21489900
H	-1.87911100	2.52079100	0.37095200
C	-1.81157300	3.56261000	-1.49217700
H	-1.09094600	4.08610500	-2.12332000
H	-2.24632300	2.74538700	-2.07439500
C	1.07843700	-0.07560600	-0.83192200
H	1.46441600	0.52514000	-1.65404900
C	-0.94943700	0.13337200	0.70440200
H	-0.54589000	-0.87486200	0.81676800
C	-2.37587800	-0.02940600	0.11437400
H	-2.99349200	0.83539700	0.37834400
C	-3.08895500	-1.30613400	0.58201200
H	-2.50020300	-2.18031500	0.27723800
H	-3.13212600	-1.33172800	1.67727100
C	-4.51101100	-1.43416600	0.02413500
H	-5.10108900	-0.56198400	0.33374000
H	-4.47337800	-1.40409100	-1.07247500
C	-5.23102000	-2.71254700	0.46864100
H	-4.64114200	-3.58399400	0.15974600
H	-5.26884000	-2.74217400	1.56432200
C	-6.65056200	-2.83256600	-0.09346600
H	-6.64204000	-2.83998700	-1.18805600
H	-7.13594900	-3.75340300	0.24171000
H	-7.27415800	-1.99189400	0.22701300
C	2.23861500	-0.28786600	0.15888600
H	2.51936700	0.69453400	0.55293300
C	3.48745000	-0.95076400	-0.43719100
H	3.25750300	-1.97370900	-0.75463700
H	3.79320100	-0.40693900	-1.33992600
C	4.66385500	-0.99103700	0.54595400
H	4.36314000	-1.53390300	1.45141000
H	4.90129800	0.03132000	0.86728400
C	5.92459400	-1.64098900	-0.03603700
H	6.21807400	-1.10304400	-0.94562300
H	5.69028500	-2.66553400	-0.34967700
C	7.10117600	-1.66441400	0.94397500
H	6.84878400	-2.22323300	1.85081700
H	7.98264700	-2.13425200	0.49866600
H	7.38199500	-0.65084400	1.24740700

C	-0.57040000	4.20366200	0.62392000
H	-1.37099600	4.90157200	0.88293400
H	-0.11719700	3.84915000	1.55367900
H	-2.61513800	4.25613800	-1.23084400
H	0.19195600	4.74546400	0.06009000
H	-2.31055200	-0.03707100	-0.97722000
H	1.89154800	-0.88127600	1.01191600
C	0.50754500	-1.38804900	-1.42845100
H	-0.57234200	-1.29040300	-1.55210500
H	0.66279100	-2.21990100	-0.73240400
C	1.10188900	-1.74555000	-2.79830900
H	0.66775000	-2.67616700	-3.17462200
H	0.88961100	-0.95959800	-3.52925900
H	2.18484400	-1.87741300	-2.75859300
C	-0.99511100	0.72738200	2.13075800
H	-1.40096600	1.74083500	2.10755100
H	-1.72734700	0.13133600	2.68521100
C	0.32322000	0.72743100	2.90645100
H	0.72027400	-0.28461900	3.02362900
H	1.08556200	1.33138400	2.41035800
H	0.17014800	1.14081100	3.90698400

L11

Sum of electronic and thermal Free Energies=

-916.578135

C	-0.17119000	1.95439300	0.15055700
O	-1.10657500	2.52906600	0.71580000
N	-0.12084200	0.59174400	0.07603200
C	0.92500300	2.79690400	-0.51430400
H	1.74639600	2.16873200	-0.85570900
C	1.48254000	3.81243600	0.49411100
H	0.67943000	4.44459500	0.87752700
H	1.95788700	3.31341500	1.34318600
C	-1.25905700	-0.15334700	0.64668600
H	-0.92641300	-1.17527400	0.83397300
H	-1.50277600	0.29410500	1.61191900
C	0.98736600	-0.16299300	-0.53361100
H	0.60890200	-1.16572200	-0.73953300
H	1.23064300	0.26908500	-1.50665700
C	2.27908500	-0.28033800	0.31222500
H	2.63895600	0.73732100	0.50839300
C	3.33111800	-0.99564800	-0.56239600
H	2.96363500	-2.00417600	-0.79567600
H	3.39080300	-0.46672800	-1.52237200
C	4.75039900	-1.10468000	0.00800100
H	5.09437200	-0.11370100	0.33021300
H	4.75062300	-1.73860600	0.90093500
C	5.75139200	-1.67967300	-1.00212600
H	5.40192100	-2.66479600	-1.33442900
H	5.76678700	-1.04391100	-1.89568500
C	7.17083800	-1.80467300	-0.44088900
H	7.19403000	-2.46416400	0.43249900
H	7.85956500	-2.21437400	-1.18504200
H	7.55894500	-0.82958900	-0.12958500
C	-2.53207600	-0.15145900	-0.22823400
H	-2.76396100	0.90077300	-0.42410000
C	-3.70363400	-0.73039300	0.59006200
H	-3.49463800	-1.77438400	0.85586100
H	-3.75677600	-0.18492700	1.54051200
C	-5.07356700	-0.64615100	-0.09405100
H	-5.07409200	-1.24336900	-1.01311100
H	-5.25931800	0.39089800	-0.40297700
C	-6.22494100	-1.11797600	0.80230100
H	-6.23850600	-0.51546600	1.71867000
H	-6.03452000	-2.15068100	1.11909800
C	-7.59370500	-1.03891100	0.11991800
H	-7.62291300	-1.66160600	-0.77992800
H	-8.39213600	-1.37896300	0.78545300
H	-7.82581900	-0.01219800	-0.18068200
C	-2.32930000	-0.83140500	-1.60033100
H	-3.18536300	-0.58782700	-2.23772200
C	-2.14950500	-2.35520800	-1.58242800
H	-1.30599800	-2.66852500	-0.96053900
H	-3.04026900	-2.86466300	-1.20550900
H	-1.96285500	-2.72799700	-2.59330100
C	2.02166800	-0.95994500	1.67718900
H	0.98743300	-0.77375400	1.97697600
C	2.91828000	-0.47587500	2.82506800
H	2.78614200	0.59802100	2.98996100
H	2.65969600	-0.98683200	3.75714600
H	3.97812900	-0.65221400	2.63457900
H	2.11373800	-2.04679000	1.56118900
H	-1.46446100	-0.36979900	-2.08884300
C	0.32365000	3.50503200	-1.74271800
H	1.08120900	4.12525900	-2.22873800
H	-0.04812900	2.78654400	-2.47852500
H	2.22957600	4.44980000	0.01405600
H	-0.50756800	4.14722200	-1.44227700

L12

Sum of electronic and thermal Free Energies=

-916.579552

C	0.17998700	2.38626000	-0.31379600
O	1.14509600	2.92893800	-0.86120200
N	0.08133300	1.02973200	-0.22939300
C	-0.91926300	3.25369400	0.31385800
H	-1.83542500	2.67505100	0.43564200
C	-1.23282500	4.44591700	-0.59960900
H	-0.33542400	5.04201100	-0.77238200
H	-1.61169300	4.11442600	-1.57021100
C	1.15023700	0.21283700	-0.82463600
H	0.69729800	-0.71292300	-1.19114800
H	1.54058600	0.75665900	-1.68279100
C	-1.00603600	0.29816800	0.43663100
H	-0.56773800	-0.61038800	0.85874600
H	-1.36969700	0.87432500	1.28611900
C	-3.24460200	-0.94772900	0.15289900
H	-2.73466400	-1.75017000	0.70517200
C	-4.10618500	-1.61530800	-0.93895300
H	-4.59364000	-0.82882600	-1.53175900
H	-3.43796000	-2.14565800	-1.62901900
C	-5.17171200	-2.60225600	-0.44735300
H	-4.69527900	-3.36684600	0.17812700
H	-5.89488100	-2.08676800	0.19298300
C	-5.92048700	-3.28091900	-1.59912400
H	-6.43504200	-2.54363900	-2.22369800
H	-5.23287800	-3.83800400	-2.24346900
C	3.33917600	-1.08899100	-0.35200200
H	2.81558400	-2.01545700	-0.62940900
C	4.31270600	-1.45033300	0.78941300
H	4.84734500	-0.55000700	1.11785100
H	3.71545000	-1.77269500	1.65169400
C	5.33034000	-2.55227800	0.46864700
H	5.99931500	-2.22554700	-0.33436300
H	4.79961600	-3.43284700	0.08584100
C	6.17121200	-2.95348800	1.68498800
H	5.54006400	-3.33390700	2.49440900
H	6.73107200	-2.09805700	2.07642700
C	4.05099200	-0.59184500	-1.63259700
H	4.72691000	-1.37800800	-1.98329400
C	4.83757700	0.71779300	-1.49304800
H	4.19022100	1.55378000	-1.21582700
H	5.62471900	0.64209800	-0.73785500
H	5.31772700	0.97662300	-2.44089600
C	-4.08922500	-0.12962900	1.16791000
H	-3.56984100	0.80192900	1.41427200
C	-4.39926300	-0.85914700	2.48105600
H	-3.47586100	-1.11495200	3.01004900
H	-5.00015000	-0.23184900	3.14610900
H	-4.94992100	-1.78758800	2.31264700
H	-5.02543800	0.17763100	0.68740400
H	3.30638100	-0.47593900	-2.42713100
C	-0.45085900	3.72417900	1.70443300
H	-1.21251200	4.35659100	2.16757500
H	-0.25695200	2.88216800	2.37441400
H	-1.99273400	5.08202200	-0.13830600
H	0.47050200	4.30584600	1.61612300
C	2.27227900	-0.10656700	0.17269600
H	2.74154300	0.83278200	0.48227300
H	1.82410200	-0.53897600	1.07454400
H	6.89315100	-3.73453800	1.43042500
H	-6.67172900	-3.98342800	-1.22747400
C	-2.15165300	-0.08503700	-0.51128200
H	-2.60167500	0.82460100	-0.92715900
H	-1.72493000	-0.63306400	-1.35808800

L13

Sum of electronic and thermal Free Energies=

-916.578980

C	0.08911000	2.57013900	-0.43686300
O	0.94581600	3.09398600	-1.15519700
N	0.04098700	1.21900500	-0.26336100
C	-0.92622900	3.45307700	0.30125100
H	-1.79627800	2.86428100	0.59432100
C	-1.40815600	4.58065500	-0.62051900
H	-0.56488300	5.18257900	-0.96307200
H	-1.91984200	4.18258300	-1.50101500
C	1.02557200	0.39058800	-0.97395700
H	0.55367700	-0.57079000	-1.19480900
H	1.25152100	0.87793800	-1.92250100
C	-0.89994600	0.51100800	0.61545100
H	-0.36952100	-0.35482100	1.02186900
H	-1.14827400	1.13668200	1.47309600
C	-2.17813700	0.04309000	-0.09309600
H	-2.71882100	0.91714300	-0.47346500
C	-3.09228700	-0.75938000	0.84032500

H	-2.54066900	-1.61889900	1.24440500
H	-3.34728500	-0.12940400	1.70132900
C	-4.39700400	-1.26386000	0.18874800
H	-4.84475300	-0.41414000	-0.34637900
C	-5.38737200	-1.69140500	1.29243400
H	-4.92953200	-2.50310300	1.87297100
H	-5.50888400	-0.85226300	1.98726500
C	-6.77391200	-2.13509000	0.81445500
H	-6.72675200	-3.03678600	0.19866800
H	-7.42139400	-2.35667300	1.66771900
H	-7.26012500	-1.35197400	0.22411900
C	2.31905800	0.17402100	-0.17879100
H	2.77071700	1.15061800	0.02403100
C	3.32404300	-0.70740800	-0.92994100
H	2.84827100	-1.65811500	-1.20680700
H	3.58448300	-0.21104900	-1.87261100
C	4.61891300	-1.00728700	-0.14510400
H	4.97256300	-0.05503300	0.27565500
C	5.70623900	-1.51796400	-1.11287700
H	5.81108200	-0.79042900	-1.92622200
H	5.34925100	-2.44586100	-1.57892900
C	7.08647400	-1.76301900	-0.49482000
H	7.06320900	-2.55363100	0.25950100
H	7.80416200	-2.06572000	-1.26275600
H	7.47391900	-0.85716600	-0.01769400
C	-0.26745100	4.01476800	1.57597900
H	-0.96797400	4.65994700	2.11227800
H	0.04622900	3.21770600	2.25564900
H	-2.10767300	5.22900900	-0.08647100
H	0.61494300	4.60648900	1.31837400
H	-1.89918500	-0.55449000	-0.96712600
H	2.07310600	-0.26956800	0.79195000
C	4.35888700	-1.98560400	1.03199800
H	3.28419500	-2.03429100	1.23418600
H	4.64556800	-2.99844600	0.72412000
C	5.07164400	-1.62513600	2.34141600
H	4.74316300	-0.64626800	2.70487600
H	4.85352200	-2.35926800	3.12292600
H	6.15657900	-1.58265000	2.21938600
C	-4.12613600	-2.39276800	-0.84130900
H	-3.06659300	-2.38950000	-1.11587900
H	-4.30159100	-3.36313400	-0.36136400
C	-4.94981700	-2.29960500	-2.13167100
H	-4.71827700	-3.12930400	-2.80629100
H	-6.02407000	-2.32161400	-1.93455600
H	-4.73217300	-1.36841900	-2.66429200

L14

Sum of electronic and thermal Free Energies= -916.579782

C	-0.17973100	1.88061000	0.27403200
O	-1.10259900	2.43241000	0.87753600
N	-0.14549500	0.52191600	0.12293700
C	0.93949500	2.70427900	-0.36152500
H	1.91365900	2.33232900	-0.03325700
C	0.83073800	4.20017700	-0.06022100
H	-0.14030700	4.56735500	-0.40281500
C	-1.30183200	-0.24214600	0.62472800
H	-0.99441200	-1.28428500	0.71991900
H	-1.53946300	0.12133700	1.62658800
C	0.96086800	-0.19427000	-0.52987000
H	0.56190900	-1.14938000	-0.87739700
H	1.26091300	0.35160900	-1.42700900
C	2.21850300	-0.46460600	0.33564600
H	2.60877200	0.50491800	0.66806400
C	3.27350100	-1.10629100	-0.59139900
H	2.87942500	-2.06384300	-0.95820700
C	4.66935500	-1.33972700	-0.00089000
H	4.61875400	-2.07461100	0.80939000
C	5.67870300	-1.83185300	-1.04596200
H	5.74965500	-1.09402000	-1.85434600
C	7.07255100	-2.08768000	-0.46522000
H	7.03996600	-2.85172100	0.31799600
H	7.76902900	-2.43076100	-1.23541200
H	7.48842800	-1.17709900	-0.02222100
C	-2.57134100	-0.13680900	-0.24952500
H	-2.78123100	0.93251700	-0.35664900
C	-3.75740400	-0.75978000	0.51337700
H	-3.80794600	-0.29152500	1.50429800
C	-5.12187000	-0.59976400	-0.16831600
H	-5.12567700	-1.12206300	-1.13190000
C	-6.28521100	-1.12352600	0.68271000
H	-6.29603300	-0.59405300	1.64310800
C	-7.64859200	-0.97220100	0.00163000
H	-7.68027100	-1.52202900	-0.94437000
H	-8.45571400	-1.35227200	0.63421500
H	-7.86490800	0.07804500	-0.21871800
C	-2.37530400	-0.70291200	-1.67321900

H	-3.22442900	-0.39186600	-2.29026100
C	-2.22155100	-2.22570600	-1.78245700
H	-1.38087000	-2.60311200	-1.19325700
H	-3.11909100	-2.75062500	-1.44484700
H	-2.04478100	-2.51630800	-2.82171400
C	1.89747600	-1.29675400	1.59865700
H	0.86247100	-1.11107300	1.89420900
C	2.77534700	-0.98942000	2.82001100
H	2.67824900	0.06206000	3.10821500
H	2.46864000	-1.59616100	3.67704600
H	3.83329500	-1.18503000	2.63828800
H	1.95619700	-2.36429500	1.35294400
H	-1.50002900	-0.21786300	-2.11878900
H	-3.56647400	-1.82499700	0.69544000
H	3.38221800	-0.46616000	-1.47624600
H	-5.29036000	0.46130000	-0.39456700
H	5.04021600	-0.40875900	0.44636000
H	5.30028200	-2.75293400	-1.50577300
H	-6.11092500	-2.18036800	0.91899100
C	1.95550700	5.00703800	-0.71448000
H	1.94272100	4.89595700	-1.80341100
H	1.85782800	6.07219000	-0.48813400
H	2.93832400	4.68052300	-0.36004100
H	0.90998700	2.54218900	-1.44617500
H	0.84599600	4.35024400	1.02336100

L15

Sum of electronic and thermal Free Energies=

-1034.471571

C	0.22153900	-1.24239100	-0.06069900
O	0.81390300	-2.19369200	0.45743900
N	0.74879000	0.01697000	-0.03443100
C	-1.10311700	-1.49566400	-0.77529200
H	-1.60218600	-0.58044900	-1.08862800
C	-2.05804800	-2.34982500	0.07148500
H	-1.52226200	-3.24151500	0.40795700
H	-2.33477300	-1.79231900	0.97472600
C	2.07811200	0.17371700	0.58471700
H	2.19996400	1.22555800	0.84662800
H	2.08498200	-0.39870400	1.51404600
C	0.07112600	1.20581900	-0.57905400
H	0.83594300	1.97381800	-0.70741200
H	-0.30064900	0.98441000	-1.58194300
C	-1.08115400	1.78439200	0.27777700
H	-1.83219000	0.99322400	0.39608200
C	-1.72244000	2.93162700	-0.53201200
H	-0.96587600	3.71207800	-0.69042800
H	-1.97302900	2.54703600	-1.52901400
C	-2.98139500	3.57429800	0.06139000
H	-3.71613600	2.79356400	0.29560300
H	-2.74064200	4.06801300	1.00872500
C	-3.62296600	4.60206700	-0.87948300
H	-2.88657200	5.37830100	-1.12073700
H	-3.87408500	4.11389000	-1.82890900
C	-4.87846900	5.25482600	-0.29387700
H	-4.65124900	5.78351500	0.63731300
H	-5.31378400	5.97812600	-0.98908000
H	-5.64438100	4.50536900	-0.07033700
C	3.25691600	-0.30186200	-0.29263000
H	3.03375600	-1.33806700	-0.56775900
C	4.54008500	-0.32368300	0.56184500
H	4.77772200	0.69049900	0.90729400
H	4.33447800	-0.90683100	1.46815800
C	5.76924700	-0.92407800	-0.13108200
H	6.03855700	-0.32590300	-1.00938200
H	5.51833500	-1.92444400	-0.50762900
C	6.99063200	-1.02528500	0.79075100
H	6.73077400	-1.62947300	1.66845700
H	7.23838900	-0.02660600	1.17067000
C	8.21921300	-1.62793900	0.10327900
H	8.52613800	-1.02477900	-0.75718600
H	9.07031000	-1.68824900	0.78743300
H	8.01147500	-2.63975600	-0.25925300
C	3.39331200	0.49654300	-1.60815800
H	4.08903400	-0.03398200	-2.26603700
C	3.86153100	1.95094300	-1.46819700
H	3.20663300	2.53815600	-0.81790100
H	4.87203000	2.01279200	-1.05614600
H	3.87516700	2.44285400	-2.44463700
C	-0.60812100	2.19929800	1.69107200
H	0.26392300	1.60119400	1.96640700
C	-1.65083600	2.01740900	2.80268900
H	-1.95305100	0.96818500	2.87826600
H	-1.23734800	2.31255700	3.77150700
H	-2.55234900	2.60874300	2.63373600
H	-0.26491600	3.24077800	1.66498500
H	2.42877400	0.47283600	-2.12643400
H	-0.84752600	-2.04404100	-1.69054900

C	-3.32687600	-2.75610600	-0.68491100
H	-3.04550200	-3.31253100	-1.58831800
H	-3.85179100	-1.85635800	-1.03049700
C	-4.28441800	-3.60753900	0.15609400
H	-4.56687300	-3.04987300	1.05851600
H	-3.75784400	-4.50550200	0.50445900
C	-5.55425700	-4.02716000	-0.59333300
H	-5.27288200	-4.58614400	-1.49404500
H	-6.07905500	-3.12967700	-0.94271700
C	-6.50515300	-4.87535700	0.25632500
H	-6.83115900	-4.32934400	1.14732700
H	-7.39940200	-5.15800000	-0.30624100
H	-6.01840900	-5.79650500	0.59226700

L16

Sum of electronic and thermal Free Energies=

-955.874408

C	-0.20269500	1.77796200	0.13119400
O	-1.11254900	2.40280500	0.68558200
N	-0.21988000	0.41345500	0.07201700
C	0.93921600	2.55976400	-0.52820400
H	1.71899300	1.88573000	-0.88328900
C	1.57125900	3.50563300	0.51599200
H	0.80069600	4.19860400	0.86536500
H	1.86945700	2.91197700	1.38763700
C	-1.39495400	-0.26695000	0.64885600
H	-1.11489800	-1.30322500	0.84330800
H	-1.61433100	0.19958600	1.61083400
C	0.84456400	-0.40501600	-0.53323400
H	0.41081000	-1.38689300	-0.73087200
H	1.10925900	0.00550000	-1.51001400
C	2.13053600	-0.58842900	0.30948100
H	2.55978600	0.40696300	0.47833200
C	3.12527300	-1.39554100	-0.55217300
H	2.69220000	-2.38564900	-0.74871600
C	4.54149700	-1.57658300	0.00738700
H	4.51126000	-2.17292000	0.92537100
C	5.48848200	-2.25727300	-0.98905800
H	5.53153100	-1.66224100	-1.90934900
C	6.90506600	-2.45078100	-0.44018300
H	6.89834900	-3.07236600	0.46083800
H	7.55454400	-2.93624800	-1.17398700
H	7.36026800	-1.49078400	-0.17651900
C	-2.66731100	-0.20665200	-0.22507000
H	-2.84792200	0.85463300	-0.42532100
C	-3.86466700	-0.72465400	0.59662500
H	-3.89243900	-0.17113500	1.54348400
C	-5.22908200	-0.58099700	-0.08871200
H	-5.25653300	-1.18315500	-1.00412600
C	-6.40140800	-0.99373200	0.80958700
H	-6.38853800	-0.38477200	1.72170700
C	-7.76452900	-0.85756000	0.12483600
H	-7.82083600	-1.48501100	-0.77039300
H	-8.57824800	-1.15601500	0.79180700
H	-7.94942900	0.17636500	-0.18366900
C	-2.49870300	-0.90157800	-1.59426800
H	-3.34178300	-0.61834100	-2.23264500
C	-2.39508700	-2.43224700	-1.56966200
H	-1.56850900	-2.78423100	-0.94578900
H	-3.31031200	-2.89485900	-1.19097200
H	-2.22679900	-2.81844800	-2.57872100
C	1.83879600	-1.21586000	1.69244400
H	0.81994100	-0.95829900	1.99209400
C	2.77087600	-0.75947100	2.82332300
H	2.70747400	0.32452100	2.96057600
H	2.48664500	-1.22892200	3.76965300
H	3.81641900	-1.00692600	2.63252900
H	1.86256700	-2.30896600	1.60459100
H	-1.61209000	-0.48548700	-2.08452100
C	0.36690600	3.31301600	-1.74421500
H	1.14984700	3.86509200	-2.26759300
H	-0.08382800	2.61952300	-2.45967100
H	-0.40303900	4.01975900	-1.42554600
H	-3.70482600	-1.77554100	0.86935700
H	3.20676500	-0.90260500	-1.52955300
H	-5.36656600	0.46161700	-0.40401900
H	4.95477800	-0.59865600	0.28528700
H	5.07157000	-3.23084900	-1.27437800
H	-6.25830200	-2.03173300	1.13385800
C	2.78962000	4.28053000	0.00562100
H	2.53096300	4.96317200	-0.80750000
H	3.22539900	4.88015500	0.80939600
H	3.56735100	3.60297100	-0.36103700

L17

Sum of electronic and thermal Free Energies=

-955.877520

C	-0.19134100	1.71742400	0.05669200

O	-1.09351000	2.35644000	0.60388800
N	-0.20525100	0.35062000	0.04017600
C	0.93741800	2.43641700	-0.68378000
H	1.89725800	1.94184900	-0.52029200
C	1.06571300	3.92785400	-0.33720400
H	0.06699400	4.36893300	-0.40888100
C	-1.38652500	-0.32045000	0.61263600
H	-1.11646100	-1.36003700	0.80247500
H	-1.60489300	0.14200600	1.57717800
C	0.86151700	-0.46560800	-0.56088600
H	0.42198300	-1.43385900	-0.80817500
H	1.16122500	-0.02059700	-1.51210400
C	2.12303300	-0.69832300	0.30883000
H	2.54734500	0.28412700	0.54959500
C	3.14438300	-1.45309600	-0.56938100
H	2.71413400	-2.42443700	-0.84878000
C	4.53874200	-1.68287400	0.02642000
H	4.47404900	-2.35110300	0.89159600
C	5.52239100	-2.28396600	-0.98562400
H	5.60772700	-1.61141200	-1.84768900
C	6.91349300	-2.53839200	-0.39772100
H	6.86536400	-3.23834500	0.44246500
H	7.59090800	-2.96180400	-1.14459000
H	7.36215800	-1.61007800	-0.02989300
C	-2.65735500	-0.24847300	-0.26337700
H	-2.83894000	0.81503000	-0.44996400
C	-3.85578300	-0.77900100	0.54865800
H	-3.88682200	-0.23830400	1.50281900
C	-5.21872000	-0.62878600	-0.13828800
H	-5.24185800	-1.21761400	-1.06243200
C	-6.39257400	-1.05793200	0.75026400
H	-6.38501900	-0.46159900	1.67072800
C	-7.75382300	-0.91732200	0.06266000
H	-7.80456100	-1.53241000	-0.84143400
H	-8.56875000	-1.22817400	0.72245100
H	-7.94161900	0.12009100	-0.23207000
C	-2.48483600	-0.92454500	-1.64143300
H	-3.32613400	-0.63268500	-2.27827600
C	-2.38072500	-2.45538300	-1.63832900
H	-1.55374700	-2.81597100	-1.01992500
H	-3.29564700	-2.92366200	-1.26592000
H	-2.21266400	-2.82717400	-2.65283800
C	1.79433000	-1.40356500	1.64495400
H	0.76987700	-1.15817400	1.93407100
C	2.69884400	-1.01759100	2.82373800
H	2.63950700	0.05789900	3.01793100
H	2.38513300	-1.53517700	3.73499700
H	3.74732900	-1.26358400	2.64831300
H	1.81622500	-2.49005100	1.49536100
H	-1.59681700	-0.50140400	-2.12313900
H	-3.69498300	-1.83323100	0.80766000
H	3.26330300	-0.89509100	-1.50701400
H	-5.35812700	0.41792000	-0.43882700
H	4.94181800	-0.73202600	0.39746300
H	5.11183000	-3.22485100	-1.37201300
H	-6.24679800	-2.09981200	1.06062500
C	1.97985100	4.63108400	-1.34972000
H	1.59905500	4.52854500	-2.37034400
H	2.05889000	5.69895600	-1.12648900
H	2.99166200	4.21139700	-1.32653600
H	0.72325200	2.32819200	-1.75525700
C	1.57296300	4.13451000	1.09655100
H	2.57255000	3.70324500	1.22236700
H	1.63868100	5.19990600	1.33638500
H	0.90443200	3.66681400	1.82211100

L18

Sum of electronic and thermal Free Energies= -995.158538

C	-0.31024600	2.01986200	0.28015200
O	-1.29422300	2.47203800	0.87429800
N	-0.13470700	0.67451800	0.12893900
C	0.70359100	2.99872200	-0.32335000
H	1.55239300	2.46664800	-0.74913900
C	1.22482300	3.94301900	0.77137300
H	0.39346200	4.47305000	1.24052100
H	1.76251000	3.39548000	1.55048100
C	-1.20523500	-0.19913100	0.64990200
H	-0.77628200	-1.19050000	0.79087500
H	-1.49384300	0.17734000	1.63313000
C	1.02802500	0.05381800	-0.53243300
H	0.74255200	-0.97437500	-0.76013100
H	1.19024100	0.53745700	-1.49526200
C	2.34684900	0.01629800	0.28574100
H	2.61117800	1.04765200	0.55032500
C	3.47271800	-0.53540200	-0.65020400
H	3.03662100	-1.38641300	-1.19461900
C	4.71579500	-1.08035300	0.08338000

