Structure and bonding in [L]M(μ-CCR)$_2$M[L] and [L]M(μ-RC$_4$R)M[L]: Requirements for C-C coupling

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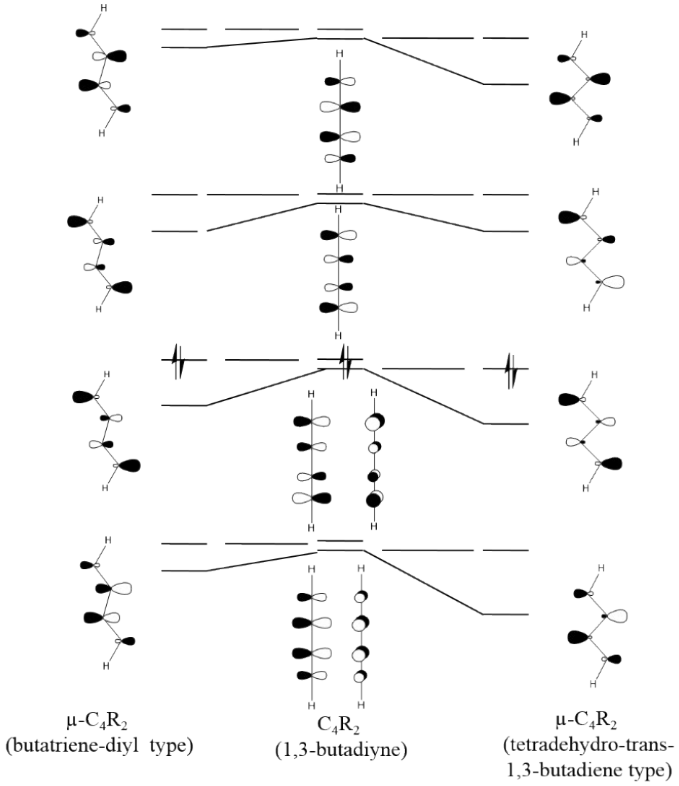
Table 1. Experimental Geometric parameters for **1**-**8**. There are 67 experimental structures available, labeled by the structure number followed by alphabets **a**, **b**, etc.

	M[L]	R	M1M2	M1C1	M1C3	C1C2	M2C2	C1C3	C2C1C3	Ref
1a	Li(tmpda)[a]	Ph	2.565	2.132	2.165	1.241	3.079	3.447	163.3	1
1b	$Al(CMe_3)_2$	Ph	2.875	2.073	2.096	1.177	2.984	3.019	172.4	2
1c	$Be(NMe_3)(C{\equiv}CMe)$	Me	2.319	1.836	1.904	1.200	2.813	2.936	165.9	3
1d	$Mg(C_5Me_4H)(thf)$	Ph	2.957	2.218	2.235	1.210	3.217	3.329	177.4	4
1e	$Ca(C_5Me_5)(thf)$	Ph	3.699	2.52	2.551	1.174	3.348	3.469	167.9	5
1f	Gd(η^5-2,4-dimethylpentadienyl)$_2$	Ph	3.853	2.565	2.512	1.210	3.364	3.307	175.4	6
1g	$ErCp_2$	^{t}Bu	3.657	2.426	2.471	1.254	3.207	3.258	162.6	7
1h	Er(η^5-2,4-dimethylpentadienyl)$_2$	Ph	3.854	2.556	2.512	1.218	3.525	3.292	175.6	6
1i	$Yb(C_5Ph_5)(thf)$	Ph	3.606	2.542	2.522	1.155	3.376	3.555	174.9	8
1j	$Sm(C_5H_4Me)_2$	^{t}Bu	3.799	2.555	2.542	1.202	3.202	3.399	160.6	9
1k	$Y(C_5Me_4SiMe_3)(X)$[b]	Ph	3.764	2.474	1.469	1.225	3.217	3.205	166.7	10
1l	$Cu(PPh_2Me)_2$	*p*-^{n}Bu-Ph	2.415	2.111	2.059	1.215	3.155	3.401	176.0	11
2a	$AlMe_2$	Ph	3.03	1.994	2.224	1.208	2.616	2.944	137.3	2
2b	Mg(β-DK$^{N\text{-}Ar}$)[a]	^{t}Bu	3.15	2.191	2.305	1.222	2.808	3.211	144.1	12
2c	Ca(β-DK$^{N\text{-}Ar}$)[a]	CH_2NMe_2	3.589	2.505	2.535	1.215	2.866	3.541	137.9	12
2d	Mn(Cp)(thf)	Ph	2.969	2.162	2.25	1.215	2.977	3.258	156.4	13
2e	Mn(β-DK$^{N\text{-}Ar}$)[a]	Ph	3.12	2.132	2.298	1.226	2.658	3.15	135.4	14
2f	$Zn[(2,6\text{-}ipr_2C_6H_3)NCMe]_2$	Ph	2.934	1.985	2.343	1.225	2.863	3.213	138.0	15
2g	$Yb(dig)(thf)_2^+$	Ph	3.845	2.586	2.662	1.168	3.127	3.572	148.5	8
2h	$Sm(C_5H_4CMe_3)_2$	Ph	3.98	2.559	2.617	1.202	3.073	3.285	148.8	16
2i	$Nd(C_5H_4CMe_3)_2$	Ph	4.025	2.603	2.641	1.204	3.116	3.332	150.4	17
2j	$Gd(C_5H_4CMe_3)_2$	Ph	3.934	2.532	2.601	1.203	3.062	3.27	149.1	17
2k	$Pt(C_6F_5)_2$	Ph	3.431	2.022	2.369	1.219	2.303	2.488	114.2	18
2l	$Pt(C_6F_5)(PPh_3)$	Ph	3.651	2.024	2.362	1.198	2.261	2.455	119.8	19
2m	$Re(CO)_4$	$SiMe_3$	3.850	2.136	2.482	1.243	2.441	2.592	122.8	20
2n	Mg((NHC^{Me})(C≡C^{t}Bu))	^{t}Bu	3.094	2.192	2.288	1.220	2.708	3.239	138.7	21
2o	$Zn(PPh_3)(Et)$	Ph	2.991	2.010	2.340	1.203	2.731	3.175	134.1	22
2p	Ir(dtbpy)(C≡CPh)[a]	$SiMe_3$	3.339	2.012	2.232	1.214	2.181	2.389	114.5	23

2q	$Ir(ppy)_2$	^{p}Tol	3.699	2.080	2.413	1.219	2.387	2.539	120.9	[24]
3a	$Zr(C_5H_4Me)_2$	Ph	3.506	2.188	2.431	1.261	2.406	3.018	119.6	[25]
3b	$ZrCp_2$	Cp-Fe-C_5H_4	3.476	2.185	2.407	1.257	2.414	3.009	121.1	[26]
3c	Zr(Y)[c]	$SiMe_3$	3.490	2.177	2.394	1.254	2.398	2.968	120.9	[27]
3d	$ZrCp_2$	^{t}Bu	3.480	2.123	2.379	1.248	2.366	2.867	120.8	A
3e	Ti(Cp)Cl	$SiMe_3$	3.155	2.046	2.206	1.252	2.240	2.855	120.6	B
3f	$TiCp_2$	$SiMe_3$	3.549	2.056	2.394	1.253	2.312	2.706	118.0	[28]
3g	TiCp2	$SnMe_3$	3.574	2.065	2.414	1.241	2.273	2.722	115.4	[29]
3h	$Ti(C_5H_3Me_2)_2$	$SnMe_3$	3.633	2.088	2.421	1.254	2.283	2.691	116.4	[29]
3i	W(Cp)NO	Ph	3.039	2.025	2.242	1.249	2.298	3.003	116.2	[30]
4a	$TiCp_2$	SCH_2Ph	4.17	2.117	2.301	1.325	2.079	1.469	127.3	[31]
4b	$Ti(C_5H_4Me)_2$	Ph	4.228	2.153	2.325	1.325	2.084	1.486	127.2	[32]
4c	$Ti(C_5H_4Me)_2$	^{t}Bu	4.226	2.160	2.324	1.322	2.085	1.508	127.4	[33]
4d	$TiCp_2$	^{t}Bu	4.197	2.143	2.307	1.320	2.086	1.488	128.1	[34]
4e	$Si(^{t}Bu)_2$	$SiMe_3$	3.960	1.899	2.314	1.362	1.899	1.497	110.0	[35]
4f	$Si(^{t}Bu)_2$	(Cyclohexylidene)methyl	3.967	1.886	2.325	1.368	1.902	1.480	108.9	[35]
4g	$Si(^{t}Bu)_2$	R[a]	3.968	1.883	2.322	1.369	1.897	1.485	108.6	[36]
4h	$Si(^{t}Bu)_2$	Me	3.955	1.887	2.316	1.339	1.899	1.485	109.5	[37]
5a	SmL_2[d]	H	5.368	2.84	2.679	1.288	2.426	1.297	155	[38]
5b	$Lu(C_5Me_5)(C{\equiv}CPh)(bipy)$ [a]	Ph	5.146	2.743	2.569	1.301	2.388	1.328	150.1	[39]
5c	$Ce(C_5Me_5)_2$	Me	5.527	2.908	2.779	1.294	2.525	1.331	147.1	[40]
5d	$Ce(C_5Me_5)_2$	^{t}Bu	5.536	2.939	2.749	1.312	2.607	1.328	154.6	[40]
5e	$Sm(C_5Me_5)_2$	CH_2CH_2Ph	5.437	2.909	2.69	1.278	2.487	1.357	152.2	[41]
5f	$Sm(C_5Me_5)_2$	Ph	5.624	2.963	2.806	1.362	2.505	1.298	147.0	[42]
5g	$La(C_5Me_5)_2$	Ph	5.635	2.95	2.824	1.361	2.577	1.263	148.6	[43]
6a	Mg(β-$DK^{N\text{-}Ar}$) [a]	$Ph^{2,6\text{-}di\text{-}ipr}$	-	2.192	-	1.518	2.184	-	-	[43]
6b	Mg(β-$DK^{N\text{-}Mes}$) [a]	^{t}Bu	-	2.148	-	1.538	2.148	-	-	[43]
6c	Mg(β-$DK^{N\text{-}Ar}$) [a]	$SiMe_3$	-	2.159	-	1.465	2.159	-	-	[43]
6d	$Al(CHSiMe_3)_2$	Ph	4.413	2.075	-	1.493	2.075			[44]
7a	$Zr(C_5Me_5)_2$	Ph		2.214	2.214	1.239		3.266		[45]
7b	$U(C_5Me_5)_2$	Ph		2.398	2.398	1.212		3.700	-	[46]
8a	$Zr(C_5Me_5)_2$	Ph	-	2.328	2.330	1.304	-	1.327	148.0	[47]
8b	$Zr(C_5Me_5)_2$	$SiMe_3$	-	2.305	2.307	1.291	-	1.336	152.5	[47]
8c	$ZrCp_2$	^{t}Bu	-	2.309	2.307	1.292	-	1.329	148.5	[47]
8d	$Zr(C_5Me_5)_2$	$(^{t}Bu)(C{\equiv}C^{t}Bu)$	-	2.320	2.339	1.285	-	1.326	153.5	[48]
8e	$TiCp_2$	Cp-Fe-C_5H_4	-	2.213	2.218	1.282	-	1.326	147.7	[49]
8f	$TiCp_2$	^{t}Bu	-	2.210	2.213	1.277	-	1.338	147.7	[50]
8g	$Th(C_5Me_5)_2$	Ph	-	2.540	2.544	1.283	-	1.342	150.3	[51]
8h	$U(C_5Me_5)_2$	$SiMe_3$	-	2.435	2.434	1.296	-	1.313	151.2	[52]

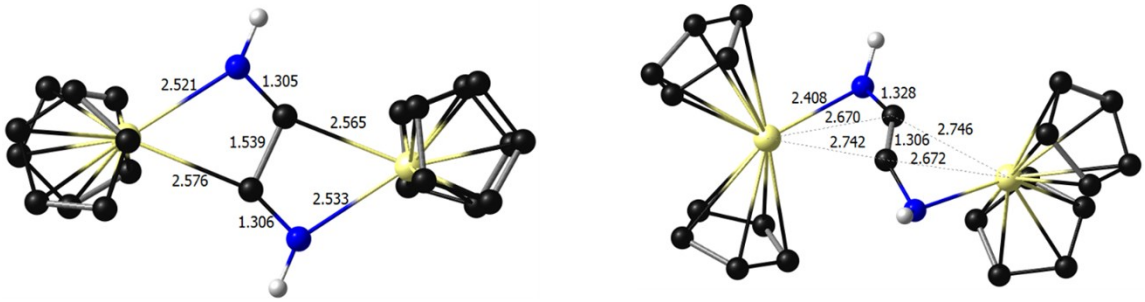
[a]*tmpda = N,N,N′,N′*-tetramethyl-1,3-propandiamin, DK = β-diketiminate, dtbpy = 4,4′-Di-*tert*-butyl-2,2′-bipyridyl; [b]X = N,N',3-triphenylprop-2-ynamidinato-N,N'; [c]Y = μ_2-η^2-Trimethylsilylethynyl)-bis((η^5-3-trimethylsilyl-cyclopentadienyl)-(η^5-cyclopentadienyl)dimethylsily; [d]L = (Et_8-calix-tetrapyrrole){Li[Li(thf)]$_2$(μ_3-OCH=CH_2). A = CCDC 181401, B = CCDC 884369. There are several more structures available if substituent attached with two acetylide groups differ. [e]Due to the presence of two C-centers, the coupled C1-C2 bonding numbering differs from the rest of the structures (C1-C3).

Scheme S1. Interaction diagram leading to μ-C_4R_2 unit starting from 1,3-butadiyene. Ligand structure similar to



that in **5** (left) and **4** (right).

Figure S1. Geometries of **6Ce** and **6Ce_2** (N-centers are pyramidal) with the hetero ligand HNCCNH. Relative energy (kcal/mol) value is given in the parethesis. H-atoms in the Cp ring are not shown for simplicity.



6Ce (0.0) **6Ce_2 (-2.8)**

Figure S2. Geometries of all the intermediates and transition state structures for the reaction pathway of C-C coupling and cleavage reactions (a) M = Th; (b) M = Zr. Bond lengths in angstroms, and bond angles in degrees. H-atoms in the Cp ring are not shown for simplicity.

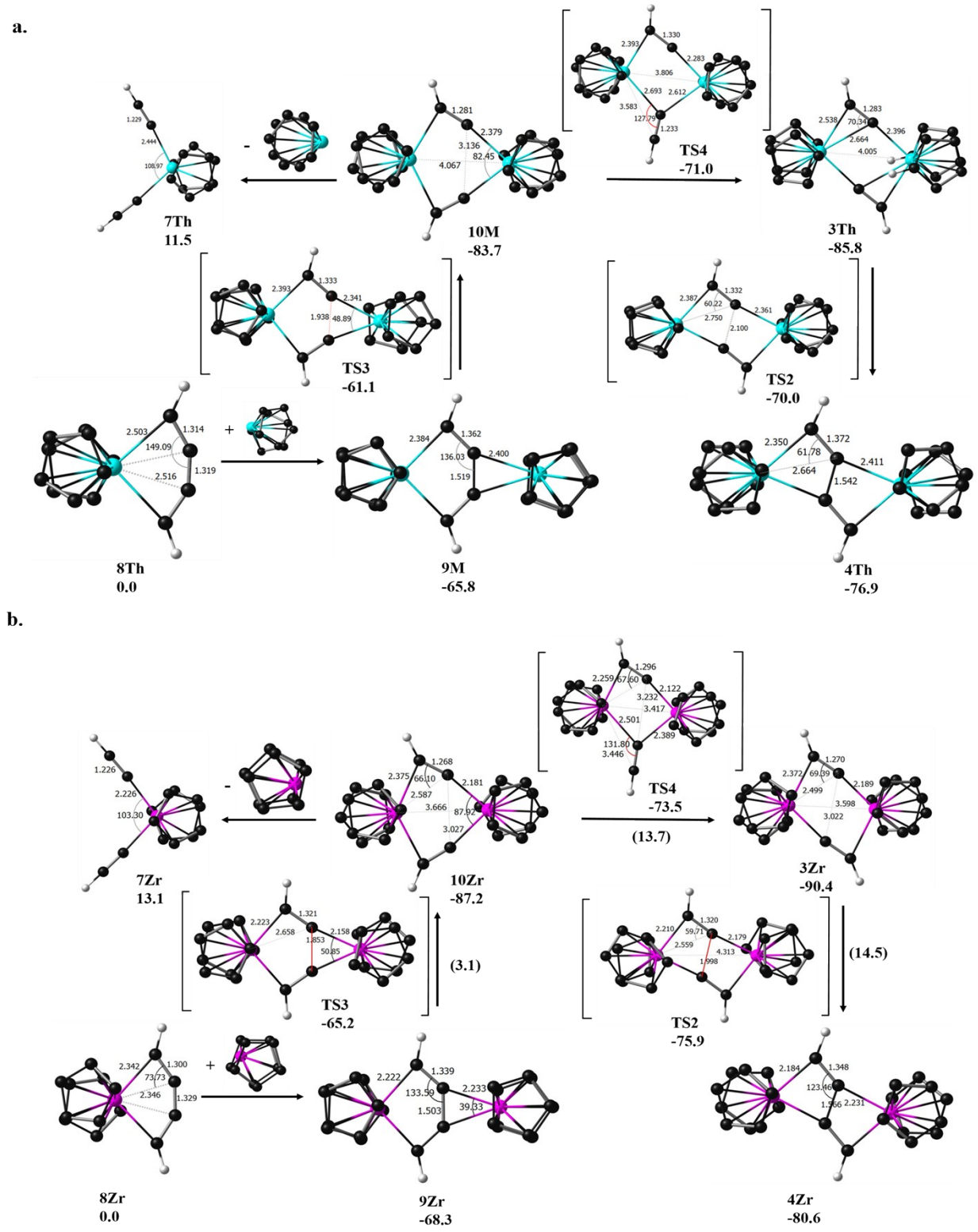


Figure S3. Geometries of all the intermediates and transition state structures for Thorium (a) R = H; (b) R = F. Bond lengths are in angstroms, and bond angles are in degrees. H-atoms in the Cp ring are not shown for simplicity.

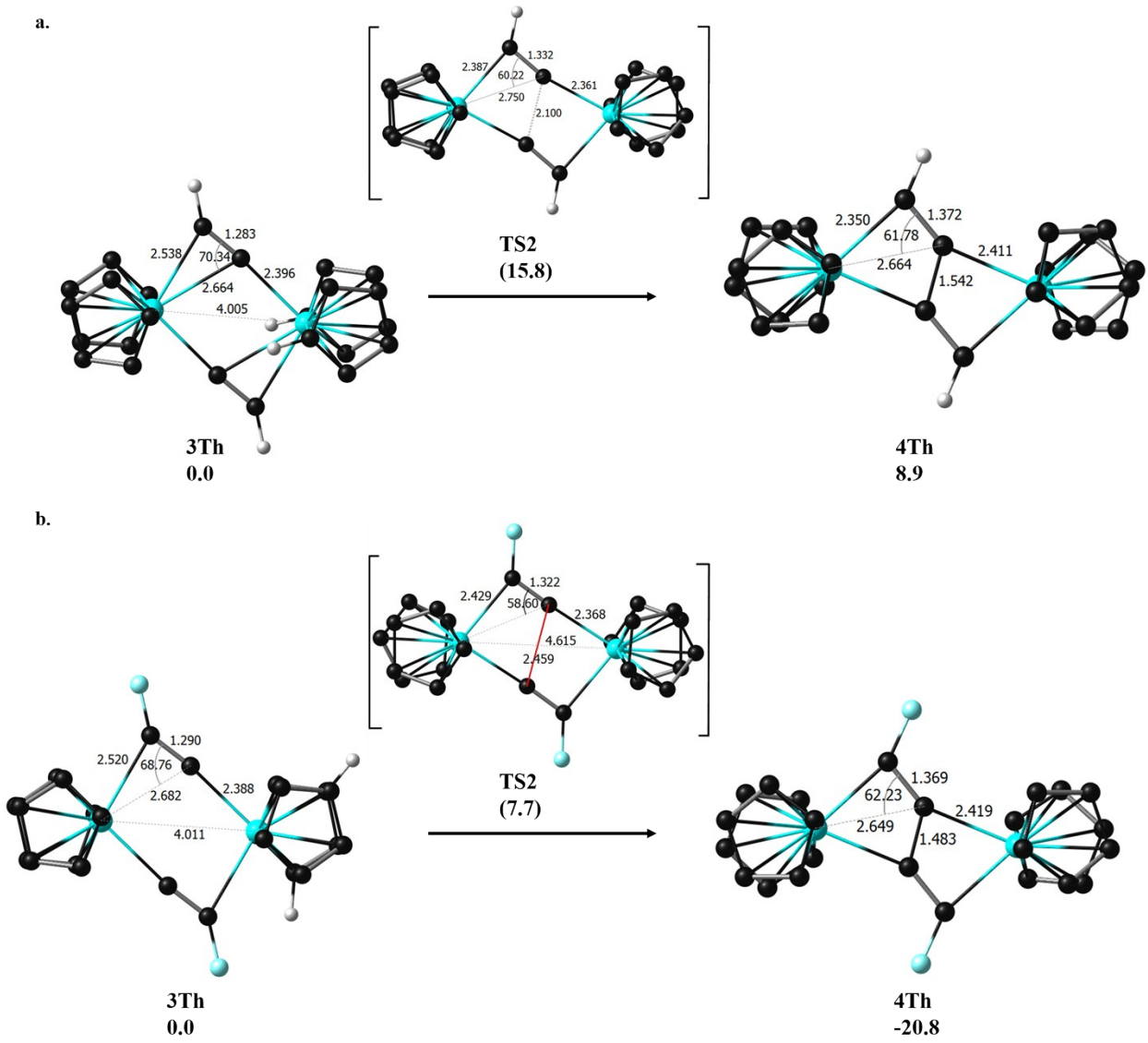


Figure S4. Geometries of all the intermediates and transition state structures for the C-C coupling reaction for Zirconium (a) R = H; (b) R = F. Bond lengths are in angstroms, and bond angles are in degrees. H-atoms in the Cp ring are not shown for simplicity.

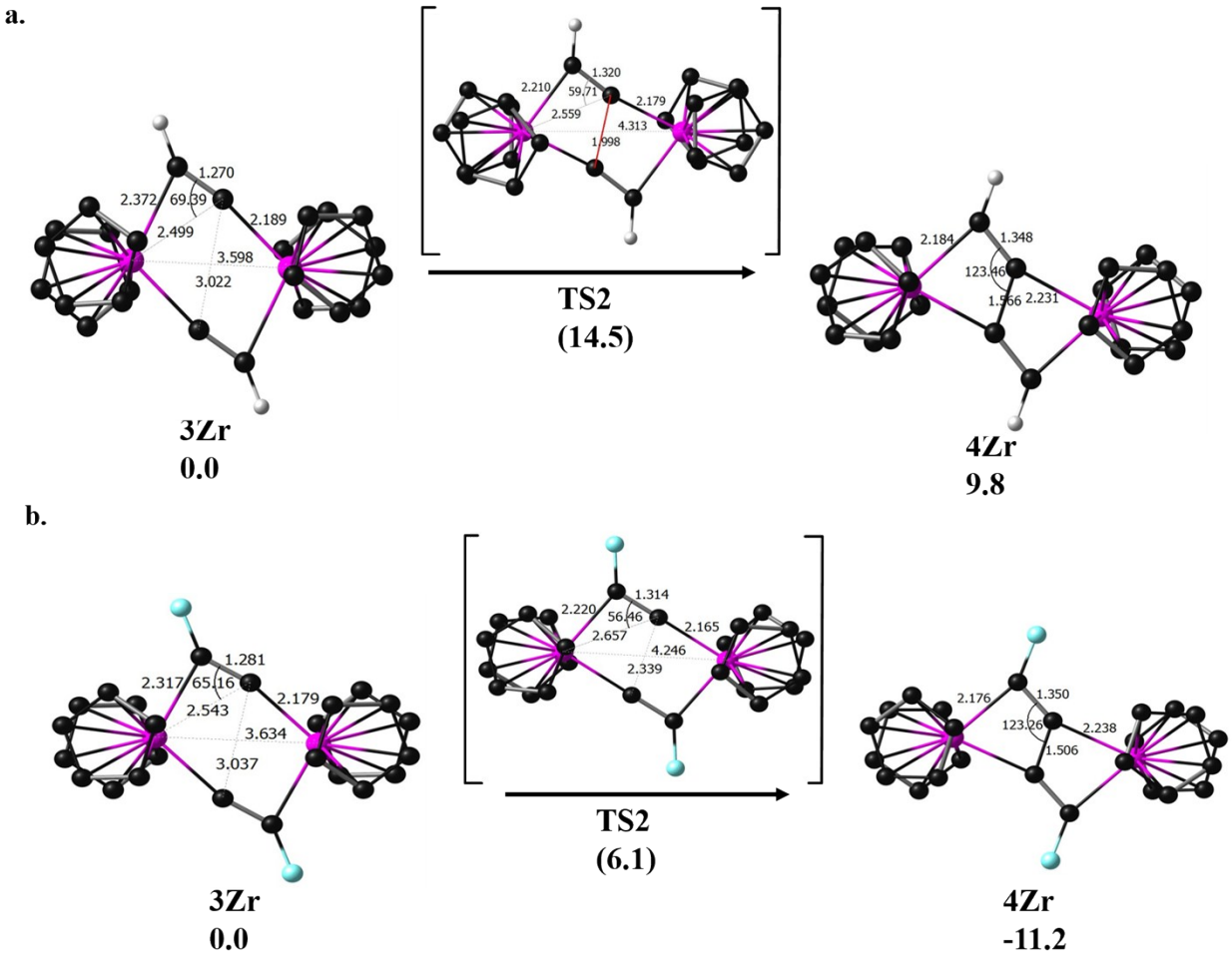
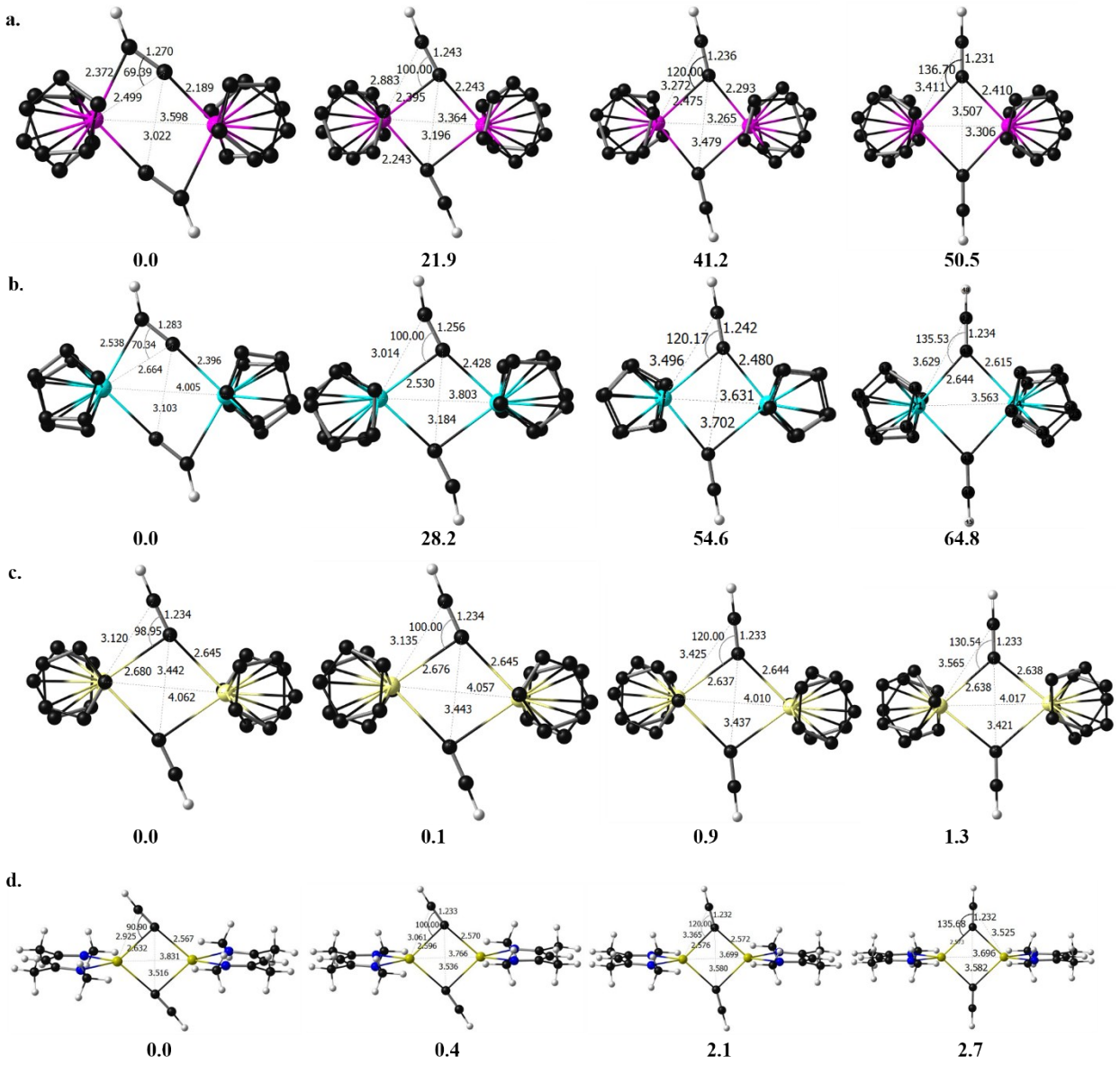


Figure S5. Variation of relative energies with M2-C1-C2 angle (θ) with important geometrical parameters. (a) M = Zr, (b) M = Th, (c) M = Ce, (d) M = Ca. Bond lengths are in angstroms, bond angles in degrees, energy values are in kcal/mol. H-atoms in the Cp ring are not shown for simplicity.



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Cartesian coordinates of all the optimized geometries obtained for TM and MG complexes and B3PW91 functional for Ln and An complexes using G09 program package.

8Zr

Total energy including ZPVE: -587.0419 a. u.
Total free energy including ZPVE: -587.0832 a. u.

N_{Img} = 0

6	-2.572768000	0.251254000	-0.177758000
6	-2.149499000	-0.643914000	-1.200189000
6	-2.315280000	-0.358304000	1.076162000
1	-3.014712000	1.226437000	-0.331763000
6	-1.612683000	-1.793889000	-0.574116000
1	-2.224160000	-0.473944000	-2.265324000
6	-1.704850000	-1.613844000	0.836324000
1	-2.526206000	0.070223000	2.045918000
1	-1.210452000	-2.662571000	-1.077847000
1	-1.390341000	-2.321011000	1.592193000
6	2.572766000	0.251247000	0.177830000
6	2.149465000	-0.643973000	1.200202000
6	2.315314000	-0.358244000	-1.076128000
1	3.014705000	1.226422000	0.331898000
6	1.612669000	-1.793917000	0.574053000
1	2.224095000	-0.474059000	2.265348000
6	1.704875000	-1.613797000	-0.836375000
1	2.526267000	0.070334000	-2.045856000
1	1.210426000	-2.662625000	1.077726000
1	1.390387000	-2.320925000	-1.592290000
6	0.014261000	1.683962000	-1.757924000
6	-0.014264000	1.683956000	1.757925000
6	0.005263000	2.386655000	-0.664293000
6	-0.005270000	2.386654000	0.664297000
1	-0.022518000	1.947906000	2.807585000
1	0.022514000	1.947915000	-2.807584000
40	0.000000000	0.137071000	-0.000001000

9Zr

Total energy including ZPVE: -1020.606 a. u.
Total free energy including ZPVE: -1020.6638 a. u.

N_{Img} = 0

6	-4.276283000	-1.738012000	-0.003635000
6	-3.488986000	-1.996702000	-1.157326000
6	-3.479045000	-2.011393000	1.139697000
1	-5.302407000	-1.394784000	0.002971000
6	-2.208469000	-2.442308000	-0.729230000
1	-3.814868000	-1.888366000	-2.184811000
6	-2.202248000	-2.451284000	0.694946000
1	-3.795887000	-1.915859000	2.171258000
1	-1.388447000	-2.730340000	-1.370679000
1	-1.376379000	-2.747153000	1.325210000
6	-2.198766000	2.455320000	-0.685749000

6	-3.472409000	2.017530000	-1.140999000
6	-2.213920000	2.438693000	0.738291000
1	-1.368872000	2.754345000	-1.309203000
6	-4.276883000	1.737634000	-0.004415000
1	-3.782443000	1.927251000	-2.175109000
6	-3.497109000	1.990287000	1.155807000
1	-1.398134000	2.723865000	1.386381000
1	-5.302823000	1.394123000	-0.019471000
1	-3.829674000	1.876465000	2.180542000
6	4.059630000	-1.644756000	-0.651828000
6	3.992599000	-1.667068000	0.772472000
6	2.873062000	-2.227893000	-1.155823000
1	4.882609000	-1.266062000	-1.242942000
6	2.765927000	-2.267566000	1.143231000
1	4.755017000	-1.309920000	1.451584000
6	2.066057000	-2.597921000	-0.046764000
1	2.617452000	-2.354740000	-2.198557000
1	2.415282000	-2.428894000	2.152857000
1	1.085226000	-3.050479000	-0.100348000
6	2.069121000	2.598178000	0.064870000
6	2.889920000	2.219717000	1.161026000
6	2.753202000	2.275043000	-1.136078000
1	1.089714000	3.051667000	0.134345000
6	4.069429000	1.639345000	0.637816000
1	2.647704000	2.339675000	2.207794000
6	3.983869000	1.670432000	-0.785272000
1	2.389997000	2.443799000	-2.140022000
1	4.899561000	1.255922000	1.215662000
1	4.736751000	1.316391000	-1.476585000
6	-0.261874000	-0.000348000	0.750410000
6	-0.262011000	0.000862000	-0.752755000
1	0.519348000	0.004170000	2.747300000
1	0.521814000	-0.003067000	-2.748903000
6	0.708316000	0.003601000	1.673848000
6	0.709176000	-0.002877000	-1.675178000
40	2.169691000	0.000142000	-0.000332000
40	-2.365050000	0.000131000	-0.001004000

10Zr

Total energy including ZPVE: -1020.6360 a. u.
Total free energy including ZPVE: -1020.6908 a. u.

$N_{Img} = 0$

6	3.784552000	-1.640885000	-0.625323000
6	3.658433000	-1.707896000	0.792088000
6	2.605607000	-2.179316000	-1.197614000
1	4.634852000	-1.251887000	-1.170151000
6	2.403831000	-2.294708000	1.093085000
1	4.395561000	-1.379137000	1.513192000

6	1.749002000	-2.576917000	-0.134797000
1	2.393269000	-2.271837000	-2.253498000
1	2.011463000	-2.482550000	2.082417000
1	0.775621000	-3.028755000	-0.246012000
6	1.882424000	2.527987000	0.617667000
6	3.052870000	1.968465000	1.199565000
6	2.023786000	2.481867000	-0.790267000
1	1.032244000	2.906554000	1.165535000
6	3.921120000	1.586285000	0.143756000
1	3.249818000	1.869813000	2.258812000
6	3.279524000	1.888212000	-1.088242000
1	1.298834000	2.815493000	-1.518802000
1	4.900922000	1.141953000	0.256859000
1	3.681820000	1.716597000	-2.078188000
6	-3.036230000	-1.902315000	1.198681000
6	-3.861955000	-1.488496000	0.123986000
6	-1.897048000	-2.552494000	0.641717000
1	-3.253313000	-1.791502000	2.252182000
6	-3.216615000	-1.835019000	-1.092449000
1	-4.818606000	-0.993716000	0.216111000
6	-2.011682000	-2.515936000	-0.761446000
1	-1.075741000	-2.968180000	1.207571000
1	-3.595131000	-1.659232000	-2.090471000
1	-1.289531000	-2.893206000	-1.471586000
6	-1.743550000	2.600237000	-0.137115000
6	-2.579609000	2.161832000	-1.201272000
6	-2.394773000	2.295428000	1.085688000
1	-0.795386000	3.104744000	-0.246069000
6	-3.729000000	1.565941000	-0.635016000
1	-2.373994000	2.274284000	-2.256003000
6	-3.612168000	1.640872000	0.783394000
1	-2.017897000	2.509139000	2.075542000
1	-4.555514000	1.136040000	-1.184603000
1	-4.334055000	1.278321000	1.503225000
6	0.333883000	-0.004581000	-1.515956000
6	0.333712000	-0.005920000	1.511449000
1	-1.224974000	-0.071024000	-3.126912000
1	-1.221957000	-0.005697000	3.126516000
6	-0.761487000	-0.034253000	-2.154202000
6	-0.760701000	0.001897000	2.152092000
40	1.903552000	0.001359000	-0.001382000
40	-1.762599000	0.002692000	-0.000430000

TS1 (M = Zr)

Total energy including ZPVE: -1020.6010 a. u.
Total free energy including ZPVE: -1020.6584 a. u.

N_{Img} = 1 (-369.2)

6	4.234257000	1.683465000	0.271668000

6	3.707729000	1.873035000	-1.035540000
6	3.242326000	2.082296000	1.205617000
1	5.217991000	1.302331000	0.512386000
6	2.396187000	2.407238000	-0.907626000
1	4.225664000	1.670705000	-1.964768000
6	2.110402000	2.533984000	0.476953000
1	3.335591000	2.058269000	2.284043000
1	1.732482000	2.666562000	-1.720108000
1	1.186044000	2.892476000	0.906086000
6	2.110333000	-2.533993000	-0.476844000
6	3.242190000	-2.082327000	-1.205650000
6	2.396280000	-2.407211000	0.907706000
1	1.185929000	-2.892486000	-0.905876000
6	4.234228000	-1.683470000	-0.271818000
1	3.335350000	-2.058319000	-2.284085000
6	3.707840000	-1.873003000	1.035460000
1	1.732659000	-2.666514000	1.720264000
1	5.217943000	-1.302350000	-0.512632000
1	4.225869000	-1.670665000	1.964633000
6	-4.104070000	1.599478000	-0.553010000
6	-3.894691000	1.705353000	0.851856000
6	-2.974895000	2.145802000	-1.208665000
1	-4.977650000	1.180502000	-1.034167000
6	-2.641132000	2.332084000	1.060457000
1	-4.580801000	1.385630000	1.624920000
6	-2.066555000	2.590663000	-0.209744000
1	-2.826232000	2.211030000	-2.277644000
1	-2.195083000	2.557187000	2.018929000
1	-1.098929000	3.037797000	-0.391348000
6	-2.066534000	-2.590655000	0.209711000
6	-2.974873000	-2.145816000	1.208658000
6	-2.641141000	-2.332058000	-1.060485000
1	-1.098900000	-3.037780000	0.391294000
6	-4.104062000	-1.599491000	0.553027000
1	-2.826201000	-2.211063000	2.277635000
6	-3.894702000	-1.705340000	-0.851847000
1	-2.195106000	-2.557141000	-2.018967000
1	-4.977637000	-1.180528000	1.034204000
1	-4.580824000	-1.385610000	-1.624898000
6	0.342730000	0.004447000	0.926509000
6	0.342731000	-0.004444000	-0.926490000
1	-0.662465000	0.012621000	2.795375000
1	-0.662452000	-0.012651000	-2.795362000
6	-0.723633000	0.011070000	1.706524000
6	-0.723627000	-0.011081000	-1.706512000
40	-2.148122000	-0.000001000	0.000004000
40	2.291694000	-0.000002000	0.000011000

3Zr

Total energy including ZPVE: -1020.6412 a. u.
Total free energy including ZPVE: -1020.6965 a. u.

N_{Img} = 0

6	-0.789900000	-0.033331000	-2.210030000
6	0.254934000	0.000432000	-1.489126000
6	-0.254950000	0.000438000	1.489132000
6	0.789883000	-0.033301000	2.210037000
6	-3.831617000	1.567537000	-0.270785000
6	-3.356548000	1.724924000	1.060331000
6	-2.094297000	2.370081000	0.998657000
6	-1.780680000	2.589962000	-0.364792000
6	-2.854592000	2.093677000	-1.153100000
6	-1.747497000	-2.550343000	0.487161000
6	-2.221491000	-2.471235000	-0.841865000
6	-3.477845000	-1.811978000	-0.825041000
6	-3.795061000	-1.517536000	0.531584000
6	-2.722507000	-1.957675000	1.342376000
6	3.831718000	1.567458000	0.270081000
6	3.355941000	1.725207000	-1.060730000
6	2.093741000	2.370404000	-0.998200000
6	1.780869000	2.589938000	0.365461000
6	2.855171000	2.093375000	1.153068000
6	1.747297000	-2.550569000	-0.485911000
6	2.721418000	-1.958232000	-1.342363000
6	3.794684000	-1.517531000	-0.532829000
6	3.478830000	-1.811376000	0.824250000
6	2.222580000	-2.470767000	0.842629000
1	2.656362000	-1.882616000	-2.418877000
1	0.814648000	-2.988234000	-0.808030000
1	4.697680000	-1.037354000	-0.883977000
1	4.099543000	-1.598912000	1.685082000
1	1.703945000	-2.815222000	1.726447000
1	3.869552000	1.423572000	-1.964076000
1	4.775151000	1.125134000	0.560800000
1	2.924141000	2.131486000	2.231339000
1	0.882288000	3.049556000	0.749434000
1	1.474766000	2.625828000	-1.846322000
1	-1.701922000	-2.815964000	-1.725027000
1	-0.815065000	-2.987654000	0.810400000
1	-2.658503000	-1.881539000	2.418920000
1	-4.698472000	-1.037334000	0.881623000
1	-4.097753000	-1.600018000	-1.686577000
1	-4.774902000	1.125309000	-0.562132000
1	-3.870647000	1.423039000	1.963315000
1	-1.475768000	2.625273000	1.847174000
1	-0.881903000	3.049691000	-0.748168000
1	-2.922981000	2.132072000	-2.231396000
40	1.797835000	-0.000189000	0.063540000
40	-1.797852000	-0.000197000	-0.063539000
1	-1.187203000	-0.054056000	-3.212166000
1	1.187214000	-0.053971000	3.212211000

TS2 (M = Zr)

Total energy including ZPVE: -1020.6142 a. u.
Total free energy including ZPVE: -1020.6687 a. u.

N_{Img} = 1 (-238.4)

40	1.672344000	-0.001362000	-0.134058000
6	0.020680000	0.007378000	2.889997000
6	-0.067605000	0.006728000	1.662604000
6	2.731216000	1.874400000	1.308060000
6	3.726256000	1.503943000	0.376764000
6	1.678434000	2.513398000	0.585650000
6	3.279336000	1.870334000	-0.923922000
6	2.027928000	2.525339000	-0.780882000
6	1.704341000	-2.601766000	-0.394377000
6	2.769998000	-2.089840000	-1.181794000
6	2.009666000	-2.362671000	0.969084000
6	3.731587000	-1.535569000	-0.298638000
6	3.258542000	-1.697524000	1.033161000
6	-0.266869000	-0.003747000	-1.562918000
6	0.841097000	0.031378000	-2.234264000
40	-1.743782000	-0.000280000	-0.039116000
6	-2.015030000	-2.427576000	-0.928774000
6	-1.695661000	-2.545656000	0.445392000
6	-3.285212000	-1.803327000	-1.030760000
6	-2.777400000	-2.010408000	1.201862000
6	-3.764223000	-1.567303000	0.288432000
6	-1.678525000	2.569590000	-0.419614000
6	-2.668273000	2.044114000	-1.294318000
6	-2.130114000	2.398207000	0.914057000
6	-3.729208000	1.546305000	-0.495483000
6	-3.393871000	1.759296000	0.872727000
1	-3.805226000	-1.571027000	-1.950911000
1	-4.712418000	-1.116263000	0.548269000
1	-4.001751000	1.492648000	1.727567000
1	-4.641248000	1.095730000	-0.863213000
1	-1.596939000	2.682920000	1.810241000
1	-0.752605000	3.028763000	-0.727680000
1	-2.621035000	2.037400000	-2.374039000
1	-1.394471000	-2.726811000	-1.760784000
1	-0.796188000	-2.975833000	0.857519000
1	-2.838127000	-1.967820000	2.280886000
1	0.819427000	-3.086082000	-0.778067000
1	2.844841000	-2.136206000	-2.258777000
1	4.670087000	-1.085977000	-0.592572000
1	3.761754000	-1.375157000	1.934985000
1	1.389630000	-2.616006000	1.817164000
1	3.814417000	1.717274000	-1.851772000

1	4.661544000	1.015790000	0.611775000
1	2.769466000	1.730967000	2.378947000
1	0.778460000	2.919708000	1.021496000
1	1.426306000	2.908140000	-1.593009000
1	0.104078000	0.008704000	3.955936000
1	1.134990000	0.054664000	-3.279307000

4Zr

Total energy including ZPVE: -1020.6228 a. u.
Total free energy including ZPVE: -1020.6809 a. u.

$N_{Img} = 0$

6	-0.759238000	-0.017525000	-1.737358000
6	0.173269000	-0.018337000	-0.763353000
6	-0.173271000	-0.018343000	0.763336000
6	0.759230000	-0.017547000	1.737344000
6	-4.194451000	1.650553000	-0.243716000
6	-3.709243000	1.724506000	1.089622000
6	-2.413560000	2.305641000	1.052529000
6	-2.103259000	2.589029000	-0.301753000
6	-3.198289000	2.182070000	-1.106312000
6	-2.084245000	-2.543639000	0.375351000
6	-2.627079000	-2.432418000	-0.927911000
6	-3.905485000	-1.822549000	-0.818665000
6	-4.160965000	-1.585578000	0.560425000
6	-3.031129000	-2.017027000	1.297689000
6	4.194103000	1.650797000	0.245115000
6	3.710366000	1.724145000	-1.088798000
6	2.414590000	2.305150000	-1.053391000
6	2.102770000	2.589109000	0.300432000
6	3.196958000	2.182638000	1.106372000
6	2.084422000	-2.543450000	-0.376332000
6	3.032052000	-2.016589000	-1.297768000
6	4.161368000	-1.585500000	-0.559494000
6	3.904821000	-1.822924000	0.819319000
6	2.626286000	-2.432732000	0.927373000
1	2.913490000	-1.967299000	-2.372365000
1	1.115489000	-2.947369000	-0.633982000
1	5.058103000	-1.141481000	-0.970508000
1	4.576326000	-1.604726000	1.639851000
1	2.147077000	-2.740665000	1.845876000
1	4.239118000	1.403342000	-1.977000000
1	5.158021000	1.266249000	0.551967000
1	3.263751000	2.271244000	2.182200000
1	1.176335000	3.011693000	0.663502000
1	1.778009000	2.493663000	-1.906746000
1	-2.148598000	-2.740097000	-1.846878000
1	-1.115142000	-2.947711000	0.632120000
1	-2.911743000	-1.968110000	2.372210000
1	-5.057351000	-1.141634000	0.972280000

1	-4.577606000	-1.604030000	-1.638608000
1	-5.158665000	1.265769000	-0.549336000
1	-4.236983000	1.404041000	1.978549000
1	-1.776067000	2.494568000	1.905107000
1	-1.177269000	3.011540000	-0.666041000
1	-3.266258000	2.270178000	-2.182109000
40	2.223256000	-0.002940000	0.116769000
40	-2.223260000	-0.002941000	-0.116778000
1	-0.491799000	-0.015383000	-2.790798000
1	0.491791000	-0.015423000	2.790784000

TS3 (M = Zr, R = H)

Total energy including ZPVE: -1020.6687 a. u.
Total free energy including ZPVE: -1020.6751 a. u.

N_{Img} = 1 (-275.1)

6	0.769250000	-0.006679000	-1.809195000
6	-0.248048000	-0.003159000	-0.967815000
6	0.247997000	0.003810000	0.967740000
6	-0.769297000	0.007236000	1.809125000
6	2.233474000	-2.418698000	0.862513000
6	2.195721000	-2.569082000	-0.544452000
6	3.398949000	-2.040466000	-1.081580000
6	4.192345000	-1.580711000	0.003700000
6	3.467741000	-1.799295000	1.204296000
6	3.913399000	1.655492000	0.839092000
6	2.654758000	2.189356000	1.212405000
6	1.980676000	2.585405000	0.026308000
6	2.821928000	2.302095000	-1.079602000
6	4.015286000	1.719323000	-0.578804000
6	-2.654431000	-2.189418000	-1.212257000
6	-1.979913000	-2.585218000	-0.026325000
6	-2.820976000	-2.302180000	1.079787000
6	-4.014660000	-1.719835000	0.579302000
6	-3.913166000	-1.655997000	-0.838609000
6	-3.469201000	1.798605000	-1.203993000
6	-4.192698000	1.580414000	-0.002635000
6	-3.398421000	2.040811000	1.081734000
6	-2.195749000	2.569376000	0.543268000
6	-2.234736000	2.418376000	-0.863596000
1	-5.177347000	1.139041000	0.074585000
1	-3.805566000	1.559967000	-2.204657000
1	-3.669028000	2.015046000	2.129075000
1	-1.378429000	2.982601000	1.117526000
1	-1.460889000	2.710970000	-1.559004000
1	-0.987308000	-3.009925000	0.025246000
1	-2.271169000	-2.275992000	-2.219853000
1	-4.666276000	-1.270128000	-1.513027000
1	-4.861863000	-1.398812000	1.171592000
1	-2.592827000	-2.492387000	2.119215000

1	2.271231000	2.276041000	2.219890000
1	4.666182000	1.269348000	1.513717000
1	4.862538000	1.397996000	-1.170859000
1	2.594158000	2.492374000	-2.119100000
1	0.988218000	3.010432000	-0.025488000
1	1.459009000	-2.711481000	1.557152000
1	1.378888000	-2.981925000	-1.119678000
1	3.670541000	-2.014266000	-2.128658000
1	5.177139000	-1.139473000	-0.072430000
1	3.803230000	-1.561166000	2.205374000
40	-2.154728000	-0.002472000	0.087586000
40	2.154685000	0.002578000	-0.087660000
1	0.667404000	-0.012432000	-2.891954000
1	-0.667460000	0.012575000	2.891886000

7Zr

Total energy including ZPVE: -587.0210 a. u.
Total free energy including ZPVE: -587.0668 a. u.

$N_{Img} = 0$

6	-2.566547000	-0.171679000	-0.284065000
6	-2.168886000	-1.164926000	0.652025000
6	-2.300853000	1.100542000	0.282069000
1	-2.982772000	-0.357725000	-1.264521000
6	-1.634815000	-0.506999000	1.786861000
1	-2.236197000	-2.233534000	0.505459000
6	-1.706082000	0.898273000	1.554490000
1	-2.481142000	2.054702000	-0.190208000
1	-1.256457000	-0.984919000	2.680575000
1	-1.395610000	1.675014000	2.240752000
6	2.566195000	0.177096000	-0.283647000
6	2.166367000	1.167221000	0.654883000
6	2.303126000	-1.097028000	0.279312000
1	2.982061000	0.366499000	-1.263604000
6	1.633954000	0.505349000	1.788199000
1	2.231573000	2.236342000	0.511005000
6	1.707930000	-0.899138000	1.552283000
1	2.485338000	-2.049652000	-0.195303000
1	1.254681000	0.980253000	2.683122000
1	1.398696000	-1.678230000	2.236445000
40	0.000002000	-0.000121000	-0.104742000
6	-0.036706000	-1.747215000	-1.484294000
6	-0.063721000	-2.655373000	-2.308056000
1	-0.088343000	-3.433848000	-3.037914000
6	0.036582000	1.743940000	-1.488101000
6	0.063478000	2.650371000	-2.313769000
1	0.087988000	3.427305000	-3.045270000

3Zr (R = F)

Total energy including ZPVE: -1219.0889 a. u.
Total free energy including ZPVE: -1219.1465 a. u.

N_{Img} = 0

6	-0.975516000	-0.036100000	-2.079898000
6	0.170453000	0.000856000	-1.508758000
6	-0.170464000	0.000852000	1.508728000
6	0.975499000	-0.036122000	2.079867000
6	-3.850075000	1.567782000	-0.047739000
6	-3.303227000	1.748196000	1.252350000
6	-2.045080000	2.391532000	1.110575000
6	-1.806621000	2.585410000	-0.270704000
6	-2.921092000	2.074605000	-0.991731000
6	-1.741389000	-2.557968000	0.577577000
6	-2.326574000	-2.444734000	-0.704523000
6	-3.572395000	-1.777602000	-0.563106000
6	-3.767683000	-1.510814000	0.820887000
6	-2.632961000	-1.978955000	1.525839000
6	3.850270000	1.567570000	0.046671000
6	3.302354000	1.748588000	-1.252872000
6	2.044392000	2.392018000	-1.109756000
6	1.807113000	2.585331000	0.271785000
6	2.922108000	2.074039000	0.991670000
6	1.741114000	-2.558191000	-0.575993000
6	2.631552000	-1.979743000	-1.525653000
6	3.767027000	-1.511018000	-0.822316000
6	3.573386000	-1.776996000	0.562071000
6	2.327791000	-2.444121000	0.705374000
1	2.472601000	-1.927783000	-2.593912000
1	0.788358000	-3.009419000	-0.808278000
1	4.631340000	-1.031790000	-1.261369000
1	4.264437000	-1.543288000	1.361479000
1	1.898728000	-2.782342000	1.638543000
1	3.768790000	1.470438000	-2.188798000
1	4.809079000	1.123006000	0.276946000
1	3.044332000	2.081838000	2.066196000
1	0.929577000	3.033715000	0.713649000
1	1.381167000	2.663885000	-1.918640000
1	-1.896365000	-2.783437000	-1.636990000
1	-0.788836000	-3.008917000	0.811255000
1	-2.475255000	-1.926327000	2.594254000
1	-4.632562000	-1.031416000	1.258632000
1	-4.262531000	-1.544460000	-1.363468000
1	-4.808720000	1.123379000	-0.279019000
1	-3.770468000	1.469659000	2.187760000
1	-1.382502000	2.662999000	1.920123000
1	-0.928689000	3.033918000	-0.711646000
1	-3.042431000	2.082880000	-2.066353000
40	1.815064000	0.000750000	-0.079792000
40	-1.815070000	0.000763000	0.079744000
9	-1.537999000	-0.053513000	-3.292054000

9 1.538033000 -0.053544000 3.291996000

4Zr (R = F)

Total energy including ZPVE: -1219.1044 a. u.
Total free energy including ZPVE: -1219.1652 a. u.