H	5.23425700	-0.25517700	0.58867400
H	4.40141300	-1.77551000	0.86663500
C	5.71441600	-1.82259600	-0.81725400
H	5.18029300	-2.59792300	-1.38062400
H	6.13882300	-1.14112900	-1.56078700
C	6.85743000	-2.46554500	-0.02485600
H	6.47811800	-3.19342500	0.69936800
H	7.55564400	-2.98662000	-0.68597100
H	7.42553200	-1.71201100	0.52998800
C	-2.46157900	-0.25629200	-0.24844700
H	-2.69240600	0.78777100	-0.48496300
C	-3.69690800	-0.74935100	0.56420800
H	-3.82467800	0.00644200	1.35242200
C	-4.98035000	-0.71509100	-0.28959500
H	-4.96621300	-1.54120300	-1.01169100
H	-4.98166600	0.20846100	-0.88285200
C	-6.29053100	-0.77487500	0.50768300
H	-6.29778600	0.03551700	1.24689200
H	-6.34307700	-1.70921900	1.07607200
C	-7.53171100	-0.66250900	-0.38358500
H	-7.56746600	-1.47727400	-1.11384800
H	-8.45183400	-0.70447900	0.20609700
H	-7.53494500	0.28035000	-0.93982800
C	-2.19884200	-0.93250600	-1.61512900
H	-3.06969300	-0.76548800	-2.25655200
C	-1.85400700	-2.42876100	-1.63993800
H	-1.04673900	-2.68483500	-0.94788200
H	-2.71328400	-3.05248200	-1.38684000
H	1.52562400	-2.71977800	-2.64195400
C	2.13650700	-0.75836000	1.60901200
H	1.09111000	-0.65459200	1.90801800
C	2.98657800	-0.27404200	2.79147500
H	2.77252400	0.77686300	3.01019900
H	2.75786900	-0.85141100	3.69219500
H	4.05810600	-0.35984500	2.60613000
H	2.29262200	-1.83013500	1.44036600
H	-1.38356300	-0.37906600	-2.09443100
C	0.01625800	3.78568000	-1.45420000
H	0.71377500	4.50486800	-1.89133600
H	-0.33002300	3.12242600	-2.25178000
H	1.90882500	4.67919100	0.34126700
H	-0.84652200	4.33165300	-1.06587400
C	-3.52094400	-2.10003400	1.28336700
H	-4.34726100	-2.27523800	1.97669300
H	-3.49806400	-2.93823300	0.58400300
H	-2.60140300	-2.13184000	1.87264500
C	3.89206200	0.52792600	-1.68356900
H	3.04226900	0.94998300	-2.22356500
H	4.41438000	1.35311400	-1.18722900
H	4.56638700	0.11314600	-2.43518800

L19

Sum of electronic and thermal Free Energies= -995.169417

C	-0.16593300	2.00991000	0.16204600
O	-1.10323800	2.58067500	0.72823200
N	-0.11167600	0.64771100	0.08459900
C	0.92843200	2.85703300	-0.49988000
H	1.75314800	2.23218900	-0.83939900
C	1.47951500	3.87412900	0.51051800
H	0.67319500	4.50343700	0.89185500
H	1.95407200	3.37644600	1.36081700
C	-1.24529500	-0.10260500	0.65786100
H	-0.90769100	-1.12336500	0.84243300
H	-1.48721200	0.34229300	1.62476600
C	0.99695600	-0.10250200	-0.52950500
H	0.61821900	-1.10348400	-0.74334600
H	1.24078800	0.33695700	-1.49893600
C	2.28976200	-0.22607500	0.31629400
H	2.64752700	0.79100500	0.51054800
C	3.32490000	-0.96326100	-0.56345800
H	2.93996500	-1.97405100	-0.75200400
C	4.77633100	-1.08764500	-0.05793200
H	4.76634400	-1.60031900	0.91145500
C	5.57781200	-1.98200300	-1.02733200
H	5.00690400	-2.90177400	-1.20005800
H	5.64588600	-1.47853800	-2.00057000
C	6.98299500	-2.36150700	-0.54745100
H	6.94489100	-2.85666900	0.42835600
H	7.45930600	-3.05125500	-1.24988400
H	7.63601900	-1.49023700	-0.45270700
C	-2.52250700	-0.10441900	-0.21171300
H	-2.75188000	0.94740400	-0.40273300
C	-3.67766000	-0.70250000	0.61789300
H	-3.74554700	-0.14441100	1.56137500
C	-5.07557400	-0.70853800	-0.03444000
H	-5.01692000	-1.27197600	-0.97503000
C	-6.06757700	-1.45730600	0.87948000

H	-6.19097400	-0.88903100	1.81068900
H	-5.61645600	-2.41466900	1.16550500
C	-7.44264600	-1.73079200	0.26048400
H	-7.34746900	-2.28818800	-0.67715600
H	-8.06176300	-2.32598200	0.93770600
H	-7.98885600	-0.80894400	0.04530000
C	-2.32317200	-0.78155800	-1.58538300
H	-3.18797600	-0.54926800	-2.21554000
C	-2.12271400	-2.30298500	-1.57182300
H	-1.26788400	-2.60571900	-0.96025900
H	-3.00177900	-2.82538400	-1.18570000
H	-1.94229600	-2.67142000	-2.58543300
C	2.02287100	-0.90416800	1.68018700
H	0.99613000	-0.68797500	1.98549200
C	2.93493200	-0.45734800	2.83105200
H	2.85129800	0.62161900	2.99427400
H	2.64684700	-0.95426200	3.76203000
H	3.98693600	-0.68376100	2.65015400
H	2.08131000	-1.99265500	1.55781900
H	-1.46889500	-0.30826900	-2.08142000
C	0.32742100	3.56341800	-1.72946300
H	1.08369800	4.18699900	-2.21317700
H	-0.03954500	2.84383800	-2.46661100
H	2.22577300	4.51416100	0.03282200
H	-0.50715000	4.20209700	-1.43082500
H	-3.42188100	-1.73172500	0.89863800
H	3.35910400	-0.46645500	-1.54298100
C	5.43932600	0.28547200	0.12436500
H	6.46008200	0.19308200	0.50258300
H	5.48428300	0.81964700	-0.83156500
H	4.88950300	0.91252000	0.82955400
C	-5.56041300	0.71136000	-0.36253200
H	-5.63338700	1.31507600	0.54937200
H	-4.87942300	1.22375000	-1.04624200
H	-6.54517100	0.70121300	-0.83562100

L20

Sum of electronic and thermal Free Energies=

-995.172692

C	-0.16608500	2.16514500	0.09494800
O	-1.13420700	2.75024500	0.59016100
N	-0.10506100	0.80117900	0.06424400
C	0.96356200	2.99590800	-0.52675200
H	1.79360900	2.35998600	-0.83083300
C	1.48598400	4.01018400	0.50237600
H	0.67287700	4.65147400	0.84801400
H	1.91888500	3.51030400	1.37335100
C	-1.26616100	0.06696000	0.60211600
H	-0.93613500	-0.94368600	0.84611100
H	-1.56243300	0.54882000	1.53554400
C	1.03289200	0.03549300	-0.47252000
H	0.66836800	-0.97418000	-0.66915000
H	1.31917200	0.44286400	-1.44447000
C	2.28558000	-0.05705600	0.43350600
H	2.63679800	0.96537600	0.62002200
C	3.37347400	-0.79569600	-0.37670100
H	3.01435000	-1.81084900	-0.58387200
C	4.77288500	-0.85892000	0.25037000
H	4.76427400	-1.50900100	1.13291700
C	5.87629200	-1.35516300	-0.70513500
H	5.86189900	-0.70714000	-1.59239700
C	7.25658500	-1.21734000	-0.04742700
H	7.32629400	-1.84704100	0.84659600
H	8.05329000	-1.52322700	-0.73204900
H	7.45177200	-0.18434800	0.25582800
C	-2.49247800	0.02301400	-0.33602400
H	-2.72136600	1.06421900	-0.58685900
C	-3.70023600	-0.53384800	0.44517700
H	-3.80537900	0.04925900	1.36884500
C	-5.03086300	-0.47663100	-0.31748000
H	-5.00266600	-1.15190100	-1.18183700
C	-6.27597200	-0.81455400	0.52537800
H	-6.27486600	-0.14827100	1.39916100
C	-7.55740300	-0.53607300	-0.27282800
H	-7.61152200	-1.17843300	-1.15896700
H	-8.44964600	-0.72742400	0.33080400
H	-7.59706900	0.50358900	-0.61149800
C	-2.21600500	-0.71185500	-1.66621000
H	-3.04506100	-0.51136900	-2.35250500
C	-2.01333600	-2.23001100	-1.57193700
H	-1.19372900	-2.50025700	-0.89992900
H	-2.91179600	-2.73780400	-1.21159400
H	-1.77581900	-2.64395900	-2.55574700
C	1.96168300	-0.70205000	1.80056800
H	0.92354300	-0.47775100	2.05834600
C	2.82928700	-0.22719800	2.97434700
H	2.74152400	0.85591700	3.10521900
H	2.50430300	-0.69904900	3.90626900

H	3.88670500	-0.45886000	2.83876800
H	2.02263100	-1.79329900	1.70639600
H	-1.33649600	-0.25662300	-2.13393600
C	0.42102100	3.70524600	-1.78114400
H	1.20215800	4.32169900	-2.23357500
H	0.07947900	2.98722500	-2.53193400
H	2.25925400	4.63893900	0.05354400
H	-0.42020400	4.35074300	-1.51857200
H	-3.48991900	-1.56158900	0.76068600
H	3.46249400	-0.30034700	-1.35256300
H	-5.15429700	0.53479900	-0.72500400
H	5.04927400	0.14148700	0.60505700
C	5.64484500	-2.79960300	-1.17237700
H	5.61423200	-3.48293100	-0.31601700
H	4.70638600	-2.90934400	-1.72117600
H	6.45310800	-3.12923500	-1.83194100
C	-6.26581400	-2.26237300	1.03726600
H	-6.24113700	-2.96878600	0.19967300
H	-5.40151700	-2.46764900	1.67351800
H	-7.16495500	-2.47403300	1.62366400

$[PaO(H_2O)_5$ (L1) $]^{3+}$-A

Sum of electronic and thermal Free Energies=

-1540.228366

O	1.27276800	-2.16884800	1.37531600
H	1.33541800	-2.07182300	2.33505300
H	1.64792000	-3.03025900	1.14926100
O	3.05174400	0.32409100	-2.23395500
O	2.45617400	-2.27771600	-1.27719900
O	1.71741100	0.42847300	2.37271800
O	2.96321900	2.10085000	-0.02905100
H	3.45050200	-0.40974700	-2.71813900
H	3.66345300	1.06996400	-2.27617500
H	3.30330100	-2.72333600	-1.15122800
H	2.52155800	0.52941600	2.89925800
H	3.81204800	2.20911300	0.41877100
H	1.91949700	-2.81752100	-1.87212700
H	1.00183700	0.89184700	2.82796900
H	2.59345200	2.97991900	-0.18139400
Pa	1.83284700	-0.13961200	-0.03262100
O	3.50364500	-0.48892400	0.55550800
C	-1.55810500	0.61675100	0.58422200
O	-0.34488000	0.18428200	0.48266600
N	-2.52228900	-0.23675700	0.86110400
C	-1.84804700	2.09015500	0.41674000
H	-2.71580800	2.19420200	-0.23898700
H	-2.16198100	2.47177500	1.39574200
C	-0.69590200	2.94262200	-0.11828300
H	0.12930600	2.93166900	0.59962600
H	-0.32517800	2.52017200	-1.05856400
C	-1.13532300	4.39369100	-0.35594300
H	-1.96685100	4.40338500	-1.06945100
H	-1.52605800	4.81008800	0.57934700
C	-0.00371400	5.28147300	-0.87909400
H	0.82062800	5.33955400	-0.16140100
H	0.39814900	4.89642200	-1.82141000
C	-2.22557700	-1.68235000	1.02871600
H	-1.27028700	-1.77145300	1.54258000
H	-2.99902500	-2.07858600	1.68639800
C	-3.92652700	0.20245200	1.05692400
H	-4.34047500	-0.44079100	1.83379000
H	-3.92034400	1.21399800	1.45816400
C	-4.79146200	0.13300700	-0.20695300
H	-4.31893000	0.70666400	-1.01126800
H	-4.85731600	-0.90205800	-0.55341500
C	-6.20148100	0.67790700	0.05428100
H	-6.66442300	0.10875000	0.86832800
H	-6.12911500	1.71420600	0.40368600
C	-7.09653600	0.61805600	-1.18616800
H	-6.67283300	1.20460500	-2.00688400
H	-7.21662500	-0.41091300	-1.53775000
C	-2.19393000	-2.46562100	-0.28862800
H	-1.41237300	-2.05855100	-0.93779700
H	-3.14345200	-2.34050200	-0.81645500
C	-1.94015400	-3.95847000	-0.04438400
H	-0.99111000	-4.08238200	0.48852600
H	-2.71987500	-4.35295400	0.61720200
C	-1.91272300	-4.77157500	-1.34142300
H	-1.11994800	-4.42279100	-2.01024300
H	-2.86243800	-4.68854300	-1.87832800
H	-8.09154800	1.01569300	-0.97082600
H	-0.35536900	6.30037800	-1.05926800
H	-1.73585200	-5.83078500	-1.13806100

$[PaO(H_2O)_5$ (L2) $]^{3+}$-A

Sum of electronic and thermal Free Energies=

-1658.126734

O	1.44246700	-3.71463900	0.47204800

H	1.25572300	-4.00281000	1.37493400
H	1.86351600	-4.45010900	0.00789900
O	4.11720900	-0.16653800	-1.25282600
O	3.34449400	-3.06122400	-1.50929900
O	1.38563800	-1.71032600	2.36704600
O	3.34713400	0.54857200	1.35550700
H	4.58699600	-0.54266600	-2.00769800
H	4.73175200	0.41440900	-0.78648800
H	4.21301900	-3.45471200	-1.35649000
H	1.93281800	-1.84626200	3.15212900
H	3.99886900	0.39444600	2.05117700
H	3.11277200	-3.20120700	-2.43691900
H	0.50761600	-1.43087400	2.65853000
H	3.01416500	1.45014300	1.45282900
Pa	2.35543600	-1.38950800	0.12139000
O	3.76413800	-2.06645300	1.02625400
C	-1.02120600	-0.88078200	-0.63116900
O	0.14841200	-1.01295200	-0.08321400
N	-1.71075400	0.21412200	-0.39898300
C	-1.51469000	-2.02432500	-1.46953300
H	-2.35533000	-1.73019800	-2.09389400
C	-1.90683300	-3.25166200	-0.61303200
H	-1.04675300	-3.55954200	-0.01651800
C	-1.16370100	1.29017500	0.46391800
H	-2.01621200	1.74181600	0.97220500
H	-0.52775800	0.83745600	1.22065300
C	-3.05854200	0.48825000	-0.95636300
H	-3.09792000	1.56544500	-1.12421200
H	-3.15232800	0.01646900	-1.93140800
C	-4.19034900	0.05834700	-0.01799800
H	-4.18333200	-1.03063500	0.08920700
C	-5.55797600	0.52256200	-0.53314700
H	-5.54781100	1.61308600	-0.64970700
C	-6.71179700	0.12435200	0.39400900
H	-6.52752900	0.53300500	1.39560000
C	-8.08147400	0.60298100	-0.10090500
H	-8.26728400	0.19208600	-1.10044300
C	-9.22986400	0.21199400	0.83369900
H	-9.08797600	0.63739400	1.83221800
H	-10.19135800	0.56843800	0.45401200
H	-9.29737800	-0.87497600	0.94319000
C	-0.39606200	2.34387100	-0.34041300
H	0.47021400	1.87139200	-0.81361400
C	0.05557400	3.51342200	0.54200700
H	0.66209500	3.13434400	1.37348200
C	0.85247200	4.57132600	-0.22986100
H	0.24011000	4.95149300	-1.05713300
C	1.30843500	5.74685300	0.64182000
H	1.92358500	5.36677600	1.46620000
C	2.09611500	6.80330900	-0.13853100
H	1.49363600	7.22439600	-0.94950200
H	2.40628000	7.62826800	0.50866100
H	2.99834000	6.37334000	-0.58508500
H	-0.82569800	3.98296000	0.99564100
H	-5.73303500	0.10549200	-1.53218000
H	1.73106000	4.10109400	-0.68946400
H	-6.72845500	-0.96712600	0.50549500
H	-8.06079600	1.69324400	-0.21716800
H	0.43080800	6.21360200	1.10475500
C	-2.37577400	-4.41369800	-1.49092000
H	-1.58606600	-4.73325900	-2.17675800
H	-3.24860300	-4.13496000	-2.08806700
H	-0.69075900	-2.29800500	-2.13411600
H	-2.70075300	-2.96887300	0.08375900
H	-4.01458500	0.47609200	0.97880300
H	-1.03113400	2.72181100	-1.14817700
H	-2.65201700	-5.27177600	-0.87369500

$[PaO(H_2O)_5$ (L3) $]^{3+}$-A

Sum of electronic and thermal Free Energies= -1697.424988

O	1.44402800	-3.71681100	0.46563800
H	1.26191500	-4.00668600	1.36893200
H	1.86392800	-4.45106400	-0.00150400
O	4.11835800	-0.16638500	-1.25743900
O	3.34671400	-3.06137000	-1.51565300
O	1.38927200	-1.71244100	2.36223000
O	3.34730500	0.54744000	1.35054300
H	4.58993700	-0.54357500	-2.01066800
H	4.73171500	0.41549300	-0.79069500
H	4.21468200	-3.45580400	-1.36215700
H	1.93764000	-1.84944700	3.14628900
H	3.99957300	0.39336000	2.04571300
H	3.11511400	-3.20188000	-2.44322600
H	0.51204200	-1.43214600	2.65529400
H	3.01337000	1.44853800	1.44892500
Pa	2.35672300	-1.39084200	0.11591300
O	3.76585000	-2.06778900	1.02008300

C	-1.02041700	-0.88265600	-0.63283800
O	0.15016600	-1.01293300	-0.08634500
N	-1.70972300	0.21283400	-0.40258800
C	-1.51593300	-2.02998100	-1.46453500
H	-2.35438700	-1.73723700	-2.09244700
C	-1.91296500	-3.24669300	-0.59634900
H	-1.05439100	-3.55349200	0.00458400
C	-1.16314000	1.28948400	0.45983700
H	-2.01598100	1.74073300	0.96793700
H	-0.52715700	0.83713700	1.21678800
C	-3.05752100	0.48591800	-0.96035800
H	-3.09656500	1.56268600	-1.13107600
H	-3.15139400	0.01152000	-1.93413200
C	-4.18954300	0.05879100	-0.02097400
H	-4.18298600	-1.02988800	0.08886000
C	-5.55709600	0.52202900	-0.53717600
H	-5.54732700	1.61242300	-0.65496900
C	-6.71096700	0.12419600	0.39008300
H	-6.52708500	0.53378300	1.39136700
C	-8.08082200	0.60164500	-0.10544600
H	-8.26604100	0.19021300	-1.10487800
C	-9.22916100	0.21009700	0.82898700
H	-9.08783200	0.63588200	1.82742100
H	-10.19083500	0.56569300	0.44896700
H	-9.29586600	-0.87689500	0.93877400
C	-0.39564100	2.34393700	-0.34356100
H	0.47111100	1.87226700	-0.81668500
C	0.05483000	3.51255400	0.54073100
H	0.66072900	3.13248200	1.37221100
C	0.85203400	4.57221200	-0.22837300
H	0.24031000	4.95392300	-1.05540000
C	1.30665100	5.74594500	0.64644700
H	1.92108700	5.36417700	1.47058300
C	2.09470700	6.80462100	-0.13049600
H	1.49285700	7.22758200	-0.94095500
H	2.40397300	7.62802700	0.51910600
H	2.99750800	6.37609500	-0.57727600
H	-0.82705800	3.98098700	0.99432100
H	-5.73168500	0.10374000	-1.53578800
H	1.73123700	4.10325600	-0.68809900
H	-6.72711000	-0.96719500	0.50251700
H	-8.06092300	1.69187500	-0.22212600
H	0.42835600	6.21123500	1.10957800
C	-2.38744400	-4.42348100	-1.45602700
H	-1.58966600	-4.70422100	-2.15291800
H	-3.23794900	-4.10605500	-2.06984400
H	-0.69154300	-2.31167000	-2.12507500
H	-2.70796500	-2.95646300	0.09756900
C	-2.78665700	-5.63835000	-0.61400500
H	-3.60143800	-5.39117800	0.07323700
H	-3.12349800	-6.46251700	-1.24799300
H	-1.94386900	-5.99886300	-0.01662800
H	-4.01371100	0.47886000	0.97483500
H	-1.03045800	2.72244700	-1.15125800

$[PaO(H_2O)_5$ (L4) $]^{3+}$-A

Sum of electronic and thermal Free Energies= -1736.721340

O	1.34815800	-3.19343400	0.54151400
H	1.14716900	-3.48055500	1.44155500
H	1.73753600	-3.94185700	0.07078800
O	4.05869500	0.29942200	-1.22159500
O	3.25769400	-2.56710400	-1.44064000
O	1.32061500	-1.18304800	2.43091900
O	3.21308500	1.12921200	1.34801900
H	4.57456700	-0.14029400	-1.90890300
H	4.64532400	0.92138800	-0.77244300
H	4.10686400	-2.99705500	-1.27761100
H	1.87951800	-1.32053800	3.20736100
H	3.87230400	1.01571800	2.04480800
H	3.01205200	-2.72992000	-2.36091300
H	0.45383800	-0.88227000	2.73500900
H	2.86051000	2.02539900	1.41848700
Pa	2.27549000	-0.88273700	0.17716700
O	3.69098000	-1.52389900	1.09683800
C	-1.08807700	-0.26432300	-0.55110800
O	0.08200200	-0.48532600	-0.03189700
N	-1.62885300	0.92495100	-0.41145800
C	-1.74967800	-1.41679200	-1.24777800
H	-2.60895500	-1.09039900	-1.82842000
C	-2.17867100	-2.52533500	-0.25917100
H	-1.29620000	-2.89731900	0.26643800
C	-0.91184300	2.00582200	0.30968600
H	-1.67820300	2.65887500	0.72727100
H	-0.36202400	1.56910300	1.14067300
C	-2.95920100	1.30930300	-0.94458100
H	-2.86743600	2.35297900	-1.24937900
H	-3.17173900	0.73721400	-1.84403400

C	-4.07739600	1.15411900	0.09072300
H	-4.20504600	0.09452800	0.33388600
C	-5.40130500	1.73950500	-0.41540000
H	-5.25080900	2.79337600	-0.67963900
C	-6.53203100	1.63513300	0.61415900
H	-6.22112500	2.13145300	1.54221000
C	-7.85044200	2.25107000	0.13191500
H	-8.16498800	1.75196600	-0.79237300
C	-8.97266100	2.16014900	1.16989800
H	-8.69701700	2.67756200	2.09434000
H	-9.89650700	2.61216000	0.79863100
H	-9.19080600	1.11848600	1.42576100
C	0.02456000	2.79322500	-0.61126100
H	0.81418200	2.12540000	-0.97136600
C	0.63931400	3.99951400	0.10772600
H	1.08948800	3.67410400	1.05480600
C	1.69265600	4.72919700	-0.73325200
H	1.23681600	5.06299300	-1.67367600
C	2.31678700	5.93200300	-0.01690400
H	2.75952300	5.59699900	0.92885700
C	3.38351700	6.64326600	-0.85443800
H	2.96377000	7.01793700	-1.79327400
H	3.80932400	7.49487400	-0.31689300
H	4.20434000	5.96424700	-1.10616000
H	-0.15809400	4.69943900	0.38371900
H	-5.69930700	1.22784800	-1.33847600
H	2.48586800	4.02324600	-1.00978000
H	-6.69622500	0.58065900	0.86938900
H	-7.68038900	3.30221100	-0.13032600
H	1.52624200	6.64325800	0.25000900
C	-2.88180400	-3.67929700	-0.98184200
H	-2.20817400	-4.09676200	-1.74028700
H	-3.75381800	-3.29129500	-1.52225700
H	-1.01259200	-1.82051200	-1.94774600
H	-2.85071800	-2.10121200	0.49387500
C	-3.33150300	-4.79470200	-0.03139100
H	-3.99320900	-4.37104300	0.73324100
H	-2.45850700	-5.18900800	0.50166000
H	-3.78711900	1.65864200	1.01809600
H	-0.52766000	3.13446400	-1.49278300
C	-4.05094900	-5.93847600	-0.75234400
H	-4.94646900	-5.57763000	-1.26780200
H	-3.40183100	-6.40348600	-1.50074200
H	-4.36161100	-6.71699700	-0.05046600

$[PaO(H_2O)_5\ (L5)\ ]^{3+}$-A

Sum of electronic and thermal Free Energies= -1776.020761

O	1.43325300	-3.68267000	0.55647500
H	1.24521000	-3.97138100	1.45889800
H	1.82674800	-4.42750400	0.08362200
O	4.09352100	-0.14043000	-1.19328700
O	3.37255000	-2.99065200	-1.40981200
O	1.33502200	-1.65580900	2.43403900
O	3.21334900	0.68580500	1.35363200
H	4.66315400	-0.60476200	-1.81931000
H	4.63809900	0.51361100	-0.73669600
H	4.20347000	-3.44061100	-1.21085600
H	1.88123100	-1.77382200	3.22261700
H	3.85624800	0.58871600	2.06770400
H	3.13629700	-3.18759100	-2.32580900
H	0.44623800	-1.40488400	2.71893100
H	2.83413600	1.57218400	1.41343800
Pa	2.30893900	-1.34733500	0.19135300
O	3.72369600	-1.95599000	1.13407500
C	-1.06023000	-0.86168600	-0.58073500
O	0.10641200	-0.98147100	-0.02183600
N	-1.74418700	0.24371000	-0.38741700
C	-1.55381100	-2.03178600	-1.38119900
H	-2.38679100	-1.75547400	-2.02357800
C	-1.96069700	-3.22033300	-0.47911700
H	-1.10312100	-3.51878300	0.12754000
C	-1.19620700	1.34424100	0.44492400
H	-2.05421900	1.84673000	0.89181600
H	-0.60962000	0.91077500	1.25168800
C	-3.09145400	0.50378100	-0.95263700
H	-3.12177500	1.57209100	-1.17242800
H	-3.19478900	-0.01512900	-1.90218200
C	-4.21937300	0.12798500	0.01348700
H	-4.21456000	-0.95410000	0.17627300
C	-5.59019000	0.56936600	-0.51258900
H	-5.57758400	1.65155500	-0.69019200
C	-6.73349100	0.22826900	0.44990100
H	-6.53582100	0.69427100	1.42355500
C	-8.10906600	0.67932200	-0.05405400
H	-8.30976700	0.20906000	-1.02411400
C	-9.24434900	0.34772800	0.91883200
H	-9.08897300	0.83455200	1.88682900

H	-10.21122400	0.67996200	0.53097300
H	-9.30955700	-0.73029100	1.09685500
C	-0.35968700	2.33413600	-0.37145000
H	0.54041800	1.82778600	-0.73284200
C	0.02474600	3.56535600	0.45807100
H	0.50263300	3.24559000	1.39239500
C	0.96168700	4.52199100	-0.28790600
H	0.48878900	4.83280200	-1.22806400
C	1.33399900	5.76652400	0.52574100
H	1.80044400	5.45454500	1.46798300
C	2.27759800	6.71350700	-0.22131800
H	1.82389000	7.07007900	-1.15141800
H	2.52573100	7.58915300	0.38477000
H	3.21525500	6.21200900	-0.48120700
H	-0.88694900	4.10047500	0.74962700
H	-5.77853100	0.09747600	-1.48444500
H	1.87772200	3.98582400	-0.56700500
H	-6.74985000	-0.85478100	0.62530100
H	-8.08878400	1.76050100	-0.23630900
H	0.41872700	6.30396000	0.80086400
C	-2.45096600	-4.41400700	-1.30568700
H	-1.65736100	-4.72584000	-1.99561200
H	-3.29868600	-4.10283800	-1.92803000
H	-0.72562400	-2.33571400	-2.02719300
H	-2.74989100	-2.90208100	0.20903600
C	-2.86900100	-5.60537000	-0.43685600
H	-3.65739400	-5.28782500	0.25732700
H	-2.01973200	-5.91700900	0.18436100
H	-4.03460600	0.59497500	0.98655600
H	-0.92416700	2.65009400	-1.25474700
C	-3.36812400	-6.80570900	-1.24956100
H	-4.21399100	-6.49143400	-1.87273600
H	-2.58004800	-7.12507200	-1.94197600
C	-3.79055500	-7.99002000	-0.37543600
H	-4.59942900	-7.70807700	0.30602100
H	-4.14413500	-8.82767800	-0.98289600
H	-2.95462600	-8.34924600	0.23301700

$[PaO(H_2O)_5$ (L6) $]^{3+}$-A

Sum of electronic and thermal Free Energies=

-1815.316946

O	-0.06606200	-3.31746600	1.02955100
H	-0.34945700	-3.59763200	1.90963800
H	-0.23376500	-4.04000000	0.41078000
O	3.76956400	-1.23559900	-0.88942900
O	1.65308500	-3.31070100	-1.21314800
O	1.25850800	-2.01044600	3.14487800
O	3.78579300	-0.59556000	1.90535800
H	3.98545200	-1.84959400	-1.60272200
H	4.60208000	-0.98022100	-0.47010000
H	2.16156800	-4.13141900	-1.23571000
H	1.80812700	-2.57942900	3.69886900
H	4.35842100	-1.13361900	2.46670800
H	1.23733400	-3.18883300	-2.07706100
H	0.78239400	-1.40007700	3.72387600
H	3.82598900	0.31250600	2.23216000
Pa	1.81787500	-1.70534700	0.72167000
O	2.86193100	-3.08471900	1.22250000
C	-0.54447000	0.67721400	-0.26662700
O	0.35454800	-0.07663700	0.29379500
N	-0.42557300	1.98113400	-0.17523500
C	-1.68066400	-0.01802100	-0.95673000
H	-2.28122700	0.68129600	-1.53337500
C	-2.58365600	-0.78695900	0.03537800
H	-1.98423400	-1.51903900	0.58087100
C	0.70272400	2.60092700	0.56441600
H	0.29721300	3.48876200	1.05204200
H	1.02512500	1.91174300	1.34155400
C	-1.38316400	2.93645900	-0.79099400
H	-0.81357600	3.84565700	-0.98299100
H	-1.69685800	2.55475900	-1.76077600
C	-2.58472300	3.24516700	0.10614700
H	-3.16731300	2.33268500	0.26650100
C	-3.48115100	4.32775500	-0.50733900
H	-2.89603600	5.24419400	-0.65005800
C	-4.71304700	4.63833700	0.34993400
H	-4.38901100	4.95139700	1.35047400
C	-5.61359500	5.72319000	-0.25206300
H	-5.93061100	5.41218900	-1.25476200
C	-6.84826000	6.02325200	0.60263600
H	-6.56277900	6.36721500	1.60176000
H	-7.46798200	6.80071500	0.14752800
H	-7.46999200	5.13067600	0.72443400
C	1.86595900	2.97687100	-0.35952500
H	2.25559500	2.07224500	-0.83682600
C	2.98978100	3.69154700	0.40046900
H	3.35467000	3.04612100	1.20865600
C	4.16338100	4.08276600	-0.50461400

H	3.79683400	4.72930400	-1.31180800
C	5.29532000	4.79890300	0.24087200
H	5.66212100	4.15161500	1.04651400
C	6.46222500	5.19092100	-0.67006600
H	6.13218800	5.86711700	-1.46489000
H	7.25234000	5.69757200	-0.10911700
H	6.90437000	4.31023400	-1.14647800
H	2.58701900	4.59094800	0.88168000
H	-3.80586700	4.00855000	-1.50515400
H	4.56288900	3.18294700	-0.98928400
H	-5.29782200	3.72036500	0.48914000
H	-5.02999900	6.64171500	-0.38678200
H	4.89471200	5.69616100	0.72765200
C	-3.73422800	-1.49734400	-0.68581900
H	-3.32213500	-2.18159100	-1.43756400
H	-4.33148000	-0.75848800	-1.23349100
H	-1.23161000	-0.72429300	-1.66137600
H	-2.98844300	-0.08843800	0.77482900
C	-4.64309600	-2.27841400	0.26977800
H	-5.04312100	-1.59380000	1.02829400
H	-4.04486600	-3.02193800	0.81133500
H	-2.22933900	3.57145200	1.08917700
H	1.50099900	3.62608700	-1.16201000
C	-5.80577900	-2.98216700	-0.43911100
H	-6.40211600	-2.23730800	-0.98165600
H	-5.40658100	-3.66657400	-1.19885000
C	-6.72004800	-3.76332700	0.51135200
H	-7.11646300	-3.07979700	1.27201800
H	-6.12510000	-4.50952300	1.05188600
C	-7.88232600	-4.45858000	-0.20351900
H	-7.51772600	-5.17625100	-0.94534400
H	-8.51612000	-5.00308000	0.50198300
H	-8.51365600	-3.73354100	-0.72686700

$[PaO(H_2O)_5$ (L7) $]^{3+}$-A

Sum of electronic and thermal Free Energies= -1854.615606

O	0.75611600	-3.88542700	-0.00491800
H	0.31528500	-4.60372600	0.46711500
H	1.41125100	-4.28099200	-0.59345000
O	3.08278200	-0.02988400	1.47245100
O	3.04590700	-2.20855700	-0.41174300
O	-0.33599900	-3.21048300	2.54060600
O	1.19573300	-0.51549900	3.42566800
H	3.93684700	-0.11817000	1.03039100
H	3.23697300	0.37271500	2.33717000
H	3.82612900	-2.74347100	-0.21567600
H	0.00239300	-3.74144300	3.27301100
H	1.53678000	-0.94007200	4.22440300
H	3.11747000	-1.89374000	-1.32308400
H	-1.29134200	-3.12468100	2.65737100
H	0.54565600	0.14516200	3.70104800
Pa	1.25261400	-1.72767600	1.25279300
O	2.34537700	-2.76062200	2.24999000
C	-0.65775800	0.85533700	-0.05112600
O	0.20130800	0.15522100	0.62737300
N	-0.51344000	2.16000800	-0.09161400
C	-1.77437600	0.11364300	-0.72989200
H	-2.33185500	0.76195000	-1.40132600
C	-2.74023300	-0.54495800	0.27961000
H	-2.17657200	-1.19800500	0.95134500
C	0.60364200	2.82468200	0.62480000
H	0.22189100	3.78960800	0.96094700
H	0.84475400	2.23605100	1.50583400
C	-1.43609000	3.06907900	-0.81840500
H	-0.84493300	3.94572700	-1.08423700
H	-1.74180100	2.60263500	-1.75281200
C	-2.64446700	3.47495600	0.02938600
H	-3.23489100	2.58450300	0.26741500
C	-3.53106200	4.50398800	-0.68199200
H	-2.94254600	5.40344800	-0.89898500
C	-4.76438500	4.88790000	0.14340400
H	-4.44090600	5.27965600	1.11609400
C	-5.66299700	5.92305600	-0.54285200
H	-5.98048000	5.53478200	-1.51804900
C	-6.89702000	6.28974900	0.28656200
H	-6.61038300	6.71070700	1.25547800
H	-7.51712800	7.02944100	-0.22719200
H	-7.51864200	5.40951900	0.47851700
C	1.83796300	3.00799800	-0.26317600
H	2.20489600	2.02421800	-0.57031800
C	2.94813000	3.77252700	0.46719200
H	3.21919000	3.23228400	1.38210200
C	4.20158200	3.97326800	-0.39139300
H	3.92981300	4.50876900	-1.30982800
C	5.31474500	4.74159600	0.33005400
H	5.58534600	4.20569200	1.24781300
C	6.56498200	4.94282100	-0.53090700

H	6.33156000	5.50526200	-1.44044900
H	7.33768500	5.49424000	0.01183200
H	6.99333500	3.98275400	-0.83577600
H	2.56614400	4.74995700	0.78610500
H	-3.85285400	4.10172800	-1.65029900
H	4.58420800	2.99458200	-0.70773100
H	-5.35113600	3.98524700	0.35568700
H	-5.07878000	6.82786100	-0.74883500
H	4.92950700	5.71766200	0.64843000
C	-3.83331700	-1.35854300	-0.42125400
H	-3.36518900	-2.12435600	-1.05160800
H	-4.39784300	-0.70356300	-1.09548100
H	-1.30253400	-0.66251300	-1.33991000
H	-3.19777400	0.22881300	0.90428200
C	-4.79620200	-2.02835600	0.56522600
H	-5.26539000	-1.25881400	1.19089500
H	-4.22516000	-2.67243500	1.24625600
H	-2.29486400	3.88601400	0.98230500
H	1.55861200	3.54758000	-1.17430300
C	-5.88766700	-2.85995200	-0.11843400
H	-6.45589800	-2.21743700	-0.80308400
H	-5.41714800	-3.63132000	-0.74150700
C	-6.85285800	-3.52671600	0.86776800
H	-7.32710900	-2.75468900	1.48762600
H	-6.28343600	-4.16425700	1.55673700
C	-7.94154800	-4.36708800	0.19051200
H	-7.46781000	-5.13905200	-0.42800300
H	-8.51130500	-3.73136400	-0.49807800
C	-8.90013300	-5.02867800	1.18480200
H	-9.66405000	-5.61898400	0.67108600
H	-8.36337600	-5.69851100	1.86423900
H	-9.41345000	-4.27945100	1.79599800

$[PaO(H_2O)_5$ (L8) $]^{3+}$-A

Sum of electronic and thermal Free Energies=

-1893.913625

O	0.74473100	-3.87812100	-0.00956300
H	0.30357500	-4.59614500	0.46259400
H	1.39982800	-4.27401300	-0.59791100
O	3.07258600	-0.02364200	1.46880400
O	3.03480900	-2.20154100	-0.41601100
O	-0.34753900	-3.20435900	2.53469200
O	1.18518100	-0.50960200	3.42209500
H	3.92583200	-0.11207600	1.02517800
H	3.22883800	0.37656200	2.33426700
H	3.81457300	-2.73728900	-0.22041400
H	-0.00956500	-3.73498800	3.26753900
H	1.52579400	-0.93520000	4.22047400
H	3.10616000	-1.88678400	-1.32738800
H	-1.30264900	-3.11661100	2.65212400
H	0.53587400	0.15156900	3.69807500
Pa	1.24151300	-1.72067500	1.24867300
O	2.33403100	-2.75411200	2.24564200
C	-0.66596600	0.86428200	-0.05676300
O	0.19075400	0.16235800	0.62294600
N	-0.51953100	2.16873500	-0.09590100
C	-1.78194900	0.12427300	-0.73848300
H	-2.33768400	0.77347600	-1.41048700
C	-2.74969000	-0.53488400	0.26870900
H	-2.18619100	-1.18402600	0.94428400
C	0.59842300	2.83067100	0.62177300
H	0.21932200	3.79721100	0.95619600
H	0.83616500	2.24227100	1.50388900
C	-1.44055600	3.08045900	-0.82140700
H	-0.84720500	3.95534400	-1.08821600
H	-1.74942500	2.61496300	-1.75521200
C	-2.64598200	3.48963000	0.02903900
H	-3.23959500	2.60102500	0.26615500
C	-3.52967400	4.52397700	-0.67821200
H	-2.93765600	5.42123100	-0.89482900
C	-4.75903100	4.91172100	0.15131000
H	-4.43106900	5.29967100	1.12402500
C	-5.65470500	5.95269100	-0.52997900
H	-5.97706300	5.56808700	-1.50503000
C	-6.88437500	6.32355400	0.30404000
H	-6.59272600	6.74117500	1.27290300
H	-7.50254400	7.06723800	-0.20627400
H	-7.50958200	5.44590200	0.49616100
C	1.83470000	3.00867400	-0.26456600
H	2.19762200	2.02325700	-0.57114000
C	2.94744700	3.76811500	0.46713700
H	3.21262600	3.22837600	1.38405100
C	4.20462100	3.95868200	-0.38834100
H	3.93907700	4.49387000	-1.30877600
C	5.32091600	4.72104200	0.33457200
H	5.58498600	4.18554600	1.25447900
C	6.57515000	4.91124600	-0.52308800
H	6.34853000	5.47329700	-1.43458500

H	7.35022400	5.45825600	0.02073100
H	6.99739200	3.94737400	-0.82449400
H	2.57073400	4.74866100	0.78270400
H	-3.85573500	4.12516400	-1.64650500
H	4.58154600	2.97670100	-0.70133900
H	-5.34939200	4.01130800	0.36309900
H	-5.06675900	6.85511800	-0.73578900
H	4.94161300	5.70059100	0.64933800
C	-3.83721700	-1.35497000	-0.43325900
H	-3.36382800	-2.12310500	-1.05680800
H	-4.40034000	-0.70559100	-1.11402600
H	-1.30916500	-0.65162600	-1.34815700
H	-3.21222000	0.23902700	0.88951700
C	-4.80258000	-2.02153300	0.55299900
H	-5.28296000	-1.24868000	1.16599200
H	-4.23155900	-2.65275000	1.24602400
H	-2.29307800	3.89720200	0.98224100
H	1.55884600	3.54938000	-1.17609800
C	-5.88156400	-2.87096800	-0.12848800
H	-6.44741800	-2.24363000	-0.82895600
H	-5.39955000	-3.64890300	-0.73433900
C	-6.85163500	-3.52824300	0.85963500
H	-7.34192300	-2.74809800	1.45617000
H	-6.28259900	-4.14295200	1.56914900
C	-7.92099200	-4.39645900	0.18728400
H	-7.43111200	-5.18104200	-0.40417100
H	-8.48809800	-3.78518600	-0.52687600
C	-8.89442900	-5.04706200	1.17664500
H	-8.32741800	-5.65373700	1.89323800
H	-9.38801000	-4.26325100	1.76406600
C	-9.95466200	-5.91958100	0.49840800
H	-10.63368700	-6.36536400	1.23068600
H	-10.55862600	-5.33404300	-0.20217200
H	-9.49197900	-6.73560900	-0.06589100

$[PaO(H_2O)_5$ (L9) $]^{3+}$-A

Sum of electronic and thermal Free Energies=

-1658.121048

O	1.54649600	-3.75794000	0.42158400
H	1.30751400	-4.02862400	1.31753800
H	1.96822900	-4.51078300	-0.01284100
O	4.13926400	-0.13623800	-1.29185800
O	3.48028800	-3.00460900	-1.55590000
O	1.36483200	-1.72580600	2.27956600
O	3.19804300	0.65992100	1.23367600
H	4.73790900	-0.57494300	-1.90931200
H	4.65107400	0.52947000	-0.81437300
H	4.31208100	-3.44656300	-1.34215500
H	1.90355600	-1.83524600	3.07456900
H	3.79293700	0.56919400	1.98920200
H	3.26592200	-3.20127600	-2.47731500
H	0.46627200	-1.50301600	2.55627700
H	2.74077400	1.50665300	1.31869900
Pa	2.36677000	-1.40566100	0.04459000
O	3.78398000	-1.97817500	1.00525700
C	-1.02547900	-0.90117800	-0.69748900
O	0.15797500	-1.07044100	-0.19022600
N	-1.68480900	0.20113200	-0.41806300
C	-1.58178300	-2.00574700	-1.56856100
H	-2.57329400	-1.71439300	-1.90725800
C	-1.72702100	-3.30440700	-0.75061500
H	-0.75686200	-3.67321500	-0.41861600
H	-2.36406700	-3.15826400	0.12437700
C	-1.09895700	1.24226100	0.46139600
H	-1.92722800	1.67170900	1.02614800
H	-0.42823000	0.76092200	1.16797300
C	-3.04048100	0.51665800	-0.93835300
H	-3.08413300	1.60366300	-1.01413700
H	-3.14020700	0.13132900	-1.95055800
C	-4.16076000	0.00413700	-0.02886300
H	-4.13090100	-1.08955900	0.00861200
C	-5.53894300	0.46918200	-0.51451300
H	-5.55524600	1.56485500	-0.56010500
H	-5.70317800	0.11367700	-1.53889900
C	-6.68352900	-0.01721100	0.38149800
H	-6.66723000	-1.11339600	0.42855900
H	-6.51596600	0.33726400	1.40635600
C	-8.06512000	0.44744500	-0.09323500
H	-8.07776400	1.54272400	-0.14549000
H	-8.23328400	0.09028800	-1.11628000
C	-9.20520000	-0.03311600	0.80920000
H	-9.08122700	0.33654100	1.83197400
H	-10.17548300	0.31545800	0.44488900
H	-9.23947200	-1.12626100	0.85381400
C	-0.36612200	2.32496100	-0.33604000
H	0.48170400	1.86794500	-0.85578700
C	0.11497400	3.46976000	0.56299000
H	-0.74919200	3.91873800	1.06707400

H	0.75623500	3.07213500	1.36013000
C	0.87449200	4.55597600	-0.20714800
H	0.23010200	4.94975300	-1.00307000
H	1.74187800	4.10746900	-0.70783100
C	1.34630000	5.71420100	0.67906400
H	1.99140700	5.32070800	1.47370400
H	0.47920900	6.15963400	1.18108400
C	2.09765700	6.79820800	-0.09927000
H	1.46476600	7.23353200	-0.87896300
H	2.42096300	7.60956500	0.55855500
H	2.98870700	6.38903700	-0.58591900
C	-0.69640200	-2.20548100	-2.81350900
H	-1.16144800	-2.95227800	-3.45988300
H	-0.59115000	-1.28122400	-3.38565700
H	-2.19011200	-4.06526800	-1.38195500
H	0.29879500	-2.56789000	-2.54705600
H	-3.99064000	0.36032300	0.99246700
H	-1.03136700	2.72634400	-1.10730500

$[PaO(H_2O)_5$ (L10) $]^{3+}$-A

Sum of electronic and thermal Free Energies= -1815.293241

O	-2.19923300	-3.19234100	-0.91955100
H	-1.97777400	-3.41082600	-1.83388200
H	-2.76798100	-3.89342800	-0.57446300
O	-3.98851200	0.54315900	1.44060200
O	-3.98304900	-2.45782300	1.14653900
O	-1.62151700	-0.93664600	-2.45423300
O	-3.04039400	1.52900700	-0.97082800
H	-4.55829300	0.15920400	2.11898100
H	-4.44183000	1.31617700	1.08014900
H	-4.91048800	-2.60008900	0.91780600
H	-2.16072400	-0.88110400	-3.25435200
H	-3.62481700	1.67401000	-1.72595700
H	-3.83434000	-2.82671100	2.02716800
H	-0.69333700	-0.97984200	-2.71840900
H	-2.47431200	2.30696000	-0.88153100
Pa	-2.56557800	-0.82700800	-0.18012000
O	-4.06722600	-0.95662600	-1.17296200
C	0.86181000	-0.91361500	0.58354700
O	-0.33672800	-0.87222600	0.07569200
N	1.69230400	0.09008900	0.38597500
C	1.20477500	-2.17406300	1.34946000
H	2.23532000	-2.11490900	1.67888700
C	1.08507000	-3.40020900	0.42191500
H	0.05755600	-3.55737500	0.09458600
H	1.72150500	-3.29843200	-0.45995900
C	1.27837200	1.24095600	-0.50764900
H	0.36114400	0.90953700	-0.98324800
C	3.10325000	0.16120100	0.94070000
H	3.43528100	1.14281800	0.60658100
C	4.04658400	-0.88166200	0.28935600
H	4.07663000	-1.79254900	0.89443400
C	5.47889700	-0.35778700	0.10991900
H	5.45966300	0.54103900	-0.51786500
H	5.88975900	-0.05025100	1.07817000
C	6.40956000	-1.39784200	-0.52446300
H	6.43561300	-2.29509500	0.10664900
H	5.99368300	-1.71340100	-1.48985000
C	7.83931300	-0.88671900	-0.73529500
H	7.81129000	0.01376800	-1.36048500
H	8.25729900	-0.57650000	0.22983700
C	8.76046600	-1.92628700	-1.38029500
H	8.38573000	-2.22955300	-2.36305600
H	9.77136300	-1.53251800	-1.51698800
H	8.83438400	-2.82621600	-0.76165200
C	0.95160400	2.47109200	0.35617000
H	0.21567700	2.17123500	1.10944800
C	0.40552300	3.67864900	-0.41724100
H	1.16669100	4.05921500	-1.10537700
H	-0.44388000	3.37566900	-1.04332300
C	-0.02901200	4.81499000	0.51614800
H	0.82280200	5.11227600	1.14054600
H	-0.79992000	4.44657400	1.20441300
C	-0.56142300	6.04400900	-0.22896500
H	-1.40975400	5.74526200	-0.85640300
H	0.21110000	6.41212000	-0.91462800
C	-0.99167100	7.17560900	0.70866700
H	-0.15351100	7.51757800	1.32386600
H	-1.36582700	8.03652300	0.14801200
H	-1.78707000	6.84751200	1.38522700
C	0.30840800	-2.30873600	2.59415700
H	0.58489900	-3.21620300	3.13435900
H	0.42377000	-1.46162400	3.27333600
H	1.41151100	-4.28459900	0.97273300
H	-0.74459900	-2.38773700	2.32008300
H	3.65243000	-1.17145100	-0.68805300
H	1.84813100	2.78630900	0.89664900

C	2.33046100	1.48550500	-1.61866700
H	2.93212400	0.58584700	-1.75306800
H	3.01817000	2.27920500	-1.31217000
C	1.71438600	1.83736200	-2.97992500
H	2.50734000	2.02696800	-3.70729700
H	1.10712600	1.01321800	-3.36348800
H	1.08400600	2.72625300	-2.93792400
C	3.20982600	0.16891400	2.47996500
H	2.86212600	-0.77611700	2.89913400
H	4.28399100	0.19965800	2.68601700
C	2.54161900	1.33123900	3.21648000
H	2.93254200	2.29587600	2.88361800
H	1.45760700	1.33904600	3.08500300
H	2.74092300	1.24687900	4.28738900

$[PaO(H_2O)_5$ (L11) $]^{3+}$-A

Sum of electronic and thermal Free Energies= -1815.294441

O	1.47958800	-3.49233100	0.39413300
H	1.20964900	-3.78024200	1.27593400
H	1.95717500	-4.22131100	-0.02347500
O	4.12678300	0.08884000	-1.26620700
O	3.37540600	-2.80539100	-1.55618300
O	1.40159700	-1.50779100	2.33443700
O	3.39035000	0.74582600	1.35867800
H	4.57344600	-0.25440300	-2.05033800
H	4.75203900	0.65586500	-0.79698400
H	4.25593100	-3.17373100	-1.40851600
H	1.95787600	-1.68937600	3.10376500
H	4.05167200	0.55799400	2.03701600
H	3.15016000	-2.93816500	-2.48645900
H	0.53700200	-1.21635000	2.65307700
H	3.08235900	1.65182600	1.48694300
Pa	2.37037700	-1.15620000	0.08917400
O	3.77540900	-1.85117400	0.98467900
C	-1.04847700	-0.55284400	-0.56711100
O	0.15304900	-0.75512400	-0.12655500
N	-1.68295400	0.55622100	-0.23907000
C	-1.64339600	-1.60463500	-1.47957300
H	-2.65982300	-1.31444800	-1.73249200
C	-1.69719000	-2.98261300	-0.79754500
H	-0.69927300	-3.35148500	-0.56499300
H	-2.27976200	-2.95154300	0.12587400
C	-0.98317600	1.64104900	0.50243300
H	-1.75190900	2.21680800	1.01443600
H	-0.35826500	1.18544000	1.26776500
C	-3.11197700	0.79446100	-0.59317200
H	-3.28056500	1.86084000	-0.45845300
H	-3.25078300	0.59042800	-1.65387400
C	-4.13520900	0.00210500	0.25074400
H	-3.92682900	-1.06539800	0.11620800
C	-5.52446700	0.29537300	-0.35854200
H	-5.71750200	1.37351100	-0.28464500
H	-5.48370900	0.06570400	-1.43048600
C	-6.71084300	-0.46305800	0.24842500
H	-6.49717400	-1.53912300	0.25304400
H	-6.85098700	-0.16802500	1.29341700
C	-8.01977300	-0.21293500	-0.51118100
H	-8.22348500	0.86445600	-0.53211300
H	-7.89544200	-0.52114900	-1.55616500
C	-9.21758500	-0.94654800	0.09899400
H	-9.38831000	-0.63121600	1.13315300
H	-10.13402300	-0.75023900	-0.46427700
H	-9.05595500	-2.02914800	0.10512400
C	-0.11964700	2.55813800	-0.39337600
H	0.62591400	1.91875100	-0.87965100
C	0.63948200	3.54229500	0.52149800
H	-0.07563000	4.19301600	1.03783200
H	1.13487200	2.96844000	1.31527700
C	1.68571400	4.40472600	-0.19498000
H	1.20516300	5.00747900	-0.97292300
H	2.40209800	3.75280200	-0.71133900
C	2.44414300	5.34090900	0.75442400
H	2.92493800	4.74936400	1.54272500
H	1.72578000	5.99643200	1.26086300
C	3.49773300	6.19349200	0.04154900
H	3.04083300	6.82055500	-0.73043700
H	4.01642800	6.85328900	0.74233100
H	4.25097300	5.56537100	-0.44452500
C	-0.91035700	3.25281900	-1.52557300
H	-0.18737700	3.67133400	-2.23158800
C	-1.87811200	4.36418500	-1.09944500
H	-2.61100100	4.02891800	-0.36016300
H	-1.35087700	5.21872900	-0.66892400
H	-2.43613000	4.72752000	-1.96597900
C	-4.02642100	0.32430600	1.76108700
H	-3.00518600	0.63347100	1.99751000
C	-4.36688200	-0.84397900	2.69577200

H	-3.69270900	-1.68768100	2.52007400
H	-4.25340500	-0.54197900	3.74056900
H	-5.38818600	-1.20362000	2.56416400
H	-4.66122700	1.18825700	1.98907700
H	-1.45330700	2.49223400	-2.09561400
C	-0.83041600	-1.63961600	-2.79128900
H	-1.27796000	-2.37426600	-3.46328300
H	-0.83950400	-0.66970800	-3.29352500
H	-2.17874100	-3.68982800	-1.47588500
H	0.20737100	-1.92897400	-2.61403400

$[PaO(H_2O)_5$ (L12) $]^{3+}$-A

Sum of electronic and thermal Free Energies= -1815.291378

O	2.59024400	-3.52693300	1.16585300
H	2.65051200	-3.97195600	2.02103700
H	3.28395600	-3.87487800	0.59026500
O	3.51691500	0.95674800	0.06697200
O	3.73967400	-1.91120000	-0.70590700
O	1.90778200	-2.12288600	3.40559100
O	2.32599200	0.85091600	2.83811900
H	3.29961300	1.46243000	-0.72536300
H	4.37203200	1.26323700	0.39092300
H	4.67520100	-1.67187200	-0.67808600
H	2.56002900	-1.97741400	4.10318300
H	3.13819800	1.02768000	3.32861100
H	3.47953600	-1.93960900	-1.63655600
H	1.04655100	-2.22866700	3.83223400
H	1.60781300	1.33024600	3.26953000
Pa	2.28272400	-1.01594900	1.16504900
O	3.93364500	-1.05543100	1.88427100
C	-0.97908300	-0.73311400	-0.22954100
O	0.18909600	-0.77678700	0.32473600
N	-1.68622900	0.37407100	-0.16147000
C	-1.45456200	-1.98057000	-0.94322200
H	-2.50638000	-1.86186600	-1.19444900
C	-1.32940300	-3.20958200	-0.02626800
H	-0.28736300	-3.42801600	0.21145400
H	-1.88009600	-3.07123900	0.90673200
C	-1.20067000	1.57348800	0.56687700
H	-2.08704400	2.02867600	1.01140200
H	-0.56303000	1.24409200	1.38153800
C	-3.03041500	0.54189700	-0.77371800
H	-3.09113100	1.59122700	-1.06560100
H	-3.08470300	-0.03753400	-1.69124100
C	-5.54505000	0.69971500	-0.24806600
H	-5.43277500	1.75626600	-0.52897800
C	-6.51244300	0.63980600	0.95294600
H	-6.60932900	-0.40652500	1.27321100
H	-6.04992400	1.17357000	1.79267200
C	-7.91204700	1.22449800	0.72780000
H	-7.82103700	2.25425500	0.36184200
H	-8.43364100	0.66331200	-0.05389600
C	-8.76128900	1.21195100	2.00319300
H	-8.89602100	0.19222500	2.37755700
H	-8.28801500	1.79693100	2.79819100
C	-0.53278100	4.03304100	0.16831900
H	-1.59382200	4.28705700	0.30047400
C	0.02715600	4.98577600	-0.90731400
H	1.07766600	4.74091600	-1.10714700
H	-0.50874100	4.79392300	-1.84508400
C	-0.09005300	6.47932400	-0.57823400
H	0.48767000	6.71250900	0.32214900
H	-1.13472400	6.71479900	-0.34119900
C	0.38893500	7.37573600	-1.72444700
H	-0.19642600	7.20348300	-2.63311900
H	1.43887000	7.18005200	-1.96459200
C	0.13149500	4.21291300	1.55316700
H	-0.14101100	5.20075800	1.93708900
C	1.65862600	4.07421400	1.59256800
H	2.00067400	3.10175600	1.23136200
H	2.14995700	4.84279200	0.99049300
H	2.02078300	4.18534500	2.61860000
C	-6.06768700	-0.07481000	-1.48791800
H	-5.23781800	-0.58716600	-1.98518400
C	-6.77647000	0.79734000	-2.53185200
H	-6.09378400	1.55133900	-2.93589600
H	-7.13516800	0.19156600	-3.36888400
H	-7.63553600	1.32355200	-2.11000200
H	-6.74136600	-0.87136900	-1.15135500
H	-0.31544100	3.50130700	2.25602700
C	-0.65853800	-2.15835500	-2.25207200
H	-1.02184000	-3.04675800	-2.77192600
H	-0.77872200	-1.30120200	-2.91823300
H	-1.74864800	-4.07583900	-0.54163800
H	0.40530300	-2.29355200	-2.04663500
C	-0.49727500	2.58113700	-0.35850900
H	0.53213800	2.25967400	-0.54108100