N_{Img} = 0

6 0.773730000 -0.027202000 1.704747000
6 -0.165197000 -0.026435000 0.734831000
6 0.165091000 -0.026714000 -0.734659000
6 -0.773722000 -0.027787000 -1.704685000
6 4.204874000 1.651726000 0.198900000
6 3.696890000 1.722380000 -1.126766000
6 2.399831000 2.300188000 -1.068989000
6 2.110942000 2.582970000 0.289773000
6 3.221059000 2.180488000 1.076703000
6 2.100206000 -2.534619000 -0.415195000
6 2.657803000 -2.430340000 0.882446000
6 3.933926000 -1.814990000 0.761538000
6 4.172284000 -1.570177000 -0.619057000
6 3.034485000 -1.999721000 -1.345284000
6 -4.204608000 1.652009000 -0.199802000
6 -3.697286000 1.722572000 1.126126000
6 -2.400122000 2.300186000 1.069019000
6 -2.110509000 2.582969000 -0.289595000
6 -3.220288000 2.180688000 -1.077094000
6 -2.100497000 -2.534341000 0.416467000
6 -3.035443000 -1.999028000 1.345653000
6 -4.172773000 -1.569914000 0.618430000
6 -3.933456000 -1.815398000 -0.761877000
6 -2.657221000 -2.430738000 -0.881599000
1 -2.900856000 -1.939426000 2.417838000
1 -1.129517000 -2.938257000 0.666009000
1 -5.063763000 -1.122368000 1.037831000
1 -4.614868000 -1.602765000 -1.575726000
1 -2.191480000 -2.746660000 -1.804474000
1 -4.211862000 1.405807000 2.023941000
1 -5.175533000 1.272808000 -0.490527000
1 -3.302695000 2.267596000 -2.152192000
1 -1.189717000 3.003400000 -0.669113000
1 -1.749148000 2.483306000 1.912579000
1 2.192717000 -2.745861000 1.805788000
1 1.129072000 -2.938702000 -0.663866000
1 2.899142000 -1.940617000 -2.417401000
1 5.062963000 -1.122793000 -1.039292000
1 4.615898000 -1.601947000 1.574810000
1 5.175882000 1.272356000 0.489125000
1 4.210973000 1.405585000 -2.024854000
1 1.748482000 2.483453000 -1.912229000
1 1.190407000 3.003526000 0.669772000

1	3.303998000	2.267324000	2.151767000
40	-2.242134000	-0.003362000	-0.098793000
40	2.242089000	-0.003379000	0.098770000
9	0.414806000	-0.016617000	3.011502000
9	-0.414616000	-0.017689000	-3.011397000

TS3 (M = Zr, R = F)

Total energy including ZPVE: -1219.0792 a. u.
Total free energy including ZPVE: -1219.1397 a. u.

N_{Img} = 1 (-147.6)

6	-0.865582000	-0.029072000	-1.805340000
6	0.266454000	-0.008987000	-1.138805000
6	-0.266452000	-0.008995000	1.138814000
6	0.865587000	-0.029072000	1.805349000
6	-4.089479000	1.628528000	-0.260214000
6	-3.680413000	1.738804000	1.097635000
6	-2.393681000	2.340348000	1.119600000
6	-2.005008000	2.584385000	-0.220167000
6	-3.049756000	2.144314000	-1.076595000
6	-2.000567000	-2.560319000	0.411166000
6	-2.603482000	-2.392076000	-0.860227000
6	-3.864977000	-1.768735000	-0.666293000
6	-4.046957000	-1.572807000	0.730731000
6	-2.892004000	-2.053963000	1.396343000
6	4.089473000	1.628515000	0.260300000
6	3.680507000	1.738749000	-1.097583000
6	2.393782000	2.340305000	-1.119665000
6	2.005014000	2.584395000	0.220068000
6	3.049697000	2.144344000	1.076588000
6	2.000521000	-2.560322000	-0.411129000
6	2.891932000	-2.053991000	-1.396342000
6	4.046914000	-1.572842000	-0.730776000
6	3.864979000	-1.768754000	0.666257000
6	2.603482000	-2.392076000	0.860240000
1	2.717879000	-2.044914000	-2.464190000
1	1.028600000	-2.989466000	-0.607032000
1	4.915881000	-1.133703000	-1.202193000
1	4.570977000	-1.509129000	1.444557000
1	2.177782000	-2.674668000	1.812963000
1	4.258985000	1.445006000	-1.963721000
1	5.031092000	1.225826000	0.609655000
1	3.051494000	2.198351000	2.156897000
1	1.064311000	3.006468000	0.543783000
1	1.809674000	2.557236000	-2.003179000
1	-2.177754000	-2.674686000	-1.812932000
1	-1.028660000	-2.989477000	0.607109000
1	-2.717990000	-2.044877000	2.464197000
1	-4.915933000	-1.133651000	1.202114000
1	-4.570942000	-1.509105000	-1.444621000

1	-5.031127000	1.225837000	-0.609485000
1	-4.258832000	1.445098000	1.963824000
1	-1.809506000	2.557302000	2.003064000
1	-1.064321000	3.006427000	-0.543965000
1	-3.051628000	2.198283000	-2.156905000
40	2.122632000	-0.002115000	-0.024357000
40	-2.122631000	-0.002112000	0.024363000
9	-1.005630000	-0.033174000	-3.155405000
9	1.005635000	-0.033174000	3.155415000

3Zr (θ = 100^o)

Total energy including ZPVE: -1020.6064 a. u.
Total free energy including ZPVE: -1020.6591 a. u.

N_{Img} = 2 (-145.1, -35.7)

40	-0.002070000	1.682056000	0.002517000
6	-2.650462000	-0.553028000	-0.012404000
6	-1.594883000	0.102135000	0.008681000
6	-1.425319000	2.586822000	-1.930814000
6	-0.600954000	3.656019000	-1.499150000
6	-0.581841000	1.616352000	-2.544988000
6	0.750752000	3.335407000	-1.814066000
6	0.750752000	2.080737000	-2.477461000
6	0.343064000	1.685882000	2.557467000
6	1.062939000	2.803353000	2.046136000
6	-1.042389000	1.932818000	2.375559000
6	0.116998000	3.731296000	1.544939000
6	-1.184840000	3.187481000	1.735999000
6	1.594883000	-0.102135000	0.008681000
6	2.650462000	0.553028000	-0.012404000
40	0.002070000	-1.682056000	0.002517000
6	1.042389000	-1.932818000	2.375559000
6	-0.343064000	-1.685882000	2.557467000
6	1.184840000	-3.187481000	1.735999000
6	-1.062939000	-2.803353000	2.046136000
6	-0.116998000	-3.731296000	1.544939000
6	0.581841000	-1.616352000	-2.544988000
6	1.425319000	-2.586822000	-1.930814000
6	-0.750752000	-2.080737000	-2.477461000
6	0.600954000	-3.656019000	-1.499150000
6	-0.750752000	-3.335407000	-1.814066000
1	2.119820000	-3.651183000	1.449982000
1	-0.347765000	-4.689115000	1.098898000
1	-1.617664000	-3.952291000	-1.617411000
1	0.941784000	-4.562480000	-1.018725000
1	-1.629353000	-1.557522000	-2.828431000
1	0.914257000	-0.690281000	-2.986398000
1	2.500978000	-2.527949000	-1.843313000
1	1.852976000	-1.271712000	2.644819000
1	-0.783642000	-0.818613000	3.023536000

1	-2.135940000	-2.931626000	2.064477000
1	0.783642000	0.818613000	3.023536000
1	2.135940000	2.931626000	2.064477000
1	0.347765000	4.689115000	1.098898000
1	-2.119820000	3.651183000	1.449982000
1	-1.852976000	1.271712000	2.644819000
1	1.617664000	3.952291000	-1.617411000
1	-0.941784000	4.562480000	-1.018725000
1	-2.500978000	2.527949000	-1.843313000
1	-0.914257000	0.690281000	-2.986398000
1	1.629353000	1.557522000	-2.828431000
1	-3.609563000	-1.022390000	-0.027483000
1	3.609563000	1.022390000	-0.027483000

3Zr (θ = 120^o)
Total energy including ZPVE: -1020.5756 a. u.
Total free energy including ZPVE: -1020.6285 a. u.

N_{Img} = 2 (-184.4, -157.2)

40	0.041492000	1.632112000	0.001243000
6	-2.934317000	-0.102622000	0.000876000
6	-1.730638000	0.176259000	0.010371000
6	-1.252596000	2.650874000	-1.953685000
6	-0.347100000	3.643304000	-1.498335000
6	-0.483088000	1.611017000	-2.550150000
6	0.978454000	3.209232000	-1.790459000
6	0.884328000	1.959120000	-2.453020000
6	0.459546000	1.610068000	2.539233000
6	1.241374000	2.672515000	1.997685000
6	-0.909806000	1.957506000	2.403835000
6	0.347100000	3.664839000	1.525914000
6	-0.983997000	3.216752000	1.764046000
6	1.730638000	-0.176259000	0.010371000
6	2.934317000	0.102622000	0.000876000
40	-0.041492000	-1.632112000	0.001243000
6	0.909806000	-1.957506000	2.403835000
6	-0.459546000	-1.610068000	2.539233000
6	0.983997000	-3.216752000	1.764046000
6	-1.241374000	-2.672515000	1.997685000
6	-0.347100000	-3.664839000	1.525914000
6	0.483088000	-1.611017000	-2.550150000
6	1.252596000	-2.650874000	-1.953685000
6	-0.884328000	-1.959120000	-2.453020000
6	0.347100000	-3.643304000	-1.498335000
6	-0.978454000	-3.209232000	-1.790459000
1	1.891992000	-3.747141000	1.508235000
1	-0.630105000	-4.603946000	1.070758000
1	-1.891432000	-3.747912000	-1.574136000
1	0.619377000	-4.576878000	-1.026383000
1	-1.723877000	-1.365557000	-2.786712000
1	0.884907000	-0.719315000	-3.002770000

1	2.330855000	-2.686244000	-1.890103000
1	1.757667000	-1.357515000	2.699931000
1	-0.852943000	-0.719409000	3.001108000
1	-2.320879000	-2.722775000	1.981316000
1	0.852943000	0.719409000	3.001108000
1	2.320879000	2.722775000	1.981316000
1	0.630105000	4.603946000	1.070758000
1	-1.891992000	3.747141000	1.508235000
1	-1.757667000	1.357515000	2.699931000
1	1.891432000	3.747912000	-1.574136000
1	-0.619377000	4.576878000	-1.026383000
1	-2.330855000	2.686244000	-1.890103000
1	-0.884907000	0.719315000	-3.002770000
1	1.723877000	1.365557000	-2.786712000
1	-3.967378000	-0.375067000	-0.008837000
1	3.967378000	0.375067000	-0.008837000

3Zr (θ = 136.7^{o})
Total energy including ZPVE: -1020.5609 a. u.
Total free energy including ZPVE: -1020.6138 a. u.

N_{Img} = 0

40	1.652754000	0.000000000	0.000000000
6	0.000000000	0.000000000	2.984374000
6	0.000000000	0.000000000	1.753567000
6	2.678918000	1.969555000	1.226602000
6	3.662332000	1.511077000	0.311339000
6	1.617922000	2.539207000	0.462320000
6	3.206286000	1.782328000	-1.011730000
6	1.951581000	2.429328000	-0.910129000
6	1.617922000	-2.539207000	-0.462320000
6	2.678918000	-1.969555000	-1.226602000
6	1.951581000	-2.429328000	0.910129000
6	3.662332000	-1.511077000	-0.311339000
6	3.206286000	-1.782328000	1.011730000
6	0.000000000	0.000000000	-1.753567000
6	0.000000000	0.000000000	-2.984374000
40	-1.652754000	0.000000000	0.000000000
6	-1.951581000	-2.429328000	-0.910129000
6	-1.617922000	-2.539207000	0.462320000
6	-3.206286000	-1.782328000	-1.011730000
6	-2.678918000	-1.969555000	1.226602000
6	-3.662332000	-1.511077000	0.311339000
6	-1.617922000	2.539207000	-0.462320000
6	-2.678918000	1.969555000	-1.226602000
6	-1.951581000	2.429328000	0.910129000
6	-3.662332000	1.511077000	-0.311339000
6	-3.206286000	1.782328000	1.011730000
1	-3.731149000	-1.551604000	-1.929395000
1	-4.606017000	-1.055347000	0.576402000
1	-3.731149000	1.551604000	1.929395000

1	-4.606017000	1.055347000	-0.576402000
1	-1.342896000	2.743592000	1.745800000
1	-0.728736000	2.992227000	-0.869514000
1	-2.739435000	1.936346000	-2.305064000
1	-1.342896000	-2.743592000	-1.745800000
1	-0.728736000	-2.992227000	0.869514000
1	-2.739435000	-1.936346000	2.305064000
1	0.728736000	-2.992227000	-0.869514000
1	2.739435000	-1.936346000	-2.305064000
1	4.606017000	-1.055347000	-0.576402000
1	3.731149000	-1.551604000	1.929395000
1	1.342896000	-2.743592000	1.745800000
1	3.731149000	1.551604000	-1.929395000
1	4.606017000	1.055347000	0.576402000
1	2.739435000	1.936346000	2.305064000
1	0.728736000	2.992227000	0.869514000
1	1.342896000	2.743592000	-1.745800000
1	0.000000000	0.000000000	4.053535000
1	0.000000000	0.000000000	-4.053535000

4'Zr

6	0.832017000	0.003234000	-1.673695000
6	-0.147029000	-0.010521000	-0.734070000
6	0.142392000	0.003730000	0.752375000
6	-0.827657000	0.108144000	1.695356000
6	4.585162000	-1.484433000	-0.298813000
6	4.046844000	-1.787544000	0.983670000
6	2.821674000	-2.508279000	0.791445000
6	2.596944000	-2.615780000	-0.611957000
6	3.654412000	-1.930112000	-1.283353000
6	2.175098000	2.503667000	0.571476000
6	2.649835000	2.489998000	-0.772606000
6	3.995450000	2.013764000	-0.756787000
6	4.359394000	1.768257000	0.602049000
6	3.220164000	2.020898000	1.417921000
6	-4.385127000	-1.797106000	0.451935000
6	-3.951718000	-1.978226000	-0.891952000
6	-2.600925000	-2.446625000	-0.862534000
6	-2.212334000	-2.563574000	0.506543000
6	-3.296486000	-2.118936000	1.318349000
6	-2.556714000	2.539878000	-0.786774000
6	-3.598277000	1.787952000	-1.421081000
6	-4.562046000	1.452104000	-0.430524000
6	-4.058793000	1.881183000	0.834853000
6	-2.845629000	2.603037000	0.605551000
40	-2.350829000	-0.004176000	0.075076000
40	2.355507000	0.003410000	-0.046178000
6	-4.808367000	-1.989027000	-2.130910000
6	-5.801862000	-1.676996000	0.943930000
6	-1.875739000	-2.998520000	-2.063507000
6	-0.956042000	-3.195198000	1.006432000

6	-3.426519000	-2.245218000	2.812947000
6	-5.995216000	1.110099000	-0.730990000
6	-4.793413000	1.875224000	2.149917000
6	-3.783013000	1.677611000	-2.911762000
6	-1.606789000	3.392881000	-1.579345000
6	-2.227977000	3.495225000	1.650672000
6	0.911891000	3.146674000	1.041882000
6	1.984440000	3.119313000	-1.962797000
6	3.222003000	2.021744000	2.924012000
6	4.913242000	2.048508000	-1.951737000
6	5.755071000	1.642650000	1.148630000
6	6.014647000	-1.141312000	-0.616699000
6	4.749918000	-1.699766000	2.312876000
6	3.914421000	-1.952713000	-2.766034000
6	1.589918000	-3.467191000	-1.330299000
6	2.160625000	-3.271187000	1.911925000
1	-2.456457000	-2.353069000	3.301476000
1	-3.923093000	-1.377891000	3.260369000
1	-4.024267000	-3.130204000	3.076449000
1	-0.071359000	-2.659221000	0.667119000
1	-0.926771000	-3.213082000	2.097688000
1	-0.882322000	-4.234637000	0.658917000
1	-1.277839000	-3.871403000	-1.784833000
1	-2.591732000	-3.325802000	-2.824953000
1	-1.203817000	-2.277541000	-2.536137000
1	-4.390597000	-1.387718000	-2.944910000
1	-4.906036000	-3.014174000	-2.514083000
1	-5.819967000	-1.628951000	-1.935452000
1	-5.925697000	-0.912661000	1.716583000
1	-6.508144000	-1.464265000	0.141176000
1	-6.106718000	-2.630900000	1.396846000
1	-6.107699000	0.352225000	-1.507516000
1	-6.542363000	0.781177000	0.152267000
1	-6.499557000	2.015483000	-1.098143000
1	-2.839607000	1.471621000	-3.427165000
1	-4.485976000	0.884390000	-3.178745000
1	-4.180039000	2.615085000	-3.329518000
1	-4.117814000	1.699816000	2.993032000
1	-5.287092000	2.841988000	2.328822000
1	-5.570585000	1.108612000	2.186038000
1	-1.108290000	2.825308000	-2.369239000
1	-2.164781000	4.202908000	-2.071300000
1	-0.838363000	3.859010000	-0.964616000
1	-1.543056000	4.219679000	1.207554000
1	-3.014412000	4.066605000	2.159764000
1	-1.677765000	2.945006000	2.419469000
1	2.496487000	2.854488000	-2.891999000
1	0.944197000	2.814059000	-2.060738000
1	2.003183000	4.216025000	-1.880817000
1	0.936477000	4.228937000	0.847885000
1	0.039025000	2.730017000	0.546800000
1	0.770697000	3.009541000	2.115402000

1	3.610645000	2.973563000	3.315363000
1	2.218510000	1.885347000	3.334854000
1	3.854116000	1.226873000	3.331943000
1	6.054465000	2.605886000	1.585510000
1	5.839368000	0.899647000	1.944699000
1	6.488467000	1.401134000	0.378992000
1	5.912738000	1.681546000	-1.710821000
1	4.534362000	1.453057000	-2.790058000
1	5.029387000	3.077248000	-2.317931000
1	6.526458000	-2.049944000	-0.964582000
1	6.114569000	-0.401702000	-1.414223000
1	6.563547000	-0.782199000	0.253523000
1	4.565913000	-2.796665000	-3.038547000
1	2.989923000	-2.055935000	-3.338268000
1	4.412005000	-1.040208000	-3.109350000
1	5.664377000	-1.107173000	2.256891000
1	4.118014000	-1.266333000	3.095961000
1	5.040738000	-2.701299000	2.660900000
1	2.925959000	-3.764800000	2.524003000
1	1.569365000	-2.639009000	2.581631000
1	1.502542000	-4.054154000	1.532312000
1	2.083983000	-4.054665000	-2.113593000
1	1.106400000	-4.174108000	-0.654053000
1	0.806962000	-2.874504000	-1.807222000
6	0.591837000	-0.012543000	-3.154358000
6	-0.569444000	0.160349000	3.171612000
1	1.005205000	-0.919174000	-3.616482000
1	-0.480058000	0.032389000	-3.398618000
1	1.091456000	0.829423000	-3.649908000
1	0.504191000	0.100015000	3.403216000
1	-0.961048000	1.088401000	3.611120000
1	-1.079217000	-0.654370000	3.700668000

8Th

Total energy including ZPVE: -948.0844 a. u.

Total free energy including ZPVE: -948.1295 a. u.

$N_{Img} = 0$

1	0.028053000	2.294788000	2.800968000
1	-0.027788000	2.296025000	-2.800386000
6	-1.877275000	-1.772592000	-0.862838000
6	-1.762145000	-1.992298000	0.533799000
6	-2.522801000	-0.527465000	-1.057894000
1	-1.556793000	-2.452895000	-1.643529000
6	-2.328796000	-0.879587000	1.199519000
1	-1.335250000	-2.868990000	1.006384000
6	-2.794771000	0.028378000	0.215345000
1	-2.766613000	-0.078255000	-2.012834000
1	-2.404798000	-0.747501000	2.272295000
1	-3.282955000	0.976925000	0.405421000
6	2.794816000	0.028209000	-0.214918000

6	2.522494000	-0.527818000	1.058165000
6	2.329008000	-0.879562000	-1.199351000
1	3.283129000	0.976744000	-0.404723000
6	1.876916000	-1.772858000	0.862756000
1	2.766106000	-0.078777000	2.013233000
6	1.762101000	-1.992333000	-0.533944000
1	2.405300000	-0.747322000	-2.272089000
1	1.556180000	-2.453252000	1.643262000
1	1.335249000	-2.868916000	-1.006772000
6	0.017769000	1.904521000	1.786979000
6	0.006483000	2.579733000	0.659971000
6	-0.006173000	2.579992000	-0.659268000
6	-0.017554000	1.905288000	-1.786578000
90	-0.000003000	0.151798000	-0.000130000

9Th

Total energy including ZPVE: -1742.7194 a. u

Total free energy including ZPVE: -1742.7848 a. u.

$N_{Img} = 0$

6	4.362483000	2.153383000	0.130332000
6	3.607248000	2.420649000	-1.038104000
6	3.495365000	2.278970000	1.245067000
1	5.419708000	1.914599000	0.167226000
6	2.277692000	2.723847000	-0.645540000
1	3.990167000	2.430776000	-2.053257000
6	2.209703000	2.638089000	0.767672000
1	3.777392000	2.159178000	2.285704000
1	1.462173000	2.987899000	-1.306452000
1	1.332528000	2.819598000	1.374070000
6	2.284418000	-2.737631000	-0.588435000
6	3.608262000	-2.436498000	-1.001085000
6	2.231006000	-2.624327000	0.823475000
1	1.463114000	-3.018426000	-1.235181000
6	4.374609000	-2.142626000	0.153620000
1	3.980430000	-2.464831000	-2.019880000
6	3.519947000	-2.249813000	1.279900000
1	1.361233000	-2.798056000	1.442668000
1	5.431083000	-1.898627000	0.174479000
1	3.812606000	-2.107967000	2.314832000
90	2.548165000	-0.000936000	-0.088740000
6	-4.356977000	1.851592000	-0.589382000
6	-4.254738000	1.865878000	0.826024000
6	-3.190936000	2.454177000	-1.118514000
1	-5.195361000	1.472847000	-1.162492000
6	-3.026078000	2.477851000	1.170037000
1	-5.000774000	1.499219000	1.521752000
6	-2.365316000	2.831649000	-0.031666000
1	-2.967505000	2.602046000	-2.168060000
1	-2.656021000	2.647535000	2.173527000
1	-1.402381000	3.322512000	-0.106908000

6	-2.377075000	-2.832888000	0.014175000
6	-3.126903000	-2.455267000	1.154661000
6	-3.114409000	-2.472431000	-1.139971000
1	-1.413326000	-3.327872000	0.023337000
6	-4.322568000	-1.845785000	0.705845000
1	-2.835269000	-2.607743000	2.186573000
6	-4.314668000	-1.856058000	-0.713284000
1	-2.811688000	-2.639756000	-2.166268000
1	-5.119164000	-1.465084000	1.334602000
1	-5.104119000	-1.484576000	-1.356551000
6	0.287345000	-0.003238000	0.702091000
6	0.260796000	-0.005480000	-0.816275000
90	-2.295552000	-0.000922000	-0.006921000
1	-0.277719000	-0.015868000	2.736513000
1	-0.382919000	0.001363000	-2.826740000
6	-0.633934000	-0.014246000	1.702023000
6	-0.701829000	0.003274000	-1.779995000

10Th

Total energy including ZPVE: -1742.7482 a. u.
Total free energy including ZPVE: -1742.8134 a. u.

$N_{Img} = 0$

6	4.078940000	2.013022000	0.445761000
6	3.751357000	2.144526000	-0.927871000
6	2.958279000	2.433149000	1.204392000
1	5.029546000	1.676354000	0.844222000
6	2.430931000	2.648702000	-1.018057000
1	4.405918000	1.922063000	-1.763391000
6	1.941400000	2.825645000	0.299127000
1	2.892958000	2.465627000	2.285430000
1	1.894209000	2.865363000	-1.933119000
1	0.964544000	3.202671000	0.573499000
6	2.023325000	-2.764423000	-0.308608000
6	3.028164000	-2.340843000	-1.213279000
6	2.507412000	-2.574936000	1.008823000
1	1.058083000	-3.169845000	-0.583601000
6	4.136004000	-1.888992000	-0.454024000
1	2.963839000	-2.373890000	-2.294367000
6	3.812446000	-2.032024000	0.919404000
1	1.977268000	-2.808501000	1.923559000
1	5.076331000	-1.524080000	-0.851989000
1	4.460079000	-1.791392000	1.755294000
90	2.114424000	0.032515000	-0.002669000
6	-3.132257000	2.192635000	-1.251132000
6	-4.172693000	1.627061000	-0.477754000
6	-2.181220000	2.751894000	-0.359137000
1	-3.078350000	2.214955000	-2.332550000
6	-3.865495000	1.834953000	0.891812000
1	-5.059652000	1.138708000	-0.863207000
6	-2.639952000	2.539431000	0.962323000

1	-1.272507000	3.265827000	-0.647026000
1	-4.475260000	1.532860000	1.735453000
1	-2.139943000	2.855498000	1.869266000
6	-2.101494000	-2.807704000	0.362078000
6	-3.058767000	-2.277890000	1.265289000
6	-2.579080000	-2.603896000	-0.954129000
1	-1.176139000	-3.297260000	0.639194000
6	-4.121989000	-1.738762000	0.504156000
1	-2.993487000	-2.301978000	2.346031000
6	-3.822797000	-1.933785000	-0.869105000
1	-2.079667000	-2.903451000	-1.866986000
1	-5.018168000	-1.276205000	0.899994000
1	-4.448930000	-1.645838000	-1.705667000
6	0.327976000	0.014465000	1.568827000
6	0.322154000	-0.000847000	-1.567196000
90	-1.952418000	-0.024692000	0.004996000
1	-1.128874000	0.058921000	3.254612000
1	-1.138816000	-0.086098000	-3.247705000
6	-0.767113000	0.035996000	2.232810000
6	-0.774406000	-0.053120000	-2.227107000

TS1 (M = Th)

Total energy including ZPVE: -1742.7122 a. u.

Total free energy including ZPVE: -1742.7773 a. u.

N_{Img} = 1 (-345.1)

6	4.271204000	2.182228000	0.110325000
6	3.577951000	2.333674000	-1.114688000
6	3.347979000	2.403076000	1.161982000
1	5.325115000	1.954943000	0.223497000
6	2.229427000	2.660664000	-0.821742000
1	4.010279000	2.247477000	-2.105799000
6	2.088629000	2.705774000	0.587361000
1	3.572216000	2.379628000	2.222948000
1	1.449663000	2.854876000	-1.547593000
1	1.181551000	2.935482000	1.131716000
6	2.626265000	-2.739730000	-0.679646000
6	3.847191000	-2.181633000	-1.133881000
6	2.638506000	-2.723722000	0.735995000
1	1.825723000	-3.114626000	-1.304160000
6	4.618913000	-1.826439000	0.000749000
1	4.152477000	-2.075471000	-2.169309000
6	3.867152000	-2.155942000	1.156314000
1	1.849193000	-3.085053000	1.382441000
1	5.616905000	-1.403185000	-0.012930000
1	4.190497000	-2.026622000	2.183615000
90	2.436157000	-0.020370000	-0.000054000
6	-4.160447000	2.006899000	-0.570465000
6	-3.999753000	2.056640000	0.837537000
6	-2.959443000	2.463673000	-1.164499000
1	-5.055864000	1.699255000	-1.097707000

6	-2.700459000	2.544832000	1.113892000
1	-4.749131000	1.789448000	1.573742000
6	-2.056037000	2.789112000	-0.123411000
1	-2.766345000	2.556765000	-2.226506000
1	-2.276550000	2.706055000	2.097436000
1	-1.052674000	3.175238000	-0.254024000
6	-2.708497000	-2.816993000	0.105603000
6	-3.487308000	-2.298518000	1.169165000
6	-3.305517000	-2.418043000	-1.114707000
1	-1.813240000	-3.418317000	0.209186000
6	-4.559247000	-1.565830000	0.606327000
1	-3.296547000	-2.442121000	2.225572000
6	-4.445433000	-1.637565000	-0.806433000
1	-2.951811000	-2.666739000	-2.107387000
1	-5.344972000	-1.061008000	1.156155000
1	-5.130314000	-1.198928000	-1.523028000
6	0.316874000	-0.250852000	0.967751000
6	0.317765000	-0.258175000	-0.970292000
90	-2.271536000	-0.033463000	-0.003824000
1	-0.544860000	-0.420896000	2.873072000
1	-0.539852000	-0.444509000	-2.875966000
6	-0.723099000	-0.303701000	1.800520000
6	-0.720498000	-0.318877000	-1.804763000

3Th (R = H)

Total energy including ZPVE: -1742.7523 a. u.

Total free energy including ZPVE: -1742.8166 a. u.

$N_{Img} = 0$

6	3.781342000	-1.874764000	-1.052673000
6	4.138358000	-1.821583000	0.318702000
6	2.510184000	-2.490607000	-1.151118000
1	4.387433000	-1.529716000	-1.882342000
6	3.084694000	-2.399042000	1.068616000
1	5.066765000	-1.431757000	0.719745000
6	2.078155000	-2.809597000	0.159210000
1	1.966234000	-2.684595000	-2.066956000
1	3.060605000	-2.526993000	2.143984000
1	1.148527000	-3.296968000	0.424770000
6	2.076858000	2.810071000	0.205308000
6	3.112827000	2.384695000	1.073925000
6	2.465691000	2.514531000	-1.123612000
1	1.155195000	3.289106000	0.510776000
6	4.141963000	1.821934000	0.279699000
1	3.123753000	2.493670000	2.151654000
6	3.739896000	1.898603000	-1.077860000
1	1.891620000	2.722483000	-2.017683000
1	5.083327000	1.426467000	0.643082000
1	4.318018000	1.568840000	-1.933290000
90	2.001252000	0.000815000	0.075122000
6	-3.738782000	-1.898328000	1.079784000

6	-4.140988000	-1.823200000	-0.277818000
6	-2.464229000	-2.513446000	1.126045000
1	-4.316996000	-1.568020000	1.934939000
6	-3.111606000	-2.386191000	-1.071570000
1	-5.082593000	-1.428579000	-0.641503000
6	-2.075255000	-2.809986000	-0.202619000
1	-1.889969000	-2.720180000	2.020272000
1	-3.122566000	-2.496276000	-2.149190000
1	-1.153326000	-3.288855000	-0.507532000
6	-2.078097000	2.809722000	-0.155397000
6	-3.080922000	2.400691000	-1.069556000
6	-2.515473000	2.488601000	1.152671000
1	-1.147438000	3.297645000	-0.416305000
6	-4.137603000	1.821986000	-0.324918000
1	-3.052449000	2.530324000	-2.144608000
6	-3.786206000	1.872922000	1.048017000
1	-1.975276000	2.681267000	2.071009000
1	-5.064297000	1.432645000	-0.730395000
1	-4.395743000	1.526511000	1.874588000
6	0.227022000	0.001168000	-1.535173000
6	-0.227084000	-0.000583000	1.534587000
90	-2.001307000	-0.000708000	-0.075417000
1	-1.058761000	0.003798000	-3.360713000
6	-0.795569000	0.002530000	-2.309159000
6	0.795604000	-0.001503000	2.308560000
1	1.058179000	-0.002195000	3.360293000

TS2 (M = Th)

Total energy including ZPVE: -1742.7290 a. u.

Total free energy including ZPVE: -1742.7931 a. u.

N_{Img} = 1 (-169.5)

6	3.736738000	-1.942314000	-0.918940000
6	3.947067000	-1.938912000	0.484787000
6	2.453686000	-2.487145000	-1.171398000
1	4.446859000	-1.614711000	-1.669913000
6	2.788104000	-2.467864000	1.100169000
1	4.843823000	-1.603319000	0.993538000
6	1.865229000	-2.805948000	0.076812000
1	2.002708000	-2.630231000	-2.144392000
1	2.638306000	-2.610635000	2.163996000
1	0.890426000	-3.252562000	0.225594000
6	2.111921000	2.753283000	0.620411000
6	3.351549000	2.217488000	1.054007000
6	2.077572000	2.693591000	-0.793003000
1	1.336207000	3.150299000	1.264082000
6	4.082812000	1.826255000	-0.094974000
1	3.689218000	2.145901000	2.081962000
6	3.291115000	2.115112000	-1.236192000
1	1.265802000	3.018577000	-1.430673000
1	5.081022000	1.403603000	-0.102391000

1	3.569158000	1.941830000	-2.269241000
90	1.948396000	-0.002066000	0.027675000
6	-3.444491000	-1.975175000	1.154229000
6	-4.092991000	-1.703649000	-0.074825000
6	-2.224597000	-2.638917000	0.865557000
1	-3.824950000	-1.743394000	2.142475000
6	-3.270095000	-2.187251000	-1.123277000
1	-5.058590000	-1.226454000	-0.192080000
6	-2.119032000	-2.770314000	-0.538022000
1	-1.505258000	-2.986280000	1.597263000
1	-3.489778000	-2.143893000	-2.182842000
1	-1.301131000	-3.226666000	-1.081171000
6	-1.934392000	2.807586000	0.006194000
6	-2.765079000	2.460475000	-1.087450000
6	-2.591146000	2.413415000	1.200388000
1	-0.977730000	3.310605000	-0.057875000
6	-3.926410000	1.838416000	-0.568925000
1	-2.552518000	2.642555000	-2.132797000
6	-3.821303000	1.814454000	0.846076000
1	-2.216115000	2.554120000	2.206955000
1	-4.764192000	1.472692000	-1.151349000
1	-4.560487000	1.419542000	1.533259000
6	0.268004000	-0.006349000	-1.517492000
6	0.044379000	-0.003234000	1.816034000
90	-1.855449000	0.002771000	-0.092460000
1	-0.903275000	0.025788000	-3.349940000
6	-0.836441000	0.016461000	-2.257641000
6	-0.112816000	-0.036999000	3.038501000
1	-0.250983000	-0.065582000	4.100050000

4Th (R = H)

Total energy including ZPVE: -1742.7366 a. u.
Total free energy including ZPVE: -1742.8025 a. u.

$N_{Img} = 0$

90	2.416573000	0.009571000	-0.092357000
90	-2.417484000	0.009699000	0.091851000
6	0.764694000	0.049414000	-1.763909000
6	-0.162317000	0.107137000	-0.753920000
6	0.161534000	0.107207000	0.753735000
6	-0.765750000	0.049597000	1.763450000
6	4.472272000	-1.953090000	0.017843000
6	3.879687000	-1.991284000	1.302856000
6	2.569824000	-2.516007000	1.167775000
6	2.355190000	-2.802046000	-0.202252000
6	3.527816000	-2.451939000	-0.914379000
6	2.530811000	2.794993000	0.295873000
6	3.002070000	2.601752000	-1.025413000
6	4.268069000	1.970766000	-0.948459000
6	4.583677000	1.781732000	0.420340000
6	3.507778000	2.288526000	1.188580000

6	-4.472051000	-1.954563000	-0.012689000
6	-3.884107000	-1.991175000	-1.299899000
6	-2.573343000	-2.514970000	-1.170020000
6	-2.353531000	-2.802052000	0.198975000
6	-3.523847000	-2.453500000	0.915662000
6	-2.527766000	2.794880000	-0.299094000
6	-3.508478000	2.289240000	-1.188123000
6	-4.582813000	1.785160000	-0.415951000
6	-4.262531000	1.975159000	0.951630000
6	-2.995223000	2.603996000	1.023864000
1	-3.453537000	2.305306000	-2.270883000
1	-1.588915000	3.253108000	-0.584658000
1	-5.497448000	1.350839000	-0.802331000
1	-4.889438000	1.709644000	1.795800000
1	-2.478609000	2.892536000	1.930512000
1	-4.360798000	-1.691080000	-2.226449000
1	-5.478516000	-1.625518000	0.219118000
1	-3.673144000	-2.568367000	1.982979000
1	-1.448494000	-3.215031000	0.627143000
1	-0.388286000	0.098901000	2.786078000
1	0.386890000	0.098626000	-2.786418000
1	-1.869469000	-2.679734000	-1.976632000
1	2.488783000	2.890215000	-1.933988000
1	1.591862000	3.255220000	0.577916000
1	3.449435000	2.305950000	2.271135000
1	5.496238000	1.346061000	0.810071000
1	4.897105000	1.702955000	-1.790322000
1	5.479236000	-1.622927000	-0.210111000
1	4.352724000	-1.691482000	2.231372000
1	1.863184000	-2.681929000	1.971718000
1	1.452047000	-3.215414000	-0.634029000
1	3.681068000	-2.565788000	-1.981250000

TS3 (M = Th, R = H)
Total energy including ZPVE: -1742.7262 a. u.
Total free energy including ZPVE: -1742.7915 a. u.

N_{Img} = 1 (-267.5)

6	-4.358349000	-1.925253000	-0.597568000
6	-3.155387000	-2.526749000	-1.042860000
6	-4.311495000	-1.841566000	0.816052000
1	-5.181930000	-1.606538000	-1.226786000
6	-2.365984000	-2.814456000	0.097522000
1	-2.891357000	-2.742079000	-2.070951000
6	-3.079292000	-2.393560000	1.245630000
1	-5.093287000	-1.450158000	1.456814000
1	-1.388108000	-3.279831000	0.093369000
1	-2.744696000	-2.489216000	2.271894000
6	-3.617262000	2.312948000	-1.060274000
6	-4.488921000	1.847173000	-0.043921000
6	-2.437199000	2.789235000	-0.438939000

1	-3.824417000	2.325408000	-2.124175000
6	-3.841920000	2.028549000	1.202415000
1	-5.483437000	1.442656000	-0.192212000
6	-2.573883000	2.614289000	0.958855000
1	-1.579678000	3.210263000	-0.949090000
1	-4.254756000	1.787184000	2.175609000
1	-1.842890000	2.885794000	1.710254000
90	-2.338732000	-0.004512000	-0.073870000
6	3.168792000	-2.508272000	1.067658000
6	2.367046000	-2.816782000	-0.058638000
6	4.366462000	-1.914449000	0.598526000
1	2.916121000	-2.705390000	2.102264000
6	3.067234000	-2.416102000	-1.221810000
1	1.389731000	-3.282754000	-0.035111000
6	4.303727000	-1.855665000	-0.815635000
1	5.197491000	-1.585457000	1.212283000
1	2.721729000	-2.530974000	-2.242446000
1	5.078808000	-1.477055000	-1.471831000
6	2.961275000	2.432244000	-1.228034000
6	2.296341000	2.807815000	-0.036238000
6	4.224738000	1.897200000	-0.873237000
1	2.574826000	2.544916000	-2.234033000
6	3.146581000	2.508763000	1.056478000
1	1.308893000	3.247783000	0.029358000
6	4.339323000	1.946347000	0.538028000
1	4.982638000	1.541361000	-1.561572000
1	2.928763000	2.693162000	2.101361000
1	5.200109000	1.632005000	1.117457000
6	-0.242898000	-0.010898000	1.013603000
6	0.243027000	-0.016570000	-1.029679000
90	2.337968000	-0.004362000	0.063238000
1	0.580419000	-0.010441000	2.944456000
6	0.777508000	-0.011870000	1.870032000
6	-0.779991000	-0.020294000	-1.883333000
1	-0.583086000	-0.024436000	-2.957808000

7Th

Total energy including ZPVE: -948.0453 a. u.
Total free energy including ZPVE: -948.0927 a. u.

$N_{Img} = 0$

6	-1.829448000	0.572040000	-1.876059000
6	-1.858145000	-0.842187000	-1.746682000
6	-2.415677000	1.129328000	-0.713634000
1	-1.453615000	1.125056000	-2.729293000
6	-2.461986000	-1.156200000	-0.505092000
1	-1.507384000	-1.556433000	-2.482827000
6	-2.795811000	0.061932000	0.135806000
1	-2.541773000	2.183777000	-0.502904000
1	-2.629076000	-2.149609000	-0.109237000
1	-3.262056000	0.161177000	1.109121000

6	2.766776000	-0.393452000	0.092094000
6	2.262045000	-1.231908000	-0.931145000
6	2.594544000	0.952678000	-0.314102000
1	3.205456000	-0.728429000	1.024353000
6	1.765641000	-0.404341000	-1.968567000
1	2.252329000	-2.315068000	-0.915021000
6	1.971531000	0.946985000	-1.585417000
1	2.878251000	1.831566000	0.250228000
1	1.338314000	-0.742148000	-2.905296000
1	1.715402000	1.822355000	-2.171535000
90	0.000105000	0.007098000	0.139940000
6	-0.011356000	2.044271000	1.489849000
6	0.014094000	-1.931129000	1.627376000
1	-0.038029000	3.818810000	2.950380000
1	0.031575000	-3.598437000	3.209278000
6	-0.025610000	2.993793000	2.269921000
6	0.023590000	-2.823716000	2.472013000

3Th (R = F)

Total energy including ZPVE: -1941.1334 a. u.

Total free energy including ZPVE: -1941.1996a. u.

$N_{Img} = 0$

6	-3.767471000	-1.872154000	1.173794000
6	-4.157002000	-1.802656000	-0.188060000
6	-2.498107000	-2.497210000	1.235455000
1	-4.351865000	-1.533132000	2.021427000
6	-3.125589000	-2.379502000	-0.968826000
1	-5.092003000	-1.403383000	-0.563269000
6	-2.100419000	-2.805752000	-0.088048000
1	-1.933537000	-2.704113000	2.136053000
1	-3.128166000	-2.495167000	-2.045990000
1	-1.180510000	-3.295660000	-0.381808000
6	-2.087922000	2.803326000	-0.141895000
6	-3.147577000	2.365128000	-0.974713000
6	-2.437366000	2.524698000	1.201452000
1	-1.175488000	3.278089000	-0.480325000
6	-4.152471000	1.811383000	-0.143934000
1	-3.189481000	2.458373000	-2.053290000
6	-3.711517000	1.906280000	1.200473000
1	-1.838178000	2.744914000	2.076056000
1	-5.103379000	1.411005000	-0.475185000
1	-4.264917000	1.588300000	2.076564000
90	-2.005250000	0.000270000	0.023736000
6	3.735858000	-1.894135000	-1.187678000
6	4.155229000	-1.807725000	0.164246000
6	2.463499000	-2.515613000	-1.213286000
1	4.302312000	-1.568371000	-2.052487000
6	3.139229000	-2.370724000	0.974950000
1	5.099737000	-1.407413000	0.513497000
6	2.093915000	-2.805396000	0.122396000

1	1.878607000	-2.731343000	-2.098652000
1	3.164692000	-2.471955000	2.053298000
1	1.178018000	-3.285971000	0.442798000
6	2.090444000	2.804446000	0.094538000
6	3.121980000	2.379564000	0.968537000
6	2.481817000	2.500426000	-1.231864000
1	1.170116000	3.289793000	0.394478000
6	4.151024000	1.808112000	0.180613000
1	3.130216000	2.492679000	2.045951000
6	3.753744000	1.879873000	-1.178863000
1	1.911485000	2.707051000	-2.128867000
1	5.089802000	1.411882000	0.549517000
1	4.334480000	1.545081000	-2.030658000
6	-0.167854000	-0.000114000	1.548896000
6	0.167701000	-0.004523000	-1.548871000
90	2.005210000	-0.001532000	-0.023707000
6	0.915930000	0.001166000	2.249147000
6	-0.916156000	-0.006315000	-2.249020000
9	1.306572000	0.003384000	3.523740000
9	-1.307000000	-0.009220000	-3.523556000

4Th (R = F)
Total energy including ZPVE: -1941.1626 a. u.
Total free energy including ZPVE: -1941.2327 a. u.

$N_{Img} = 0$

90	2.423749000	-0.005389000	-0.095852000
90	-2.424630000	-0.005587000	0.097273000
6	0.757941000	-0.019796000	-1.750466000
6	-0.149559000	-0.013702000	-0.725198000
6	0.148541000	-0.013503000	0.727055000
6	-0.759026000	-0.019356000	1.752304000
6	4.568308000	-1.850255000	-0.142191000
6	4.067017000	-1.920245000	1.180616000
6	2.780117000	-2.513375000	1.131843000
6	2.488313000	-2.808854000	-0.221755000
6	3.590326000	-2.397690000	-1.010256000
6	2.384982000	2.725514000	0.548575000
6	2.766306000	2.686869000	-0.814461000
6	4.070755000	2.138002000	-0.887205000
6	4.500196000	1.847189000	0.432073000
6	3.455855000	2.206312000	1.318323000
6	-4.570019000	-1.850077000	0.121862000
6	-4.049169000	-1.926891000	-1.192975000
6	-2.763120000	-2.519670000	-1.122134000
6	-2.491353000	-2.808119000	0.237143000
6	-3.604853000	-2.392811000	1.007113000
6	-2.384806000	2.724480000	-0.550967000
6	-3.455229000	2.204494000	-1.320780000
6	-4.500305000	1.846823000	-0.434810000
6	-4.071770000	2.139369000	0.884393000

6	-2.767121000	2.687780000	0.811853000
1	-3.474612000	2.114281000	-2.401166000
1	-1.444009000	3.091708000	-0.941556000
1	-5.464975000	1.441826000	-0.717023000
1	-4.650482000	1.994853000	1.790112000
1	-2.171468000	3.021666000	1.652212000
1	-4.554636000	-1.609024000	-2.098056000
1	-5.545816000	-1.468496000	0.399753000
1	-3.705465000	-2.490171000	2.081877000
1	-1.588329000	-3.263633000	0.624688000
1	-2.108424000	-2.723696000	-1.960710000
1	2.170147000	3.019760000	-1.654850000
1	1.444573000	3.093551000	0.939343000
1	3.476031000	2.117642000	2.398825000
1	5.464909000	1.442162000	0.714092000
1	4.648712000	1.992009000	-1.793164000
1	5.539841000	-1.470027000	-0.436453000
1	4.585881000	-1.597895000	2.076465000
1	2.137819000	-2.713337000	1.980962000
1	1.579687000	-3.266433000	-0.593468000
1	3.675094000	-2.500541000	-2.085848000
9	-0.246295000	-0.008117000	3.012795000
9	0.245284000	-0.008916000	-3.010978000

TS3 (M = Th, R = F)

Total energy including ZPVE: -1941.1195 a.u.

Total free energy including ZPVE: -1941.1873 a. u.

N_{Img} = (-148.4)

6	-2.972966000	2.416556000	-1.278046000
6	-4.219217000	1.867968000	-0.883967000
6	-2.279114000	2.807150000	-0.107893000
1	-2.615347000	2.525052000	-2.295236000
6	-4.294756000	1.926259000	0.530126000
1	-4.992220000	1.498911000	-1.548365000
6	-3.094692000	2.505850000	1.010806000
1	-1.294997000	3.257941000	-0.073619000
1	-5.134362000	1.605069000	1.136315000
1	-2.849975000	2.699019000	2.048186000
6	-2.458180000	-2.771336000	0.467354000
6	-3.649330000	-2.251107000	1.030476000
6	-2.542792000	-2.641691000	-0.939514000
1	-1.629083000	-3.193433000	1.021829000
6	-4.474685000	-1.801627000	-0.030128000
1	-3.891243000	-2.220980000	2.086747000
6	-3.787974000	-2.037639000	-1.247036000
1	-1.792706000	-2.952093000	-1.656230000
1	-5.465088000	-1.372969000	0.069427000
1	-4.161058000	-1.821784000	-2.242116000
90	-2.298369000	0.000684000	0.000969000
6	4.474637000	1.801660000	0.030133000

6	3.649272000	2.251121000	-1.030470000
6	3.787925000	2.037662000	1.247042000
1	5.465047000	1.373018000	-0.069422000
6	2.458114000	2.771330000	-0.467348000
1	3.891182000	2.220995000	-2.086742000
6	2.542732000	2.641690000	0.939521000
1	4.161016000	1.821816000	2.242121000
1	1.629007000	3.193410000	-1.021822000
1	1.792642000	2.952080000	1.656239000
6	3.094777000	-2.505807000	-1.010855000
6	4.294822000	-1.926176000	-0.530178000
6	2.279225000	-2.807163000	0.107847000
1	2.850054000	-2.698966000	-2.048236000
6	4.219298000	-1.867914000	0.883916000
1	5.134407000	-1.604937000	-1.136372000
6	2.973075000	-2.416562000	1.277999000
1	1.295128000	-3.257997000	0.073576000
1	4.992293000	-1.498838000	1.548312000
1	2.615474000	-2.525095000	2.295191000
6	-0.268345000	-0.003387000	-1.188834000
6	0.268333000	0.003342000	1.188850000
90	2.298359000	-0.000693000	-0.000956000
6	0.830702000	-0.002999000	-1.924599000
6	-0.830714000	0.002965000	1.924616000
9	0.834888000	-0.004079000	-3.282033000
9	-0.834899000	0.004049000	3.282049000

3Th ($\theta = 100^o$)

Total energy including ZPVE: -1742.7073 a. u.

Total free energy including ZPVE: -1742.7719 a. u.

N_{Img} = 1 (-301.4)

6	3.665195000	-1.817739000	-1.067104000
6	4.030578000	-1.803432000	0.304220000
6	2.393737000	-2.426824000	-1.176495000
1	4.262802000	-1.440499000	-1.888993000
6	2.983128000	-2.404177000	1.043740000
1	4.959803000	-1.422619000	0.712165000
6	1.968063000	-2.785663000	0.128582000
1	1.843967000	-2.590426000	-2.094103000
1	2.968698000	-2.564794000	2.114781000
1	1.046215000	-3.293270000	0.382635000
6	1.975487000	2.795998000	0.423889000
6	3.169107000	2.320665000	1.027016000
6	2.078897000	2.595960000	-0.973322000
1	1.140191000	3.243165000	0.948255000
6	4.007243000	1.824466000	-0.003360000
1	3.407250000	2.360386000	2.083163000
6	3.329472000	1.989761000	-1.239052000
1	1.330263000	2.847901000	-1.713064000
1	5.001943000	1.414289000	0.126630000

1	3.707888000	1.717897000	-2.217499000
90	1.896642000	0.006806000	0.132577000
6	-3.329983000	-1.989363000	1.238674000
6	-4.007084000	-1.824512000	0.002545000
6	-2.079195000	-2.595503000	0.973808000
1	-3.708971000	-1.717237000	2.216829000
6	-3.168342000	-2.320892000	-1.027220000
1	-5.001696000	-1.414346000	-0.128093000
6	-1.975004000	-2.795896000	-0.423293000
1	-1.330911000	-2.847171000	1.713998000
1	-3.405904000	-2.360919000	-2.083485000
1	-1.139455000	-3.243406000	-0.946963000
6	-1.968249000	2.785633000	-0.127499000
6	-2.982788000	2.404416000	-1.043353000
6	-2.394584000	2.426188000	1.177205000
1	-1.046436000	3.293724000	-0.380735000
6	-4.030565000	1.803254000	-0.304640000
1	-2.967831000	2.565458000	-2.114323000
6	-3.665921000	1.817023000	1.066881000
1	-1.845350000	2.589521000	2.095182000
1	-4.959531000	1.422516000	-0.713237000
1	-4.263930000	1.439381000	1.888292000
6	0.177551000	-0.009261000	-1.581906000
6	-0.177468000	0.009251000	1.581855000
90	-1.896591000	-0.006750000	-0.132666000
1	-0.509649000	-0.011630000	-3.781426000
6	-0.352235000	-0.009167000	-2.721018000
6	0.352342000	0.009083000	2.720950000
1	0.509792000	0.011396000	3.781349000

3Th ($\theta = 120^o$)

Total energy including ZPVE: -1742.6654 a. u.

Total free energy including ZPVE: -1742.7268 a. u.

N_{Img} = 3 (-238.3, -162.1, -12.1)

6	-3.526898000	-1.925387000	0.986916000
6	-3.850534000	-1.840217000	-0.393516000
6	-2.246722000	-2.509937000	1.102465000
1	-4.158154000	-1.608069000	1.809098000
6	-2.765162000	-2.372560000	-1.132983000
1	-4.778348000	-1.459145000	-0.806566000
6	-1.767550000	-2.783862000	-0.205233000
1	-1.721400000	-2.705043000	2.028137000
1	-2.716158000	-2.478049000	-2.209735000
1	-0.832734000	-3.267201000	-0.452807000
6	-1.796686000	2.777932000	-0.236753000
6	-2.795083000	2.351044000	-1.155483000
6	-2.266272000	2.513273000	1.075913000
1	-0.867617000	3.258098000	-0.495079000
6	-3.872500000	1.818659000	-0.406558000
1	-2.751726000	2.448471000	-2.233506000

6	-3.543521000	1.919286000	0.971859000
1	-1.737676000	2.721444000	1.996903000
1	-4.798308000	1.426295000	-0.811919000
1	-4.169151000	1.605620000	1.799799000
90	-1.797293000	-0.003865000	-0.073706000
6	3.293472000	-2.090454000	-1.118624000
6	3.897382000	-1.811120000	0.137736000
6	2.034419000	-2.684093000	-0.874782000
1	3.724023000	-1.891589000	-2.093303000
6	3.005685000	-2.238085000	1.157196000
1	4.883618000	-1.389109000	0.289674000
6	1.847696000	-2.769414000	0.525393000
1	1.329502000	-2.995345000	-1.635180000
1	3.184837000	-2.195441000	2.224788000
1	0.987055000	-3.184205000	1.033632000
6	1.797151000	2.782004000	0.497095000
6	2.964492000	2.287670000	1.141471000
6	1.985679000	2.667838000	-0.902428000
1	0.929543000	3.192796000	0.997343000
6	3.864684000	1.856798000	0.131318000
1	3.145297000	2.275174000	2.209590000
6	3.256591000	2.092873000	-1.131424000
1	1.275958000	2.951423000	-1.671621000
1	4.858600000	1.456977000	0.293241000
1	3.691847000	1.879785000	-2.100867000
6	-0.211356000	0.006439000	1.832451000
6	0.241521000	-0.010471000	-1.841492000
90	1.830847000	0.007124000	0.061568000
1	0.221323000	0.004230000	4.103702000
6	0.020613000	0.006212000	3.052563000
6	0.011135000	-0.078168000	-3.058877000
1	-0.189567000	-0.137883000	-4.108316000

3Th (θ = 135.5°)

Total energy including ZPVE: -1742.6490 a. u.

Total free energy including ZPVE: -1742.7084 a. u.