H	-0.99867500	2.56859300	-1.33137000
H	0.29921500	8.43438900	-1.46571900
H	-9.75385600	1.63441800	1.82430900
C	-4.15769500	0.20323500	0.21034600
H	-4.18551400	-0.87847600	0.38322800
H	-3.92174600	0.66575000	1.17367700

$[PaO(H_2O)_5$ (L13) $]^{3+}$-A

Sum of electronic and thermal Free Energies= -1815.298653

O	-2.04900200	-3.59733600	-0.26382200
H	-1.81781100	-4.01615400	-1.10349000
H	-2.56982100	-4.22955600	0.24905800
O	-4.31330700	0.28640000	1.05058400
O	-4.02699500	-2.54887300	1.42843000
O	-1.54812500	-1.72107900	-2.31267800
O	-3.26067500	0.95196300	-1.44078300
H	-4.98268300	-0.06301900	1.65196800
H	-4.70480800	1.02595300	0.56766900
H	-4.89016900	-2.90807000	1.18566300
H	-2.04277300	-1.87308900	-3.12869100
H	-3.83096600	0.88258600	-2.21730400
H	-3.89319500	-2.70431900	2.37299700
H	-0.61357500	-1.62452800	-2.53857600
H	-2.73132200	1.75453800	-1.53646000
Pa	-2.64198600	-1.15984900	-0.16949600
O	-4.04288900	-1.64757400	-1.19797800
C	0.75856900	-0.87567900	0.69084500
O	-0.42084500	-0.96609000	0.15800800
N	1.51280600	0.16159000	0.40145200
C	1.20609500	-1.99775500	1.60194200
H	2.19356200	-1.75808800	1.98913100
C	1.31582700	-3.31373800	0.80533100
H	0.34016100	-3.63440900	0.44059600
H	1.99344700	-3.21543900	-0.04543100
C	1.04456700	1.22396300	-0.52210200
H	1.91525300	1.53097200	-1.10400700
H	0.31919000	0.79449800	-1.20890900
C	2.88003100	0.36487100	0.94944900
H	3.05163100	1.44098800	0.93132600
H	2.89776700	0.06550100	1.99569800
C	3.96072300	-0.35665700	0.13886900
H	3.79216600	-1.43708700	0.18534600
C	5.36414600	-0.03834000	0.67027500
H	5.54205800	1.04339800	0.61697800
H	5.40167000	-0.30494700	1.73298100
C	6.50029100	-0.77643400	-0.06845500
H	6.21086200	-1.83487600	-0.13394900
C	7.79148200	-0.70193600	0.77257300
H	8.07414400	0.35288800	0.88466600
H	7.56556600	-1.06541700	1.78173500
C	8.98580600	-1.48945000	0.22476200
H	9.31974600	-1.10791700	-0.74348200
H	9.83503100	-1.42619900	0.91098100
H	8.73844600	-2.54833800	0.09964100
C	0.44276800	2.41957200	0.22367000
H	-0.47349600	2.09814500	0.72959200
C	0.13307300	3.57565800	-0.73576200
H	1.05098600	3.87059100	-1.26013100
H	-0.55399400	3.21627400	-1.51125900
C	-0.47830600	4.81819400	-0.05535400
H	-1.28323400	4.46702000	0.60571700
C	-1.12069600	5.72412500	-1.12695300
H	-1.82788700	5.12061000	-1.70785100
H	-0.33917200	6.03832900	-1.83090000
C	-1.85176300	6.96248200	-0.59934800
H	-1.17367700	7.65440100	-0.09346800
H	-2.32227500	7.50949800	-1.42119900
H	-2.63875700	6.68682100	0.10955000
C	0.24929300	-2.13601100	2.80026700
H	0.65393100	-2.87983300	3.48931600
H	0.14186500	-1.19453600	3.34317400
H	1.70972100	-4.08988000	1.46435400
H	-0.73915600	-2.47685600	2.48630500
H	3.86928300	-0.06844300	-0.91257900
H	1.13629500	2.74963100	1.00246000
C	0.56745600	5.56769100	0.81355900
H	1.42924400	4.91699900	0.99271000
H	0.95817300	6.41936000	0.24444600
C	0.04604400	6.05103900	2.17244000
H	-0.28324700	5.20551300	2.78455200
H	0.82711600	6.57874000	2.72762900
H	-0.80295500	6.73030200	2.06635900
C	6.69515600	-0.24111900	-1.51274800
H	5.82187900	0.34970500	-1.80687600
H	7.53839100	0.45952100	-1.52364600
C	6.91433600	-1.32747000	-2.57322700
H	7.05847100	-0.88682100	-3.56411900

H	7.78993400	-1.94227300	-2.35191100
H	6.04885300	-1.99513600	-2.62867100

$[PaO(H_2O)_5$ (L14) $]^{3+}$-A

Sum of electronic and thermal Free Energies= -1815.297757

O	1.31723200	-3.42228500	0.45288700
H	1.14594100	-3.71663700	1.35698100
H	1.76098500	-4.14292800	-0.01412800
O	3.95719100	0.14636300	-1.26818200
O	3.19421000	-2.76546500	-1.53179400
O	1.26380100	-1.42378900	2.35845800
O	3.20650700	0.83011900	1.35523900
H	4.28764800	-0.10097000	-2.14076400
H	4.64530700	0.65870600	-0.82570100
H	4.09083700	-3.09968100	-1.40134600
H	1.82782400	-1.57510800	3.12867500
H	3.86020300	0.67042100	2.04778700
H	2.97058500	-2.87581300	-2.46549500
H	0.39747900	-1.13498900	2.67483300
H	2.90718200	1.74471600	1.43151700
Pa	2.20833100	-1.08693600	0.10175400
O	3.62340400	-1.76579300	0.99443200
C	-1.22188400	-0.56034000	-0.51180900
O	-0.00600200	-0.70137000	-0.08669200
N	-1.87990700	0.54765100	-0.23260300
C	-1.79679600	-1.68842400	-1.32246200
H	-2.73408400	-1.39775600	-1.79133100
C	-1.98815100	-2.99877000	-0.52724900
H	-1.02958200	-3.30994800	-0.11196000
C	-1.19813800	1.67584900	0.46006700
H	-1.97542700	2.25112400	0.95968300
H	-0.55667100	1.25757800	1.23301300
C	-3.31683200	0.73302300	-0.58153500
H	-3.50888200	1.80109900	-0.50102600
H	-3.45982200	0.46842000	-1.62845900
C	-4.31557100	-0.03834900	0.30944500
H	-4.10903000	-1.10795900	0.19458300
C	-5.72186100	0.23396200	-0.26940500
H	-5.92022200	1.31211400	-0.21238000
C	-6.88290400	-0.51983000	0.39019500
H	-6.98662000	-0.20902000	1.43486200
C	-8.22027200	-0.28907100	-0.32440000
H	-8.13275500	-0.61197200	-1.36862400
C	-9.38919400	-1.02157100	0.34085500
H	-9.52288100	-0.69275200	1.37627400
H	-10.32766500	-0.83923300	-0.18985300
H	-9.21988000	-2.10291600	0.35605100
C	-0.36155000	2.58310000	-0.47084900
H	0.38357300	1.94491000	-0.95939700
C	0.40648900	3.59176600	0.41030400
H	0.93366500	3.03416300	1.19540200
C	1.41965900	4.45658600	-0.34920600
H	0.90811600	5.04299100	-1.11994000
C	2.19783500	5.41570200	0.56058900
H	2.72368100	4.84110400	1.33244300
C	3.20354100	6.28145000	-0.20365200
H	2.70168200	6.89521600	-0.95827000
H	3.74127600	6.95490700	0.46921200
H	3.94516700	5.66301600	-0.71911300
C	-1.18279400	3.24628900	-1.59989900
H	-0.47935300	3.66780800	-2.32374200
C	-2.16380900	4.34579700	-1.17354000
H	-2.88477900	4.00495600	-0.42515900
H	-1.64621000	5.21185300	-0.75432500
H	-2.73549100	4.69358800	-2.03756000
C	-4.17291800	0.32094800	1.80899000
H	-3.15399600	0.65958100	2.01159900
C	-4.46053400	-0.83452500	2.77698200
H	-3.76538200	-1.66233000	2.60734800
H	-4.33567100	-0.50550400	3.81226600
H	-5.47322200	-1.22666400	2.67363500
H	-4.82232700	1.17405100	2.03601500
H	-1.72060300	2.46693600	-2.14937800
H	-0.30293300	4.23955000	0.93798800
H	-5.70983500	-0.01882800	-1.33682700
H	2.12712100	3.80493500	-0.87816400
H	-6.66320500	-1.59459500	0.40426900
H	-8.43222200	0.78651200	-0.35314000
H	1.48870100	6.06213600	1.09109200
C	-2.55571700	-4.10723400	-1.41691300
H	-1.88707000	-4.32178600	-2.25552900
H	-2.68266200	-5.02925200	-0.84481800
H	-3.53118500	-3.83030300	-1.82678800
H	-1.07394700	-1.86526500	-2.12620900
H	-2.66167800	-2.82064200	0.31551400

$[PaO(H_2O)_5$ (L15) $]^{3+}$-A

Sum of electronic and thermal Free Energies=
-1933.191441

O	1.19069500	-3.42355300	0.49138000
H	1.00349600	-3.71950100	1.39180700
H	1.63251900	-4.14717200	0.02725600
O	3.83741600	0.15885700	-1.20353400
O	3.08009000	-2.76112200	-1.48622800
O	1.13903600	-1.42941800	2.40743000
O	3.07408500	0.82205300	1.41785800
H	4.19291500	-0.09208500	-2.06515800
H	4.50030100	0.69817400	-0.75448200
H	3.97299600	-3.10333400	-1.35109500
H	1.70187600	-1.58738100	3.17717400
H	3.72115300	0.65561600	2.11528200
H	2.85905200	-2.87162100	-2.42051500
H	0.27894100	-1.12323300	2.72462800
H	2.70468800	1.70333900	1.55855900
Pa	2.08948400	-1.09216200	0.15225000
O	3.50418100	-1.77464900	1.04315500
C	-1.33081300	-0.50923200	-0.46361500
O	-0.11862400	-0.69320700	-0.04430200
N	-1.94575600	0.62368500	-0.18705500
C	-1.94564700	-1.61496700	-1.27513000
H	-2.89107500	-1.30365200	-1.71248100
C	-2.12819200	-2.93957800	-0.50454900
H	-1.16877400	-3.25200000	-0.08954000
H	-2.80948600	-2.78356900	0.33754400
C	-1.21502600	1.73589000	0.48118800
H	-1.96633800	2.35316500	0.97012700
H	-0.58729400	1.31012900	1.26165500
C	-3.38007100	0.85305000	-0.52162200
H	-3.53908400	1.92650100	-0.44187100
H	-3.54212800	0.59054200	-1.56619200
C	-4.38863600	0.11204600	0.38355700
H	-4.19567000	-0.96230800	0.28852000
C	-5.79258500	0.39102400	-0.19750200
H	-5.97793600	1.47240700	-0.16102500
H	-5.78626000	0.11735100	-1.25979500
C	-6.96068200	-0.33643300	0.47898000
H	-6.75284100	-1.41311800	0.51312100
H	-7.05846500	-0.00462600	1.51773400
C	-8.29688300	-0.10472500	-0.23747100
H	-8.49873300	0.97218800	-0.28358400
H	-8.21387700	-0.44550600	-1.27637500
C	-9.47171500	-0.81534300	0.44095500
H	-9.60034700	-0.46945700	1.47143600
H	-10.40928900	-0.63194800	-0.09097600
H	-9.31299700	-1.89795100	0.47238500
C	-0.34727300	2.58832400	-0.47322000
H	0.37415000	1.91151000	-0.94540400
C	0.45402900	3.59405800	0.38083000
H	-0.23374900	4.28781900	0.87777300
H	0.94620900	3.04465000	1.19397200
C	1.51000100	4.39050100	-0.39493100
H	1.03029300	4.96566600	-1.19410500
H	2.19951200	3.69420700	-0.88938200
C	2.31084100	5.35473500	0.48965400
H	2.80634300	4.79209300	1.28994000
H	1.61871200	6.04557600	0.98552700
C	3.35624000	6.15462800	-0.29280600
H	2.88596500	6.75623600	-1.07692700
H	3.90908100	6.83400000	0.36158500
H	4.08171400	5.49124100	-0.77419000
C	-1.14756500	3.25106600	-1.61768000
H	-0.43235000	3.63180900	-2.35244800
C	-2.09132100	4.39142500	-1.21440400
H	-2.81282000	4.09290700	-0.44864500
H	-1.54390800	5.25348000	-0.82608000
H	-2.66230600	4.73072700	-2.08217500
C	-4.23786200	0.49813200	1.87581200
H	-3.21508100	0.83142000	2.06860100
C	-4.53416300	-0.63546000	2.86669700
H	-3.84699200	-1.47273500	2.71210200
H	-4.40474900	-0.28746800	3.89519500
H	-5.55066400	-1.02006000	2.77233500
H	-4.87844400	1.36169600	2.08781000
H	-1.71218000	2.47669500	-2.14690600
H	-1.24734200	-1.78083100	-2.10296900
C	-2.67974600	-4.04194400	-1.41608400
H	-1.99940900	-4.17903500	-2.26560900
H	-3.64033000	-3.72194400	-1.83785500
C	-2.86333500	-5.38083200	-0.69324800
H	-3.55017600	-5.24655200	0.15189000
H	-1.90381800	-5.69472900	-0.26292700
C	-3.39524500	-6.49325500	-1.60457700
H	-2.70819500	-6.62503000	-2.44903200
H	-4.35301100	-6.17820000	-2.03581100
C	-3.57677400	-7.83082600	-0.88139400

H	-4.28628200	-7.73848300	-0.05312000
H	-3.95460100	-8.60176700	-1.55860900
H	-2.62836300	-8.18736400	-0.46716600

$[PaO(H_2O)_5$ (L16) $]^{3+}$-A

Sum of electronic and thermal Free Energies= -1854.591627

O	1.37632300	-3.44043700	0.39709300
H	1.16414200	-3.71508900	1.29863600
H	1.85387900	-4.16539500	-0.02747300
O	3.96780200	0.17615700	-1.31903500
O	3.25442200	-2.72538000	-1.59744900
O	1.27656100	-1.42436900	2.29518700
O	3.19880700	0.84748900	1.28892700
H	4.43926400	-0.18322900	-2.08103600
H	4.57901700	0.75161500	-0.84170600
H	4.13242500	-3.09347200	-1.43538000
H	1.84422200	-1.57550900	3.06276400
H	3.85046700	0.67782800	1.98125900
H	3.03301700	-2.88137700	-2.52491000
H	0.40395800	-1.16058400	2.61586400
H	2.86330700	1.74506400	1.40960100
Pa	2.21248400	-1.08313700	0.03520900
O	3.63400300	-1.74139600	0.93326300
C	-1.23021600	-0.58655600	-0.54708600
O	-0.01009100	-0.73679300	-0.13602300
N	-1.87964100	0.52192900	-0.24711200
C	-1.83189700	-1.70399900	-1.37102000
H	-2.84358900	-1.42047000	-1.65425300
C	-1.92122600	-3.00904200	-0.54012300
H	-0.91307900	-3.37516100	-0.34035500
H	-2.37147100	-2.78174700	0.43115100
C	-1.18587300	1.63840100	0.45274400
H	-1.95546500	2.20984400	0.96820000
H	-0.53859600	1.20860000	1.21452500
C	-3.31851500	0.72462400	-0.58195700
H	-3.49874900	1.79402900	-0.49308800
H	-3.47292300	0.46947100	-1.62943800
C	-4.31920700	-0.04108300	0.31289800
H	-4.10753200	-1.11167400	0.21317200
C	-5.72172400	0.22177000	-0.28024400
H	-5.92118700	1.30046500	-0.23976000
C	-6.89069900	-0.52379500	0.37456500
H	-7.01389600	-0.19328800	1.41093000
C	-8.21572600	-0.31131100	-0.36832200
H	-8.10786100	-0.65335800	-1.40455400
C	-9.39451100	-1.03542100	0.28856800
H	-9.54860300	-0.68809200	1.31505100
H	-10.32338700	-0.86605900	-0.26293300
H	-9.22223000	-2.11573000	0.32674300
C	-0.35658600	2.55633800	-0.47458200
H	0.38568500	1.92521800	-0.97608500
C	0.41468700	3.55631100	0.41319600
H	0.95135200	2.98985600	1.18582100
C	1.41586600	4.43998700	-0.34032700
H	0.89507100	5.02951100	-1.10232700
C	2.18595600	5.39760400	0.57791800
H	2.71721300	4.82119800	1.34468700
C	3.18348800	6.27956600	-0.17842900
H	2.67603000	6.89455600	-0.92828700
H	3.71393600	6.95272200	0.50047600
H	3.93165700	5.67292200	-0.69838100
C	-1.18548200	3.23145600	-1.59110100
H	-0.48644500	3.65740900	-2.31661200
C	-2.16035300	4.33004700	-1.14874900
H	-2.87647100	3.98639500	-0.39698500
H	-1.63718800	5.19192300	-0.72793100
H	-2.73785000	4.68522900	-2.00587100
C	-4.18354800	0.33691000	1.80788900
H	-3.15793000	0.65295500	2.01389000
C	-4.50745000	-0.79460800	2.79271000
H	-3.83791500	-1.64591800	2.63710700
H	-4.37318600	-0.45299000	3.82271800
H	-5.53135800	-1.15732900	2.69502200
H	-4.81353800	1.20962800	2.01485600
H	-1.72918000	2.45842200	-2.14350000
C	-1.01220200	-1.86867800	-2.66835800
H	-1.50976600	-2.58357400	-3.32411000
H	-0.93259700	-0.92347400	-3.20969100
H	-0.00618000	-2.24088700	-2.46408700
H	-0.29374700	4.19143800	0.95737900
H	-5.69910000	-0.04458400	-1.34419200
H	2.12841600	3.80256600	-0.87949600
H	-6.66787100	-1.59732400	0.41276600
H	-8.43062200	0.76277800	-0.42129000
H	1.47097100	6.03249900	1.11444300
C	-2.75004900	-4.09695400	-1.22940900
H	-2.30129900	-4.41864500	-2.17177500

H	-2.82408200	-4.97555600	-0.58417000
H	-3.76631000	-3.75096900	-1.43955700

$[PaO(H_2O)_5$ (L17) $]^{3+}$-A

Sum of electronic and thermal Free Energies=

-1854.590340

O	1.36556600	-3.47460100	0.51072500
H	1.05087000	-3.73920000	1.38495600
H	1.86418500	-4.21343300	0.13768100
O	3.90522400	0.18261100	-1.17371600
O	3.26362300	-2.70797200	-1.45863100
O	1.16890100	-1.45656800	2.39360900
O	3.00557300	0.93815200	1.37103600
H	4.45867200	-0.19584300	-1.86810000
H	4.43978400	0.82425900	-0.68858800
H	4.13478500	-3.08800800	-1.28730400
H	1.73249900	-1.61014100	3.16372800
H	3.61505900	0.80966700	2.10938200
H	3.02647200	-2.90283800	-2.37489600
H	0.30225100	-1.17000700	2.71072700
H	2.53439200	1.76745800	1.52209700
Pa	2.14391600	-1.11163500	0.14539600
O	3.57033900	-1.68578700	1.09013900
C	-1.30097400	-0.60538500	-0.46816500
O	-0.08165100	-0.78174800	-0.06800800
N	-1.92313000	0.52015600	-0.17277800
C	-1.92084500	-1.68127200	-1.32227100
H	-2.98528200	-1.50702000	-1.45772400
C	-1.68767000	-3.13659000	-0.86174400
H	-0.61242300	-3.29677400	-0.77632800
C	-1.19849100	1.63951200	0.48991500
H	-1.95595400	2.25663200	0.96886400
H	-0.57453400	1.22405700	1.27904200
C	-3.35916800	0.74818600	-0.50500000
H	-3.50984500	1.82469500	-0.46192600
H	-3.52917800	0.45260600	-1.53917400
C	-4.37035600	0.04933400	0.43208800
H	-4.17424200	-1.02766600	0.39231600
C	-5.77126000	0.29744400	-0.17120300
H	-5.96174100	1.37845700	-0.18255600
C	-6.94355000	-0.40761200	0.52170500
H	-7.06194800	-0.02686500	1.54120900
C	-8.26966900	-0.22474800	-0.22686200
H	-8.16472100	-0.61116700	-1.24770000
C	-9.44784900	-0.91863900	0.46299100
H	-9.59819700	-0.52910400	1.47478500
H	-10.37813100	-0.77042200	-0.09220000
H	-9.27741500	-1.99680500	0.54515600
C	-0.33086000	2.49657700	-0.46127000
H	0.43518600	1.83793700	-0.88729300
C	0.39471200	3.56187800	0.38828300
H	0.87640000	3.06637100	1.24226500
C	1.44447800	4.38005200	-0.37299900
H	0.97000100	4.91036700	-1.20552100
C	2.17080500	5.40279200	0.51023100
H	2.66650400	4.88355600	1.33922500
C	3.20186300	6.23278700	-0.25961900
H	2.72907700	6.79396600	-1.07169700
H	3.70169500	6.95194600	0.39488200
H	3.97222100	5.59375500	-0.70260800
C	-1.11464900	3.09780200	-1.65081800
H	-0.38810700	3.47507800	-2.37616500
C	-2.10078500	4.22451300	-1.31342700
H	-2.82846800	3.93598400	-0.54972800
H	-1.58725100	5.11753600	-0.94949900
H	-2.66305900	4.51109800	-2.20549200
C	-4.22725500	0.50696700	1.90439500
H	-3.19863700	0.82450100	2.09165100
C	-4.55948300	-0.56589000	2.95048000
H	-3.89688400	-1.42947700	2.84195300
H	-4.42245300	-0.16855100	3.95994800
H	-5.58630100	-0.92526500	2.87288000
H	-4.84871400	1.39550300	2.06447000
H	-1.64090200	2.29068300	-2.17025900
H	-0.34083100	4.24000600	0.83538500
H	-5.75409400	-0.02053100	-1.22099700
H	2.18013500	3.70064500	-0.82212100
H	-6.72643500	-1.47929600	0.61133800
H	-8.48317600	0.84638200	-0.32535100
H	1.43178400	6.07174000	0.96699300
C	-2.22729000	-4.09218300	-1.93458400
H	-1.74644900	-3.92067000	-2.90158900
H	-2.04380900	-5.13035900	-1.64674000
H	-3.30696200	-3.96839800	-2.06756200
H	-1.45508700	-1.54549600	-2.30759200
C	-2.32054200	-3.42612300	0.50454800
H	-3.40862200	-3.31448300	0.46901600
H	-2.10329300	-4.45261700	0.81092200

H	-1.93683900	-2.76235200	1.28465000

$[PaO(H_2O)_5$ (L18) $]^{3+}$-A

Sum of electronic and thermal Free Energies= -1893.873819

O	1.47645300	-3.35078100	0.48714600
H	1.23573200	-3.61967700	1.38332700
H	1.92082000	-4.09729100	0.06406100
O	4.04407900	0.29310900	-1.21519700
O	3.39839900	-2.58236100	-1.49742000
O	1.29817500	-1.31476700	2.35107200
O	3.15575500	1.05591300	1.34000300
H	4.64037700	-0.13080900	-1.84513400
H	4.55454200	0.95490100	-0.73063200
H	4.23766800	-3.01080200	-1.28529200
H	1.84519800	-1.44055300	3.13801600
H	3.76158900	0.91505800	2.07929800
H	3.19255500	-2.77037500	-2.42262500
H	0.41012900	-1.06636400	2.64025500
H	2.66088600	1.86624200	1.51949500
Pa	2.27740400	-0.99304600	0.10901500
O	3.69964100	-1.57778400	1.05364800
C	-1.15093300	-0.57503100	-0.58483700
O	0.05662500	-0.66701600	-0.11903000
N	-1.88085700	0.47846400	-0.27535900
C	-1.65220800	-1.68812900	-1.48011200
H	-2.65559400	-1.43396300	-1.81154900
C	-1.72429600	-3.02706000	-0.72256100
H	-0.73525300	-3.35504600	-0.40579400
H	-2.36715200	-2.95977500	0.15727600
C	-1.29086700	1.60606300	0.49831300
H	-2.11935700	2.09159000	1.00744600
H	-0.63807200	1.18429500	1.26162700
C	-3.30757800	0.62830600	-0.68972300
H	-3.54628300	1.67851700	-0.53765800
H	-3.37231500	0.44864800	-1.75988300
C	-4.33095200	-0.23039700	0.09403200
H	-4.07771800	-1.28681600	-0.05015900
C	-5.72977400	0.01356400	-0.56781600
H	-5.81376900	1.09718600	-0.73532300
C	-6.92986500	-0.38405800	0.31657000
H	-6.93748900	-1.47262500	0.45593800
H	-6.81382600	0.05711100	1.30983200
C	-8.29583700	0.06259000	-0.22633100
H	-8.26249200	1.13810900	-0.43987700
H	-8.51077000	-0.43339200	-1.17749000
C	-9.43720500	-0.22625200	0.75421000
H	-9.28439200	0.29505800	1.70443600
H	-10.40025800	0.09578400	0.34854200
H	-9.50920600	-1.29666400	0.97148500
C	-0.49299100	2.60736500	-0.36929700
H	0.27365800	2.01476900	-0.88141900
C	0.30757000	3.57684100	0.55515000
H	0.97278400	2.91830900	1.13179100
C	1.20959700	4.51404500	-0.27323500
H	0.59223600	5.27934300	-0.75813400
H	1.67175700	3.93463700	-1.08207200
C	2.32551600	5.20885300	0.51914100
H	2.94154200	4.45199200	1.02059000
H	1.89587200	5.82884400	1.31178200
C	3.22169100	6.07901400	-0.36771200
H	2.64319800	6.86897200	-0.85662800
H	4.01231500	6.55799100	0.21607800
H	3.69922200	5.48367500	-1.15220000
C	-1.31528700	3.25693200	-1.50858500
H	-0.61145200	3.75538000	-2.18076500
C	-2.42710100	4.25303800	-1.14955500
H	-3.10663100	3.88130300	-0.37782700
H	-2.02387300	5.20360700	-0.79702100
H	-3.03004000	4.46600900	-2.03619900
C	-4.24844300	0.06824000	1.61159000
H	-3.23067500	0.37765800	1.85992000
C	-4.58038600	-1.11800100	2.52669900
H	-3.88935600	-1.94709100	2.34723700
H	-4.48109800	-0.82791900	3.57638100
H	-5.59294700	-1.49520300	2.38127200
H	-4.88365500	0.92740400	1.85269600
H	-1.74349700	2.44709600	-2.10811100
C	-0.76335500	-1.79235300	-2.73617800
H	-1.21389400	-2.51216400	-3.42223900
H	-0.68235600	-0.83517800	-3.25567800
H	-2.14302300	-3.78344500	-1.38941300
H	0.24015900	-2.14710900	-2.49360200
C	-0.52180000	4.34359900	1.60208700
H	0.13933600	4.85021900	2.30798300
H	-1.15852300	5.10235000	1.14571700
H	-1.15890800	3.67984600	2.19072300
C	-5.81909900	-0.69150100	-1.93437100

H	-5.00061100	-0.42421500	-2.60585500
H	-5.80276000	-1.77857300	-1.80335000
H	-6.74321100	-0.43331600	-2.45413800

$[PaO(H_2O)_5$ (L19) $]^{3+}$-A

Sum of electronic and thermal Free Energies= -1893.886918

O	1.40717300	-3.48735100	0.52393400
H	1.19724800	-3.75632700	1.42779400
H	1.86273700	-4.22546900	0.09697700
O	4.04470400	0.00371300	-1.33497600
O	3.25556100	-2.87754800	-1.52033200
O	1.32617700	-1.31135800	2.34040300
O	3.29280000	0.79398100	1.27867600
H	4.36503800	-0.26164100	-2.20584300
H	4.72594800	0.54890200	-0.92218300
H	4.14758400	-3.21935300	-1.37717900
H	1.86067600	-1.43519100	3.13604500
H	3.96302000	0.63912300	1.95659300
H	3.03021700	-3.02297500	-2.44867400
H	0.42022800	-1.11910500	2.61526600
H	2.96530000	1.69651200	1.38558300
Pa	2.28376100	-1.16672700	0.07826600
O	3.70134800	-1.81093900	0.99144300
C	-1.16102100	-0.68833900	-0.53985400
O	0.06164600	-0.82726000	-0.13371300
N	-1.81309100	0.42304400	-0.25819200
C	-1.76495600	-1.82205000	-1.34174800
H	-2.77548100	-1.54339400	-1.62988900
C	-1.84244500	-3.11638600	-0.51112400
H	-0.84860200	-3.47302000	-0.24427000
H	-2.41979800	-2.97570400	0.40481800
C	-1.11977100	1.55565900	0.41457600
H	-1.88363000	2.11525500	0.95123400
H	-0.44210000	1.14178200	1.15796600
C	-3.25537200	0.61397500	-0.58610500
H	-3.43763000	1.68419100	-0.51558100
H	-3.41636900	0.33942000	-1.62753400
C	-4.25112900	-0.13649500	0.32936800
H	-4.04687200	-1.20741500	0.23239300
C	-5.65572400	0.15935600	-0.24854200
H	-5.82863200	1.23954300	-0.16335900
C	-6.86910900	-0.57232200	0.36007900
H	-6.90752900	-0.35053300	1.43291800
C	-8.16354000	-0.00367700	-0.25896200
H	-8.12690000	1.08968500	-0.19079300
H	-8.17997300	-0.24231800	-1.33023200
C	-9.46045200	-0.49155200	0.39550700
H	-9.46392200	-0.27668700	1.46908300
H	-10.32762500	0.00852800	-0.04461100
H	-9.60625800	-1.56739800	0.27077900
C	-0.33463300	2.48304500	-0.54188400
H	0.38657200	1.85438300	-1.07408700
C	0.45597100	3.48259400	0.33037500
H	1.06985500	2.90825500	1.03835900
C	1.36352100	4.48554700	-0.41230800
H	0.72807100	5.10215800	-1.06024300
C	2.01997800	5.43622100	0.61003600
H	2.71549300	4.86174700	1.23571800
H	1.24014400	5.80846000	1.28401000
C	2.75336600	6.63448600	-0.00192900
H	2.08413600	7.22083700	-0.63967800
H	3.13025600	7.29796900	0.78119700
H	3.60856500	6.32774800	-0.60901000
C	-1.21291400	3.16245200	-1.61678800
H	-0.54741400	3.62216500	-2.35346800
C	-2.19830400	4.22921700	-1.12175900
H	-2.88775000	3.85424800	-0.36000200
H	-1.68209300	5.09161100	-0.69398700
H	-2.80529800	4.59229500	-1.95485000
C	-4.08364300	0.25629300	1.81701000
H	-3.04014700	0.52107000	2.00521000
C	-4.45130500	-0.83366000	2.83304100
H	-3.84848000	-1.73283600	2.67453400
H	-4.25726600	-0.48214900	3.85007500
H	-5.50103300	-1.12484300	2.78143700
H	-4.66465900	1.16469600	2.01390500
H	-1.75550500	2.38945900	-2.17018900
C	-0.94925500	-2.02441300	-2.63483600
H	-1.43815100	-2.78853900	-3.24205000
H	-0.89422400	-1.10693500	-3.22463900
H	-2.33855100	-3.88502600	-1.10713600
H	0.06534800	-2.36415100	-2.41797500
H	-0.24714100	4.04913400	0.95171300
H	-5.64075100	-0.06247600	-1.32392300
C	-6.77275400	-2.09373000	0.17770500
H	-7.62066100	-2.60743100	0.63616500
H	-6.76119800	-2.35256500	-0.88710200

H	-5.86628600	-2.50338000	0.62901000
C	2.40307000	3.79010600	-1.30274900
H	3.07529200	3.16100200	-0.70887700
H	1.93265800	3.15365500	-2.05597200
H	3.02016900	4.51562700	-1.83675800

$[PaO(H_2O)_5$ (L20) $]^{3+}$-A

Sum of electronic and thermal Free Energies=

-1893.890365

O	1.33800700	-3.42420000	0.40689000
H	1.15608900	-3.71288800	1.31072200
H	1.79928800	-4.14314200	-0.04522300
O	3.94269400	0.18643400	-1.30087100
O	3.22009300	-2.71684900	-1.58318300
O	1.24956400	-1.41362800	2.31096900
O	3.18136100	0.85065600	1.31208400
H	4.40929900	-0.16855100	-2.06792100
H	4.55610900	0.76102200	-0.82533200
H	4.09846200	-3.08494500	-1.42304700
H	1.81481900	-1.56820700	3.07964200
H	3.83478700	0.67313900	2.00083100
H	3.00303000	-2.85940300	-2.51388700
H	0.37517900	-1.15371000	2.62998400
H	2.83961500	1.74324100	1.44983600
Pa	2.18766200	-1.07005200	0.05349700
O	3.60658200	-1.73788200	0.94841600
C	-1.25278200	-0.55121400	-0.53133400
O	-0.03304200	-0.70864000	-0.12336100
N	-1.89773000	0.55880400	-0.22883800
C	-1.86229700	-1.66528100	-1.35661100
H	-2.87146500	-1.37584000	-1.63852100
C	-1.94635400	-2.97427400	-0.54926600
H	-0.95434900	-3.34318000	-0.29159500
H	-2.52060500	-2.84602700	0.37055100
C	-1.20293400	1.66980900	0.47911500
H	-1.97310200	2.23895900	0.99639800
H	-0.55833700	1.23428400	1.24005400
C	-3.33574300	0.76798200	-0.56509800
H	-3.51245300	1.83714000	-0.46777600
H	-3.48836800	0.52238400	-1.61511100
C	-4.34183500	-0.00156300	0.32070700
H	-4.14452500	-1.07274800	0.20071600
C	-5.74386200	0.29149200	-0.26061700
H	-5.93078400	1.36798300	-0.17523100
C	-6.90744700	-0.48809400	0.36618100
H	-7.05460700	-0.17624100	1.40631800
C	-8.24796700	-0.33491600	-0.37965800
H	-8.07866500	-0.61739200	-1.42777400
C	-9.29431000	-1.29627500	0.20157000
H	-9.49951900	-1.05990700	1.25157900
H	-10.23951600	-1.22853900	-0.34492400
H	-8.95143300	-2.33414500	0.15375700
C	-0.36962700	2.59244000	-0.43999300
H	0.37856400	1.96423500	-0.93647600
C	0.38987200	3.59497800	0.45612300
H	0.92434400	3.03061500	1.23197700
C	1.39551400	4.47443000	-0.29830000
H	0.87200600	5.09786400	-1.03243500
C	2.25254500	5.39544200	0.59318400
H	2.75051900	4.76876100	1.34542700
C	3.34462800	6.07693700	-0.24345300
H	2.90087700	6.71490100	-1.01572300
H	3.98479900	6.70693600	0.38093900
H	3.98142900	5.34133300	-0.74369700
C	-1.19200000	3.26711500	-1.56163500
H	-0.48865600	3.69649300	-2.28093800
C	-2.17358700	4.36220700	-1.12529400
H	-2.89297900	4.01641200	-0.37769500
H	-1.65610500	5.22603900	-0.70168200
H	-2.74719300	4.71503700	-1.98599900
C	-4.19433100	0.34805800	1.82146000
H	-3.16206800	0.64116100	2.02850400
C	-4.53569100	-0.79302500	2.78916000
H	-3.88973600	-1.65796900	2.61046700
H	-4.38116700	-0.47354400	3.82342200
H	-5.56947700	-1.12781300	2.69717500
H	-4.80720600	1.22872300	2.04549100
H	-1.72910800	2.49331000	-2.11944000
C	-1.05058600	-1.84860700	-2.65519200
H	-1.55247100	-2.59018600	-3.27962200
H	-0.98314000	-0.91822900	-3.22307800
H	-2.44922600	-3.72865300	-1.15775400
H	-0.04068900	-2.20973700	-2.45090500
H	-0.33166000	4.21842200	0.99285100
H	-5.72370800	0.06750700	-1.33463200
H	2.06674700	3.82311400	-0.87187000
H	-6.64777800	-1.55316000	0.39370700
C	-8.77219300	1.10832400	-0.35736500

H	-8.92801200	1.44700500	0.67325200
H	-8.08183500	1.80577200	-0.83797100
H	-9.73060600	1.18118200	-0.87963700
C	1.41244700	6.44401300	1.33684100
H	0.87590500	7.08375300	0.62724500
H	0.67483900	5.98693500	2.00074500
H	2.05086200	7.08849300	1.94801000

$[PaO(H_2O)_6]^{3+}$

Sum of electronic and thermal Free Energies=

-975.162285

O	2.34891700	0.75324700	-0.40316200
H	2.54498200	1.56211800	-0.89376900
H	3.01148100	0.09080100	-0.64264800
O	0.00726800	0.35674500	2.69809300
O	-1.54661100	-1.94354900	-0.28778900
O	1.59527600	-1.91666900	-0.32151500
O	0.00103900	2.33331800	-0.68878300
O	-2.37457700	0.68899200	-0.31826800
H	0.80333800	0.77317500	3.05857000
H	-0.74206800	0.86597200	3.03910700
H	-1.54634100	-2.47194000	-1.09700200
H	-1.84904500	-2.51213700	0.43520900
H	1.61786800	-2.41375400	-1.14994900
H	-0.03849800	2.59394700	-1.61932200
H	-2.99643000	0.00399200	-0.59899500
H	1.90745800	-2.50088100	0.38450700
H	0.00054500	3.13492700	-0.14757000
H	-2.62051000	1.51170100	-0.76116700
Pa	0.01697800	-0.02312400	0.04592500
O	-0.01415800	-0.21819800	-1.73345800

$[PaO(H_2O)_5]^{3+}$

Sum of electronic and thermal Free Energies=

-898.724726

O	-2.37315900	0.69741500	0.06534700
H	-2.66995600	1.59669700	0.25561500
H	-3.00549200	0.07545900	0.44819900
O	1.64327200	-1.84320400	0.23103800
O	-1.54427000	-1.88759700	0.34373200
O	-0.01899100	2.37055400	0.40227100
O	2.34446500	0.79780900	0.10890200
H	1.64169000	-2.25788800	1.10425500
H	1.92878100	-2.51061000	-0.40847000
H	-1.52851300	-2.25596400	1.23696700
H	-0.07368400	2.65522800	1.32411400
H	2.97275400	0.14151400	0.44007200
H	-1.86959600	-2.57257100	-0.25677000
H	-0.01346700	3.15624400	-0.16264700
H	2.53441700	1.63955600	0.54329800
Pa	-0.00483400	-0.00144200	-0.28330700
O	0.01405200	-0.07703300	1.50574400

$[PaO(H_2O)_5(L_1)]^{3+}$-E

Sum of electronic and thermal Free Energies=

-1540.230337

O	-3.57525700	0.21873700	1.94964300
H	-3.17710800	0.14851600	2.82855900
H	-4.31538600	-0.40153100	1.90562700
O	-1.63915200	-1.05894900	-2.15327600
O	-4.14214900	-0.85450800	-0.46443200
O	-0.93630400	0.28538600	2.43719900
O	-3.86378500	1.81646500	-0.27439300
H	-1.73236300	-2.01497100	-2.24862100
H	-1.72010400	-0.66359500	-3.03171100
H	-4.30649800	-1.78902800	-0.64426200
H	-0.40939800	-0.46258500	2.74755400
H	-3.79497900	2.57408100	-0.87124200
H	-4.81574700	-0.33071500	-0.91937700
H	-0.56513800	1.08201700	2.83932800
H	-4.28122500	2.12800100	0.54074400
Pa	-1.89751100	0.11825500	0.03975300
O	-1.70073200	-1.60345900	0.54476700
C	1.58644000	0.58754700	-0.20905400
O	0.32321400	0.35108700	-0.27785100
N	2.44007700	-0.28823900	-0.70141800
C	2.01366900	1.89304400	0.40609500
H	1.31168200	2.09871500	1.21595600
H	3.00489800	1.81348900	0.85052300
C	1.97224800	3.05435700	-0.61233500
H	2.64335800	2.83488000	-1.44958400
H	0.96267500	3.13077100	-1.02850700
C	2.37213000	4.38790800	0.02861100
H	1.69707500	4.60195700	0.86486300
H	3.37607800	4.29387300	0.45754700
C	2.34606700	5.55145800	-0.96560100
H	3.04043000	5.37917100	-1.79348100
H	1.34687000	5.68641200	-1.39050800

C	1.94695500	-1.55837800	-1.29436300
H	1.04969700	-1.33009800	-1.86875800
H	2.71508600	-1.88885100	-1.99340800
C	3.90540400	-0.05595100	-0.71728600
H	4.26382000	-0.42833300	-1.67819900
H	4.09116900	1.01570100	-0.71015700
C	4.65314900	-0.73845600	0.43266900
H	4.22908600	-0.41015800	1.38776900
H	4.50907900	-1.82095700	0.37712300
C	6.15394100	-0.42501400	0.39428900
H	6.56362100	-0.73616900	-0.57338300
H	6.30014200	0.65916000	0.45847100
C	6.92639300	-1.11479800	1.52217100
H	6.55865000	-0.79888300	2.50308100
H	6.82410000	-2.20253900	1.46215800
C	1.65800600	-2.65326100	-0.25963300
H	0.89216300	-2.30288700	0.43725400
H	2.55915800	-2.85236600	0.32665500
C	1.19167000	-3.95303800	-0.92681300
H	0.29377500	-3.75808900	-1.52377100
H	1.95930000	-4.29613400	-1.62990900
C	0.89367500	-5.06116300	0.08702500
H	0.10453900	-4.75712600	0.78115100
H	1.78169700	-5.30597100	0.67749600
H	7.99182500	-0.87639900	1.47222900
H	2.63186600	6.48818000	-0.48034300
H	0.56391600	-5.97470000	-0.41439200

$[PaO(H_2O)_6(L1)]^{3+}$

Sum of electronic and thermal Free Energies=

-1616.668646

O	-0.77562500	-2.43864500	-1.01282600
H	-0.86242100	-2.59716800	-1.96229100
H	-0.93402200	-3.27839800	-0.56170300
O	-3.40112900	0.43609000	1.79121700
O	-0.79808900	-0.06840100	2.33866800
O	-2.16613100	-2.20972100	1.46902500
O	-1.41274400	-0.23703800	-2.56393600
O	-3.29507900	1.60670300	-0.81898400
H	-4.02513300	-0.20670000	2.15380200
H	-3.92164700	1.21357700	1.54503900
H	0.11140800	0.12941700	2.59473600
H	-2.88166100	-2.85703700	1.43079100
H	-2.14444200	-0.34595500	-3.18591900
H	-4.07494700	1.39857700	-1.34887800
H	-1.38299300	0.42501500	2.93057900
H	-1.72361800	-2.27555500	2.32611500
H	-0.71214000	0.24656900	-3.02121300
H	-3.05510800	2.52501700	-0.99858200
Pa	-1.79356200	-0.32703800	-0.09903300
O	-3.30669200	-1.08798400	-0.73540700
C	1.50421000	0.90135900	-0.45429700
O	0.36388700	0.30182000	-0.35220200
N	2.57167500	0.19424100	-0.75989200
C	1.57187800	2.39566500	-0.23521500
H	2.35490300	2.59558700	0.50248600
H	1.90989100	2.85443700	-1.17078100
C	0.26111900	3.04940000	0.20713000
H	-0.50513300	2.88345300	-0.55739200
H	-0.10086800	2.58095600	1.12679100
C	0.42887900	4.55643800	0.43561000
H	1.20638700	4.72115500	1.19010600
H	0.79089500	5.02310100	-0.48755800
C	-0.86817900	5.23613300	0.88007400
H	-1.65677200	5.11062900	0.13175700
H	-1.23199400	4.81574700	1.82261900
C	2.47739400	-1.27297800	-0.97589000
H	1.58608600	-1.47241700	-1.56799100
H	3.34405700	-1.54242900	-1.57970300
C	3.90303700	0.80407800	-0.98959200
H	4.22486000	0.47010500	-1.97930900
H	3.79545200	1.88368900	-1.03604600
C	4.94506800	0.42374600	0.06591800
H	4.58226600	0.71831400	1.05618700
H	5.08082500	-0.66148800	0.08367900
C	6.29545100	1.09385000	-0.21818200
H	6.63061800	0.81773100	-1.22447000
H	6.16769900	2.18216500	-0.22246200
C	7.37041600	0.70737800	0.80110900
H	7.07684300	0.99705100	1.81450500
H	7.54491800	-0.37274900	0.79974000
C	2.45182000	-2.09921300	0.31486400
H	1.52960300	-1.89274200	0.86412600
H	3.28225200	-1.80250500	0.96147600
C	2.54489000	-3.60134400	0.01754500
H	1.73681400	-3.88722000	-0.66432000
H	3.48222200	-3.80680600	-0.51185900
C	2.47358900	-4.45847400	1.28406100

H	1.52972300	-4.30122700	1.81482200
H	3.28804700	-4.21379400	1.97243500
H	8.32000800	1.19896300	0.57500300
H	-0.71865300	6.30839100	1.02951300
H	2.54780900	-5.52211300	1.04370300

In Figure 4(a)

$[PaO(H_2O)_5]^{3+}(H_2O)$ (fixing Pa-O(H_2O) 3.28Å)

Sum of electronic and thermal Free Energies=

-975.161462

O	-2.44197900	-0.49299600	-0.33408400
H	-2.77791700	-1.34689900	-0.63662800
H	-3.05183800	0.19364400	-0.63611600
O	0.05413900	-0.18127600	3.32537100
O	1.77477900	1.73290000	-0.36294900
O	-1.32681500	2.10403900	-0.44913200
O	-0.18104200	-2.30715600	-0.67458700
O	2.22813700	-0.97743200	-0.13701700
H	-0.83282700	-0.44758100	3.59548400
H	0.60235500	-0.95530800	3.50201700
H	1.87155800	2.14572900	-1.23132400
H	2.12019600	2.34855000	0.29851400
H	-1.30791300	2.51787600	-1.32247700
H	-0.25076800	-2.56341400	-1.60413700
H	2.97090700	-0.42059300	-0.40679300
H	-1.58693900	2.77592300	0.19697000
H	-0.34805900	-3.08850100	-0.12861900
H	2.35618800	-1.85764300	-0.51493500
Pa	-0.04276800	0.04944900	0.05493200
O	0.04117800	0.16218200	-1.73010500

In Figure 4(a)

$[PaO(H_2O)_5]^{3+}(H_2O)$ (fixing Pa-O(H_2O) 3.78Å)

Sum of electronic and thermal Free Energies=

-975.164848

O	-2.44502100	-0.48968600	-0.30873300
H	-2.78114900	-1.34333400	-0.61167100
H	-3.05029100	0.19761100	-0.61852500
O	-0.01494300	-0.16165600	3.85473100
O	1.77406500	1.73087700	-0.33809800
O	-1.32622000	2.10775100	-0.43082800
O	-0.18484600	-2.30855000	-0.64681000
O	2.22444500	-0.98103600	-0.10819100
H	-0.82074600	-0.68992600	3.84490100
H	0.68976300	-0.81740300	3.81015500
H	1.87731300	2.13713300	-1.20880100
H	2.12227700	2.34764900	0.32073100
H	-1.30516000	2.51775700	-1.30591600
H	-0.25610200	-2.56496200	-1.57617400
H	2.96933700	-0.42887500	-0.38141300
H	-1.58611800	2.78287200	0.21181400
H	-0.35339400	-3.08942800	-0.10069400
H	2.34868100	-1.86396500	-0.48097800
Pa	-0.04432600	0.04987900	0.08076900
O	0.04080700	0.15902700	-1.70523300

In Figure 4(b)

$[PaO(H_2O)_5]^{3+}(H_2O)$ (fixing Pa-O(H_2O) 2.96Å)

Sum of electronic and thermal Free Energies=

-975.159371

O	-2.38495600	-0.60768500	-0.28581500
H	-2.60216600	-1.44610300	-0.71542800
H	-3.03852800	0.05459800	-0.54716800
O	0.01148900	-0.22130700	2.76998600
O	1.74166900	1.70733900	-0.33693700
O	-1.30892900	1.98629000	-0.41124000
O	-0.40111000	-2.38709000	-0.67747100
O	2.57598300	-1.28163400	-0.65243300
H	-0.24390100	0.56180600	3.27715600
H	-0.45187400	-0.97304200	3.16491900
H	1.89796200	2.07468400	-1.21589200
H	2.18522200	2.26968100	0.31173000
H	-1.30198100	2.38766000	-1.29043400
H	-0.08661400	-2.62913100	-1.55917600
H	3.27969200	-1.08794900	-0.02050600
H	-1.59466100	2.65628700	0.22569500
H	-0.30975300	-3.16714000	-0.11170100
H	2.87284000	-0.89710500	-1.48654000
Pa	-0.00116000	-0.03803100	0.10478800
O	0.11208500	0.05223400	-1.67735000

In Figure 4(b)

$[PaO(H_2O)_5]^{3+}(H_2O)$ (fixing Pa-O(H_2O) 3.16Å)

Sum of electronic and thermal Free Energies=

-975.153308

O	-2.37914500	-0.52406900	-0.32754300
H	-2.62009100	-1.36473700	-0.73997300
H	-3.01584900	0.15228700	-0.59651200

O	-0.03425800	-0.20481200	2.79495700
O	1.77185800	1.68387000	-0.28594700
O	-1.28113200	2.06184300	-0.50781000
O	-0.42754900	-2.35305200	-0.63635000
O	2.80321100	-1.28854800	-0.40506200
H	-0.87681000	-0.09948300	3.25814100
H	0.40471500	-0.97520800	3.18195400
H	1.93852100	2.03356700	-1.17068200
H	2.16033800	2.29065200	0.35882200
H	-1.19797200	2.43896100	-1.39373700
H	-0.16729600	-2.61001700	-1.53112800
H	3.37730700	-0.51284300	-0.43077900
H	-1.54095400	2.77016300	0.09761600
H	-0.38738100	-3.14196900	-0.07712000
H	2.81626800	-1.62797600	-1.30844600
Pa	-0.03069200	-0.00156200	0.14106900
O	0.17919800	0.03966300	-1.63288700

In Figure 4(b)

$[PaO(H_2O)_5]^{3+}(H_2O)$ (fixing Pa-O(H_2O) 3.36Å)

Sum of electronic and thermal Free Energies=

-975.161086

O	-2.22805800	-0.54093700	-0.67676400
H	-2.28613000	-1.34077100	-1.21636800
H	-2.78487100	0.14527100	-1.06893100
O	-0.02229200	-0.03783100	2.92827500
O	1.46783200	2.12096300	0.05472000
O	-1.48098200	2.02982100	-0.57663200
O	-0.15030100	-2.23087800	-0.45803500
O	2.30802300	-1.90496400	-1.06011100
H	-0.69525700	-0.57361700	3.36915900
H	0.82079400	-0.23418800	3.35955400
H	1.94362900	2.31324000	-0.76302900
H	1.82807800	2.67725900	0.75776600
H	-1.21009800	2.49496700	-1.37958800
H	0.76933200	-2.39695600	-0.81185200
H	3.02470900	-2.48561100	-0.77630000
H	-1.84353400	2.69201800	0.02891200
H	-0.36323100	-2.93059800	0.17596000
H	2.52518000	-1.63025500	-1.95960700
Pa	-0.02605100	0.12338800	0.25422600
O	0.43649300	0.22877800	-1.47037400

$Pa(OH)_2(NO_3)_3(H_2O)_2$

Sum of electronic and thermal Free Energies=

-1587.504757

Pa	0.06221300	-0.04063200	0.12287100
O	1.51140600	1.92756600	-0.13972800
O	-0.34482700	1.84736400	1.96238300
O	2.53495900	0.07375800	-0.51735000
O	1.09054100	-2.30026400	-0.40615700
O	1.05318900	-0.52305600	1.83068500
O	-1.02662100	-2.23945900	-0.03673400
O	-2.43735700	0.13404400	-0.65804000
O	0.06972100	-0.07624900	-1.90713200
O	-1.34134500	1.97973200	-0.47941600
H	0.40187300	2.04149100	2.54299000
H	-0.65140500	2.69119200	1.60450000
H	1.50219900	-0.78651400	2.64264000
H	-0.04043600	-0.07665600	-2.86519500
N	0.00426800	-2.95866300	-0.33399400
O	-0.07132400	-4.14407100	-0.52180100
N	2.61349500	1.34023300	-0.47758200
N	-2.43399100	1.39580700	-0.82872500
O	-3.37088800	2.00438200	-1.28146600
O	3.61668900	1.95694400	-0.72620700
O	-1.75360000	-0.44166100	1.91661600
H	-1.74914700	0.32319600	2.51128000
H	-2.65523100	-0.52907700	1.57936600

$Pa(OH)_2(NO_3)_3(H_2O)$(L1)

Sum of electronic and thermal Free Energies=

-2152.559164

C	-1.91216100	0.28967100	0.56232100
N	-2.81699600	-0.66896100	0.73638600
C	-2.23713300	1.75254400	0.72409000
H	-3.21161700	1.90624900	1.18332200
H	-1.47991500	2.14809800	1.40607500
C	-2.14893500	2.52558300	-0.60870700
H	-1.19094300	2.30670400	-1.08632800
H	-2.93162700	2.17452100	-1.29018800
C	-2.28702900	4.03734800	-0.40050400
H	-3.23407600	4.25158600	0.10834900
H	-1.48947400	4.37611200	0.27000200
C	-2.22101600	4.82386400	-1.71244100
H	-1.26787300	4.65738300	-2.22382200
H	-3.02229400	4.52404000	-2.39489000

C	-2.42506100	-2.09146200	0.60650200
H	-1.34084900	-2.14353900	0.65263100
H	-2.82878800	-2.61134500	1.47896600
C	-4.22709500	-0.40198200	1.10842300
H	-4.61057700	-1.34063600	1.50948200
H	-4.24887100	0.31612200	1.92936500
C	-5.12093300	0.06729600	-0.04443500
H	-4.75815100	1.02354600	-0.43241600
H	-5.05899700	-0.64918300	-0.86879100
C	-6.58061400	0.22024700	0.40022100
H	-6.94507600	-0.74045200	0.78183400
H	-6.63233300	0.92449700	1.23865100
C	-7.49505800	0.70264800	-0.72923500
H	-7.17422300	1.67805100	-1.10723400
H	-7.48856900	0.00130200	-1.56913100
C	-2.91935300	-2.75184200	-0.68449300
H	-2.55664900	-2.17552000	-1.54235600
H	-4.01331500	-2.73258700	-0.72565800
C	-2.43330700	-4.20215900	-0.79214700
H	-1.33844900	-4.21307000	-0.76179400
H	-2.77439400	-4.76490000	0.08469500
C	-2.91865200	-4.89896800	-2.06619400
H	-2.56813900	-4.37435000	-2.96031100
H	-4.01168500	-4.93248900	-2.10704300
H	-8.52780500	0.80143700	-0.38505800
H	-2.31990800	5.89793800	-1.53410600
H	-2.55158900	-5.92742700	-2.11770900
O	-0.71773500	-0.01405600	0.24692800
Pa	1.59039400	0.03797900	0.00271400
O	0.94546200	0.60994600	-1.89003800
O	3.19563900	0.40306800	1.21438800
O	2.65417100	2.37032700	-0.65690200
O	0.97419200	2.30899900	0.69058500
O	3.51078100	-0.28664200	-1.58253200
O	3.23698300	-1.98994900	-0.29526000
O	0.76924500	0.07592200	2.53716900
O	1.20524100	-1.82323800	1.61348300
O	0.69105600	-2.09976100	-1.18082500
H	1.35459400	0.96770700	-2.68655900
H	3.96722700	0.75170500	1.67340200
N	1.83740100	3.02727400	0.04620800
N	3.94437900	-1.43097000	-1.19502400
N	0.83670200	-1.17831500	2.67109500
H	0.38052100	-1.95631400	-2.08344500
H	1.28518400	-2.86138400	-1.20028000
O	1.83734600	4.23415700	0.12699700
O	4.94298700	-1.93150900	-1.65523200
O	0.57719300	-1.75621700	3.70239900