N_{Img} = 4 (-453.0, -384.7, -63.4, -36.4)

6	-3.371049000	2.053991000	-1.002986000
6	-3.816609000	1.784551000	0.320370000
6	-2.091159000	2.646427000	-0.920982000
1	-3.919703000	1.847960000	-1.915294000
6	-2.805032000	2.221450000	1.219197000
1	-4.781426000	1.374584000	0.594601000
6	-1.733536000	2.749305000	0.444847000
1	-1.483106000	2.947298000	-1.764846000
1	-2.853878000	2.193670000	2.300649000
1	-0.821864000	3.179078000	0.836127000
6	-1.719471000	-2.769512000	0.443684000
6	-2.802898000	-2.262831000	1.215003000
6	-2.067347000	-2.665495000	-0.923786000
1	-0.807303000	-3.191412000	0.842481000

6	-3.812863000	-1.839464000	0.312442000
1	-2.857448000	-2.240549000	2.296426000
6	-3.355644000	-2.089948000	-1.010372000
1	-1.453801000	-2.959248000	-1.766362000
1	-4.781519000	-1.435720000	0.582795000
1	-3.903451000	-1.889416000	-1.924222000
90	-1.780734000	-0.006241000	-0.000980000
6	3.365612000	2.057834000	1.005417000
6	3.815756000	1.787115000	-0.316215000
6	2.085126000	2.648338000	0.918547000
1	3.911601000	1.853921000	1.919802000
6	2.806291000	2.221482000	-1.218794000
1	4.782092000	1.378485000	-0.587085000
6	1.731711000	2.748953000	-0.448482000
1	1.473944000	2.949163000	1.760148000
1	2.858567000	2.192548000	-2.300061000
1	0.820135000	3.175583000	-0.843450000
6	1.720670000	-2.768872000	-0.450547000
6	2.809027000	-2.261166000	-1.214075000
6	2.060123000	-2.667964000	0.919163000
1	0.810350000	-3.188599000	-0.855978000
6	3.813842000	-1.840391000	-0.304372000
1	2.870128000	-2.236470000	-2.295109000
6	3.348323000	-2.093479000	1.015057000
1	1.441345000	-2.963056000	1.757413000
1	4.784507000	-1.436925000	-0.567781000
1	3.890575000	-1.895565000	1.932775000
6	-0.020439000	-0.026530000	-1.933969000
6	0.021440000	-0.026008000	1.933513000
90	1.782101000	-0.006103000	0.000798000
1	-0.019602000	0.463300000	-4.185543000
6	-0.022037000	0.240103000	-3.138501000
6	0.022895000	0.240283000	3.138126000
1	0.020383000	0.463296000	4.185218000

4'Th

90	-2.491280000	0.003691000	-0.026283000
90	2.494752000	0.002769000	0.011182000
6	-0.827514000	-0.145779000	-1.715870000
6	0.124237000	0.034213000	-0.746014000
6	-0.122209000	0.021938000	0.731912000
6	0.830498000	-0.164749000	1.699785000
6	-4.722715000	1.803438000	-0.522722000
6	-4.054251000	2.304359000	0.626456000
6	-2.781306000	2.800549000	0.214161000
6	-2.664278000	2.604159000	-1.190620000
6	-3.847517000	1.953811000	-1.639174000
6	-2.564325000	-2.673881000	0.981182000
6	-3.105035000	-2.753877000	-0.333788000
6	-4.385573000	-2.124361000	-0.318912000
6	-4.636661000	-1.662500000	1.003308000

6	-3.495258000	-1.969666000	1.794878000
6	4.791504000	1.725319000	0.501385000
6	4.102175000	2.283384000	-0.608935000
6	2.857962000	2.800527000	-0.140383000
6	2.776428000	2.555541000	1.259259000
6	3.956343000	1.862012000	1.649443000
6	2.449916000	-2.661258000	-0.936040000
6	3.371299000	-2.019800000	-1.809396000
6	4.556154000	-1.735958000	-1.072801000
6	4.352493000	-2.169295000	0.267071000
6	3.050824000	-2.742838000	0.353011000
6	-5.343640000	-2.151196000	-1.475042000
6	-5.945005000	-1.194563000	1.568990000
6	-3.386210000	-1.758204000	3.278035000
6	-2.580067000	-3.543741000	-1.498283000
6	-1.337267000	-3.363228000	1.505803000
6	2.537530000	-3.495131000	1.546135000
6	1.152635000	-3.288759000	-1.340581000
6	5.362995000	-2.217695000	1.376637000
6	5.845324000	-1.296420000	-1.702091000
6	3.220950000	-1.822716000	-3.290338000
6	6.240458000	1.338794000	0.543325000
6	4.635346000	2.481678000	-1.999012000
6	1.939281000	3.667080000	-0.949376000
6	1.716091000	3.080681000	2.182718000
6	4.356344000	1.504156000	3.052541000
6	-1.566003000	3.136796000	-2.063366000
6	-1.864693000	3.608829000	1.084018000
6	-4.622566000	2.474785000	2.006180000
6	-6.179830000	1.464084000	-0.633105000
6	-4.218213000	1.650989000	-3.062867000
6	-0.488243000	-0.125913000	-3.175231000
6	0.488587000	-0.169151000	3.159142000
1	-0.498700000	-2.678786000	1.671207000
1	-1.554642000	-3.852292000	2.462136000
1	-1.004987000	-4.146064000	0.818821000
1	-1.528248000	-3.805668000	-1.377560000
1	-3.141768000	-4.481136000	-1.616191000
1	-2.668870000	-2.995761000	-2.442046000
1	-4.907059000	-1.739748000	-2.393532000
1	-5.646136000	-3.180722000	-1.708151000
1	-6.256116000	-1.589425000	-1.262745000
1	-5.839281000	-0.330162000	2.233010000
1	-6.662965000	-0.931342000	0.790440000
1	-6.401046000	-1.993680000	2.168858000
1	-2.346768000	-1.779399000	3.614705000
1	-3.814139000	-0.800001000	3.593295000
1	-3.925794000	-2.539833000	3.831769000
1	-6.628526000	1.240768000	0.336464000
1	-6.730679000	2.318271000	-1.050025000
1	-6.371841000	0.615723000	-1.296790000
1	-3.338183000	1.491566000	-3.691541000

1	-4.840257000	0.753126000	-3.142084000
1	-4.793054000	2.474561000	-3.508718000
1	-0.590937000	2.703243000	-1.827406000
1	-1.766760000	2.930394000	-3.117419000
1	-1.483646000	4.225923000	-1.958671000
1	-0.878743000	3.723590000	0.630836000
1	-2.268805000	4.618565000	1.244047000
1	-1.720987000	3.162309000	2.073355000
1	-3.910879000	2.187411000	2.789855000
1	-4.887731000	3.523603000	2.196341000
1	-5.529946000	1.883517000	2.152787000
1	1.138762000	0.506905000	3.728339000
1	-0.557774000	0.114872000	3.351728000
1	0.651538000	-1.168046000	3.586729000
1	0.558110000	0.158557000	-3.366748000
1	-0.656976000	-1.116590000	-3.620094000
1	-1.138819000	0.560507000	-3.731635000
1	1.769908000	3.275370000	-1.957547000
1	0.963828000	3.774484000	-0.472312000
1	2.357676000	4.677083000	-1.064700000
1	5.504144000	1.849432000	-2.200384000
1	3.884678000	2.266398000	-2.769091000
1	4.952501000	3.521634000	-2.155488000
1	6.841139000	2.178839000	0.918074000
1	6.435597000	0.493405000	1.209146000
1	6.631102000	1.085793000	-0.444065000
1	4.899591000	2.328840000	3.534315000
1	3.492482000	1.273693000	3.681950000
1	5.018818000	0.632997000	3.078681000
1	1.677787000	4.176815000	2.145114000
1	0.719329000	2.703202000	1.939844000
1	1.924580000	2.802389000	3.218615000
1	6.235193000	-2.087432000	-2.356574000
1	5.734485000	-0.403093000	-2.326537000
1	6.616364000	-1.087886000	-0.958332000
1	6.291870000	-1.709981000	1.107084000
1	4.993095000	-1.763331000	2.303912000
1	5.622377000	-3.256280000	1.620430000
1	3.763746000	-2.598617000	-3.848221000
1	2.175886000	-1.870023000	-3.604847000
1	3.621905000	-0.858742000	-3.624037000
1	1.286417000	-4.355637000	-1.567156000
1	0.408877000	-3.208492000	-0.547168000
1	0.728704000	-2.811490000	-2.226774000
1	2.735728000	-2.968283000	2.485144000
1	1.461484000	-3.665153000	1.487529000
1	3.018878000	-4.480731000	1.620544000

3U (spin multiplicity = 1, open shell)
Total energy including ZPVE: -1881.1447 a. u.
Total free energy including ZPVE: -1881.2080 a. u.

N_{Img} = 0

6	3.740477000	1.644652000	1.031679000
6	3.943383000	1.792012000	-0.364838000
6	2.490000000	2.220983000	1.352508000
1	4.428997000	1.184449000	1.729589000
6	2.822029000	2.465510000	-0.905484000
1	4.816923000	1.465926000	-0.917700000
6	1.920448000	2.722032000	0.154563000
1	2.043051000	2.268415000	2.337552000
1	2.682977000	2.745966000	-1.941584000
1	0.967332000	3.225843000	0.063334000
6	2.023228000	-2.635806000	-0.467412000
6	3.204025000	-2.117761000	-1.068534000
6	2.155408000	-2.508966000	0.940736000
1	1.191420000	-3.080503000	-0.998351000
6	4.057367000	-1.670320000	-0.027677000
1	3.423403000	-2.100429000	-2.129642000
6	3.405949000	-1.906636000	1.204678000
1	1.433427000	-2.820946000	1.682456000
1	5.038341000	-1.228474000	-0.152648000
1	3.792844000	-1.657547000	2.185751000
6	-3.444579000	1.885105000	-1.187041000
6	-4.065539000	1.667552000	0.064448000
6	-2.188059000	2.492086000	-0.963172000
1	-3.856267000	1.622455000	-2.154374000
6	-3.187683000	2.130515000	1.076875000
1	-5.042089000	1.225562000	0.220194000
6	-2.021917000	2.639259000	0.439840000
1	-1.485896000	2.796611000	-1.726618000
1	-3.380307000	2.127001000	2.143236000
1	-1.178776000	3.093269000	0.944241000
6	-1.908193000	-2.719367000	-0.162505000
6	-2.803265000	-2.470267000	0.904780000
6	-2.489191000	-2.218036000	-1.354941000
1	-0.952118000	-3.219089000	-0.080113000
6	-3.931770000	-1.800722000	0.374245000
1	-2.655255000	-2.752613000	1.939106000
6	-3.740132000	-1.648945000	-1.023418000
1	-2.049437000	-2.261053000	-2.343442000
1	-4.802799000	-1.480464000	0.934414000
1	-4.436510000	-1.191148000	-1.715029000
6	0.224634000	-0.219736000	1.425250000
6	-0.223842000	0.225988000	-1.426971000
1	-0.941775000	-0.445460000	3.305496000
6	-0.778808000	-0.279067000	2.244383000
6	0.779766000	0.288600000	-2.245357000
1	0.944327000	0.458826000	-3.305572000
92	-1.881294000	0.012158000	0.134931000
92	1.882552000	-0.010512000	-0.136236000

3U (spin multiplicity = 3)
Total energy including ZPVE: -1881.2145 a. u.
Total free energy including ZPVE: -1881.2791 a. u.

N_{Img} = 0

6	-3.756415000	-1.769027000	1.002464000
6	-4.019417000	-1.793376000	-0.389348000
6	-2.481345000	-2.343694000	1.217508000
1	-4.421006000	-1.386289000	1.767730000
6	-2.906977000	-2.383694000	-1.037523000
1	-4.923102000	-1.439139000	-0.871481000
6	-1.953950000	-2.719467000	-0.044437000
1	-1.995084000	-2.476257000	2.175458000
1	-2.808508000	-2.563769000	-2.100800000
1	-0.998387000	-3.194718000	-0.222246000
6	-2.136201000	2.693897000	-0.426338000
6	-3.309677000	2.166033000	-1.022332000
6	-2.235119000	2.511664000	0.973659000
1	-1.315497000	3.159673000	-0.956787000
6	-4.135337000	1.660906000	0.013717000
1	-3.544361000	2.174716000	-2.080423000
6	-3.467028000	1.868391000	1.243469000
1	-1.499356000	2.805876000	1.710698000
1	-5.113145000	1.212070000	-0.110251000
1	-3.836784000	1.591576000	2.223931000
6	3.648411000	-1.776677000	-1.129777000
6	4.137679000	-1.675048000	0.195086000
6	2.386163000	-2.416828000	-1.085448000
1	4.157933000	-1.437334000	-2.023700000
6	3.176535000	-2.246362000	1.063997000
1	5.087313000	-1.244271000	0.489556000
6	2.092674000	-2.701402000	0.272318000
1	1.761310000	-2.652035000	-1.936846000
1	3.259770000	-2.335928000	2.140417000
1	1.203933000	-3.192723000	0.646902000
6	1.889693000	2.706723000	-0.068430000
6	2.794820000	2.450406000	0.989967000
6	2.492549000	2.279037000	-1.280433000
1	0.912513000	3.160521000	0.031768000
6	3.952319000	1.853817000	0.435139000
1	2.632180000	2.677303000	2.036158000
6	3.767384000	1.749371000	-0.966627000
1	2.057810000	2.355371000	-2.268514000
1	4.834086000	1.544253000	0.984395000
1	4.485128000	1.351519000	-1.673434000
6	-0.231420000	0.015749000	1.453933000
6	0.255304000	-0.042844000	-1.458623000
1	1.022939000	0.039693000	3.304875000
6	0.775312000	0.023232000	2.250047000
6	-0.758554000	-0.038009000	-2.244715000

1	-1.019599000	-0.048201000	-3.296251000
92	1.954516000	0.002504000	0.104145000
92	-1.952391000	-0.008359000	-0.101044000

3U (spin multiplicity = 5)
Total energy including ZPVE: -1881.2268 a. u.
Total free energy including ZPVE: -1881.2924 a. u.

$N_{Img} = 0$

6	-3.766768000	-1.775314000	0.993120000
6	-4.011615000	-1.808132000	-0.401933000
6	-2.489465000	-2.337565000	1.226525000
1	-4.445251000	-1.397160000	1.748214000
6	-2.886756000	-2.392994000	-1.033384000
1	-4.912264000	-1.464137000	-0.896883000
6	-1.943496000	-2.715545000	-0.027199000
1	-2.013812000	-2.461839000	2.190941000
1	-2.773564000	-2.577033000	-2.094465000
1	-0.981265000	-3.182390000	-0.190573000
6	-2.099631000	2.703723000	-0.291084000
6	-3.192960000	2.233027000	-1.060723000
6	-2.375956000	2.440894000	1.073337000
1	-1.216154000	3.189324000	-0.684885000
6	-4.144477000	1.677743000	-0.169933000
1	-3.291392000	2.307182000	-2.137165000
6	-3.637208000	1.801813000	1.145714000
1	-1.738001000	2.685455000	1.912600000
1	-5.100537000	1.248264000	-0.443804000
1	-4.134112000	1.476971000	2.052232000
6	3.637371000	-1.801784000	-1.145523000
6	4.144358000	-1.677875000	0.170249000
6	2.376053000	-2.440773000	-1.073482000
1	4.134506000	-1.476908000	-2.051902000
6	3.192608000	-2.233172000	1.060780000
1	5.100376000	-1.248460000	0.444373000
6	2.099411000	-2.703706000	0.290858000
1	1.738264000	-2.685217000	-1.912905000
1	3.290793000	-2.307423000	2.137237000
1	1.215783000	-3.189227000	0.684422000
6	1.943487000	2.715528000	0.026707000
6	2.886285000	2.393209000	1.033394000
6	2.490059000	2.337325000	-1.226694000
1	0.981157000	3.182359000	0.189535000
6	4.011452000	1.808254000	0.402585000
1	2.772584000	2.577430000	2.094387000
6	3.767274000	1.775167000	-0.992582000
1	2.014854000	2.461412000	-2.191356000
1	4.911855000	1.464337000	0.898041000
1	4.446132000	1.396905000	-1.747283000
6	-0.235844000	0.029042000	1.455304000

6	0.235869000	-0.029025000	-1.455381000
1	1.039660000	0.028299000	3.293212000
6	0.776188000	0.023003000	2.242365000
6	-0.776184000	-0.022952000	-2.242415000
1	-1.039674000	-0.028210000	-3.293259000
92	1.962070000	0.004920000	0.091993000
92	-1.962073000	-0.004912000	-0.092040000

3U (Spin multiplicity = 7)
Total energy including ZPVE: -1881.2122 a. u.
Total free energy including ZPVE: -1881.2806 a. u.

$N_{Img} = 0$

6	-3.742407000	1.743198000	-1.036899000
6	-4.065715000	1.721416000	0.342344000
6	-2.481653000	2.372386000	-1.182981000
1	-4.364078000	1.368619000	-1.841148000
6	-3.002749000	2.331484000	1.051507000
1	-4.979023000	1.331013000	0.774650000
6	-2.023014000	2.730770000	0.108607000
1	-1.963536000	2.554464000	-2.115967000
1	-2.956816000	2.492493000	2.121641000
1	-1.095346000	3.237549000	0.340891000
6	-1.999051000	-2.730741000	0.126002000
6	-3.001540000	-2.326366000	1.042063000
6	-2.431712000	-2.391328000	-1.179558000
1	-1.073304000	-3.227665000	0.385303000
6	-4.053408000	-1.732664000	0.302012000
1	-2.977787000	-2.473368000	2.115063000
6	-3.699557000	-1.769981000	-1.069258000
1	-1.891680000	-2.579736000	-2.098706000
1	-4.979336000	-1.344760000	0.708800000
1	-4.305065000	-1.409080000	-1.891969000
6	3.742479000	1.740419000	1.039746000
6	4.068365000	1.718825000	-0.338895000
6	2.482192000	2.371123000	1.183742000
1	4.362236000	1.364852000	1.845015000
6	3.007410000	2.330327000	-1.049778000
1	4.982034000	1.327568000	-0.769645000
6	2.026397000	2.730458000	-0.108551000
1	1.962580000	2.553480000	2.115840000
1	2.963636000	2.491772000	-2.119936000
1	1.099662000	3.238169000	-0.342503000
6	1.995636000	-2.730729000	-0.126830000
6	2.998059000	-2.327135000	-1.043295000
6	2.429585000	-2.392567000	1.178648000
1	1.069081000	-3.226293000	-0.385815000
6	4.051158000	-1.735153000	-0.303566000
1	2.973415000	-2.473445000	-2.116373000
6	3.698143000	-1.772846000	1.067902000
1	1.889838000	-2.580688000	2.098018000

1	4.977351000	-1.348269000	-0.710714000
1	4.304605000	-1.413101000	1.890412000
6	-0.141577000	0.007366000	-1.603952000
6	0.141656000	0.005225000	1.603642000
1	1.273163000	0.065438000	-3.395084000
6	0.819940000	0.039029000	-2.418517000
6	-0.819522000	0.032284000	2.418712000
1	-1.272936000	0.054494000	3.395278000
92	1.941883000	0.001015000	-0.080368000
92	-1.941811000	0.001242000	0.080149000

4U (Spin multiplicity = 5)
Total energy including ZPVE: -1881.2240 a. u.
Total free energy including ZPVE: -1881.291 a. u.

$N_{Img} = 0$

92	-2.345025000	0.000056000	0.001405000
92	2.345329000	-0.000009000	-0.001051000
6	-0.857721000	0.000558000	-1.712213000
6	0.114503000	0.000332000	-0.751364000
6	-0.114042000	-0.000028000	0.751276000
6	0.857870000	-0.000366000	1.712447000
6	-4.246861000	1.868288000	-0.761702000
6	-4.370838000	1.776535000	0.645218000
6	-3.184795000	2.295398000	1.220443000
6	-2.331160000	2.710687000	0.167074000
6	-2.990058000	2.449028000	-1.059266000
6	-2.330988000	-2.710920000	0.159646000
6	-2.996330000	-2.445643000	-1.062478000
6	-4.251522000	-1.865696000	-0.756595000
6	-4.367904000	-1.777826000	0.651199000
6	-3.178920000	-2.298544000	1.218671000
6	4.252143000	1.866116000	0.755401000
6	4.367324000	1.778322000	-0.652502000
6	3.177750000	2.298839000	-1.218931000
6	2.330649000	2.710969000	-0.159163000
6	2.997098000	2.445793000	1.062383000
6	2.330302000	-2.710545000	-0.169017000
6	3.185126000	-2.294716000	-1.221217000
6	4.370865000	-1.776910000	-0.644418000
6	4.245489000	-1.869823000	0.762304000
6	2.988155000	-2.450292000	1.058164000
1	2.975028000	-2.379172000	-2.281781000
1	1.352564000	-3.160584000	-0.286207000
1	5.230252000	-1.396455000	-1.182940000
1	4.991503000	-1.564711000	1.487149000
1	2.603201000	-2.668745000	2.045785000
1	5.222656000	1.399495000	-1.198602000
1	5.003254000	1.558040000	1.473687000
1	2.619188000	2.660742000	2.053501000
1	1.352192000	3.161625000	-0.267619000

1	0.557772000	-0.000736000	2.761248000
1	-0.557993000	0.000738000	-2.761118000
1	2.960052000	2.387127000	-2.277638000
1	-2.617690000	-2.660806000	-2.053268000
1	-1.352770000	-3.161888000	0.268981000
1	-2.962215000	-2.386956000	2.277572000
1	-5.223635000	-1.398828000	1.196550000
1	-5.001954000	-1.557544000	-1.475554000
1	-4.993412000	1.562155000	-1.485556000
1	-5.229536000	1.396161000	1.184896000
1	-2.973698000	2.380794000	2.280734000
1	-1.353473000	3.161188000	0.282904000
1	-2.606068000	2.666712000	-2.047432000

4U (Spin multiplicity = 7)
Total energy including ZPVE: -1881.2205 a. u.
Total free energy including ZPVE: -1881.2856 a. u.

$N_{Img} = 0$

92	2.530851000	0.000001000	0.084814000
92	-2.530854000	-0.000002000	-0.084829000
6	0.873335000	-0.000071000	-1.691975000
6	0.015341000	-0.000006000	-0.689925000
6	-0.015322000	0.000083000	0.689879000
6	-0.873311000	0.000115000	1.691937000
6	4.602377000	-1.758041000	0.505706000
6	3.480351000	-2.339707000	1.145882000
6	2.553974000	-2.729714000	0.144759000
6	3.106414000	-2.391565000	-1.115947000
6	4.369131000	-1.786905000	-0.892007000
6	2.553864000	2.729716000	0.144837000
6	3.106237000	2.391637000	-1.115908000
6	4.368993000	1.787027000	-0.892069000
6	4.602334000	1.758130000	0.505623000
6	3.480321000	2.339721000	1.145889000
6	-4.369006000	-1.786998000	0.892068000
6	-4.602293000	-1.758177000	-0.505637000
6	-3.480248000	-2.339788000	-1.145833000
6	-2.553821000	-2.729718000	-0.144727000
6	-3.106247000	-2.391579000	1.115986000
6	-2.554006000	2.729711000	-0.144764000
6	-3.480395000	2.339704000	-1.145875000
6	-4.602408000	1.758026000	-0.505683000
6	-4.369140000	1.786883000	0.892024000
6	-3.106425000	2.391552000	1.115947000
1	-3.364419000	2.491097000	-2.214148000
1	-1.604382000	3.223637000	-0.312725000
1	-5.495300000	1.387890000	-0.994479000
1	-5.054993000	1.443387000	1.657214000
1	-2.654674000	2.586348000	2.080140000
1	-5.495213000	-1.388107000	-0.994428000

1	-5.054873000	-1.443536000	1.657261000
1	-2.654471000	-2.586328000	2.080176000
1	-1.604166000	-3.223582000	-0.312694000
1	-0.620693000	0.000177000	2.749542000
1	0.620727000	-0.000149000	-2.749582000
1	-3.364273000	-2.491185000	-2.214105000
1	2.654421000	2.586438000	-2.080070000
1	1.604222000	3.223584000	0.312863000
1	3.364392000	2.491067000	2.214174000
1	5.495266000	1.388021000	0.994363000
1	5.054822000	1.443588000	-1.657308000
1	5.495261000	-1.387908000	0.994517000
1	3.364359000	-2.491096000	2.214154000
1	1.604345000	-3.223634000	0.312708000
1	2.654672000	-2.586357000	-2.080145000
1	5.054998000	-1.443413000	-1.657187000

TS3/4 (**M = U;** spin multiplicity = 5)
Total energy including ZPVE: -1881.2099 a. u.
Total free energy including ZPVE: -1881.2740 a. u.

N_{Img} = 2 (-249.4, -9.6)
(9.6 corresponds to rotation of Cp ring and thus not considered)

6	-4.298489000	-1.810546000	-0.550606000
6	-3.119010000	-2.401527000	-1.066775000
6	-4.186653000	-1.762077000	0.859655000
1	-5.147469000	-1.469587000	-1.131821000
6	-2.276931000	-2.717575000	0.028053000
1	-2.904980000	-2.593725000	-2.110795000
6	-2.936714000	-2.324212000	1.218670000
1	-4.935258000	-1.379899000	1.543351000
1	-1.303113000	-3.185936000	-0.033774000
1	-2.554526000	-2.443511000	2.225531000
6	-2.244412000	2.714732000	-0.146885000
6	-3.231644000	2.336776000	-1.091632000
6	-2.735127000	2.413609000	1.146983000
1	-1.284612000	3.158690000	-0.377976000
6	-4.333292000	1.802799000	-0.378758000
1	-3.162475000	2.456070000	-2.166082000
6	-4.025300000	1.846278000	1.001904000
1	-2.216636000	2.591588000	2.081236000
1	-5.257732000	1.438754000	-0.811263000
1	-4.672854000	1.521492000	1.807961000
92	-2.260572000	-0.002736000	-0.059435000
6	3.011653000	-2.452822000	1.038008000
6	2.262609000	-2.712629000	-0.135655000
6	4.233973000	-1.852522000	0.648935000
1	2.708190000	-2.684444000	2.051189000
6	3.024279000	-2.276528000	-1.248758000
1	1.283630000	-3.172296000	-0.177719000
6	4.244195000	-1.744933000	-0.762640000

1	5.031899000	-1.543593000	1.314635000
1	2.728528000	-2.350814000	-2.288738000
1	5.052091000	-1.345146000	-1.363440000
6	3.195564000	2.350949000	1.095324000
6	4.322398000	1.808499000	0.429688000
6	2.241718000	2.713081000	0.111159000
1	3.087513000	2.484753000	2.164744000
6	4.064085000	1.832662000	-0.961445000
1	5.230575000	1.450173000	0.900084000
6	2.778561000	2.394654000	-1.160160000
1	1.273557000	3.158476000	0.301053000
1	4.740928000	1.499101000	-1.739253000
1	2.294115000	2.559425000	-2.114996000
6	-0.241272000	-0.020853000	1.036486000
6	0.241788000	-0.016781000	-1.041923000
92	2.261134000	-0.003314000	0.054533000
1	0.676966000	-0.030117000	2.945557000
6	0.793286000	-0.027160000	1.860781000
6	-0.792667000	-0.018370000	-1.866608000
1	-0.675636000	-0.015847000	-2.951303000

2Ce (spin multiplicity 1, open shell)
Total energy including ZPVE: -1877.5036 a. u.
Total free energy including ZPVE: -1877.5688 a. u.