$Pa(OH)_2(NO_3)_3(H_2O)$(L2)

Sum of electronic and thermal Free Energies= -2270.455003

C	-1.55853000	-0.63857200	-0.60421600
N	-2.41858400	0.36148100	-0.44548800
C	-1.91801600	-1.89506500	-1.35847500
H	-2.86873900	-1.79718400	-1.87754100
C	-1.95228400	-3.14378700	-0.45209600
H	-0.97209300	-3.27874900	0.00685900
C	-2.03507500	1.56811900	0.32096300
H	-2.92452500	1.88698300	0.86892300
H	-1.27302500	1.29056900	1.04440900
C	-3.79867300	0.36604400	-0.97924200
H	-4.05837300	1.41335600	-1.14035400
H	-3.81659100	-0.10828000	-1.95890000
C	-4.81134300	-0.28374800	-0.03134700
H	-4.56463500	-1.34295400	0.09521800
C	-6.24949400	-0.14465500	-0.54359600
H	-6.48738700	0.91880300	-0.66947100
C	-7.28288600	-0.78736000	0.38835800
H	-7.19852800	-0.33782000	1.38598300
C	-8.72573200	-0.64319000	-0.10879500
H	-8.80998200	-1.09211000	-1.10583300
C	-9.75289800	-1.28545500	0.82807500
H	-9.71578400	-0.83270700	1.82398900
H	-10.77057700	-1.16603700	0.44615100
H	-9.56452600	-2.35743800	0.94442100
C	-1.52677400	2.69727300	-0.58227100
H	-0.61373200	2.36068900	-1.08244100
C	-1.25075300	3.98252700	0.20689800
H	-0.53148500	3.77096000	1.00583100
C	-0.71133700	5.11754900	-0.67123300
H	-1.42729300	5.32462700	-1.47709100
C	-0.43507900	6.41143300	0.10290900
H	0.28632800	6.20468100	0.90235700
C	0.09513600	7.54264100	-0.78307700
H	-0.62099900	7.79410700	-1.57183200
H	0.28272400	8.45016500	-0.20241800
H	1.03446600	7.25731600	-1.26736900

H	-2.17474000	4.31281000	0.69805200
H	-6.32725000	-0.59836700	-1.53941800
H	0.21371100	4.78668600	-1.16047700
H	-7.04779100	-1.85223900	0.51092900
H	-8.95909300	0.42123400	-0.23209300
H	-1.35681300	6.73826700	0.59923200
C	-2.32658400	-4.39971800	-1.24254600
H	-1.60501600	-4.58972800	-2.04256500
H	-3.31630200	-4.30433900	-1.69870100
H	-1.13830000	-2.03187900	-2.11179600
H	-2.67031900	-2.98894100	0.35939600
H	-4.72596400	0.17906200	0.95783100
H	-2.26506200	2.90295400	-1.36554600
H	-2.34185500	-5.27635200	-0.59027800
O	-0.39400800	-0.56158600	-0.09443400
Pa	1.93144900	-0.48088200	0.07270200
O	1.57396500	0.75858000	-1.55941600
O	3.32744200	-0.59087900	1.56513600
O	3.04961300	1.90255200	0.44983100
O	1.17872500	1.42720200	1.40871400
O	4.05631400	-0.33348200	-1.22624500
O	3.68044300	-2.35570300	-0.59182000
O	0.72564700	-1.30053300	2.28945300
O	1.35609300	-2.77073000	0.84380900
O	1.37049900	-1.98210000	-1.96691900
H	2.06593700	1.39818400	-2.08703100
H	4.07516800	-0.37592300	2.13316500
N	2.12779000	2.28782300	1.21916300
N	4.48025000	-1.54628100	-1.15606800
N	0.79496700	-2.52279600	1.98259500
H	1.39023400	-1.51385700	-2.81111300
H	1.87437500	-2.79866100	-2.07998700
O	2.10665500	3.37407800	1.75309200
O	5.55483600	-1.87559000	-1.60057400
O	0.37055300	-3.41477700	2.68159500

$Pa(OH)_2(NO_3)_3(H_2O)$(L3)

Sum of electronic and thermal Free Energies= -2309.75284

C	-1.54486900	-0.39115000	-0.59982500
N	-2.33090500	0.66854700	-0.44404800
C	-1.99812000	-1.62527900	-1.34032400
H	-2.94710500	-1.46688000	-1.84719600
C	-2.09958500	-2.85943400	-0.42058900
H	-1.12558600	-3.04635300	0.03498900
C	-1.85947600	1.84922800	0.31366300
H	-2.72062800	2.23142800	0.86632700
H	-1.11375500	1.52180200	1.03334900
C	-3.71000600	0.76551300	-0.97225600
H	-3.90157200	1.82844500	-1.12555900
H	-3.76127600	0.29976600	-1.95496300
C	-4.75974000	0.17642700	-0.02498200
H	-4.57879600	-0.89639000	0.09785300
C	-6.18736400	0.40446200	-0.53454900
H	-6.36270000	1.48092700	-0.65208900
C	-7.25585900	-0.18415600	0.39353800
H	-7.14559200	0.25272700	1.39427100
C	-8.68817900	0.04536400	-0.10171000
H	-8.79781900	-0.39020900	-1.10222500
C	-9.75004900	-0.54509900	0.83054400
H	-9.68810900	-0.10220400	1.82963900
H	-10.75926000	-0.36612400	0.44940100
H	-9.62208400	-1.62675900	0.93923600
C	-1.27997800	2.93884700	-0.59526400
H	-0.39568400	2.54020500	-1.10136100
C	-0.91002100	4.20050000	0.19378500
H	-0.21401000	3.93369600	0.99689800
C	-0.27745600	5.29042500	-0.67884800
H	-0.96610200	5.55089000	-1.49306300
C	0.08677800	6.55975700	0.09970500
H	0.77262600	6.29668900	0.91385200
C	0.72597900	7.64229000	-0.77474900
H	0.05043600	7.95061500	-1.57908900
H	0.97464800	8.53241900	-0.19010000
H	1.64911400	7.28017000	-1.23840800
H	-1.80875200	4.60106400	0.67949700
H	-6.29251400	-0.03637500	-1.53368100
H	0.62579100	4.89048500	-1.15711400
H	-7.08179000	-1.26156300	0.50848900
H	-8.86127500	1.12216900	-0.21654500
H	-0.81537300	6.96096300	0.57708400
C	-2.54754600	-4.10991600	-1.18505900
H	-1.84450500	-4.29919200	-2.00456300
H	-3.52260600	-3.92531100	-1.65048100
H	-1.24002600	-1.81878300	-2.10322500
H	-2.80391600	-2.65660800	0.39389000
C	-2.63324100	-5.34709900	-0.28680700
H	-3.35661700	-5.19881700	0.52091500

H	-2.94393700	-6.22780600	-0.85503100
H	-1.66461800	-5.56872000	0.17157400
H	-4.64433000	0.62958100	0.96562000
H	-2.00698600	3.19555500	-1.37403700
O	-0.37436100	-0.39329300	-0.09781900
Pa	1.94813100	-0.49282000	0.07299500
O	1.68183500	0.72984600	-1.58981900
O	3.33188200	-0.67909200	1.56985400
O	3.24811800	1.79954000	0.38862800
O	1.35267500	1.50166400	1.36939000
O	4.08372300	-0.52883600	-1.22211600
O	3.54723200	-2.50484900	-0.55764200
O	0.68291300	-1.17193400	2.30420400
O	1.20436600	-2.71757100	0.89428300
O	1.26749400	-1.99329800	-1.92984400
H	2.22720900	1.32117100	-2.12130600
H	4.09795700	-0.51704000	2.13094400
N	2.36750400	2.27635800	1.15564500
N	4.40942600	-1.76999600	-1.13327900
N	0.66090900	-2.40269000	2.02479400
H	1.31043800	-1.54194500	-2.78231700
H	1.71781700	-2.84205500	-2.03121400
O	2.44161800	3.37144200	1.66605500
O	5.45418700	-2.19122800	-1.57120200
O	0.16917800	-3.24436300	2.74196000

$Pa(OH)_2(NO_3)_3(H_2O)$(L4)

Sum of electronic and thermal Free Energies= -2349.049928

C	1.50458700	-0.07880600	0.49261800
N	2.13659800	1.08275300	0.36503800
C	2.13391100	-1.26121600	1.18706900
H	3.06109700	-0.98925000	1.68618700
C	2.38993100	-2.43885800	0.22314000
H	1.44058500	-2.75845000	-0.21026600
C	1.50666400	2.20709900	-0.36258100
H	2.30442300	2.70901600	-0.91513600
H	0.80221800	1.79882500	-1.08272300
C	3.48662600	1.35518400	0.90743500
H	3.53630800	2.43299900	1.06729000
H	3.58677700	0.89596800	1.88990400
C	4.61704500	0.91484700	-0.02724400
H	4.58147400	-0.17156600	-0.15721800
C	5.99324100	1.32674700	0.50811700
H	6.02475700	2.41715500	0.62383300
C	7.14923400	0.87919300	-0.39334500
H	7.00641800	1.29492400	-1.39889000
C	8.52748700	1.29460000	0.13362900
H	8.66750200	0.88189600	1.14004900
C	9.67989600	0.84179700	-0.76754400
H	9.58613100	1.26680100	-1.77188800
H	10.64741200	1.15274600	-0.36375600
H	9.69643300	-0.24796800	-0.86922000
C	0.80032000	3.19253100	0.57468000
H	-0.01543700	2.66926400	1.08251000
C	0.25357500	4.40959900	-0.18094000
H	-0.42406600	4.07000700	-0.97223000
C	-0.48792700	5.39499600	0.72934000
H	0.18969600	5.73860100	1.52170000
C	-1.05068000	6.61083200	-0.01555000
H	-1.73432700	6.26573500	-0.80026600
C	-1.78264500	7.59536700	0.90099700
H	-1.11433700	7.98567600	1.67522100
H	-2.17417000	8.44791600	0.33907000
H	-2.62640100	7.11302200	1.40470100
H	1.08048900	4.92999600	-0.68058300
H	6.13395900	0.90596700	1.51150500
H	-1.30932600	4.87095100	1.23462700
H	7.11948200	-0.21207200	-0.50540000
H	8.55690400	2.38530200	0.24385800
H	-0.23221200	7.12980400	-0.52911000
C	3.04880400	-3.62621800	0.93257100
H	2.41121800	-3.94762500	1.76576300
H	4.00010000	-3.30741200	1.37656000
H	1.42270600	-1.58297000	1.95141100
H	3.02633500	-2.10618900	-0.60419100
C	3.29880200	-4.81610700	-0.00128900
H	3.94065200	-4.49438000	-0.83001500
H	2.34834600	-5.12464000	-0.45264100
H	4.45714200	1.35532000	-1.01732400
H	1.49812500	3.52859000	1.35018400
C	3.94122100	-6.01190900	0.70737800
H	4.91023500	-5.74138900	1.13845000
H	3.30621300	-6.37599300	1.52117100
H	4.10494500	-6.84283300	0.01576400
O	0.34055700	-0.22803600	-0.00278000
Pa	-1.96038100	-0.59847600	-0.07753700
O	-1.76436400	0.65207400	1.57548000

O	-3.38576000	-0.93751500	-1.50946200
O	-3.53030100	1.53109000	-0.32767700
O	-1.65659800	1.44945900	-1.38994200
O	-4.01179600	-0.89012400	1.31367800
O	-3.27909100	-2.78656400	0.60602600
O	-0.72686700	-1.11847300	-2.36122800
O	-0.98771900	-2.71708800	-0.93815300
O	-1.03497900	-1.99511500	1.90395500
H	-2.35052200	1.17880300	2.13089100
H	-4.19895000	-0.83156400	-2.01495600
N	-2.74290000	2.10395800	-1.12934000
N	-4.19496000	-2.16070800	1.22548300
N	-0.53724300	-2.33679400	-2.08922900
H	-1.10764600	-1.54415500	2.75459400
H	-1.35931400	-2.89678300	2.02691400
O	-2.96224900	3.18344900	-1.63150700
O	-5.16367300	-2.70274700	1.70327800
O	0.02561900	-3.10931900	-2.83104600

$Pa(OH)_2(NO_3)_3(H_2O)$(L5)

Sum of electronic and thermal Free Energies= -2388.349787

C	1.30395200	-0.24150900	-0.63073000
N	2.01111400	-1.33722600	-0.37151200
C	1.87760300	0.94691500	-1.36669400
H	2.53864200	0.62808700	-2.17403500
C	2.61161500	1.93654100	-0.43720400
H	1.94767500	2.19975700	0.39095500
C	1.35705100	-2.47737900	0.31152500
H	2.13607200	-3.01622400	0.85217500
H	0.65263500	-2.08053900	1.03966500
C	3.41822400	-1.53976500	-0.76581200
H	3.48111400	-2.53379700	-1.21606000
H	3.68023300	-0.82476800	-1.54183200
C	4.40576000	-1.43143700	0.40310400
H	4.32674500	-0.43761600	0.85445700
C	5.84737100	-1.68305700	-0.05450500
H	5.91558900	-2.68035300	-0.50626100
C	6.86860400	-1.57183600	1.08316300
H	6.60848700	-2.28552900	1.87523800
C	8.31142700	-1.82358000	0.63064700
H	8.56762200	-1.11420000	-0.16553200
C	9.33014900	-1.70284000	1.76767700
H	9.11951400	-2.42277700	2.56490600
H	10.34770800	-1.88821500	1.41268300
H	9.30924100	-0.70228400	2.21102000
C	0.63756700	-3.41188800	-0.66677700
H	-0.12288700	-2.83966100	-1.20526000
C	-0.02021000	-4.59222000	0.05707600
H	-0.72763100	-4.20406000	0.79842100
C	-0.75724600	-5.54382700	-0.89163600
H	-0.05305800	-5.93084100	-1.63957400
C	-1.42898500	-6.72057400	-0.17463400
H	-2.13388600	-6.33245700	0.57052200
C	-2.16445600	-7.66796600	-1.12680400
H	-1.47795500	-8.09982600	-1.86208500
H	-2.63387700	-8.49379300	-0.58495500
H	-2.95059800	-7.14165100	-1.67759500
H	0.74237600	-5.15313700	0.61231300
H	6.10789500	-0.96805800	-0.84472700
H	-1.51698000	-4.98053300	-1.44853800
H	6.80053900	-0.57392700	1.53459100
H	8.37923100	-2.82256400	0.18332200
H	-0.67090000	-7.28167800	0.38511400
C	3.03532200	3.20856900	-1.17959400
H	2.14440800	3.69366900	-1.59711800
H	3.66898500	2.93790400	-2.03341300
H	1.02703400	1.45471900	-1.82269600
H	3.49382700	1.45693700	-0.00334800
C	3.78464700	4.20291500	-0.28621500
H	4.67782300	3.71723000	0.12725500
H	3.15339400	4.46568300	0.57240300
H	4.14057200	-2.15260900	1.18254300
H	1.35169900	-3.78517000	-1.40980000
C	4.20138400	5.48484300	-1.01653100
H	4.82845100	5.22129800	-1.87685700
H	3.30841200	5.97145200	-1.42706600
C	4.95445500	6.47235200	-0.12065900
H	5.87073800	6.02463000	0.27710900
H	5.23682300	7.37432700	-0.67072400
H	4.33982100	6.78072600	0.73104500
O	0.09576100	-0.18624900	-0.23746600
Pa	-1.98805700	0.77639500	0.16979500
O	-0.75330900	2.43984800	0.27686800
O	-3.89502700	0.32112300	-0.41387200
O	-1.73662600	1.41778500	-2.17497200
O	-1.91629800	-0.72797500	-2.05363600
O	-3.34379000	2.99823200	-0.24444500

O	-3.24278900	2.20333100	1.75659900
O	-2.04106300	-1.68456900	0.73430100
O	-3.08497200	-0.51156400	2.20619300
O	-0.75323400	0.73168100	2.43352300
H	-0.65456500	3.36741000	0.03666600
H	-4.80281800	0.34159500	-0.73514900
N	-1.81179500	0.28053200	-2.79996500
N	-3.67963000	3.12699800	0.96838000
N	-2.75877700	-1.67173300	1.79677600
H	-0.21879500	1.52437000	2.56987300
H	-1.30209300	0.61227600	3.21939000
O	-1.77452600	0.22874700	-4.00753200
O	-4.35953700	4.04014900	1.37942500
O	-3.09359300	-2.68833500	2.36059900

$Pa(OH)_2(NO_3)_3(H_2O)$(L6)

Sum of electronic and thermal Free Energies= -2427.648006

C	1.00155600	-0.78654400	-0.58457300
N	1.09251500	-2.10509400	-0.45039300
C	2.07995000	0.02824300	-1.25470300
H	2.81549200	-0.60329300	-1.74777900
C	2.79059600	0.98527500	-0.27491100
H	2.05489100	1.66904300	0.15207000
C	0.02244700	-2.86561000	0.23284000
H	0.51329900	-3.66486800	0.79267900
H	-0.46959600	-2.20605900	0.94308800
C	2.22997300	-2.91261300	-0.94581600
H	1.83806800	-3.91670100	-1.11354200
H	2.54786800	-2.54139200	-1.91916400
C	3.40410500	-2.96659700	0.03579200
H	3.80980000	-1.95919200	0.17349300
C	4.51441100	-3.90718500	-0.44702300
H	4.10716900	-4.91893100	-0.56442500
C	5.71775200	-3.95069600	0.50123800
H	5.38208500	-4.26043700	1.49908300
C	6.83237100	-4.89154600	0.02936400
H	7.16254900	-4.58513100	-0.97054200
C	8.03560000	-4.92292200	0.97613800
H	7.74251400	-5.25818100	1.97606700
H	8.81175200	-5.60173300	0.61196900
H	8.48336300	-3.92928600	1.07799200
C	-0.99895800	-3.44471500	-0.75196500
H	-1.49497300	-2.61602800	-1.26618400
C	-2.04033600	-4.32546800	-0.05141100
H	-2.53145100	-3.74723000	0.73935600
C	-3.10244000	-4.86919000	-1.01374900
H	-2.61121700	-5.44205700	-1.81103700
C	-4.15309300	-5.75332500	-0.33252000
H	-4.64617200	-5.17876500	0.46063600
C	-5.20840800	-6.29122800	-1.30325200
H	-4.74859900	-6.89865900	-2.08939900
H	-5.94375800	-6.91546500	-0.78799000
H	-5.74888600	-5.47339600	-1.79041200
H	-1.53508200	-5.16441500	0.44349100
H	4.85024200	-3.59198000	-1.44275000
H	-3.60576400	-4.02759300	-1.50671600
H	6.12494800	-2.93801600	0.61518400
H	6.42668700	-5.90454600	-0.07963000
H	-3.65152200	-6.59286500	0.16388400
C	3.89360900	1.79317100	-0.96644300
H	3.45673100	2.35855600	-1.79898000
H	4.62619500	1.10724200	-1.40979600
H	1.57951200	0.62250000	-2.02289300
H	3.21921500	0.41340200	0.55529500
C	4.61183800	2.75991100	-0.01786500
H	5.05618100	2.19129700	0.80888900
H	3.87523300	3.43491600	0.43622600
H	3.03917800	-3.29516300	1.01493800
H	-0.48010200	-4.03320100	-1.51720700
C	5.70235100	3.58888200	-0.70527400
H	6.43773300	2.91284300	-1.16074700
H	5.25743700	4.15764800	-1.53201700
C	6.42506200	4.55657100	0.23890800
H	6.87101800	3.98865700	1.06435200
H	5.68980100	5.23076900	0.69478200
C	7.51059400	5.38283400	-0.45712000
H	7.08839600	5.98489500	-1.26803500
H	8.00342600	6.06471700	0.24154600
H	8.28073500	4.73707900	-0.89103700
O	-0.01086600	-0.16869000	-0.11987000
Pa	-1.94024800	1.14087500	-0.05879800
O	-2.29183000	-0.06409800	-1.71717400
O	-3.09833800	2.04250000	1.37123500
O	-4.26472000	-0.13050200	0.18837700
O	-2.52630500	-0.85212300	1.23878000
O	-3.66405300	2.28204400	-1.45680000
O	-2.20740300	3.68912600	-0.72804800

O	-0.61457800	1.09066200	2.23561100
O	-0.17497900	2.65321500	0.81663400
O	-0.48862300	2.02811500	-2.01521800
H	-3.03286700	-0.28588200	-2.29262300
H	-3.89050600	2.27257600	1.86879700
N	-3.78802600	-0.98831900	0.98003500
N	-3.29553300	3.51090500	-1.35833600
N	0.06761800	2.11881000	1.96910000
H	-0.73125400	1.67539600	-2.88063800
H	-0.38789400	2.98404800	-2.11248200
O	-4.43773100	-1.88200600	1.47493900
O	-3.94141100	4.41331000	-1.83730600
O	0.89662200	2.58586900	2.71677400

$Pa(OH)_2(NO_3)_3(H_2O)$(L7)

Sum of electronic and thermal Free Energies= -2466.946014

C	0.99122900	-0.77888700	-0.58176200
N	1.08689500	-2.09726300	-0.44883600
C	2.06680400	0.04003600	-1.25113400
H	2.80213100	-0.58896500	-1.74774200
C	2.77890000	0.99525000	-0.27048600
H	2.04460100	1.68023600	0.15709000
C	0.01839300	-2.86254000	0.23156700
H	0.51105300	-3.66133100	0.79045800
H	-0.47679100	-2.20603800	0.94240100
C	2.22789200	-2.90034800	-0.94334400
H	1.83946600	-3.90535400	-1.11364200
H	2.54681900	-2.52652700	-1.91534100
C	3.40004600	-2.95243800	0.04075100
H	3.80309300	-1.94423200	0.18025500
C	4.51370000	-3.88994800	-0.44035100
H	4.10911600	-4.90253800	-0.55965500
C	5.71480500	-3.93144400	0.51083400
H	5.37735700	-4.24278400	1.50758200
C	6.83281200	-4.86929000	0.04101000
H	7.16487700	-4.56123000	-0.95776700
C	8.03365000	-4.89869700	0.99088300
H	7.73873800	-5.23547700	1.98976300
H	8.81230500	-5.57541100	0.62815800
H	8.47886700	-3.90412500	1.09474300
C	-0.99953500	-3.44288600	-0.75614600
H	-1.49824500	-2.61469100	-1.26854500
C	-2.03824800	-4.33009500	-0.05986800
H	-2.53323400	-3.75636000	0.73179100
C	-3.09626300	-4.87556100	-1.02573600
H	-2.60098600	-5.44344300	-1.82408900
C	-4.14387900	-5.76693300	-0.34933900
H	-4.64132600	-5.19733200	0.44468500
C	-5.19469900	-6.30690100	-1.32380500
H	-4.73053200	-6.91012600	-2.11062500
H	-5.92832400	-6.93583300	-0.81180500
H	-5.73781100	-5.49016500	-1.80987000
H	-1.53022000	-5.16831600	0.43341100
H	4.85119300	-3.57303600	-1.43497200
H	-3.60268100	-4.03468900	-1.51676600
H	6.11936400	-2.91791900	0.62664000
H	6.42976400	-5.88313000	-0.06992100
H	-3.63918100	-6.60559500	0.14537200
C	3.88343000	1.80046800	-0.96271500
H	3.44685700	2.36962300	-1.79284500
H	4.61150200	1.11210100	-1.40974700
H	1.56390700	0.63576100	-2.01655300
H	3.20678900	0.42217800	0.55924600
C	4.61009300	2.76157300	-0.01482900
H	5.05268200	2.18915900	0.81021700
H	3.87967000	3.44159100	0.44166200
H	3.03375100	-3.28275800	1.01879900
H	-0.47725900	-4.02692100	-1.52248900
C	5.70487100	3.58222000	-0.70587000
H	6.42953600	2.89923900	-1.16785100
H	5.26006700	4.15724000	-1.52818300
C	6.44391700	4.53894100	0.23651200
H	6.89022100	3.96467500	1.05876800
H	5.72060700	5.22293000	0.69944300
C	7.53819500	5.35852800	-0.45683500
H	7.09172800	5.93329800	-1.27735000
H	8.25971000	4.67498100	-0.92088900
O	-0.02371600	-0.16524900	-0.11694300
Pa	-1.95690200	1.13808700	-0.05254100
O	-2.30656800	-0.06625100	-1.71182000
O	-3.11649700	2.03453100	1.37973300
O	-4.27680500	-0.14148500	0.19642400
O	-2.53445200	-0.85835100	1.24351500
O	-3.68675100	2.27472600	-1.44673000
O	-2.23379300	3.68624200	-0.71913800
O	-0.62840400	1.09035500	2.24013600
O	-0.19493200	2.65492000	0.82146300

O	-0.51123800	2.03233400	-2.01014700
H	-3.04715400	-0.28933200	-2.28735000
H	-3.91065400	2.25922500	1.87659400
N	-3.79588200	-0.99906400	0.98577100
N	-3.32256500	3.50481000	-1.34740600
N	0.05059700	2.12053100	1.97334000
H	-0.75336800	1.67776100	-2.87495700
H	-0.41539600	2.98868200	-2.10805400
O	-4.44145500	-1.89645400	1.47937900
O	-3.97278900	4.40544000	-1.82383200
O	0.87925500	2.58947200	2.72021400
C	8.27479700	6.31032500	0.49039400
H	9.04935600	6.87657100	-0.03453200
H	7.58486000	7.03048700	0.94175100
H	8.75835900	5.76082400	1.30433700

$Pa(OH)_2(NO_3)_3(H_2O)$(L8)

Sum of electronic and thermal Free Energies= -2506.244321

C	0.99177200	-0.78114000	-0.57604600
N	1.08645400	-2.09980100	-0.44532000
C	2.06812500	0.03809800	-1.24370000
H	2.80359100	-0.59066800	-1.74038500
C	2.78017500	0.99284400	-0.26254800
H	2.04589100	1.67744100	0.16567200
C	0.01653500	-2.86564800	0.23220500
H	0.50787300	-3.66616600	0.78977800
H	-0.47875600	-2.21032500	0.94406000
C	2.22749700	-2.90272700	-0.93999000
H	1.83869200	-3.90723800	-1.11232300
H	2.54764300	-2.52753300	-1.91105400
C	3.39860600	-2.95702200	0.04521200
H	3.80186000	-1.94920000	0.18695300
C	4.51237700	-3.89409200	-0.43647400
H	4.10742600	-4.90622800	-0.55837400
C	5.71232800	-3.93822000	0.51604200
H	5.37355700	-4.25160900	1.51169800
C	6.83045000	-4.87555000	0.04545400
H	7.16391100	-4.56535900	-0.95219900
C	8.03009400	-4.90778100	0.99673300
H	7.73381200	-5.24684200	1.99443700
H	8.80889500	-5.58396400	0.63333200
H	8.47562700	-3.91366200	1.10354500
C	-1.00069900	-3.44286900	-0.75808700
H	-1.49836700	-2.61310200	-1.26893500
C	-2.04062000	-4.33139300	-0.06537100
H	-2.53629300	-3.75956200	0.72724600
C	-3.09774900	-4.87380800	-1.03395600
H	-2.60171800	-5.43937200	-1.83348900
C	-4.14617800	-5.76704100	-0.36134000
H	-4.64436800	-5.19978400	0.43390500
C	-5.19611000	-6.30388500	-1.33849800
H	-4.73129000	-6.90488500	-2.12663300
H	-5.93039400	-6.93416700	-0.82911000
H	-5.73856200	-5.48559800	-1.82268500
H	-1.53353900	-5.17114300	0.42627600
H	4.85121800	-3.57529000	-1.43003400
H	-3.60353900	-4.03140700	-1.52300400
H	6.11721000	-2.92513800	0.63456900
H	6.42702300	-5.88892600	-0.06832700
H	-3.64211400	-6.60727600	0.13134400
C	3.88392600	1.79825800	-0.95572400
H	3.44664700	2.36544500	-1.78684400
H	4.61255600	1.10981600	-1.40175300
H	1.56573700	0.63445200	-2.00898200
H	3.20867900	0.41949100	0.56667000
C	4.61028000	2.76225400	-0.01048800
H	5.05330100	2.19263000	0.81625900
H	3.87980600	3.44362200	0.44390600
H	3.03115700	-3.28897600	1.02227500
H	-0.47780600	-4.02518100	-1.52533200
C	5.70442500	3.58043400	-0.70533500
H	6.42970700	2.89557900	-1.16352900
H	5.25909500	4.15029800	-1.53093700
C	6.44289000	4.54371400	0.23122700
H	6.88860200	3.97453600	1.05719000
H	5.71864600	5.22997900	0.68901400
C	7.53643600	5.35792800	-0.46898300
H	7.09074600	5.92680100	-1.29541300
H	8.26037000	4.67137100	-0.92732600
O	-0.02316000	-0.16760300	-0.11104800
Pa	-1.95569000	1.13669900	-0.04650300
O	-2.30512500	-0.06569900	-1.70724300
O	-3.11560100	2.03226700	1.38607300
O	-4.27653300	-0.14158100	0.19968800
O	-2.53522300	-0.86103100	1.24671400
O	-3.68407900	2.27583100	-1.44050500
O	-2.23067000	3.68566100	-0.71055700

O	-0.62868300	1.08611100	2.24703600
O	-0.19356400	2.65182900	0.83012500
O	-0.50840700	2.03214600	-2.00242100
H	-3.04551300	-0.28774900	-2.28342300
H	-3.91007700	2.25667700	1.88255300
N	-3.79657700	-1.00062800	0.98803000
N	-3.31917600	3.50557600	-1.33968100
N	0.05101300	2.11619800	1.98162300
H	-0.75040000	1.67877200	-2.86775900
H	-0.41187100	2.98854400	-2.09914400
O	-4.44292000	-1.89847800	1.47979500
O	-3.96853900	4.40712100	-1.81555000
O	0.87957300	2.58389700	2.72938000
C	8.27900600	6.32342800	0.46212900
H	7.55609600	7.00977500	0.91975000
H	8.72526100	5.75590900	1.28777300
C	9.36846900	7.13163500	-0.24878800
H	8.94654200	7.73358100	-1.05995600
H	9.87618300	7.81193000	0.44075200
H	10.12645500	6.47341000	-0.68541900

$Pa(OH)_2(NO_3)_3(H_2O)$(L9)

Sum of electronic and thermal Free Energies=

-2270.450612

Pa	-1.91984700	-0.45822700	-0.12735400
O	-3.96120100	-2.10730200	0.44202100
O	-1.79008900	-1.84868900	2.03934700
O	-4.12226800	-0.01489400	0.92422100
O	-2.80929600	1.95720900	-0.76435700
O	-1.59563600	0.86187600	1.44608800
O	-0.92024700	1.27196400	-1.54098100
O	-0.55821800	-1.58427800	-2.10997500
O	-3.14082500	-0.59629700	-1.75590500
O	-1.52550600	-2.84549100	-0.65335000
H	-1.87896600	-1.33740900	2.85338900
H	-2.35795000	-2.62590000	2.12324900
H	-2.08128400	1.57054500	1.88414100
H	-3.75971200	-0.54155700	-2.49186300
N	-1.81526700	2.20768500	-1.49783600
O	-1.68105100	3.23446200	-2.12416900
N	-4.69565000	-1.16901300	0.87181900
N	-0.80534100	-2.76050200	-1.72351400
O	-0.40707600	-3.75094800	-2.29340700
O	-5.84450100	-1.32347800	1.21599200
O	0.38789900	-0.71505600	0.30207800
C	1.58402600	-0.81701200	0.71795700
N	2.46738900	0.15016900	0.48077700
C	1.99959300	-2.04929600	1.51355400
C	2.09246200	1.36026800	-0.28088100
C	3.87004500	0.12110500	0.95219600
H	3.08128700	-2.15220300	1.44126900
C	1.38116000	-3.33318500	0.94653700
C	1.63515300	-1.85321200	3.00026500
H	1.31480200	1.09873700	-0.99264200
C	1.62658500	2.50667600	0.62409900
H	4.14944000	1.15894500	1.14250800
C	4.83329400	-0.50099000	-0.06424200
H	0.29569000	-3.32393300	1.02906900
H	1.65060500	-3.47771700	-0.10246100
H	1.76379700	-4.18759200	1.50988800
H	2.00105200	-2.70595500	3.57642500
H	2.08194600	-0.94680000	3.41583000
H	0.55359600	-1.79553400	3.12462000
H	0.69035300	2.21279500	1.10780100
C	1.42813800	3.81111500	-0.15737400
H	4.55293500	-1.54506000	-0.24021600
C	6.29030200	-0.42541800	0.40668400
H	2.38342600	4.11534500	-0.60348700
H	0.73936000	3.63698100	-0.99142500
C	0.88889500	4.95240800	0.71268200
H	6.55852000	0.62307800	0.58600500
H	6.38828800	-0.93820100	1.37157400
C	7.27835200	-1.03591900	-0.59358200
H	1.57930800	5.13034300	1.54726200
H	-0.06302400	4.64310300	1.16299500
C	0.67820400	6.26139000	-0.05667700
H	7.01241100	-2.08569400	-0.77112800
H	7.17610500	-0.52586100	-1.55988600
C	8.73843000	-0.95609700	-0.13336500
H	-0.01881200	6.08276700	-0.88411700
H	1.62630000	6.56691400	-0.51553900
C	0.14737100	7.39841700	0.82147400
H	9.00227900	0.09323800	0.04538600
H	8.84018100	-1.46563400	0.83239200
C	9.72141200	-1.56514900	-1.13741100
H	0.84104300	7.62255300	1.63803900
H	0.00564200	8.31619600	0.24394400
H	-0.81632000	7.13456400	1.26868500

H	9.66554300	-1.05398700	-2.10372600
H	10.75259500	-1.49110300	-0.78105300
H	9.50396500	-2.62399600	-1.30983500
H	2.36278100	2.66910600	1.41947400
H	4.72890500	0.01654000	-1.02369600
H	2.97811400	1.65906800	-0.84602200
H	3.92757900	-0.38960300	1.91137800

$Pa(OH)_2(NO_3)_3(H_2O)$(L10)

Sum of electronic and thermal Free Energies= -2427.621408

Pa	-2.27204500	-0.51067000	0.03839500
O	-4.03412700	-2.52185400	-0.33407500
O	-2.09992500	-2.58906800	1.54004500
O	-4.58081300	-0.83326300	0.88687800
O	-3.54791400	1.81292000	0.23704400
O	-2.28130100	0.14020700	2.00518300
O	-1.51345200	1.75898600	-0.46839400
O	-0.69221000	-0.66718600	-2.13160300
O	-3.38134900	-0.16062400	-1.64727900
O	-1.36024200	-2.47290900	-1.16199200
H	-2.34548100	-2.49533200	2.46861300
H	-2.48854800	-3.41314400	1.21817800
H	-2.88865100	0.53778900	2.63987100
H	-4.09902600	0.20521400	-2.17569700
N	-2.56086600	2.46930700	-0.19251300
O	-2.56466200	3.66990000	-0.34366200
N	-4.94182000	-1.93822900	0.32713900
N	-0.67102800	-1.92749800	-2.11287000
O	-0.06081800	-2.60172100	-2.91099100
O	-6.06656700	-2.36896600	0.44342700
O	0.02692900	-0.50113800	0.53014800
C	1.25396500	-0.61392000	0.86139000
N	2.18153900	0.19642900	0.35313800
C	1.60000900	-1.70264800	1.86733800
C	1.77178300	1.31005700	-0.56996700
C	3.65061200	0.13809800	0.68492400
H	2.66015600	-1.65750300	2.08934900
C	1.29970200	-3.09303900	1.27634500
C	0.84567700	-1.46125500	3.18756400
H	0.73699700	1.10820200	-0.82052600
C	1.82977900	2.63654900	0.21510400
H	4.05795800	0.96695900	0.10837100
C	4.32210700	-1.13525500	0.12471100
H	0.23432400	-3.21981900	1.09243700
H	1.83725100	-3.25413900	0.33866700
H	1.62256800	-3.85870500	1.98592200
H	1.09338000	-2.25822700	3.89238900
H	1.13049800	-0.50900000	3.64140200
H	-0.23175100	-1.45452500	3.03364100
H	1.21377600	2.51758600	1.11312500
C	1.34878700	3.87576800	-0.55073400
H	4.02982300	-2.01386400	0.70480100
C	5.85430100	-1.05823200	0.08986600
H	2.01328500	4.07444600	-1.39842500
H	0.35200400	3.68606900	-0.96044100
C	1.29843800	5.12281600	0.34103500
H	6.16471000	-0.16467900	-0.46561200
H	6.24734200	-0.94625200	1.10591100
C	6.48766500	-2.29897600	-0.55151100
H	2.28860300	5.29702800	0.78202200
H	0.61678600	4.93783300	1.18113500
C	0.84894200	6.38616800	-0.40186600
H	6.16665400	-3.19369100	-0.00292000
H	6.10686900	-2.41323400	-1.57432800
C	8.01951200	-2.25160100	-0.58458800
H	-0.14031400	6.21138000	-0.84142500
H	1.52892500	6.57124700	-1.24215600
C	0.79700300	7.62664100	0.49488900
H	8.34051200	-1.35817400	-1.13359700
H	8.39794800	-2.13445500	0.43802800
C	8.64725100	-3.49470800	-1.22170700
H	1.78116100	7.84726000	0.92045900
H	0.47012800	8.50910500	-0.06221800
H	0.10129300	7.48207700	1.32760000
H	8.31169800	-3.61994500	-2.25600900
H	9.73879700	-3.42960300	-1.23160700
H	8.37278200	-4.40091100	-0.67246200
H	2.85464000	2.81518700	0.55912300
H	3.95354400	-1.30050800	-0.89190300
C	2.59289900	1.28991500	-1.88316300
H	3.45599600	1.95850900	-1.80059400
H	2.99094700	0.28463900	-2.03699300
C	1.76869100	1.65767100	-3.12519200
H	0.95869300	0.93988600	-3.27037200
H	1.32899100	2.65367300	-3.05137100
H	2.40336900	1.64009000	-4.01534400
C	3.96690600	0.44289700	2.17702700

H	4.27211300	-0.47517300	2.68767300
H	3.05708100	0.78618900	2.67344700
C	5.05646300	1.50617000	2.36740100
H	4.75409100	2.46553500	1.93868000
H	5.24898600	1.66416200	3.43155900
H	5.99841400	1.21365700	1.89895400

$Pa(OH)_2(NO_3)_3(H_2O)$(L11)

Sum of electronic and thermal Free Energies= -2427.625162

Pa	-1.94130800	-0.87143900	-0.15030300
O	-3.42258800	-3.04029800	0.37110600
O	-1.70107400	-1.98855300	2.15551900
O	-4.29164100	-1.08444600	0.60928100
O	-3.44466100	1.08103400	-1.13419700
O	-2.23603600	0.60236800	1.28278800
O	-1.35424200	0.97347500	-1.64532300
O	-0.03552900	-1.59013000	-1.86010300
O	-2.82539700	-1.50556200	-1.87381600
O	-0.77133300	-3.04436000	-0.44981800
H	-1.98167200	-1.44095700	2.89938500
H	-2.06317700	-2.87372600	2.29306900
H	-2.94686800	1.18408400	1.57665600
H	-3.24316800	-1.80521400	-2.68825600
N	-2.49542500	1.56618000	-1.80591100
O	-2.61034300	2.51221600	-2.55201300
N	-4.46493600	-2.36203900	0.61686700
N	0.03036700	-2.77354600	-1.42418100
O	0.78641300	-3.60945600	-1.86900300
O	-5.54389600	-2.85580400	0.84778200
O	0.26128300	-0.39037400	0.57981200
C	1.48199300	-0.27007700	0.90921200
N	2.20779900	0.75362500	0.45301300
C	2.07924800	-1.25735700	1.90562300
C	1.55005100	1.84985800	-0.30185800
C	3.67296300	0.86032200	0.66849500
H	3.15621700	-1.11715200	1.93826200
C	1.81430500	-2.72108500	1.53094100
C	1.52795600	-0.92475300	3.30888900
H	2.32746800	2.34628000	-0.88168300
H	0.84655700	1.41080100	-1.00511100
C	0.80456400	2.86680800	0.59284000
H	3.94330500	1.88756700	0.42909900
H	3.89755300	0.72667300	1.72676400
C	4.52468700	-0.10448000	-0.18689400
H	0.75056700	-2.95081500	1.54697900
H	2.20868600	-2.96242300	0.54115900
H	2.31718600	-3.36595100	2.25549800
H	1.99700200	-1.58504500	4.04192700
H	1.74477000	0.10686500	3.59563600
H	0.44977700	-1.07930700	3.34782500
H	0.02261200	2.30318500	1.11402400
C	0.10088700	3.89336900	-0.31806900
C	1.69183700	3.51791400	1.67804400
H	4.20996800	-1.12706000	0.05279500
C	5.99179300	0.05472800	0.26550200
C	4.31771200	0.11022000	-1.70799200
H	0.84965200	4.49266000	-0.85005200
H	-0.44967900	3.34990500	-1.09130900
C	-0.87303700	4.82790900	0.41066800
H	1.03618900	4.02016100	2.39616000
C	2.73937700	4.52608900	1.18745500
H	2.18792100	2.72679600	2.24940800
H	6.31172800	1.08497700	0.06045400
H	6.03401700	-0.06622900	1.35527700
C	6.99939400	-0.91432500	-0.36413400
H	3.36344600	0.61193700	-1.88503800
C	4.31571100	-1.18115500	-2.53700900
H	5.08889400	0.79420200	-2.08050900
H	-0.33359100	5.44507100	1.13829500
H	-1.58583300	4.22521800	0.98845900
C	-1.64873400	5.74679600	-0.54148300
H	3.40601900	4.10547500	0.42920800
H	2.27524000	5.41544400	0.75427100
H	3.36465500	4.85732500	2.02083800
H	6.65792100	-1.94622400	-0.21408000
H	7.04673600	-0.75709500	-1.44704500
C	8.41027200	-0.76224700	0.21839800
H	3.47811500	-1.82356300	-2.24876800
H	4.20777500	-0.95615100	-3.60185600
H	5.23519600	-1.75593600	-2.41015900
H	-2.20978200	5.13146700	-1.25425500
H	-0.93709200	6.33267700	-1.13596700
C	-2.60869400	6.69503600	0.18288200
H	8.74844700	0.27145500	0.07743600
H	8.37202700	-0.92641000	1.30200600
C	9.42692400	-1.72120500	-0.40776800
H	-2.06983800	7.34989200	0.87518800

H	-3.15003800	7.33110300	-0.52310300
H	-3.35005700	6.13762600	0.76434100
H	9.51448400	-1.55493000	-1.48613600
H	10.42031200	-1.59079900	0.03042800
H	9.13070500	-2.76408200	-0.25656700

$Pa(OH)_2(NO_3)_3(H_2O)$(L12)

Sum of electronic and thermal Free Energies= -2427.621827

C	-0.04541900	2.46995800	-0.80161200
N	0.08828800	1.16918200	-0.54812500
C	-1.12963500	3.26108000	-0.07757900
H	-1.94641000	2.58192700	0.15957000
C	-1.71952200	4.39188000	-0.92778500
H	-1.00230900	5.20788500	-1.02427000
H	-2.02829200	4.03461200	-1.91359100
C	1.18445900	0.36197200	-1.13039400
H	0.73172500	-0.56464900	-1.49368700
H	1.58739500	0.89705600	-1.98220900
C	-0.86202500	0.39710300	0.28848000
H	-0.29607400	-0.43592300	0.70527500
H	-1.18257000	0.99748200	1.13643100
C	-2.98254300	-1.04961500	0.32037300
H	-2.34620000	-1.75790000	0.86933600
C	-3.87682000	-1.87316900	-0.63032600
H	-4.48931300	-1.18020700	-1.22324700
H	-3.22956500	-2.39618300	-1.34525900
C	-4.79467900	-2.90568200	0.03506100
H	-4.19298400	-3.57625400	0.66027000
H	-5.49673600	-2.40358800	0.70827000
C	-5.58399700	-3.73248800	-0.98528600
H	-6.21827200	-3.09173800	-1.60603300
H	-4.91214800	-4.28030400	-1.65367400
C	3.22158800	-1.10143000	-0.53460300
H	2.57788200	-1.93061700	-0.86206500
C	4.01670000	-1.61467900	0.68420600
H	4.63980900	-0.80692300	1.08793600
H	3.29947000	-1.86295900	1.47639000
C	4.89134200	-2.84718900	0.42279400
H	5.67209100	-2.60727400	-0.30622300
H	4.27727200	-3.63323200	-0.03403900
C	5.54595300	-3.38872000	1.69775100
H	4.79173000	-3.67919100	2.43606500
H	6.18937500	-2.63427200	2.16170800
C	4.11688600	-0.73817100	-1.74271900
H	4.58429500	-1.65592200	-2.11487700
C	5.21145700	0.30180200	-1.47065800
H	4.79740400	1.24457400	-1.10593100
H	5.93707200	-0.05426500	-0.73397600
H	5.76113900	0.52063600	-2.39054800
C	-3.79965800	-0.23242200	1.35813700
H	-3.35143700	0.75813100	1.48719000
C	-3.91043900	-0.88324900	2.74241100
H	-2.92018400	-1.01479800	3.18952000
H	-4.50180300	-0.26182000	3.42109300
H	-4.38356300	-1.86680600	2.69490100
H	-4.80205900	-0.04556800	0.95600700
H	3.48436000	-0.37556400	-2.55830400
C	-0.55051100	3.80453400	1.24821800
H	-1.33259300	4.34006400	1.79116000
H	-0.18010300	3.00259400	1.89067000
H	-2.60558200	4.78800900	-0.42723600
H	0.26915300	4.49654100	1.04911900
C	2.28294700	0.04571900	-0.10075600
H	2.84863300	0.95744700	0.10796800
H	1.80933200	-0.24951800	0.84094400
H	6.16254100	-4.26722600	1.48776500
H	-6.23103000	-4.46251900	-0.49115200
C	-2.04988500	-0.14805000	-0.51553500
H	-2.62605600	0.68125000	-0.94160200
H	-1.65763500	-0.72083000	-1.36162300
O	0.73955900	3.06415600	-1.60880100
Pa	2.33728100	4.61926400	-2.43042500
O	1.39503400	5.74674600	-0.96880900
O	4.26943600	4.50514900	-3.12237900
O	4.09150800	5.40065100	-0.57451200
O	3.28890400	3.40090200	-0.54110400
O	2.88805500	7.01205800	-2.81038000
O	2.49420500	5.99832600	-4.66651100
O	2.84104800	2.14613100	-3.31954200
O	1.56278400	3.42876200	-4.47974400
O	0.16094000	5.49947100	-3.46829500
H	1.49091300	6.61804200	-0.56705700
H	5.17131700	4.84176900	-3.07517500
N	4.07840800	4.27780500	-0.00239200
N	2.82803700	7.07891400	-4.09626900
N	2.13300100	2.27566200	-4.35652100
H	-0.64577300	5.49163300	-2.93816600

H	-0.06746900	5.14982100	-4.33971700
O	4.73656500	4.00894200	0.97581100
O	3.07095800	8.10160900	-4.69357800
O	1.98217600	1.40353600	-5.18006400

$Pa(OH)_2(NO_3)_3(H_2O)$(L13)

Sum of electronic and thermal Free Energies= -2427.628706

Pa	-2.26758000	-0.65616700	-0.16480600
O	-4.33421400	-2.25489000	0.45100300
O	-2.19780600	-1.91348900	2.08511900
O	-4.48806500	-0.13762300	0.81161900
O	-3.11105800	1.72947900	-0.95526700
O	-1.96360600	0.74742600	1.34079300
O	-1.21882700	0.97655600	-1.65793100
O	-0.87762500	-1.90286000	-2.05323100
O	-3.46098600	-0.87065700	-1.80563400
O	-1.88341600	-3.07131800	-0.54650400
H	-2.30644400	-1.35247300	2.86327300
H	-2.76502300	-2.68637600	2.20554500
H	-2.44775400	1.49177300	1.71695300
H	-4.08083600	-0.83569800	-2.54203900
N	-2.10343200	1.92246400	-1.68814800
O	-1.94893300	2.90558800	-2.37651900
N	-5.06987600	-1.28860600	0.81065600
N	-1.13913800	-3.05305200	-1.60341900
O	-0.73363100	-4.07710100	-2.10448500
O	-6.22751900	-1.41510900	1.13672200
O	0.02767800	-0.90988900	0.32586200
C	1.20885200	-0.98697900	0.78793300
N	2.10206000	-0.03652500	0.52263500
C	1.59543300	-2.17113800	1.66712900
C	1.75798700	1.12145900	-0.32872800
C	3.48770700	-0.03706300	1.04244600
H	2.67810300	-2.28315300	1.62904100
C	0.98346400	-3.48265100	1.15961500
C	1.19398700	-1.88657700	3.12977900
H	1.00777100	0.81261300	-1.05104600
C	1.25953300	2.32694700	0.47842100
H	3.76033900	1.01047400	1.18334800
C	4.48480600	-0.71412500	0.09554500
H	-0.10389300	-3.46045500	1.20810000
H	1.28289200	-3.69129300	0.12974000
H	1.34152200	-4.30446500	1.78417600
H	1.54072300	-2.70526500	3.76434200
H	1.63465500	-0.95917600	3.50345800
H	0.10996100	-1.81782900	3.22285300
H	0.29602400	2.07181600	0.92865500
C	1.11993500	3.56738300	-0.41362400
H	4.21692000	-1.77013500	-0.02035900
C	5.92226400	-0.59621300	0.61785800
H	2.11634000	3.87042100	-0.76290500
H	0.55204300	3.29059400	-1.30860800
C	0.43000400	4.78762100	0.22992200
H	6.20358600	0.46248200	0.66813900
H	5.95103300	-0.96432700	1.65060500
C	6.97574800	-1.37845700	-0.19376300
H	-0.58517600	4.47879400	0.51791200
C	0.28300100	5.90539500	-0.82479800
H	6.66305800	-2.43261500	-0.19107800
C	8.33870200	-1.31529800	0.52762400
H	-0.03443500	5.45549000	-1.77196300
H	1.26936700	6.34898000	-1.01270500
C	-0.71641600	7.00444400	-0.44899100
H	8.68385900	-0.27559200	0.57342200
H	8.18284200	-1.62330000	1.56800800
C	9.43683100	-2.19154700	-0.08425300
H	-0.44386200	7.50824000	0.48260100
H	-0.77117100	7.76838100	-1.22971300
H	-1.72072700	6.58877200	-0.31923700
H	9.72398400	-1.85467200	-1.08364100
H	10.33678500	-2.17443500	0.53688700
H	9.11004200	-3.23337000	-0.16595600
H	1.95773300	2.52628700	1.29726100
H	4.39700500	-0.25887700	-0.89491500
H	2.66499300	1.38306600	-0.87831800
H	3.51196700	-0.49300100	2.03014700
C	7.04858900	-0.95074600	-1.67779200
H	7.74538300	-1.61607700	-2.19732600
H	6.07525000	-1.13125000	-2.14575400
C	7.46417700	0.50349300	-1.93436800
H	7.49357700	0.70796200	-3.00817100
H	6.76443600	1.21432100	-1.48602400
H	8.45781100	0.71982100	-1.53284800
C	1.15800300	5.29424700	1.50260500
H	2.22404800	5.04761500	1.42624200
H	1.11183900	6.38729700	1.53447700
C	0.59695500	4.76139900	2.82732400

H	-0.44836400	5.06087300	2.95285400
H	0.63444000	3.67115000	2.88322500
H	1.15932400	5.15659600	3.67861500

$Pa(OH)_2(NO_3)_3(H_2O)$(L14)

Sum of electronic and thermal Free Energies= -2427.628254

C	-1.42408700	-0.33588200	-0.55748900
N	-2.16086800	0.74126900	-0.28501700
C	-1.96180700	-1.47736500	-1.38836200
H	-2.91248700	-1.21827400	-1.84920200
C	-2.10062200	-2.80823600	-0.62144100
H	-1.12208600	-3.11043200	-0.24856300
C	-1.54072900	1.89857000	0.40825000
H	-2.34373700	2.42840200	0.92065400
H	-0.86185900	1.51151500	1.16634100
C	-3.58872700	0.86219800	-0.66983500
H	-3.83983800	1.91668100	-0.56767700
H	-3.69596200	0.62280500	-1.72818500
C	-4.58462200	0.02687500	0.16526300
H	-4.32190200	-1.02996400	0.04515900
C	-5.97746500	0.24221000	-0.46666900
H	-6.23743900	1.30575000	-0.38409100
C	-7.12925500	-0.59588100	0.10108600
H	-7.31852900	-0.32049600	1.14389900
C	-8.42877300	-0.42502400	-0.69600100
H	-8.25072900	-0.70910000	-1.74019500
C	-9.59279200	-1.24687500	-0.13498400
H	-9.81730400	-0.96020700	0.89726400
H	-10.50226500	-1.10400100	-0.72513900
H	-9.35852600	-2.31614100	-0.13817200
C	-0.75858400	2.85020700	-0.52576500
H	0.03323400	2.24755900	-0.98288100
C	-0.07549200	3.92980600	0.33943100
H	0.45963200	3.43260700	1.15461400
C	0.91425100	4.81990300	-0.42332100
H	0.39500900	5.37287300	-1.21451700
C	1.64643100	5.82081700	0.47926500
H	2.18707000	5.27136100	1.25788700
C	2.62446900	6.71738200	-0.28565900
H	2.10758300	7.30273500	-1.05294600
H	3.12961200	7.41931800	0.38383300
H	3.39509800	6.12260600	-0.78647100
C	-1.59876900	3.43755400	-1.68294600
H	-0.90918100	3.88640200	-2.40465200
C	-2.65037600	4.48777000	-1.30071500
H	-3.36298800	4.12176900	-0.55597300
H	-2.19001800	5.39038700	-0.89127400
H	-3.22609100	4.78475800	-2.18140000
C	-4.51420000	0.37191800	1.67224000
H	-3.51053300	0.73048900	1.91529300
C	-4.81576200	-0.79682000	2.61971700
H	-4.09678500	-1.60856100	2.47302700
H	-4.73973700	-0.47410000	3.66188500
H	-5.81500100	-1.20949900	2.47302400
H	-5.19151900	1.20882300	1.87933800
H	-2.07992300	2.61656800	-2.22423900
H	-0.83617400	4.55939100	0.81668500
H	-5.90069600	0.03098800	-1.54073200
H	1.65298900	4.18427300	-0.92879600
H	-6.84636700	-1.65603600	0.10466000
H	-8.70512200	0.63625300	-0.71105800
H	0.90840600	6.44549400	0.99720200
C	-2.66915600	-3.91157400	-1.51734200
H	-2.02450900	-4.08498200	-2.38409900
H	-2.75042700	-4.85233100	-0.96729700
H	-3.66572500	-3.65277200	-1.88719200
H	-1.23442600	-1.61935800	-2.19196500
H	-2.74860900	-2.66944200	0.24908200
O	-0.22755900	-0.41125000	-0.13366200
Pa	2.08086300	-0.79044300	0.02648300
O	1.95087600	0.58890200	-1.52949200
O	3.38844700	-1.29149000	1.50966900
O	1.70590000	1.11162700	1.52149300
O	3.62268400	1.29273500	0.55453800
O	4.21554500	-0.92513100	-1.25868800
O	3.46046700	-2.88685400	-0.79609900
O	0.71341500	-1.52872000	2.18657400
O	1.11071300	-2.98943600	0.65134100
O	1.24318100	-2.02706400	-2.09407800
H	2.56355400	1.15263300	-2.01599000
H	3.98542600	-1.50860100	2.23362000
N	2.81588500	1.76684000	1.40069000
N	4.40520800	-2.19720500	-1.29278700
N	0.58668400	-2.72414200	1.80398300
H	1.33048200	-1.49989900	-2.89829500
H	1.60172500	-2.90356800	-2.28515000
O	3.03774700	2.75548100	2.06241400

O	5.40484200	-2.68364500	-1.76609100
O	0.01576600	-3.57727800	2.44536600

$Pa(OH)_2(NO_3)_3(H_2O)$(L15)