N_{Img} = 1 (-2.3)

6	-0.612419000	-0.047218000	2.779479000
6	0.023415000	-0.021971000	1.721643000
6	3.923074000	1.779676000	0.961208000
6	4.062109000	1.834448000	-0.448384000
6	2.680448000	2.365867000	1.301153000
6	2.904665000	2.454268000	-0.977546000
6	2.049446000	2.779756000	0.102861000
6	3.470829000	-2.159317000	-1.016387000
6	4.224239000	-1.708084000	0.094146000
6	2.275228000	-2.742816000	-0.527146000
6	3.487537000	-1.998499000	1.267883000
6	2.285778000	-2.644542000	0.883179000
6	-0.020535000	0.012613000	-1.719239000
6	0.617939000	0.003803000	-2.775767000
6	-2.645667000	-2.395489000	-1.276741000
6	-2.084283000	-2.791390000	-0.039137000
6	-3.892312000	-1.778234000	-1.013913000
6	-2.986531000	-2.425446000	0.988923000
6	-4.104228000	-1.798557000	0.387865000
6	-2.264795000	2.728947000	0.591213000
6	-2.203394000	2.671600000	-0.819965000
6	-3.487050000	2.140474000	1.001441000
6	-3.387952000	2.047685000	-1.285068000

6	-4.185520000	1.727565000	-0.159839000
1	-4.578452000	-1.385379000	-1.755318000
1	-4.981903000	-1.427271000	0.904278000
1	-5.165742000	1.267156000	-0.184487000
1	-3.649637000	1.873874000	-2.322848000
1	-3.842597000	2.057054000	2.022648000
1	-1.512760000	3.150905000	1.247031000
1	-1.397057000	3.042160000	-1.440958000
1	-2.200516000	-2.544233000	-2.253258000
1	-1.136157000	-3.297446000	0.097939000
1	-2.852045000	-2.613347000	2.047897000
1	3.772659000	-2.103500000	-2.056571000
1	5.200189000	-1.239612000	0.054737000
1	3.802085000	-1.793573000	2.285106000
1	1.516165000	-3.003940000	1.555305000
1	1.495311000	-3.190667000	-1.131278000
1	2.712773000	2.661700000	-2.023863000
1	4.917828000	1.489090000	-1.017182000
1	4.652095000	1.381089000	1.657103000
1	2.283094000	2.484257000	2.302224000
1	1.087458000	3.271984000	0.026860000
1	-1.124164000	-0.067383000	3.720165000
1	1.131752000	-0.003115000	-3.715523000
58	2.033332000	-0.004253000	0.002807000
58	-2.029826000	0.004838000	-0.000579000

2Ce (spin multiplicity 3)
Total energy including ZPVE: -1877.5037 a. u.
Total free energy including ZPVE: -1877.5730 a. u.

$N_{Img} = 0$

6	-0.609448000	-0.035583000	2.780660000
6	0.026970000	-0.012767000	1.723119000
6	3.938709000	1.776638000	0.965056000
6	4.077518000	1.834051000	-0.444869000
6	2.703542000	2.377203000	1.307535000
6	2.927228000	2.469736000	-0.971035000
6	2.076982000	2.801838000	0.111064000
6	3.435814000	-2.154409000	-1.023253000
6	4.196723000	-1.713629000	0.087209000
6	2.237372000	-2.729981000	-0.532178000
6	3.461799000	-2.004349000	1.262229000
6	2.253600000	-2.637959000	0.878415000
6	-0.017939000	0.014972000	-1.718946000
6	0.617679000	0.040638000	-2.776897000
6	-2.634492000	-2.413102000	-1.266370000
6	-2.075409000	-2.802544000	-0.025692000
6	-3.883024000	-1.797196000	-1.009257000
6	-2.980788000	-2.433810000	0.998567000
6	-4.098289000	-1.811770000	0.392040000

6	-2.265187000	2.720356000	0.582127000
6	-2.201650000	2.657793000	-0.828723000
6	-3.487194000	2.131718000	0.992820000
6	-3.384647000	2.030430000	-1.293191000
6	-4.183430000	1.713458000	-0.167916000
1	-4.568100000	-1.408832000	-1.754015000
1	-4.977881000	-1.439796000	0.904689000
1	-5.163008000	1.251653000	-0.192221000
1	-3.644472000	1.852107000	-2.330671000
1	-3.844210000	2.051758000	2.013791000
1	-1.514728000	3.145909000	1.237397000
1	-1.394841000	3.026926000	-1.449884000
1	-2.186876000	-2.565626000	-2.241198000
1	-1.126842000	-3.306476000	0.115882000
1	-2.848655000	-2.617048000	2.058668000
1	3.734515000	-2.096898000	-2.064216000
1	5.176842000	-1.254004000	0.046770000
1	3.780467000	-1.805347000	2.279337000
1	1.481987000	-2.991468000	1.551288000
1	1.450562000	-3.166643000	-1.135421000
1	2.737187000	2.683993000	-2.016334000
1	4.929713000	1.482516000	-1.015178000
1	4.664261000	1.369175000	1.659449000
1	2.308220000	2.497869000	2.309164000
1	1.120420000	3.305081000	0.037196000
1	-1.121682000	-0.052704000	3.721141000
1	1.129315000	0.059924000	-3.717656000
58	2.035571000	0.007457000	0.002838000
58	-2.026296000	-0.005735000	0.000768000

2Ce (θ = 100°) (spin multiplicity 3)
Total energy including ZPVE: -1877.5036 a. u.
Total free energy including ZPVE: -1877.5735 a. u.

$N_{Img} = 0$

6	-0.511224000	0.009347000	2.806984000
6	0.073360000	0.008172000	1.719805000
6	3.947298000	1.776909000	0.838871000
6	4.079127000	1.793243000	-0.572755000
6	2.718213000	2.396008000	1.170392000
6	2.930093000	2.420787000	-1.110998000
6	2.088044000	2.790055000	-0.034402000
6	3.415339000	-2.173647000	-1.093251000
6	4.180175000	-1.737265000	0.016374000
6	2.215392000	-2.744627000	-0.600633000
6	3.445941000	-2.025606000	1.192285000
6	2.234232000	-2.653491000	0.809953000
6	-0.073361000	-0.008176000	-1.719800000
6	0.511223000	-0.009367000	-2.806979000
6	-2.718214000	-2.396005000	-1.170386000
6	-2.088049000	-2.790049000	0.034411000

6	-3.947298000	-1.776901000	-0.838870000
6	-2.930101000	-2.420777000	1.111004000
6	-4.079134000	-1.793234000	0.572755000
6	-2.215391000	2.744633000	0.600627000
6	-2.234228000	2.653494000	-0.809959000
6	-3.415341000	2.173657000	1.093243000
6	-3.445936000	2.025609000	-1.192293000
6	-4.180174000	1.737273000	-0.016384000
1	-4.673898000	-1.384737000	-1.541016000
1	-4.925676000	-1.419372000	1.137164000
1	-5.162308000	1.282145000	0.025475000
1	-3.766900000	1.828881000	-2.209138000
1	-3.712699000	2.116396000	2.134626000
1	-1.425461000	3.177178000	1.202745000
1	-1.462399000	3.004112000	-1.484086000
1	-2.329125000	-2.547835000	-2.170156000
1	-1.134296000	-3.297091000	0.118107000
1	-2.735880000	-2.605893000	2.161146000
1	3.712693000	-2.116381000	-2.134635000
1	5.162308000	-1.282136000	-0.025487000
1	3.766908000	-1.828881000	2.209130000
1	1.462406000	-3.004113000	1.484082000
1	1.425460000	-3.177171000	-1.202750000
1	2.735869000	2.605904000	-2.161139000
1	4.925668000	1.419383000	-1.137167000
1	4.673901000	1.384745000	1.541013000
1	2.329127000	2.547836000	2.170164000
1	1.134290000	3.297096000	-0.118093000
1	-0.979985000	0.012919000	3.769979000
1	0.980013000	-0.013029000	-3.769960000
58	2.027296000	-0.005880000	-0.062749000
58	-2.027299000	0.005885000	0.062752000

2Ce (θ = 120^{o}) (spin multiplicity 3)
Total energy including ZPVE: -1877.5022 a. u.
Total free energy including ZPVE: -1877.5665 a. u.

N_{Img} = 3 (-61.7, -50.9, -3.9)

6	-0.251339000	0.023886000	2.928863000
6	-0.015462000	0.017729000	1.718178000
6	3.953545000	1.791482000	0.831558000
6	4.039769000	1.786836000	-0.583788000
6	2.735285000	2.415185000	1.192907000
6	2.874106000	2.406867000	-1.094012000
6	2.066632000	2.791909000	0.003367000
6	3.425293000	-2.138471000	-1.041904000
6	4.157427000	-1.736800000	0.102015000
6	2.212393000	-2.725342000	-0.602029000
6	3.389660000	-2.061096000	1.247030000
6	2.190468000	-2.677799000	0.810480000
6	0.015463000	-0.017728000	-1.718198000

6	0.251342000	-0.023894000	-2.928882000
6	-2.735307000	-2.415183000	-1.192914000
6	-2.066637000	-2.791910000	-0.003385000
6	-3.953561000	-1.791479000	-0.831546000
6	-2.874094000	-2.406868000	1.094007000
6	-4.039763000	-1.786833000	0.583801000
6	-2.212378000	2.725341000	0.602022000
6	-2.190480000	2.677800000	-0.810487000
6	-3.425271000	2.138471000	1.041919000
6	-3.389680000	2.061098000	-1.247017000
6	-4.157426000	1.736802000	-0.101988000
1	-4.702819000	-1.410382000	-1.515833000
1	-4.866938000	-1.402783000	1.169646000
1	-5.139401000	1.279399000	-0.102191000
1	-3.681638000	1.896782000	-2.278331000
1	-3.750636000	2.046260000	2.072295000
1	-1.440908000	3.139471000	1.239815000
1	-1.399592000	3.048963000	-1.450789000
1	-2.378975000	-2.583299000	-2.202357000
1	-1.110896000	-3.298375000	0.056622000
1	-2.644005000	-2.571620000	2.140188000
1	3.750678000	-2.046263000	-2.072275000
1	5.139402000	-1.279396000	0.102236000
1	3.681598000	-1.896776000	2.278350000
1	1.399568000	-3.048960000	1.450767000
1	1.440936000	-3.139475000	-1.239836000
1	2.644033000	2.571619000	-2.140196000
1	4.866954000	1.402788000	-1.169620000
1	4.702793000	1.410386000	1.515857000
1	2.378936000	2.583299000	2.202345000
1	1.110891000	3.298372000	-0.056654000
1	-0.448834000	0.030566000	3.981276000
1	0.448867000	-0.030582000	-3.981290000
58	2.005017000	-0.004277000	0.012757000
58	-2.005015000	0.004277000	-0.012773000

2Ce (θ = 130.5°) (spin multiplicity 3)
Total energy including ZPVE: -1877.5017 a. u.
Total free energy including ZPVE: -1877.5691 a. u.

$N_{Img} = 0$

6	0.001565000	0.000082000	2.944157000
6	-0.000580000	-0.000035000	1.710675000
6	3.982266000	1.834114000	0.709188000
6	3.981910000	1.833848000	-0.708786000
6	2.780615000	2.441589000	1.145915000
6	2.780183000	2.441428000	-1.145144000
6	2.036409000	2.813556000	0.000499000
6	3.431533000	-2.066474000	-1.144880000
6	4.178013000	-1.696516000	0.000414000
6	2.231369000	-2.679988000	-0.706443000

6	3.431592000	-2.066907000	1.145609000
6	2.231405000	-2.680254000	0.706999000
6	0.000587000	0.000020000	-1.710668000
6	-0.001559000	-0.000077000	-2.944150000
6	-2.780590000	-2.441667000	-1.145868000
6	-2.036406000	-2.813567000	-0.000413000
6	-3.982219000	-1.834106000	-0.709200000
6	-2.780188000	-2.441385000	1.145208000
6	-3.981947000	-1.833890000	0.708811000
6	-2.231369000	2.679989000	0.706393000
6	-2.231400000	2.680228000	-0.707048000
6	-3.431535000	2.066483000	1.144838000
6	-3.431584000	2.066870000	-1.145650000
6	-4.178009000	1.696501000	-0.000451000
1	-4.776588000	-1.460968000	-1.345350000
1	-4.776070000	-1.460555000	1.345151000
1	-5.155367000	1.229265000	-0.000508000
1	-3.739048000	1.935798000	-2.177266000
1	-3.738931000	1.935031000	2.176424000
1	-1.453986000	3.080062000	1.345891000
1	-1.454035000	3.080515000	-1.346436000
1	-2.484860000	-2.604343000	-2.175671000
1	-1.072707000	-3.308334000	-0.000518000
1	-2.484074000	-2.603750000	2.174947000
1	3.738926000	-1.935000000	-2.176465000
1	5.155371000	-1.229281000	0.000475000
1	3.739060000	-1.935857000	2.177226000
1	1.454043000	-3.080555000	1.346381000
1	1.453983000	-3.080048000	-1.345945000
1	2.484056000	2.603836000	-2.174873000
1	4.776012000	1.460510000	-1.345149000
1	4.776669000	1.460979000	1.345296000
1	2.484912000	2.604220000	2.175733000
1	1.072711000	3.308324000	0.000643000
1	0.003265000	0.000337000	4.014975000
1	-0.003409000	-0.000017000	-4.014968000
58	2.008357000	0.017001000	0.000756000
58	-2.008352000	-0.017015000	-0.000751000

5Ce (spin multiplicity 3)
Total energy including ZPVE: -1877.5093 a. u.
Total free energy including ZPVE: -1877.5782 a. u.

$N_{Img} = 0$

58	2.668117000	-0.001126000	0.090688000
58	-2.682158000	0.002427000	-0.070450000
6	0.769044000	-0.010795000	1.759029000
6	0.017891000	-0.010165000	0.686672000
6	-0.029534000	-0.007923000	-0.664202000
6	-0.782485000	-0.005135000	-1.735289000
6	4.811234000	1.776313000	-0.055491000

6	4.034943000	2.055747000	-1.205657000
6	2.819094000	2.649960000	-0.779629000
6	2.846195000	2.738304000	0.632111000
6	4.073234000	2.192139000	1.080960000
6	2.618597000	-2.768229000	-0.323369000
6	3.246582000	-2.594930000	0.932445000
6	4.508163000	-1.986871000	0.710335000
6	4.662424000	-1.793569000	-0.684665000
6	3.492544000	-2.272251000	-1.322617000
6	-4.452966000	1.999573000	-0.841810000
6	-4.686004000	1.829585000	0.545906000
6	-3.546828000	2.304533000	1.240025000
6	-2.612754000	2.772297000	0.281849000
6	-3.174429000	2.588147000	-1.003717000
6	-2.669473000	-2.720179000	0.572554000
6	-3.749230000	-2.176977000	1.314418000
6	-4.761611000	-1.797681000	0.400973000
6	-4.304355000	-2.098866000	-0.906229000
6	-3.014829000	-2.676323000	-0.798708000
1	-3.805877000	-2.100835000	2.395141000
1	-1.752007000	-3.123439000	0.985397000
1	-5.726311000	-1.376076000	0.656289000
1	-4.861671000	-1.951210000	-1.824879000
1	-2.405679000	-3.032915000	-1.620316000
1	-5.588468000	1.433983000	0.996346000
1	-5.148344000	1.756363000	-1.637701000
1	-2.712140000	2.861237000	-1.944611000
1	-1.645986000	3.212587000	0.496483000
1	-3.425823000	2.338569000	2.317554000
1	2.841886000	-2.892938000	1.892327000
1	1.647537000	-3.218530000	-0.492891000
1	3.311646000	-2.288752000	-2.392111000
1	5.531313000	-1.374216000	-1.177799000
1	5.243805000	-1.748006000	1.470468000
1	5.804208000	1.342864000	-0.046369000
1	4.333652000	1.879730000	-2.233331000
1	2.022432000	3.005003000	-1.423669000
1	2.068633000	3.156606000	1.259459000
1	4.404740000	2.134879000	2.112054000
1	-0.423704000	0.000127000	-2.761675000
1	0.407887000	-0.010672000	2.784639000

TS4 (**M = Ce**) (spin multiplicity 3)
Total energy including ZPVE: -1877.4647 a. u.
Total free energy including ZPVE: -1877.5351 a. u.

N_{Img} = 1 (-407.8)

6	-0.692182000	0.013030000	1.843562000
6	0.217609000	0.010751000	0.974866000
6	4.587307000	1.782474000	0.678570000
6	4.368693000	2.006377000	-0.702781000

6	3.447288000	2.244498000	1.381506000
6	3.096000000	2.611906000	-0.852132000
6	2.526795000	2.759017000	0.435365000
6	3.631283000	-2.362801000	-1.058202000
6	4.651993000	-1.829641000	-0.231671000
6	2.574198000	-2.798106000	-0.222191000
6	4.220430000	-1.928558000	1.113615000
6	2.936830000	-2.528970000	1.117942000
6	-0.217349000	0.026221000	-1.013598000
6	0.694286000	0.028821000	-1.880429000
6	-2.963743000	-2.535789000	-1.113015000
6	-2.591428000	-2.787793000	0.228010000
6	-4.244510000	-1.927161000	-1.103016000
6	-3.638212000	-2.336960000	1.069082000
6	-4.662853000	-1.809032000	0.245503000
6	-3.047302000	2.623608000	0.857536000
6	-2.518421000	2.772223000	-0.445546000
6	-4.326128000	2.024922000	0.744678000
6	-3.468531000	2.267079000	-1.366179000
6	-4.588454000	1.807263000	-0.630806000
1	-4.823051000	-1.638063000	-1.973349000
1	-5.610541000	-1.408271000	0.586190000
1	-5.496591000	1.387256000	-1.046962000
1	-3.369514000	2.261520000	-2.446305000
1	-5.003876000	1.805312000	1.562453000
1	-2.567716000	2.935320000	1.778115000
1	-1.557252000	3.205627000	-0.693762000
1	-2.383488000	-2.782762000	-1.994692000
1	-1.667175000	-3.248474000	0.555504000
1	-3.665403000	-2.417626000	2.150333000
1	3.671405000	-2.456852000	-2.138061000
1	5.606372000	-1.439427000	-0.565838000
1	4.788952000	-1.633249000	1.988239000
1	2.343010000	-2.762034000	1.994347000
1	1.650003000	-3.257618000	-0.551435000
1	2.648884000	2.932579000	-1.785991000
1	5.071376000	1.788929000	-1.499787000
1	5.479657000	1.356113000	1.121315000
1	3.313132000	2.232804000	2.457793000
1	1.561074000	3.194540000	0.661061000
1	-1.022226000	0.009306000	2.866353000
1	1.027186000	0.035804000	-2.902392000
58	2.555168000	0.000487000	-0.014928000
58	-2.560993000	0.007313000	-0.021800000

5'Ce (spin multiplicity 3)

58	-2.846092000	-0.000096000	0.019717000
58	2.865409000	-0.003145000	-0.052323000
6	-0.915837000	0.008736000	1.658264000
6	-0.559837000	-0.020230000	3.113502000
6	-0.110738000	0.035824000	0.619009000

6	0.155051000	0.103516000	-0.687390000
6	0.965307000	0.174407000	-1.718352000
6	0.627575000	0.274202000	-3.173623000
6	-5.044644000	-1.747663000	0.427643000
6	-4.566614000	-2.034715000	-0.880829000
6	-3.290951000	-2.660719000	-0.755878000
6	-2.984272000	-2.763080000	0.629829000
6	-4.053326000	-2.172852000	1.358388000
6	-6.434383000	-1.326654000	0.807223000
6	-5.316137000	-1.883738000	-2.174188000
6	-2.521327000	-3.247434000	-1.905803000
6	-1.841871000	-3.516975000	1.242417000
6	-4.212939000	-2.171485000	2.852093000
6	-2.636727000	2.693349000	-0.697570000
6	-3.035997000	2.723562000	0.667554000
6	-4.379728000	2.260105000	0.742048000
6	-4.816364000	1.956407000	-0.580374000
6	-3.730806000	2.205600000	-1.467016000
6	-1.345705000	3.231237000	-1.237931000
6	-2.243674000	3.299471000	1.804472000
6	-5.232498000	2.271944000	1.979521000
6	-6.230660000	1.700206000	-1.012717000
6	-3.794791000	2.107205000	-2.965561000
6	4.825176000	-2.024020000	-0.457386000
6	4.311898000	-2.250571000	0.851294000
6	2.957630000	-2.672233000	0.722758000
6	2.640607000	-2.724159000	-0.663717000
6	3.785248000	-2.304853000	-1.392123000
6	6.261209000	-1.798310000	-0.833324000
6	5.089633000	-2.222897000	2.136935000
6	2.061108000	-3.109566000	1.846676000
6	1.354997000	-3.236094000	-1.237316000
6	3.946416000	-2.298787000	-2.885784000
6	2.950643000	2.680073000	0.784450000
6	3.979038000	2.030015000	1.524578000
6	5.027106000	1.693930000	0.624126000
6	4.625956000	2.098661000	-0.682358000
6	3.348401000	2.721906000	-0.580350000
6	1.753861000	3.350900000	1.393698000
6	4.013423000	1.873550000	3.018893000
6	6.398787000	1.240820000	1.029942000
6	5.468939000	2.043558000	-1.925846000
6	2.637821000	3.428098000	-1.698987000
1	-1.065677000	-0.848858000	3.623342000
1	-0.917085000	0.893170000	3.605472000
1	0.515487000	-0.109685000	3.318872000
1	1.048537000	1.193585000	-3.599047000
1	-0.448730000	0.268102000	-3.393116000
1	1.086002000	-0.549566000	-3.734269000
1	-6.987397000	-0.917315000	-0.040492000
1	-6.448842000	-0.577343000	1.605874000
1	-7.006405000	-2.188529000	1.177086000

1	-6.206645000	-1.261066000	-2.058565000
1	-5.652308000	-2.858068000	-2.554154000
1	-4.706187000	-1.436792000	-2.969666000
1	-1.498112000	-3.508844000	-1.627313000
1	-2.461382000	-2.567788000	-2.765167000
1	-2.999392000	-4.165957000	-2.273155000
1	-2.157446000	-4.524882000	1.545008000
1	-1.449522000	-3.021815000	2.135859000
1	-1.009916000	-3.640468000	0.546272000
1	-4.731671000	-1.276768000	3.213977000
1	-3.248508000	-2.222270000	3.365754000
1	-4.801584000	-3.034936000	3.193025000
1	-1.361387000	4.329089000	-1.277876000
1	-1.145564000	2.875771000	-2.252641000
1	-0.494654000	2.936983000	-0.618947000
1	-2.573954000	2.904642000	2.770377000
1	-2.354298000	4.392007000	1.852286000
1	-1.175967000	3.085134000	1.710646000
1	-6.107766000	1.624298000	1.879637000
1	-5.606781000	3.281795000	2.195709000
1	-4.683137000	1.944978000	2.869756000
1	-6.849598000	1.317276000	-0.198535000
1	-6.297872000	0.990679000	-1.843543000
1	-6.699802000	2.632093000	-1.357660000
1	-2.808016000	1.949580000	-3.413997000
1	-4.199468000	3.025339000	-3.413289000
1	-4.441040000	1.286889000	-3.297282000
1	6.857491000	-1.439990000	0.008479000
1	6.376770000	-1.078231000	-1.650816000
1	6.721713000	-2.735343000	-1.175321000
1	5.322657000	-3.239392000	2.481077000
1	4.545074000	-1.735302000	2.954806000
1	6.042203000	-1.699246000	2.024446000
1	2.412845000	-2.737877000	2.814691000
1	2.021806000	-4.204844000	1.925357000
1	1.030757000	-2.764070000	1.714883000
1	1.275441000	-4.325649000	-1.121001000
1	1.269731000	-3.014905000	-2.304399000
1	0.486074000	-2.787545000	-0.746727000
1	2.985880000	-2.207001000	-3.400939000
1	4.415194000	-3.226156000	-3.243056000
1	4.581111000	-1.474626000	-3.230414000
1	1.059802000	3.705667000	0.629193000
1	2.055368000	4.226832000	1.983711000
1	1.191877000	2.694060000	2.067454000
1	4.630723000	1.024251000	3.330756000
1	3.013131000	1.728846000	3.442921000
1	4.432802000	2.763791000	3.508233000
1	6.950751000	0.797109000	0.198414000
1	6.377664000	0.508507000	1.843123000
1	6.993526000	2.092211000	1.388710000
1	5.977998000	2.999823000	-2.108067000

1	6.247511000	1.278045000	-1.858210000
1	1.550900000	3.373564000	-1.599766000
1	2.895335000	3.002314000	-2.673904000
1	2.910499000	4.492001000	-1.735068000
1	4.877004000	1.829166000	-2.823020000

6Ce (spin multiplicity 3)
Total energy including ZPVE: -1910.8539 a. u.
Total free energy including ZPVE: -1910.9218 a. u.

$N_{Img} = 0$

58	2.722159000	-0.019443000	-0.231519000
58	-2.703238000	-0.007319000	0.142492000
6	-0.294535000	-0.040263000	-0.769493000
6	0.311638000	-0.038426000	0.644949000
6	4.801627000	-1.797924000	0.327331000
6	3.901444000	-1.939879000	1.411315000
6	2.727629000	-2.569493000	0.927063000
6	2.899680000	-2.810871000	-0.456372000
6	4.180774000	-2.332951000	-0.828010000
6	2.631352000	2.601520000	0.751887000
6	2.805428000	2.754394000	-0.643916000
6	4.104890000	2.296997000	-0.975742000
6	4.735548000	1.864847000	0.216830000
6	3.823078000	2.048182000	1.283700000
6	-4.820588000	-1.832212000	0.255346000
6	-4.417011000	-1.835794000	-1.102183000
6	-3.140254000	-2.445386000	-1.177861000
6	-2.754890000	-2.817310000	0.132296000
6	-3.791712000	-2.437921000	1.018261000
6	-2.541241000	2.710033000	-0.532080000
6	-3.675729000	2.218457000	-1.225394000
6	-4.675814000	1.913884000	-0.271118000
6	-4.156011000	2.209160000	1.013954000
6	-2.839236000	2.704953000	0.850530000
1	-3.772597000	2.124049000	-2.301453000
1	-1.617695000	3.051226000	-0.983367000
1	-5.671447000	1.544081000	-0.486034000
1	-4.689331000	2.111979000	1.953624000
1	-2.181174000	3.039781000	1.643860000
1	-4.998963000	-1.467452000	-1.939581000
1	-5.764597000	-1.461068000	0.637892000
1	-3.809554000	-2.611981000	2.088748000
1	-1.834277000	-3.318627000	0.406814000
1	-0.247303000	-0.084727000	2.507552000
1	0.276545000	-0.099546000	-2.626808000
1	-2.570326000	-2.623251000	-2.082285000
1	2.080304000	3.170108000	-1.333920000
1	1.751093000	2.881339000	1.317320000
1	4.016832000	1.838119000	2.329524000
1	5.748463000	1.489805000	0.301788000

1	4.554265000	2.313597000	-1.963186000
1	5.800929000	-1.382337000	0.379019000
1	4.092853000	-1.651970000	2.438858000
1	1.860201000	-2.840063000	1.516419000
1	2.185180000	-3.295526000	-1.111524000
1	4.624735000	-2.400445000	-1.815744000
7	-0.619017000	-0.088673000	1.558780000
7	0.643594000	-0.099742000	-1.676171000

6Ce_2 (spin multiplicity 3)
Total energy including ZPVE: -1910.8686 a. u.
Total free energy including ZPVE: -1910.936 a. u.