Sum of electronic and thermal Free Energies= -2545.522446

C	-1.42459900	-0.24313000	-0.49483500
N	-2.22098900	0.75499600	-0.11253500
C	-1.94271700	-1.45144600	-1.23518400
H	-2.93029800	-1.27450700	-1.65746300
C	-1.96273400	-2.72621000	-0.36359300
H	-0.99275700	-2.84444800	0.12304900
H	-2.70396100	-2.61596400	0.43416500
C	-1.63681300	1.92046800	0.59968500
H	-2.43299600	2.35042400	1.20684800
H	-0.86934400	1.54352100	1.27303100
C	-3.67825300	0.78518400	-0.38975300
H	-3.98223000	1.82370500	-0.26920300
H	-3.84188100	0.53717000	-1.43873300
C	-4.57416600	-0.10276400	0.50399100
H	-4.29807100	-1.14754100	0.32619900
C	-6.02046200	0.09507300	-0.00285800
H	-6.29944100	1.14725200	0.14121300
C	-7.09982900	-0.79409800	0.62623000
H	-7.20843100	-0.55902700	1.68998000
C	-8.46537700	-0.63244500	-0.05367800
H	-8.36972300	-0.88030300	-1.11764100
C	-9.55838500	-1.50015000	0.57689100
H	-9.70170100	-1.24925200	1.63267500
H	-10.51755300	-1.36396500	0.06967500
H	-9.30021200	-2.56243100	0.52105800
C	-1.01141400	2.99501000	-0.31636600
H	-0.25251200	2.48739000	-0.91687200
C	-0.27364200	4.01866300	0.57215100
H	0.39053500	3.46753100	1.24712800
C	0.56377000	5.04653200	-0.19912200
H	-0.08522100	5.67250000	-0.82220000
C	1.39169500	5.95459000	0.71871300
H	2.05623800	5.33578500	1.33369900
C	2.22257500	6.98819800	-0.04730100
H	1.58197200	7.64730800	-0.64185900
H	2.80534900	7.61569400	0.63286400
H	2.92262700	6.50039700	-0.73292100
C	-2.00470200	3.63804400	-1.30987600
H	-1.42623500	4.21401500	-2.03860800
C	-3.07669800	4.55210800	-0.70292100
H	-3.67503900	4.04877600	0.06200200
H	-2.63747800	5.43881300	-0.23937400
H	-3.76531500	4.89589500	-1.47915600
C	-4.38591000	0.19456200	2.01065300
H	-3.36857200	0.55436600	2.18427500
C	-4.59971000	-1.00678400	2.94166700
H	-3.89269500	-1.80831400	2.70719600
H	-4.43463300	-0.71677300	3.98316200
H	-5.60570600	-1.42218500	2.86944700
H	-5.05105000	1.01695100	2.29960800
H	-2.48522100	2.84463600	-1.89150800
H	-0.99260100	4.54157800	1.21473100
H	-6.02877200	-0.07510800	-1.08689700
H	1.23527200	4.51800200	-0.88670000
H	-6.79136900	-1.84549500	0.56863000
H	-8.76621300	0.42139200	-0.01114500
H	0.72126800	6.47021400	1.41701100
C	-2.28241800	-3.97286300	-1.19522600
H	-1.52394300	-4.07904400	-1.97944600
H	-3.24407800	-3.83570600	-1.70544400
O	-0.18049000	-0.19330200	-0.23466400
Pa	2.06075200	-0.85822100	-0.01606300
O	1.13335100	-1.91963900	1.51199400
O	3.67013600	-1.13666000	-1.24594200
O	2.58331700	-3.44633200	-0.23488800
O	1.09354000	-2.54397500	-1.50317500
O	3.83625700	-1.52239600	1.61321300
O	4.07883100	0.52368200	0.98941300
O	1.49488200	0.15985500	-2.40182100
O	2.23204400	1.47349800	-0.86017200
O	1.55482300	0.82953800	1.88846800
H	1.36370500	-2.63604600	2.11489800
H	4.41273900	-1.52050800	-1.72450100
N	1.73838600	-3.61232700	-1.15715100
N	4.55107400	-0.45446800	1.65068600
N	1.84917700	1.32960100	-2.08520300
H	1.18854200	0.44438000	2.69433000
H	2.26221500	1.43231300	2.15214400
O	1.52633000	-4.67619400	-1.69263900
O	5.58566800	-0.39640100	2.27216400
O	1.83543900	2.26380700	-2.85627700
C	-2.32973800	-5.25737200	-0.36072200

H	-1.36532000	-5.39568200	0.14445500
H	-3.07992200	-5.14903000	0.43309300
C	-2.64776500	-6.50840600	-1.18783000
H	-1.89574600	-6.61692600	-1.97860000
H	-3.60888600	-6.36853800	-1.69723800
C	-2.69638000	-7.79004800	-0.35097100
H	-2.92215400	-8.66256100	-0.97040700
H	-1.73835300	-7.97341900	0.14579500
H	-3.46515500	-7.72517600	0.42552600
H	-1.24899200	-1.60970800	-2.06416500

$Pa(OH)_2(NO_3)_3(H_2O)$(L16)

Sum of electronic and thermal Free Energies= -2466.920848

C	-1.39809800	-0.27096400	-0.64154600
N	-2.16034000	0.73490100	-0.20538400
C	-1.99340900	-1.40640900	-1.46102700
H	-3.06177200	-1.23549800	-1.57617800
C	-1.82204700	-2.75579600	-0.72386400
H	-0.76000400	-2.98689600	-0.64377200
H	-2.19765200	-2.64762900	0.29890400
C	-1.53791300	1.88660200	0.49581100
H	-2.29622200	2.29999900	1.16059200
H	-0.72827500	1.50486200	1.11243500
C	-3.63170200	0.78378100	-0.40009400
H	-3.92345100	1.81690300	-0.22060800
H	-3.86170400	0.58071800	-1.44608100
C	-4.47123800	-0.13715700	0.51565700
H	-4.17626100	-1.17356700	0.31576900
C	-5.94130900	0.03149800	0.07142000
H	-6.23686200	1.07659500	0.23317100
C	-6.97546600	-0.88453000	0.73681700
H	-7.05387900	-0.65242200	1.80383400
C	-8.36678800	-0.75712900	0.10313200
H	-8.30009000	-1.00232100	-0.96364900
C	-9.41614200	-1.65222000	0.76851300
H	-9.53121500	-1.40503300	1.82860900
H	-10.39453500	-1.54041500	0.29301800
H	-9.13311400	-2.70761300	0.70330900
C	-0.97803000	2.98415200	-0.43625400
H	-0.23358500	2.49999600	-1.07429600
C	-0.23058000	4.01695600	0.43344400
H	0.47151500	3.47667200	1.07762500
C	0.55141400	5.07427800	-0.35610800
H	-0.13490300	5.67886300	-0.96022000
C	1.37097400	6.00727600	0.54384900
H	2.07132100	5.40930800	1.13955000
C	2.14702000	7.07069700	-0.23884000
H	1.46967100	7.71043700	-0.81344200
H	2.72627300	7.71474200	0.42878600
H	2.84470100	6.60906500	-0.94467500
C	-2.02195300	3.61544000	-1.38463700
H	-1.48132400	4.19755300	-2.13726500
C	-3.07734000	4.52054600	-0.73623500
H	-3.63972100	4.01581700	0.05464800
H	-2.62856700	5.41367700	-0.29467000
H	-3.80035100	4.85450600	-1.48510700
C	-4.22587600	0.14582400	2.01689400
H	-3.20823700	0.52095400	2.15185500
C	-4.38111400	-1.06995500	2.94068000
H	-3.67595200	-1.85901200	2.66228100
H	-4.17168100	-0.79123800	3.97729400
H	-5.38415900	-1.49735400	2.90942800
H	-4.89185200	0.95363600	2.34296400
H	-2.51801600	2.81738900	-1.94644800
C	-1.36771000	-1.38986500	-2.87069800
H	-1.86376400	-2.12799200	-3.50302800
H	-1.49599600	-0.41212200	-3.34224600
H	-0.30434300	-1.62124000	-2.83267300
H	-0.93879700	4.51502500	1.10701800
H	-5.99029600	-0.13282400	-1.01243400
H	1.22299500	4.57019700	-1.06120300
H	-6.64295200	-1.92781600	0.66747200
H	-8.69237500	0.28883300	0.15658500
H	0.70160500	6.49794100	1.26092700
C	-2.55982400	-3.91295000	-1.40399800
H	-2.15202900	-4.13214400	-2.39341200
H	-2.46934900	-4.82200000	-0.80394300
H	-3.62622000	-3.69555900	-1.51942000
O	-0.14849200	-0.27887900	-0.40561500
Pa	2.07577700	-0.86491500	0.15525400
O	0.97222500	-1.99546600	1.49967100
O	3.86626200	-1.01894000	-0.81470700
O	2.80248400	-3.41098800	0.03209300
O	1.49316600	-2.59340500	-1.47127200
O	3.60821600	-1.45832700	2.02647500
O	3.88624200	0.60041000	1.45961800
O	1.83861000	0.18178400	-2.26999000

O	2.24489300	1.49190000	-0.60709700
O	1.26854300	0.70619000	2.04477500
H	1.11432700	-2.72701800	2.11155400
H	4.71336000	-1.30346600	-1.17422100
N	2.14682500	-3.62064100	-1.02459800
N	4.27981400	-0.37033500	2.17639000
N	2.07225300	1.35911100	-1.88010000
H	0.83786200	0.26809500	2.78952800
H	1.88746000	1.35485700	2.40462100
O	2.10746800	-4.68500900	-1.59574100
O	5.20770400	-0.29445600	2.94786200
O	2.13283500	2.31013600	-2.62852300

$Pa(OH)_2(NO_3)_3(H_2O)$(L17)

Sum of electronic and thermal Free Energies= -2466.919548

C	-1.37032100	-0.29452100	-0.76178700
N	-2.07879400	0.75670500	-0.35250600
C	-1.97863900	-1.38769300	-1.61326100
H	-3.03098200	-1.20089100	-1.81727700
C	-1.80396700	-2.83209600	-1.08155800
H	-0.75139000	-2.96712700	-0.84372500
C	-1.40874100	1.87513700	0.36161300
H	-2.15831300	2.32421400	1.01266500
H	-0.62932000	1.45105200	0.99131900
C	-3.52990000	0.92105500	-0.62548900
H	-3.72996600	1.98660300	-0.53465900
H	-3.72399300	0.66271000	-1.66570400
C	-4.50665500	0.15476000	0.29754700
H	-4.33730900	-0.91638500	0.15174100
C	-5.92427900	0.49079900	-0.22092300
H	-6.10492300	1.56379300	-0.07452300
C	-7.09834300	-0.29768200	0.37415600
H	-7.24437900	-0.02585000	1.42383700
C	-8.41125300	-0.05127300	-0.38034100
H	-8.28377100	-0.34206600	-1.43003900
C	-9.60079700	-0.80723600	0.21855300
H	-9.77578500	-0.50888000	1.25705200
H	-10.51936000	-0.61379500	-0.34238400
H	-9.42641300	-1.88786400	0.20938600
C	-0.77342800	2.94695400	-0.55589000
H	-0.03230500	2.42742100	-1.16931400
C	-0.01327600	3.94433300	0.34426000
H	0.65217800	3.37003500	0.99609300
C	0.82606400	4.98295600	-0.41038800
H	0.17849700	5.63855500	-1.00331300
C	1.68452200	5.84786000	0.52139200
H	2.35109100	5.19896900	1.10202700
C	2.51536000	6.89680100	-0.22338100
H	1.87326600	7.58279500	-0.78498900
H	3.11630100	7.49427500	0.46788200
H	3.19889000	6.42463400	-0.93617200
C	-1.75747800	3.63340400	-1.53019000
H	-1.16667400	4.20071900	-2.25616500
C	-2.79284300	4.57737700	-0.90384000
H	-3.38603800	4.09471800	-0.12170200
H	-2.32037600	5.45412300	-0.45433700
H	-3.48979200	4.93639300	-1.66570900
C	-4.26893600	0.47710500	1.79025800
H	-3.19543200	0.60036600	1.95581800
C	-4.74806800	-0.58676900	2.78790700
H	-4.28687700	-1.55541300	2.57467600
H	-4.46305200	-0.30377900	3.80513400
H	-5.82923800	-0.72486800	2.77647400
H	-4.72678500	1.44573800	2.02561700
H	-2.26785200	2.86601700	-2.12073100
H	-0.71991000	4.46232600	1.00441000
H	-5.93158700	0.32947300	-1.30646400
H	1.47972100	4.47085500	-1.12845200
H	-6.86982900	-1.37058800	0.35799800
H	-8.62719500	1.02404900	-0.38528700
H	1.03375100	6.34709700	1.24944700
C	-2.16260700	-3.82249400	-2.19777400
H	-1.52060300	-3.68286900	-3.07210600
H	-2.03689300	-4.85169100	-1.85075400
H	-3.20320000	-3.70368100	-2.51863800
H	-1.45059100	-1.31074500	-2.57088800
C	-2.61866000	-3.11125900	0.18519000
H	-3.69423100	-3.04012100	-0.00486800
H	-2.41396600	-4.12384400	0.54358100
H	-2.36305400	-2.42298800	0.99462100
O	-0.12537400	-0.37369700	-0.49321900
Pa	2.08945200	-0.73976900	0.14464600
O	1.89782300	1.09501500	1.09650500
O	3.35690600	-2.33990900	0.45122800
O	1.79939300	-1.21003900	2.60379700
O	0.58330900	-2.41999900	1.30824000
O	4.25163100	-0.10186000	1.64455700

O	4.27615000	0.26803200	-0.47808800
O	1.37568300	-2.74371400	-1.43637700
O	2.68484200	-1.24815300	-2.25137500
O	2.00273500	1.18984000	-1.65455300
H	2.27222200	1.47728800	1.89883400
H	4.10743900	-2.59754100	0.99859900
N	0.94212200	-2.15666900	2.50641800
N	4.89898600	0.33316400	0.65151700
N	2.05870900	-2.36294500	-2.42940500
H	2.53332700	1.93952200	-1.35691700
H	2.37229400	0.91032400	-2.50291400
O	0.50766700	-2.74623000	3.46509600
O	6.02028200	0.78407900	0.72673800
O	2.13298900	-2.97666300	-3.46718900

$Pa(OH)_2(NO_3)_3(H_2O)$(L18)

Sum of electronic and thermal Free Energies= -2506.203873

C	-1.29434900	-0.44361100	-0.97622800
N	-2.05611600	0.55479600	-0.52357300
C	-1.85172500	-1.42997800	-1.99634300
H	-2.93697300	-1.38110300	-1.97385600
C	-1.45287800	-2.88045200	-1.70340100
H	-0.37859900	-3.02666300	-1.80411600
H	-1.75996200	-3.18792800	-0.70115300
C	-1.45423200	1.64777100	0.28117400
H	-2.25843300	2.07250700	0.87824000
H	-0.73181800	1.21042300	0.96713600
C	-3.51113500	0.65375600	-0.81615800
H	-3.78666500	1.69206700	-0.63837300
H	-3.66170400	0.47552400	-1.87710700
C	-4.42095600	-0.26210800	0.03404900
H	-4.14649900	-1.30248400	-0.18233900
C	-5.91990400	-0.09307800	-0.37081200
H	-6.28149200	0.81924400	0.12343800
C	-6.75021700	-1.28611700	0.15843100
H	-6.60951100	-2.13441800	-0.52460500
H	-6.36292900	-1.61570200	1.12794900
C	-8.24958000	-1.00316100	0.32043000
H	-8.38029200	-0.18061300	1.03387300
H	-8.67372600	-0.65534100	-0.62747900
C	-9.03666200	-2.22580500	0.80216400
H	-8.66156500	-2.58330200	1.76648000
H	-10.09824600	-1.99320200	0.92372000
H	-8.95652100	-3.05238200	0.08906600
C	-0.75928300	2.73123000	-0.57862600
H	-0.06204900	2.18727300	-1.22425200
C	0.15913200	3.61544900	0.32045100
H	0.90658400	2.91679400	0.71192200
C	0.93926300	4.64919600	-0.51731800
H	0.27519200	5.47031900	-0.81479000
H	1.26773800	4.16949300	-1.44787600
C	2.17468400	5.23341300	0.18197800
H	2.82043300	4.41056000	0.51225700
H	1.87571800	5.77073000	1.08770700
C	2.97430800	6.17954100	-0.71928700
H	2.36364000	7.02985300	-1.03935200
H	3.85157100	6.57687800	-0.20115300
H	3.32365800	5.66551400	-1.62042600
C	-1.71457900	3.47649800	-1.53989600
H	-1.10499400	4.06812800	-2.22915000
C	-2.79378500	4.38938000	-0.93980900
H	-3.37354900	3.89809300	-0.15339400
H	-2.36698600	5.29725200	-0.51028400
H	-3.49772000	4.69726400	-1.71798900
C	-4.24156300	-0.02240400	1.55697000
H	-4.02050800	1.03577400	1.73250500
C	-3.19069500	-0.90035200	2.24753600
H	-2.18670700	-0.75563900	1.84488800
H	-3.15046900	-0.68096000	3.31822200
H	-3.44014300	-1.96004200	2.13608000
H	-5.19938800	-0.19736000	2.05298900
H	-2.19947800	2.72470600	-2.17179400
C	-1.39001900	-0.99129400	-3.40321600
H	-1.84172500	-1.64863200	-4.14958200
H	-1.69229700	0.03444600	-3.62793700
H	-1.95398800	-3.53585700	-2.41962100
H	-0.30558400	-1.06459900	-3.49063700
C	-0.51884400	4.25659700	1.54567100
H	0.23059600	4.71528200	2.19467200
H	-1.23147600	5.03483300	1.26596800
H	-1.04912400	3.51896500	2.15270900
C	-6.15509200	0.07118500	-1.88289400
H	-5.74923800	1.00627100	-2.27446000
H	-5.70970500	-0.75737200	-2.44441000
H	-7.22479200	0.07433700	-2.10370400
O	-0.08152900	-0.54908500	-0.61167000
Pa	2.18780000	-0.82337800	0.01034800

O	2.21115900	0.98528400	-1.01251000
O	3.25415500	-1.66494400	1.53530100
O	3.23681900	1.07900800	1.54970900
O	1.22318900	0.39728100	1.89953700
O	4.54895800	-0.33299300	-0.65462400
O	4.04584100	-2.38693400	-1.05211800
O	0.54667500	-2.34750000	1.41243800
O	1.53346400	-3.19818700	-0.30352200
O	2.03071600	-1.36132100	-2.51302000
H	2.84286600	1.69660600	-1.17044400
H	3.87577200	-1.83580500	2.25099800
N	2.20174500	1.16641700	2.26313800
N	4.94863100	-1.49266000	-1.03951500
N	0.75385700	-3.37795900	0.71028100
H	2.15279300	-0.59508200	-3.08762300
H	2.59069600	-2.06993600	-2.85665400
O	2.09706900	1.90556300	3.21502900
O	6.09406000	-1.70125600	-1.36420100
O	0.26609200	-4.45884500	0.94767600

$Pa(OH)_2(NO_3)_3(H_2O)$(L19)

Sum of electronic and thermal Free Energies=

-2506.215331

C	-1.30778600	-0.25983300	-0.94846100
N	-2.00316700	0.77429300	-0.46869700
C	-1.93505900	-1.20996600	-1.96276200
H	-3.00531300	-1.02730600	-2.00258900
C	-1.72924500	-2.68745100	-1.60443800
H	-0.67444900	-2.95597800	-1.61187100
H	-2.14381500	-2.92675400	-0.62239300
C	-1.31688100	1.83959100	0.30552400
H	-2.07963300	2.33244200	0.90749000
H	-0.61166200	1.37200700	0.98832900
C	-3.46741400	0.91951200	-0.66983900
H	-3.71230500	1.94603400	-0.40267800
H	-3.70276100	0.81751900	-1.72925500
C	-4.33593400	-0.04667700	0.16876800
H	-4.04139200	-1.06636700	-0.10028100
C	-5.80160600	0.17809300	-0.26572900
H	-6.07337200	1.20790200	-0.00058000
C	-6.87576300	-0.76901200	0.30609600
H	-6.81339800	-0.74454300	1.40107400
C	-8.27534700	-0.24230700	-0.07453100
H	-8.32999200	0.81808400	0.19754600
H	-8.38552000	-0.28333600	-1.16607800
C	-9.44601500	-0.97789900	0.58656100
H	-9.34958800	-0.96991700	1.67716400
H	-10.39598100	-0.49812400	0.33491400
H	-9.51269800	-2.02051500	0.26599200
C	-0.56599800	2.87221800	-0.56923000
H	0.20955100	2.31112900	-1.09933500
C	0.12036200	3.88017700	0.37740500
H	0.71345600	3.32281400	1.11004400
C	1.03076000	4.94035400	-0.27720000
H	0.43931500	5.50156600	-1.01209100
C	1.49597200	5.94938700	0.79368800
H	2.14031300	5.42876600	1.51357000
H	0.61780500	6.28468300	1.35791900
C	2.22649800	7.18201300	0.24961700
H	1.60587900	7.71894300	-0.47532700
H	2.46714000	7.87813800	1.05812200
H	3.16535700	6.92113200	-0.24566200
C	-1.45138600	3.54744600	-1.64086600
H	-0.79518000	4.06212200	-2.34986200
C	-2.49706600	4.54820000	-1.13071200
H	-3.15918300	4.11656900	-0.37491400
H	-2.03180700	5.43143900	-0.68680500
H	-3.12688200	4.89057700	-1.95610300
C	-4.10766700	0.13083800	1.69173100
H	-3.13105200	0.58866600	1.86608600
C	-4.14832900	-1.16863700	2.50699400
H	-3.35454700	-1.85087200	2.18805400
H	-3.99531600	-0.95921000	3.56947400
H	-5.09968900	-1.69473800	2.40805900
H	-4.84533500	0.84101100	2.08263800
H	-1.94951300	2.76893400	-2.22744300
C	-1.35922500	-0.88301800	-3.35742300
H	-1.85897100	-1.50474900	-4.10372300
H	-1.51903400	0.16344800	-3.62711500
H	-2.24696800	-3.30418200	-2.34290000
H	-0.29096500	-1.09546700	-3.39350900
H	-0.65186900	4.40115300	0.95606300
H	-5.85526000	0.12240900	-1.36132500
C	-6.66706200	-2.21687400	-0.16154700
H	-7.40668300	-2.89142900	0.27567700
H	-6.75575900	-2.28437100	-1.25176400
H	-5.68097300	-2.59693700	0.11488700
C	2.22115000	4.30738600	-1.01298300

H	2.85781500	3.75434100	-0.31356600
H	1.89641700	3.61189800	-1.79024000
H	2.84065500	5.06613800	-1.49653600
O	-0.09032800	-0.42277200	-0.62611100
Pa	2.09848700	-0.98901800	0.08328500
O	2.43177600	0.49165100	-1.33315300
O	2.98410700	-1.65931700	1.79321400
O	3.65310400	0.91719900	1.08159800
O	1.56446800	0.85034100	1.60611100
O	4.43883300	-1.26090500	-0.68825100
O	3.51478800	-3.19378200	-0.47117100
O	0.18322600	-1.67716600	1.79257300
O	0.86845100	-3.13029200	0.35594700
O	1.81954000	-2.06999500	-2.23570900
H	3.15052500	1.06662800	-1.62057300
H	3.48265400	-1.89066100	2.58417100
N	2.71796900	1.41850700	1.76170800
N	4.57546100	-2.54272200	-0.71180300
N	0.08238200	-2.85238800	1.34156000
H	2.11931100	-1.52372700	-2.97302300
H	2.15137400	-2.96536600	-2.38307300
O	2.85750900	2.36096900	2.50847900
O	5.63921500	-3.06441200	-0.95181400
O	-0.69096200	-3.67449800	1.78151900

$Pa(OH)_2(NO_3)_3(H_2O)$(L20)

Sum of electronic and thermal Free Energies=

-2506.219687

C	-1.40604600	-0.12636200	-0.87775700
N	-2.10792800	0.89254300	-0.37584400
C	-2.02916800	-1.06226800	-1.90770400
H	-3.10205500	-0.89310300	-1.93426800
C	-1.80146300	-2.54443600	-1.58373900
H	-0.74360300	-2.79981600	-1.60755500
H	-2.20301000	-2.81019500	-0.60310100
C	-1.42362800	1.94743500	0.41425800
H	-2.18815900	2.43709500	1.01648100
H	-0.72392300	1.47030900	1.09625400
C	-3.57171000	1.03778200	-0.57865800
H	-3.81996000	2.05935800	-0.29543500
H	-3.80352100	0.95238400	-1.64043700
C	-4.43962200	0.05630500	0.24073600
H	-4.14457800	-0.96194500	-0.03930200
C	-5.90443100	0.26213800	-0.20137200
H	-6.19859800	1.28746000	0.05179100
C	-6.92003900	-0.72848600	0.38244800
H	-6.99784700	-0.59496900	1.46787200
C	-8.33356900	-0.62232200	-0.22428400
H	-8.23471100	-0.72300700	-1.31381700
C	-9.21670200	-1.77511100	0.27373900
H	-9.34651500	-1.72478200	1.36054000
H	-10.21065100	-1.73713900	-0.18180000
H	-8.77447800	-2.74696700	0.03507300
C	-0.66483300	2.98098000	-0.44982400
H	0.10870300	2.42248600	-0.98873600
C	0.05366900	3.97356500	0.48788100
H	0.60038800	3.40277100	1.24453200
C	1.03984800	4.90313300	-0.23373400
H	0.49926500	5.58172100	-0.90521800
C	1.93548700	5.74557800	0.69601000
H	2.46056500	5.05152200	1.36543000
C	2.99280000	6.50194100	-0.12060900
H	2.51898800	7.20838500	-0.81128700
H	3.66224100	7.07201200	0.53053000
H	3.60462300	5.81513900	-0.71312200
C	-1.54527600	3.67420700	-1.51458400
H	-0.88494000	4.18632900	-2.22119800
C	-2.57761200	4.68263300	-0.99334700
H	-3.23823300	4.25406500	-0.23434300
H	-2.10015000	5.55977400	-0.55012000
H	-3.20998000	5.03452300	-1.81277400
C	-4.22309500	0.21012900	1.76771300
H	-3.25378200	0.67720700	1.95809900
C	-4.25481700	-1.10782400	2.55299500
H	-3.44185200	-1.76698400	2.23364000
H	-4.12722100	-0.92165700	3.62317600
H	-5.19371400	-1.64863400	2.41977000
H	-4.97279200	0.90298700	2.16681200
H	-2.05422900	2.90586100	-2.10514700
C	-1.46994900	-0.69781000	-3.29989400
H	-1.96471700	-1.31333700	-4.05457300
H	-1.64954700	0.35073200	-3.54821100
H	-2.31926800	-3.15132600	-2.33028900
H	-0.39853000	-0.89093500	-3.34835000
H	-0.69019300	4.56251900	1.03475800
H	-5.94870600	0.19205900	-1.29580500
O	-0.18605900	-0.28456600	-0.56182100
Pa	2.01555400	-0.83293200	0.12180500

O	2.32600700	0.68761200	-1.25521000
O	2.92568700	-1.53025000	1.80862100
O	3.56471200	1.06320300	1.16274000
O	1.47560300	0.96797000	1.68281100
O	4.35246700	-1.06488700	-0.67356600
O	3.44867500	-3.01136600	-0.49403200
O	0.12392100	-1.57792200	1.83291300
O	0.80879900	-2.99209600	0.35782200
O	1.73604400	-1.86266500	-2.22049000
H	3.03380700	1.27751300	-1.53951000
H	3.45854100	-1.74428700	2.58188900
N	2.62665000	1.53828300	1.85612500
N	4.50112800	-2.34437000	-0.72747900
N	0.02873800	-2.74331800	1.35573400
H	2.01718400	-1.29580300	-2.94949600
H	2.08313500	-2.74829600	-2.39003500
O	2.75900500	2.45640000	2.63389500
O	5.56801600	-2.85008400	-0.98723900
O	-0.73437200	-3.58149000	1.78314600
H	-6.55164900	-1.74876500	0.22109000
H	1.68751500	4.29121700	-0.87429200
C	-9.00021500	0.73011800	0.06669900
H	-9.09116800	0.89197500	1.14677200
H	-8.43545300	1.56722600	-0.35075800
H	-10.00653700	0.76651700	-0.36079300
C	1.12734500	6.72077900	1.56429000
H	0.55067900	7.41053200	0.93745900
H	0.42647800	6.20132700	2.22217100
H	1.78969700	7.32008200	2.19606900