$N_{Img} = 0$

58	2.558316000	-0.055619000	-0.083027000
58	-2.559891000	-0.056298000	0.094537000
6	0.016453000	-0.638468000	-0.657493000
6	-0.015319000	-0.655083000	0.648487000
6	5.085699000	-1.186685000	-0.384531000
6	4.532022000	-1.827716000	0.750141000
6	3.479363000	-2.668667000	0.307718000
6	3.380719000	-2.543137000	-1.097451000
6	4.369796000	-1.623722000	-1.526065000
6	1.846995000	2.427009000	0.965723000
6	2.512720000	2.728694000	-0.244706000
6	3.881491000	2.395759000	-0.086817000
6	4.063444000	1.902232000	1.228546000
6	2.805517000	1.913964000	1.876814000
6	-5.075930000	-1.206370000	0.354514000
6	-4.503615000	-1.847136000	-0.770673000
6	-3.448668000	-2.676268000	-0.312794000
6	-3.367590000	-2.544999000	1.093097000
6	-4.369816000	-1.632573000	1.506740000
6	-1.861627000	2.438036000	-0.960606000
6	-2.811423000	1.920180000	-1.877596000
6	-4.071940000	1.895240000	-1.235764000
6	-3.900491000	2.384231000	0.082829000
6	-2.534870000	2.729421000	0.247925000
1	-2.610297000	1.628848000	-2.902721000
1	-0.807311000	2.588017000	-1.159536000
1	-5.007532000	1.574031000	-1.678231000
1	-4.685558000	2.518410000	0.818945000
1	-2.089702000	3.155586000	1.139836000
1	-4.837016000	-1.746999000	-1.797670000
1	-5.918743000	-0.525570000	0.339285000
1	-4.585280000	-1.342488000	2.529414000
1	-2.673295000	-3.067452000	1.740090000
1	-2.827419000	-3.317458000	-0.927764000
1	2.059488000	3.151077000	-1.134220000
1	0.792433000	2.568049000	1.169725000
1	2.612219000	1.618283000	2.902235000

1	5.003988000	1.587445000	1.665090000
1	4.661364000	2.536487000	-0.827173000
1	5.923250000	-0.499283000	-0.382291000
1	4.878789000	-1.723007000	1.772261000
1	2.872865000	-3.315096000	0.931905000
1	2.683350000	-3.073582000	-1.734738000
1	4.569198000	-1.334577000	-2.552258000
7	0.784373000	-0.314801000	-1.691273000
7	-0.784833000	-0.356131000	1.689625000
1	0.652782000	-0.918336000	-2.498389000
1	-0.650590000	-0.978318000	2.481967000

2Ca

Total energy including ZPVE: -2276.5380 a. u.
Total free energy including ZPVE: -2276.6095 a. u.

$N_{Img} = 0$

20	1.915366000	0.020651000	0.015782000
7	3.680453000	1.624864000	0.080992000
7	3.723746000	-1.536343000	0.054031000
6	5.977488000	2.514010000	-0.043218000
1	5.766889000	3.198157000	-0.873259000
1	7.002869000	2.158480000	-0.148175000
1	5.917194000	3.107630000	0.876507000
6	4.982980000	1.360855000	-0.015727000
6	5.562211000	0.071212000	-0.092241000
1	6.642015000	0.086772000	-0.176904000
6	5.018542000	-1.234928000	-0.038424000
6	6.044445000	-2.359516000	-0.086837000
1	6.001657000	-2.971041000	0.822110000
1	7.059499000	-1.973900000	-0.185911000
1	5.852176000	-3.034367000	-0.928878000
6	0.029797000	-0.010155000	1.757470000
6	-0.787278000	-0.023359000	2.682776000
20	-1.915366000	-0.020651000	-0.015782000
7	-3.680453000	-1.624864000	-0.080992000
7	-3.723746000	1.536343000	-0.054031000
6	-5.977488000	-2.514010000	0.043218000
1	-5.766889000	-3.198157000	0.873259000
1	-7.002869000	-2.158480000	0.148175000
1	-5.917194000	-3.107630000	-0.876507000
6	-4.982980000	-1.360855000	0.015727000
6	-5.562211000	-0.071212000	0.092241000
1	-6.642015000	-0.086772000	0.176904000
6	-5.018542000	1.234928000	0.038424000
6	-6.044445000	2.359516000	0.086837000
1	-6.001657000	2.971041000	-0.822110000
1	-7.059499000	1.973900000	0.185911000
1	-5.852176000	3.034367000	0.928878000
6	-0.029797000	0.010155000	-1.757470000
6	0.787278000	0.023359000	-2.682776000

1	1.435840000	0.034572000	-3.534492000
1	-1.435840000	-0.034572000	3.534492000
6	-3.268629000	-3.023214000	-0.191104000
6	-3.351051000	2.947371000	-0.139223000
6	3.268629000	3.023214000	0.191104000
6	3.351051000	-2.947371000	0.139223000
1	-2.175546000	-3.076749000	-0.283495000
1	-3.537961000	-3.630777000	0.685928000
1	-3.678384000	-3.531157000	-1.076573000
1	-2.259671000	3.033211000	-0.227322000
1	-3.772752000	3.458546000	-1.017224000
1	-3.639655000	3.532179000	0.747039000
1	3.537961000	3.630777000	-0.685928000
1	2.175546000	3.076749000	0.283495000
1	3.678384000	3.531157000	1.076573000
1	3.772752000	-3.458546000	1.017224000
1	2.259671000	-3.033211000	0.227322000
1	3.639655000	-3.532179000	-0.747039000

2Ca (θ = 100°)

Total energy including ZPVE: -2276.5374 a. u.

Total free energy including ZPVE: -2276.6098 a. u.

$N_{Img} = 0$

20	1.883107000	0.000787000	0.016585000
7	3.667124000	1.584250000	0.081778000
7	3.669970000	-1.579306000	0.085955000
6	5.978362000	2.441270000	0.001607000
1	5.798469000	3.115745000	-0.843457000
1	7.001143000	2.070608000	-0.071856000
1	5.902736000	3.049293000	0.910737000
6	4.967955000	1.301766000	0.020105000
6	5.531917000	0.004005000	-0.025845000
1	6.613644000	0.004910000	-0.082462000
6	4.970306000	-1.294632000	0.023694000
6	5.982780000	-2.432349000	0.008608000
1	5.907918000	-3.038063000	0.919339000
1	7.004915000	-2.060036000	-0.065471000
1	5.804444000	-3.109428000	-0.834707000
6	0.002067000	0.002079000	1.768230000
6	-0.677415000	0.003432000	2.797401000
20	-1.883107000	-0.000787000	-0.016585000
7	-3.667124000	-1.584250000	-0.081778000
7	-3.669970000	1.579306000	-0.085955000
6	-5.978362000	-2.441270000	-0.001607000
1	-5.798469000	-3.115745000	0.843457000
1	-7.001143000	-2.070608000	0.071856000
1	-5.902736000	-3.049293000	-0.910737000
6	-4.967955000	-1.301766000	-0.020105000
6	-5.531917000	-0.004005000	0.025845000
1	-6.613644000	-0.004910000	0.082462000

6	-4.970306000	1.294632000	-0.023694000
6	-5.982780000	2.432349000	-0.008608000
1	-5.907918000	3.038063000	-0.919339000
1	-7.004915000	2.060036000	0.065471000
1	-5.804444000	3.109428000	0.834707000
6	-0.002067000	-0.002079000	-1.768230000
6	0.677415000	-0.003432000	-2.797401000
1	1.225748000	-0.004616000	-3.716407000
1	-1.225748000	0.004616000	3.716407000
6	-3.272193000	-2.989709000	-0.158443000
6	-3.277575000	2.985251000	-0.166480000
6	3.272193000	2.989709000	0.158443000
6	3.277575000	-2.985251000	0.166480000
1	-2.177990000	-3.059795000	-0.221774000
1	-3.572072000	-3.578541000	0.721362000
1	-3.666588000	-3.506876000	-1.045547000
1	-2.183464000	3.057151000	-0.229420000
1	-3.672420000	3.499124000	-1.055303000
1	-3.578998000	3.576095000	0.711444000
1	3.572072000	3.578541000	-0.721362000
1	2.177990000	3.059795000	0.221774000
1	3.666588000	3.506876000	1.045547000
1	3.672420000	-3.499124000	1.055303000
1	2.183464000	-3.057151000	0.229420000
1	3.578998000	-3.576095000	-0.711444000

2Ca ($\theta = 120^o$)
Total energy including ZPVE: -2276.5345 a. u.
Total free energy including ZPVE: -2276.605 a. u.

N_{Img} = 2 (-69.9, -57.1)

20	1.849107000	0.000284000	0.027846000
7	3.631776000	1.585098000	0.062803000
7	3.635175000	-1.580596000	0.067068000
6	5.942615000	2.441379000	-0.030749000
1	5.763090000	3.106281000	-0.883459000
1	6.965477000	2.070111000	-0.099782000
1	5.866332000	3.059495000	0.871477000
6	4.932365000	1.301970000	-0.001001000
6	5.496434000	0.004099000	-0.041679000
1	6.578122000	0.005195000	-0.098678000
6	4.935180000	-1.294848000	0.002735000
6	5.947878000	-2.432163000	-0.023441000
1	5.872488000	-3.047973000	0.880434000
1	6.969975000	-2.058894000	-0.092997000
1	5.770211000	-3.099788000	-0.874416000
6	-0.024469000	0.003148000	1.789977000
6	-0.341067000	0.005689000	2.980431000
20	-1.849107000	-0.000284000	-0.027846000
7	-3.631776000	-1.585098000	-0.062803000
7	-3.635175000	1.580596000	-0.067068000

6	-5.942615000	-2.441379000	0.030749000
1	-5.763090000	-3.106281000	0.883459000
1	-6.965477000	-2.070111000	0.099782000
1	-5.866332000	-3.059495000	-0.871477000
6	-4.932365000	-1.301970000	0.001001000
6	-5.496434000	-0.004099000	0.041679000
1	-6.578122000	-0.005195000	0.098678000
6	-4.935180000	1.294848000	-0.002735000
6	-5.947878000	2.432163000	0.023441000
1	-5.872488000	3.047973000	-0.880434000
1	-6.969975000	2.058894000	0.092997000
1	-5.770211000	3.099788000	0.874416000
6	0.024469000	-0.003148000	-1.789977000
6	0.341067000	-0.005689000	-2.980431000
1	0.605386000	-0.007864000	-4.016953000
1	-0.605386000	0.007864000	4.016953000
6	-3.237014000	-2.991404000	-0.122233000
6	-3.243435000	2.987565000	-0.130462000
6	3.237014000	2.991404000	0.122233000
6	3.243435000	-2.987565000	0.130462000
1	-2.142907000	-3.062552000	-0.186133000
1	-3.535416000	-3.568483000	0.765752000
1	-3.632840000	-3.520070000	-1.001925000
1	-2.149427000	3.060909000	-0.193715000
1	-3.639712000	3.512703000	-1.012073000
1	-3.543761000	3.566712000	0.755521000
1	3.535416000	3.568483000	-0.765752000
1	2.142907000	3.062552000	0.186133000
1	3.632840000	3.520070000	1.001925000
1	3.639712000	-3.512703000	1.012073000
1	2.149427000	-3.060909000	0.193715000
1	3.543761000	-3.566712000	-0.755521000

2Ca (θ = 135.7°)
Total energy including ZPVE: -2276.5337 a. u.
Total free energy including ZPVE: -2276.6055 a. u.

N_{Img} = 2 (-88.6, -73.7)

20	-1.847765000	0.000006000	-0.001981000
7	-3.631735000	1.583753000	-0.004856000
7	-3.631734000	-1.583743000	-0.004839000
6	-5.945727000	2.436605000	-0.000630000
1	-5.815290000	3.080031000	0.877269000
1	-6.970225000	2.063386000	0.002858000
1	-5.820303000	3.077123000	-0.881386000
6	-4.933461000	1.298562000	-0.001675000
6	-5.497218000	0.000004000	0.000739000
1	-6.580385000	0.000004000	0.003656000
6	-4.933460000	-1.298553000	-0.001662000
6	-5.945725000	-2.436597000	-0.000605000
1	-5.820298000	-3.077126000	-0.881353000

1	-6.970223000	-2.063379000	0.002877000
1	-5.815289000	-3.080013000	0.877301000
6	0.001729000	0.000000000	-1.791129000
6	0.036709000	-0.000034000	-3.022352000
20	1.847773000	0.000006000	0.001981000
7	3.631742000	-1.583743000	0.004855000
7	3.631743000	1.583753000	0.004840000
6	5.945733000	-2.436597000	0.000630000
1	5.815297000	-3.080021000	-0.877270000
1	6.970231000	-2.063379000	-0.002855000
1	5.820306000	-3.077117000	0.881384000
6	4.933468000	-1.298553000	0.001676000
6	5.497226000	0.000004000	-0.000737000
1	6.580393000	0.000004000	-0.003653000
6	4.933469000	1.298562000	0.001663000
6	5.945735000	2.436605000	0.000609000
1	5.820308000	3.077133000	0.881356000
1	6.970233000	2.063386000	-0.002873000
1	5.815300000	3.080021000	-0.877298000
6	-0.001719000	0.000017000	1.791129000
6	-0.036699000	0.000002000	3.022351000
1	-0.066374000	-0.000081000	4.091575000
1	0.065537000	-0.000688000	-4.091598000
6	3.237369000	-2.991484000	0.008693000
6	3.237372000	2.991495000	0.008666000
6	-3.237364000	2.991495000	-0.008696000
6	-3.237361000	-2.991484000	-0.008665000
1	2.141581000	-3.065382000	0.011367000
1	3.583506000	-3.545642000	-0.876380000
1	3.587429000	-3.541783000	0.894622000
1	2.141584000	3.065394000	0.011340000
1	3.587433000	3.541801000	0.894591000
1	3.583509000	3.545645000	-0.876412000
1	-3.583501000	3.545653000	0.876377000
1	-2.141577000	3.065394000	-0.011373000
1	-3.587426000	3.541793000	-0.894626000
1	-3.587422000	-3.541791000	-0.894590000
1	-2.141573000	-3.065382000	-0.011340000
1	-3.583497000	-3.545635000	0.876413000

5Ca

Total energy including ZPVE: -2276.5011 a. u.
Total free energy including ZPVE: -2276.5687 a. u.

$N_{Img} = 0$

20	2.541048000	-0.067245000	-0.707148000
7	4.158394000	1.578288000	-0.126811000
7	4.355618000	-1.570869000	-0.372441000
6	6.301029000	2.512569000	0.657343000
1	6.415061000	3.218978000	-0.172995000
1	7.294989000	2.179314000	0.956638000

1	5.864969000	3.075054000	1.491021000
6	5.411148000	1.342040000	0.261748000
6	6.025200000	0.068883000	0.345059000
1	7.051990000	0.106539000	0.687824000
6	5.574965000	-1.241485000	0.055413000
6	6.611719000	-2.337279000	0.262246000
1	6.262759000	-3.078955000	0.989931000
1	7.559049000	-1.932364000	0.618945000
1	6.803757000	-2.878746000	-0.671283000
6	3.699278000	2.966777000	-0.166733000
6	4.076912000	-2.982689000	-0.636403000
6	0.076456000	-0.103148000	0.665646000
6	-0.378553000	-0.100854000	1.911996000
20	-2.541702000	-0.068629000	0.709140000
7	-4.357087000	-1.570756000	0.372243000
7	-4.157091000	1.578377000	0.127491000
6	-6.612994000	-2.335222000	-0.265456000
1	-6.806306000	-2.877091000	0.667572000
1	-7.559693000	-1.929434000	-0.622839000
1	-6.263871000	-3.076727000	-0.993244000
6	-5.575643000	-1.240291000	-0.057052000
6	-6.024481000	0.070494000	-0.346945000
1	-7.050827000	0.109028000	-0.690938000
6	-5.409531000	1.343167000	-0.262667000
6	-6.298034000	2.514440000	-0.659175000
1	-5.860510000	3.076746000	-1.492205000
1	-7.291869000	2.181983000	-0.959776000
1	-6.412583000	3.220787000	0.171145000
6	-4.079845000	-2.982860000	0.636227000
6	-0.077024000	-0.102395000	-0.663997000
6	0.377979000	-0.098540000	-1.910316000
1	-0.339589000	-0.096548000	-2.734336000
1	0.339081000	-0.099681000	2.735969000
6	-3.696919000	2.966500000	0.168188000
1	-3.046401000	-3.092757000	0.990502000
1	-4.723374000	-3.415889000	1.416097000
1	-4.175226000	-3.621122000	-0.254688000
1	-3.720862000	3.463713000	-0.812680000
1	-4.269824000	3.595349000	0.865509000
1	-2.653368000	2.996006000	0.507724000
1	4.172376000	-3.621130000	0.254379000
1	3.043109000	-3.091608000	-0.989924000
1	4.719474000	-3.416210000	-1.416792000
1	4.271673000	3.595227000	-0.864839000
1	2.655261000	2.997160000	-0.504773000
1	3.725012000	3.463933000	0.814126000

TS4 (M = Ca; R = H)
Total energy including ZPVE: -2276.4641 a. u.
Total free energy including ZPVE: -2276.4641 a. u.

N_{Img} = 1 (-469.2)

20	-2.449635000	0.000100000	0.277348000
7	-4.205707000	-1.582139000	-0.008529000
7	-4.205920000	1.582109000	-0.008503000
6	-6.460917000	-2.437570000	-0.521281000
1	-6.128559000	-3.107869000	-1.322289000
1	-7.453047000	-2.066709000	-0.779533000
1	-6.552707000	-3.050098000	0.383201000
6	-5.472637000	-1.298502000	-0.311607000
6	-6.017664000	-0.000136000	-0.458589000
1	-7.069837000	-0.000204000	-0.715723000
6	-5.472812000	1.298301000	-0.311584000
6	-6.461246000	2.437241000	-0.521224000
1	-6.553132000	3.049714000	0.383285000
1	-7.453321000	2.066255000	-0.779507000
1	-6.128966000	3.107623000	-1.322195000
6	-3.828633000	-2.989173000	0.128154000
6	-0.266173000	0.000252000	1.476027000
6	0.694678000	0.000247000	2.366805000
20	2.539056000	0.000096000	0.731473000
7	4.224624000	1.580822000	0.120866000
7	4.224491000	-1.580824000	0.121007000
6	6.317489000	2.437309000	-0.863117000
1	6.606256000	3.045344000	0.002297000
1	7.228583000	2.066689000	-1.333711000
1	5.819476000	3.112197000	-1.568872000
6	5.395721000	1.298076000	-0.447973000
6	5.895421000	-0.000108000	-0.712042000
1	6.867942000	-0.000171000	-1.189172000
6	5.395615000	-1.298227000	-0.447851000
6	6.317293000	-2.437574000	-0.862884000
1	5.819239000	-3.112470000	-1.568602000
1	7.228432000	-2.067070000	-1.333482000
1	6.605982000	-3.045569000	0.002583000
6	0.209850000	0.000157000	-0.362474000
6	-0.367310000	0.000120000	-1.467805000
6	3.888528000	2.986580000	0.342315000
6	3.888275000	-2.986533000	0.342578000
6	-3.829054000	2.989198000	0.128179000
1	2.907730000	-3.054932000	0.831555000
1	3.816472000	-3.571392000	-0.586806000
1	4.600265000	-3.508214000	0.999306000
1	2.907995000	3.055104000	0.831299000
1	4.600570000	3.508259000	0.998987000
1	3.816761000	3.571361000	-0.587120000
1	-4.384522000	-3.515249000	0.917943000
1	-3.955764000	-3.568143000	-0.798708000
1	-2.766343000	-3.058925000	0.396613000
1	-4.385045000	3.515198000	0.917949000
1	-2.766783000	3.059104000	0.396671000
1	-3.956241000	3.568142000	-0.798691000
1	0.350456000	0.000295000	3.403559000

1	-0.631274000	0.000097000	-2.504909000

2Ca (R = CH_2OMe)
Total energy including ZPVE: -2584.1126 a. u.
Total free energy including ZPVE: -2584.1898 a. u.

N_{Img} = 0

20	-1.935040000	0.108354000	0.842849000
8	-1.907556000	1.043861000	3.176249000
7	-3.552016000	-1.534168000	1.548635000
7	-3.935323000	1.377587000	0.394153000
6	-5.640236000	-2.318132000	2.601505000
1	-5.818915000	-3.162993000	1.925842000
1	-6.609994000	-1.928155000	2.913075000
1	-5.133653000	-2.724775000	3.484393000
6	-4.795536000	-1.248611000	1.918688000
6	-5.453617000	-0.005927000	1.720577000
1	-6.459761000	0.021018000	2.122459000
6	-5.112219000	1.147217000	0.965402000
6	-6.234685000	2.167196000	0.812528000
1	-6.535346000	2.259941000	-0.237807000
1	-5.916401000	3.164814000	1.136502000
1	-7.116814000	1.885774000	1.388939000
6	0.827879000	0.587895000	1.357861000
6	0.272072000	0.941039000	2.403894000
6	-0.542713000	1.313586000	3.557421000
1	-0.289545000	0.726126000	4.453199000
1	-0.437041000	2.378563000	3.814922000
20	1.935040000	-0.108354000	-0.842849000
8	1.907556000	-1.043861000	-3.176249000
7	3.552016000	1.534168000	-1.548635000
7	3.935323000	-1.377587000	-0.394153000
6	5.640236000	2.318132000	-2.601505000
1	5.818915000	3.162993000	-1.925842000
1	6.609994000	1.928155000	-2.913075000
1	5.133653000	2.724775000	-3.484393000
6	4.795536000	1.248611000	-1.918688000
6	5.453617000	0.005927000	-1.720577000
1	6.459761000	-0.021018000	-2.122459000
6	5.112219000	-1.147217000	-0.965402000
6	6.234685000	-2.167196000	-0.812528000
1	6.535346000	-2.259941000	0.237807000
1	5.916401000	-3.164814000	-1.136502000
1	7.116814000	-1.885774000	-1.388939000
6	-0.827879000	-0.587895000	-1.357861000
6	-0.272072000	-0.941039000	-2.403894000
6	0.542713000	-1.313586000	-3.557421000
1	0.289545000	-0.726126000	-4.453199000
1	0.437041000	-2.378563000	-3.814922000
6	-2.877834000	1.332602000	4.178890000
6	3.073854000	2.901755000	-1.733685000

6	3.792894000	-2.569593000	0.437452000
6	2.877834000	-1.332602000	-4.178890000
6	-3.073854000	-2.901755000	1.733685000
6	-3.792894000	2.569593000	-0.437452000
1	3.849553000	-1.070636000	-3.756282000
1	2.859475000	-2.398339000	-4.443011000
1	2.692370000	-0.736689000	-5.082601000
1	-2.859475000	2.398339000	4.443011000
1	-3.849553000	1.070636000	3.756282000
1	-2.692370000	0.736689000	5.082601000
1	-2.789389000	2.584117000	-0.881467000
1	-4.502095000	2.604015000	-1.277732000
1	-3.908178000	3.512533000	0.120200000
1	-2.056552000	-2.988481000	1.332164000
1	-3.027147000	-3.213405000	2.789438000
1	-3.679750000	-3.651585000	1.203565000
1	4.502095000	-2.604015000	1.277732000
1	2.789389000	-2.584117000	0.881467000
1	3.908178000	-3.512533000	-0.120200000
1	3.027147000	3.213405000	-2.789438000
1	2.056552000	2.988481000	-1.332164000
1	3.679750000	3.651585000	-1.203565000

5Ca (R = CH_2OMe)
Total energy including ZPVE: -2584.0912 a. u.
Total free energy including ZPVE: -2584.1689 a. u.

$N_{Img} = 0$

20	2.459761000	-0.277075000	-0.452926000
7	4.544773000	-1.455177000	-0.490414000
7	3.896823000	1.628969000	-0.622492000
6	6.941651000	-1.808994000	-0.027295000
1	6.765084000	-2.561814000	0.749426000
1	7.828372000	-1.236821000	0.247307000
1	7.166223000	-2.357124000	-0.949877000
6	5.726530000	-0.909313000	-0.213616000
6	5.985643000	0.479022000	-0.082459000
1	7.015063000	0.706128000	0.167904000
6	5.194413000	1.629821000	-0.328942000
6	5.944260000	2.953799000	-0.254644000
1	5.939510000	3.458550000	-1.227910000
1	6.983174000	2.812447000	0.044890000
1	5.472271000	3.640526000	0.457370000
6	-0.021036000	-0.871509000	-0.652005000
6	0.281561000	-0.598940000	-1.908863000
6	-0.881639000	-0.385380000	-2.819187000
1	-0.759748000	0.530117000	-3.417541000
1	-1.000881000	-1.219827000	-3.528426000
20	-2.460306000	-0.280560000	0.452096000
7	-3.894000000	1.627810000	0.624554000
7	-4.547258000	-1.455140000	0.489242000

6	-5.939065000	2.956583000	0.257883000
1	-5.465596000	3.643364000	-0.453095000
1	-6.978105000	2.817395000	-0.042227000
1	-5.933832000	3.460137000	1.231770000
6	-5.191526000	1.631228000	0.330885000
6	-5.984766000	0.482019000	0.083274000
1	-7.013779000	0.711160000	-0.166901000
6	-5.728113000	-0.906867000	0.213198000
6	-6.944896000	-1.804212000	0.026449000
1	-7.170008000	-2.352953000	0.948533000
1	-7.830735000	-1.230184000	-0.247123000
1	-6.770029000	-2.556496000	-0.751179000
6	0.021102000	-0.873119000	0.649821000
6	-0.281860000	-0.604056000	1.907348000
6	0.881077000	-0.390893000	2.818114000
1	1.001747000	-1.226972000	3.525184000
1	0.757753000	0.522862000	3.418826000
8	-2.147856000	-0.249866000	-2.075594000
8	2.147016000	-0.251435000	2.074761000
6	4.478718000	-2.904919000	-0.665705000
6	3.255965000	2.906427000	-0.926577000
6	-3.250941000	2.903795000	0.930150000
6	-4.483922000	-2.905126000	0.663518000
1	-3.697402000	3.422640000	1.791154000
1	-2.198624000	2.726983000	1.187301000
1	-3.256849000	3.612069000	0.087064000
1	-4.760098000	-3.468181000	-0.241314000
1	-3.456500000	-3.197690000	0.914804000
1	-5.120553000	-3.274246000	1.480948000
1	3.450937000	-3.195259000	-0.918072000
1	5.115349000	-3.274799000	-1.482785000
1	4.752950000	-3.469071000	0.239038000
1	2.203211000	2.731819000	-1.183482000
1	3.263476000	3.613881000	-0.082816000
1	3.702996000	3.425316000	-1.787263000
6	-3.270848000	-0.037124000	-2.927454000
6	3.269854000	-0.039869000	2.927122000
1	-4.156666000	0.074663000	-2.297157000
1	-3.141644000	0.873282000	-3.528938000
1	-3.416094000	-0.888496000	-3.606437000
1	3.415824000	-0.892826000	3.603954000
1	4.155583000	0.074167000	2.297101000
1	3.139896000	0.868911000	3.530900000

6Ca

20	-2.679843000	0.000139000	-0.083551000
7	-4.480534000	-1.579831000	0.002894000
7	-4.480789000	1.579930000	0.001134000
6	-6.792844000	-2.437377000	0.062444000
1	-6.681870000	-3.088811000	-0.812251000
1	-7.817802000	-2.065635000	0.079547000

1	-6.646111000	-3.070054000	0.945585000
6	-5.782306000	-1.297892000	0.030756000
6	-6.347740000	-0.000099000	0.036690000
1	-7.430774000	-0.000177000	0.058327000
6	-5.782516000	1.297769000	0.029537000
6	-6.793258000	2.437103000	0.060393000
1	-6.646255000	3.070818000	0.942737000
1	-7.818138000	2.065185000	0.078381000
1	-6.682812000	3.087558000	-0.815104000
6	-0.250524000	-0.000458000	0.728515000
20	2.679801000	-0.001404000	0.083017000
7	4.479450000	1.579861000	-0.001472000
7	4.481899000	-1.579824000	-0.002805000
6	6.791177000	2.439104000	-0.059207000
1	6.679370000	3.089578000	0.816097000
1	7.816406000	2.068106000	-0.076255000
1	6.644358000	3.072560000	-0.941770000
6	5.781434000	1.298871000	-0.029054000
6	6.347791000	0.001484000	-0.035972000
1	7.430835000	0.002337000	-0.057104000
6	5.783454000	-1.296772000	-0.030342000
6	6.794965000	-2.435396000	-0.061915000
1	6.648989000	-3.068084000	-0.945176000
1	7.819609000	-2.062774000	-0.078740000
1	6.684359000	-3.087051000	0.812663000
6	0.250477000	-0.001149000	-0.729043000
1	-0.416844000	-0.001618000	-2.544235000
1	0.416807000	-0.000454000	2.543702000
7	0.742932000	-0.000862000	1.578104000
7	-0.742974000	-0.001166000	-1.578640000
6	-4.083668000	2.986799000	0.007932000
6	-4.083135000	-2.986615000	0.011200000
6	4.081083000	2.986379000	-0.008564000
6	4.085740000	-2.986955000	-0.011300000
1	-2.987822000	3.057620000	-0.011388000
1	-4.448023000	3.549570000	-0.864664000
1	-4.414753000	3.531473000	0.904787000
1	-2.987272000	-3.057235000	-0.007629000
1	-4.414469000	-3.530466000	0.908460000
1	-4.447063000	-3.550306000	-0.860984000
1	4.412470000	3.531370000	-0.905114000
1	2.985164000	3.056228000	0.009812000
1	4.444211000	3.549437000	0.864366000
1	4.449940000	-3.550385000	0.860944000
1	2.989929000	-3.058544000	0.007275000
1	4.417746000	-3.530482000	-0.908507000

2Mn

Total energy (spin = 11): -1129.6495 a. u

Total energy (antiferromagnetic state): -1129.65296 a. u.

$N_{Img} = 0$

25	-1.631180000	0.000035000	-0.265242000
6	-4.337223000	1.280847000	0.012421000
7	-3.047801000	1.507317000	-0.235649000
7	-3.047693000	-1.507404000	-0.235492000
6	-4.912231000	-0.000104000	0.163033000
6	-0.029142000	0.000556000	1.587486000
6	-4.337100000	-1.281034000	0.012588000
6	-1.007436000	0.000819000	2.337845000
1	-5.974366000	-0.000138000	0.375539000
25	1.631177000	-0.000052000	0.265182000
7	3.047831000	-1.507305000	0.235707000
6	4.337263000	-1.280812000	-0.012300000
6	4.912244000	0.000145000	-0.162953000
6	4.337080000	1.281068000	-0.012571000
7	3.047658000	1.507416000	0.235454000
6	0.029075000	-0.000624000	-1.587617000
6	1.007499000	-0.000972000	-2.337808000
1	5.974382000	0.000197000	-0.375443000
1	-1.834639000	0.001165000	3.014237000
1	1.834729000	-0.001285000	-3.014167000
6	-2.589426000	2.881683000	-0.428723000
6	-2.589152000	-2.881715000	-0.428541000
6	2.589470000	-2.881678000	0.428758000
6	2.589077000	2.881723000	0.428445000
6	-5.289207000	2.458286000	0.134948000
6	-5.289002000	-2.458535000	0.135353000
6	5.288962000	2.458585000	-0.135337000
6	5.289261000	-2.458237000	-0.134844000
1	-1.525227000	2.870010000	-0.680386000
1	-3.111295000	3.390725000	-1.251025000
1	-2.707568000	3.498747000	0.473631000
1	-4.956280000	3.158443000	0.909433000
1	-5.336934000	3.023419000	-0.803203000
1	-6.299039000	2.128942000	0.382459000
1	-4.955942000	-3.158577000	0.909878000
1	-6.298816000	-2.129203000	0.382971000
1	-5.336833000	-3.023746000	-0.802741000
1	-2.707249000	-3.498797000	0.473804000
1	-3.110922000	-3.390796000	-1.250876000
1	-1.524943000	-2.869901000	-0.680165000
1	3.111284000	-3.390700000	1.251107000
1	1.525251000	-2.870025000	0.680337000
1	2.707697000	-3.498749000	-0.473580000
1	5.337080000	-3.023314000	0.803335000
1	4.956281000	-3.158447000	-0.909260000
1	6.299066000	-2.128888000	-0.382463000
1	6.298795000	2.129264000	-0.382891000
1	4.955925000	3.158585000	-0.909909000
1	5.336734000	3.023836000	0.802735000
1	3.110791000	3.390834000	1.250797000
1	2.707211000	3.498784000	-0.473909000

1 1.524855000 2.869892000 0.680009000

2Mn (symm)

Total energy (antiferromagnetic state): -1129.6392 a. u.

$N_{Img} = 0$

25	0.061089000	1.612159000	0.000000000
6	-0.021139000	4.318887000	1.282535000
7	0.082624000	3.010798000	1.516108000
7	0.082624000	3.010798000	-1.516108000
6	-0.085860000	4.906027000	0.000000000
6	-1.536444000	0.048026000	0.000000000
6	-0.021139000	4.318887000	-1.282535000
6	-2.770113000	0.086183000	0.000000000
1	-0.175201000	5.985439000	0.000000000
25	-0.061089000	-1.612159000	0.000000000
7	-0.082624000	-3.010798000	-1.516108000
6	0.021139000	-4.318887000	-1.282535000
6	0.085860000	-4.906027000	0.000000000
6	0.021139000	-4.318887000	1.282535000
7	-0.082624000	-3.010798000	1.516108000
6	1.536444000	-0.048026000	0.000000000
6	2.770113000	-0.086183000	0.000000000
1	0.175201000	-5.985439000	0.000000000
1	-3.838853000	0.122716000	0.000000000
1	3.838853000	-0.122716000	0.000000000
6	0.168578000	2.537089000	2.895842000
6	0.168578000	2.537089000	-2.895842000
6	-0.168578000	-2.537089000	-2.895842000
6	-0.168578000	-2.537089000	2.895842000
6	-0.068687000	5.279820000	2.458279000
6	-0.068687000	5.279820000	-2.458279000
6	0.068687000	-5.279820000	2.458279000
6	0.068687000	-5.279820000	-2.458279000
1	0.294928000	1.451036000	2.892740000
1	1.025823000	2.961519000	3.436948000
1	-0.737407000	2.760573000	3.477223000
1	-0.904483000	5.044004000	3.126614000
1	0.845941000	5.211941000	3.058604000
1	-0.179154000	6.312019000	2.124097000
1	-0.904483000	5.044004000	-3.126614000
1	-0.179154000	6.312019000	-2.124097000
1	0.845941000	5.211941000	-3.058604000
1	-0.737407000	2.760573000	-3.477223000
1	1.025823000	2.961519000	-3.436948000
1	0.294928000	1.451036000	-2.892740000
1	-1.025823000	-2.961519000	-3.436948000
1	-0.294928000	-1.451036000	-2.892740000
1	0.737407000	-2.760573000	-3.477223000
1	-0.845941000	-5.211941000	-3.058604000
1	0.904483000	-5.044004000	-3.126614000

1	0.179154000	-6.312019000	-2.124097000
1	0.179154000	-6.312019000	2.124097000
1	0.904483000	-5.044004000	3.126614000
1	-0.845941000	-5.211941000	3.058604000
1	-1.025823000	-2.961519000	3.436948000
1	0.737407000	-2.760573000	3.477223000
1	-0.294928000	-1.451036000	2.892740000

3W

Total energy including ZPVE: -936.0054 a. u.
Total free energy including ZPVE: -936.0567 a. u.

$N_{Img} = 0$

74	-1.562991000	0.249481000	0.025489000
7	-1.730919000	2.024621000	-0.118733000
8	-1.972947000	3.194707000	-0.233475000
6	-3.845488000	-0.297399000	0.453937000
1	-4.480778000	0.420103000	0.954822000
6	-2.738241000	-1.479575000	-1.190374000
1	-2.367320000	-1.794312000	-2.155507000
6	-3.104699000	-1.346974000	1.069827000
1	-3.057213000	-1.546206000	2.131178000
6	-3.612642000	-0.375372000	-0.955519000
1	-4.044902000	0.269033000	-1.708519000
6	-2.425754000	-2.082678000	0.058930000
1	-1.766681000	-2.925510000	0.214055000
6	-0.781592000	0.280883000	2.168602000
6	-0.223457000	0.065964000	-1.481952000
74	1.563045000	-0.249470000	-0.025510000
7	1.730998000	-2.024615000	0.118684000
8	1.972047000	-3.194864000	0.233841000
6	3.845547000	0.297405000	-0.453962000
1	4.480837000	-0.420096000	-0.954850000
6	2.738304000	1.479576000	1.190353000
1	2.367386000	1.794312000	2.155488000
6	3.104751000	1.346978000	-1.069848000
1	3.057260000	1.546212000	-2.131198000
6	3.612705000	0.375375000	0.955494000
1	4.044968000	-0.269032000	1.708491000
6	2.425802000	2.082675000	-0.058949000
1	1.766723000	2.925503000	-0.214070000
6	0.781645000	-0.280863000	-2.168623000
6	0.223511000	-0.065944000	1.481932000
1	-1.238140000	0.548195000	3.103150000
1	1.238194000	-0.548169000	-3.103173000

3W (Symm)

Total energy including ZPVE: -935.9181 a. u.
Total free energy including ZPVE: -935.9668 a. u.

$N_{Img} = 4$ (-541.8, -444.4, -32.8, -26.1)

74	-0.859121000	-1.319001000	0.000000000
7	-2.524593000	-0.649589000	0.000000000
8	-3.683845000	-0.334086000	0.000000000
6	-1.326198000	-3.532692000	0.715180000
1	-2.179112000	-3.729641000	1.350024000
6	0.000000000	-3.241578000	-1.150346000
1	0.325416000	-3.165463000	-2.178266000
6	0.000000000	-3.241578000	1.150346000
1	0.325416000	-3.165463000	2.178266000
6	-1.326198000	-3.532692000	-0.715180000
1	-2.179112000	-3.729641000	-1.350024000
6	0.826962000	-3.072899000	0.000000000
1	1.880416000	-2.830058000	0.000000000
6	0.000000000	0.000000000	2.712179000
6	0.000000000	0.000000000	-1.470083000
74	0.859121000	1.319001000	0.000000000
7	2.524593000	0.649589000	0.000000000
8	3.683845000	0.334086000	0.000000000
6	1.326198000	3.532692000	-0.715180000
1	2.179112000	3.729641000	-1.350024000
6	0.000000000	3.241578000	1.150346000
1	-0.325416000	3.165463000	2.178266000
6	0.000000000	3.241578000	-1.150346000
1	-0.325416000	3.165463000	-2.178266000
6	1.326198000	3.532692000	0.715180000
1	2.179112000	3.729641000	1.350024000
6	-0.826962000	3.072899000	0.000000000
1	-1.880416000	2.830058000	0.000000000
6	0.000000000	0.000000000	-2.712179000
6	0.000000000	0.000000000	1.470083000
1	0.000000000	0.000000000	3.781610000
1	0.000000000	0.000000000	-3.781610000

2Mo-Ti

Total energy including ZPVE: -1119.4252 a. u.
Total free energy including ZPVE: -1119.4808 a. u.

$N_{Img} = 0$

42	1.618729000	0.012647000	-0.022588000
22	-1.664002000	0.010782000	0.024777000
8	1.678475000	-3.199321000	0.112032000
8	4.274608000	-0.154779000	-1.826263000
8	3.540645000	0.075673000	2.509629000
6	-0.290803000	0.047054000	-1.501287000
6	0.662816000	0.039804000	-2.307940000
6	0.111206000	0.032629000	1.509884000
6	-0.781590000	-0.009371000	2.370527000
6	-1.529116000	-2.320273000	-0.755836000

1	-0.668238000	-2.651908000	-1.313532000
6	-1.684032000	-2.364924000	0.640960000
1	-0.947376000	-2.714693000	1.347558000
6	-2.944736000	-1.791839000	0.965370000
1	-3.361966000	-1.687400000	1.957639000
6	-3.583691000	-1.441238000	-0.250945000
1	-4.570859000	-1.014900000	-0.350714000
6	-2.695772000	-1.723354000	-1.312994000
1	-2.873123000	-1.542651000	-2.364044000
6	1.616446000	-2.046964000	0.046059000
6	3.315997000	-0.087542000	-1.185482000
6	2.849214000	0.047370000	1.583781000
8	1.863181000	3.216085000	-0.139215000
6	-2.004447000	2.142558000	-1.101273000
1	-1.485384000	2.349251000	-2.024372000
6	-1.538237000	2.441377000	0.202337000
1	-0.604472000	2.918338000	0.451025000
6	-2.521054000	2.014132000	1.130257000
1	-2.460069000	2.114783000	2.203467000
6	-3.581888000	1.430628000	0.407447000
1	-4.482978000	1.015819000	0.836096000
6	-3.256416000	1.493704000	-0.977891000
1	-3.863573000	1.128494000	-1.794482000
6	1.731040000	2.068607000	-0.100268000
1	1.218305000	0.042820000	-3.222027000
1	-1.383736000	-0.061752000	3.251275000

2Mo-Ti (symm)
Total energy including ZPVE: -1119.3971 a. u
Total free energy including ZPVE: -1119.4536 a. u.

N_{Img} = 2 (-228.7, -182.4)

42	-1.541002000	0.000051000	-0.005430000
22	1.562563000	0.000205000	0.001022000
8	-1.774076000	3.198545000	0.162628000
8	-3.819546000	0.117007000	-2.198561000
8	-3.706177000	-0.123229000	2.292305000
6	0.170243000	-0.017066000	-1.657184000
6	0.192027000	-0.022533000	-2.889427000
6	0.136292000	0.015443000	1.637477000
6	0.231658000	0.023239000	2.866804000
6	1.459022000	2.345241000	-0.658714000
1	0.597373000	2.706225000	-1.196555000
6	1.612554000	2.310524000	0.741817000
1	0.882370000	2.634088000	1.466617000
6	2.870014000	1.715174000	1.032769000
1	3.278024000	1.538733000	2.018716000
6	3.511028000	1.436849000	-0.202987000
1	4.501230000	1.027876000	-0.331892000
6	2.626394000	1.785656000	-1.246260000
1	2.806317000	1.662523000	-2.304674000

6	-1.644341000	2.049959000	0.095691000
6	-2.985415000	0.068519000	-1.393336000
6	-2.915881000	-0.072395000	1.443954000
8	-1.772010000	-3.197957000	-0.187155000
6	1.622860000	-2.304503000	-0.758335000
1	0.899603000	-2.625456000	-1.491132000
6	1.457581000	-2.347368000	0.640978000
1	0.592178000	-2.712878000	1.169616000
6	2.620395000	-1.791920000	1.241286000
1	2.792733000	-1.677019000	2.301857000
6	3.512506000	-1.434634000	0.207509000
1	4.501154000	-1.025290000	0.346974000
6	2.881599000	-1.705889000	-1.035209000
1	3.296455000	-1.521016000	-2.016775000
6	-1.642880000	-2.049661000	-0.114552000
1	0.181604000	-0.031071000	-3.958315000
1	0.297184000	0.033892000	3.933724000

2Ni-Ti

Total energy including ZPVE: -1228.8728 a. u.
Total free energy including ZPVE: -1228.9263 a. u.

$N_{Img} = 0$

28	1.175551000	-0.013507000	-0.239142000
22	-1.546255000	-0.000043000	0.020888000
15	3.341153000	-0.009095000	0.072163000
6	0.367175000	-0.004705000	1.416986000
6	-0.380562000	0.003326000	2.407087000
6	-0.254509000	-0.019489000	-1.550156000
6	0.832128000	-0.019183000	-2.212097000
6	-3.335362000	1.476059000	-0.572765000
6	-2.181029000	1.947656000	-1.237464000
6	-1.261093000	2.395375000	-0.245331000
6	-1.865873000	2.224991000	1.018886000
6	-3.135088000	1.631587000	0.828932000
6	-1.314351000	-2.386176000	0.225819000
6	-1.851973000	-2.156118000	-1.063062000
6	-3.130274000	-1.569063000	-0.905569000
6	-3.406293000	-1.484090000	0.487758000
6	-2.286832000	-1.986296000	1.183832000
1	-4.220350000	1.074442000	-1.045139000
1	-2.018032000	1.959341000	-2.304576000
1	-0.267256000	2.774326000	-0.430097000
1	-1.403097000	2.444424000	1.968686000
1	-3.835765000	1.364555000	1.608109000
1	-0.330947000	-2.774696000	0.443995000
1	-1.356385000	-2.350317000	-2.001386000
1	-3.785534000	-1.261061000	-1.708418000
1	-4.307886000	-1.087785000	0.933761000
1	-2.176089000	-2.042650000	2.256287000
6	3.975010000	-1.322314000	1.212624000

6	4.003917000	1.528285000	0.863571000
6	4.476971000	-0.197337000	-1.378072000
1	5.054129000	-1.233963000	1.379800000
1	3.449263000	-1.244782000	2.167627000
1	3.758547000	-2.306493000	0.787673000
1	3.804795000	2.385621000	0.214586000
1	3.484178000	1.693328000	1.810829000
1	5.081910000	1.460696000	1.046820000
1	5.530894000	-0.178695000	-1.079368000
1	4.263208000	-1.143537000	-1.882722000
1	4.290234000	0.613017000	-2.087996000
1	1.346287000	-0.027805000	-3.156250000
1	-0.888999000	0.022543000	3.345898000

Al_2Me_4
Total energy including ZPVE: -644.4121 a. u.
Total free energy including ZPVE: -644.4467 a. u.

N_{Img} = 5 (-43, -40, -40, -24.6, -24.6)
(planar structure was considered as starting point as the experimental structure with bulky ligand is planar)

13	-1.321432000	-0.000027000	-0.008163000
6	-2.381135000	1.675900000	0.000624000
6	-2.381302000	-1.675848000	0.000255000
1	-3.125341000	1.679536000	-0.807261000
1	-1.781036000	-2.585886000	-0.099738000
13	1.321421000	-0.000028000	0.008110000
6	2.381162000	1.675875000	-0.000602000
6	2.381283000	-1.675855000	-0.000239000
1	3.125006000	1.679656000	0.807617000
1	1.780958000	-2.585928000	0.099066000
1	3.125463000	-1.679230000	0.807671000
1	2.951796000	1.763521000	-0.936194000
1	1.780734000	2.585949000	0.098072000
1	2.951532000	-1.763873000	-0.936033000
1	-3.126048000	-1.678965000	-0.807129000
1	-1.780724000	2.585937000	-0.098485000
1	-2.951346000	1.763754000	0.936457000
1	-2.950886000	-1.764181000	0.936428000

HNC
Total energy including ZPVE: -93.3844a. u.
Total free energy including ZPVE: -93.4039 a. u.

N_{Img} = 0

6	0.000000000	0.000000000	-0.743703000
1	0.000000000	0.000000000	1.431677000
7	0.000000000	0.000000000	0.432935000

INT1

Total energy including ZPVE: -737.8231 a. u.
Total free energy including ZPVE: -737.8689 a. u.

N_{Img} =

13	0.957584000	0.649336000	0.004189000
6	1.730168000	1.365234000	-1.697380000
6	1.737250000	1.342525000	1.711872000
1	1.340962000	2.374417000	-1.884613000
1	1.498598000	0.731805000	2.590819000
13	-1.596683000	-0.002234000	0.005319000
6	-2.298131000	-1.870197000	0.007907000
6	-3.049838000	1.358527000	-0.007450000
1	-2.772328000	-2.091593000	0.975394000
1	-2.723980000	2.365492000	0.274084000
1	-3.880526000	1.077793000	0.653184000
1	-3.082838000	-2.003926000	-0.748966000
1	-1.543805000	-2.646883000	-0.161260000
1	-3.475555000	1.435006000	-1.019028000
1	1.346233000	2.347753000	1.916029000
1	1.485213000	0.768122000	-2.583883000
1	2.822776000	1.451992000	-1.650908000
1	2.829358000	1.433083000	1.661139000
6	1.673144000	-1.339421000	-0.011191000
7	1.944913000	-2.475906000	-0.020158000
1	2.094229000	-3.464061000	-0.027048000

INT2

Total energy including ZPVE: -737.8547 a. u.
Total free energy including ZPVE: -737.8981 a. u.

N_{Img} = 0

13	1.749704000	-0.000002000	-0.044676000
7	0.827312000	0.000009000	1.650632000
6	2.506631000	1.733292000	-0.600475000
6	2.506681000	-1.733295000	-0.600414000
1	3.556929000	1.828597000	-0.296860000
1	1.967444000	-2.586437000	-0.173701000
6	-0.141722000	-0.000048000	0.796871000
13	-1.916621000	-0.000012000	0.086202000
6	-2.693960000	1.739222000	-0.410377000
6	-2.694051000	-1.739184000	-0.410442000
1	-2.894509000	1.794795000	-1.487011000
1	-2.050332000	-2.584752000	-0.148293000
1	-2.894440000	-1.794766000	-1.487105000
1	-3.656738000	1.892417000	0.093600000
1	-2.050128000	2.584738000	-0.148343000
1	-3.656918000	-1.892282000	0.093391000
1	3.557017000	-1.828528000	-0.296910000

1	1.967310000	2.586447000	-0.173897000
1	2.486998000	1.849693000	-1.691252000
1	2.486928000	-1.849791000	-1.691178000
1	0.657701000	0.000067000	2.662318000

INT3

Total energy including ZPVE: -831.2443 a. u.
Total free energy including ZPVE: -831.2937 a. u.

N_{Img} = 0

13	-1.578943000	-0.363801000	-0.000273000
7	-0.610424000	-2.135537000	-0.003632000
6	-0.927577000	1.926828000	0.003063000
6	-2.492666000	-0.194760000	-1.748583000
6	-2.491955000	-0.200669000	1.748944000
1	-3.108514000	-1.080567000	-1.949337000
1	-1.792055000	-0.109542000	2.589267000
6	0.309848000	-1.232785000	-0.002113000
7	-0.459129000	2.998929000	0.003931000
13	2.051818000	-0.455286000	-0.000845000
6	2.803569000	0.134168000	-1.728050000
6	2.804683000	0.126842000	1.728361000
1	2.953271000	1.220623000	-1.758412000
1	2.172822000	-0.149190000	2.578800000
1	2.954269000	1.213173000	1.763305000
1	3.789451000	-0.317104000	-1.898942000
1	2.171002000	-0.138092000	-2.579181000
1	3.790761000	-0.325031000	1.896524000
1	-3.106413000	-1.087876000	1.947744000
1	-1.793047000	-0.102526000	-2.589019000
1	-3.161177000	0.674433000	-1.791835000
1	-3.161699000	0.667445000	1.794736000
1	-0.053028000	3.912331000	0.004590000
1	-0.351572000	-3.131441000	-0.005538000

TS5

Total energy including ZPVE: -737.8206 a.u.
Total free energy including ZPVE: -737.8656 a. u.

N_{Img} = 1 (-90.5)

13	-1.230758000	-0.000104000	-0.423831000
6	-2.121348000	1.728775000	-0.860466000
6	-2.121442000	-1.729159000	-0.859571000
1	-2.087719000	1.907394000	-1.942444000
1	-1.644705000	-2.592879000	-0.382424000
13	1.425613000	-0.000098000	-0.365111000
6	2.490266000	-1.677908000	-0.317423000
6	2.490297000	1.677709000	-0.318020000

1	1.897784000	-2.578190000	-0.123941000
1	1.897655000	2.578264000	-0.126319000
1	2.987276000	1.825276000	-1.287890000
1	2.985858000	-1.826632000	-1.287831000
1	3.291032000	-1.632575000	0.432018000
1	3.290025000	1.633121000	0.432584000
1	-2.087807000	-1.908354000	-1.941454000
1	-1.644543000	2.592714000	-0.383784000
1	-3.179026000	1.731215000	-0.570761000
1	-3.179125000	-1.731374000	-0.569883000
6	-0.936986000	0.000409000	1.604749000
7	-0.455624000	0.000678000	2.691218000
1	-0.675175000	0.000937000	3.674234000

TS6

Total energy including ZPVE: -831.2376 a. u.
Total free energy including ZPVE: -831.2845 a. u.

N_{Img} = 1 (-174.5)

13	-1.804437000	-0.000047000	-0.107496000
7	-0.810488000	-0.000460000	-1.887172000
6	-0.568902000	0.000594000	1.703126000
6	-2.721882000	1.741518000	0.065309000
6	-2.721741000	-1.741594000	0.066221000
1	-3.442318000	1.891146000	-0.748779000
1	-2.031112000	-2.593700000	0.036891000
6	0.102216000	-0.000230000	-0.981498000
7	0.510635000	0.000830000	2.227773000
13	1.976937000	-0.000145000	-0.429693000
6	2.855749000	1.729180000	-0.100254000
6	2.855487000	-1.729412000	-0.099243000
1	3.344492000	1.750261000	0.881789000
1	2.160063000	-2.574085000	-0.142185000
1	3.344740000	-1.749812000	0.882559000
1	3.642199000	1.918359000	-0.842744000
1	2.160567000	2.573997000	-0.144242000
1	3.641497000	-1.919410000	-0.841991000
1	-3.442395000	-1.891554000	-0.747613000
1	-2.031290000	2.593651000	0.035864000
1	-3.283807000	1.816351000	1.004956000
1	-3.283404000	-1.816112000	1.006049000
1	0.834997000	0.001159000	3.185099000
1	-0.563326000	-0.000691000	-2.888367000

6Al

Total energy including ZPVE: -831.3257 a. u
Total free energy including ZPVE: -831.3693 a. u.

N_{Img} = 0

13	-2.212398000	-0.000002000	0.019115000
7	-0.802422000	0.000044000	-1.471603000
6	-0.252046000	0.000028000	0.713708000
6	-3.169295000	1.721958000	0.134293000
6	-3.169087000	-1.722078000	0.134344000
1	-3.941894000	1.807385000	-0.640756000
1	-2.509595000	-2.591278000	0.027873000
6	0.252040000	0.000023000	-0.713718000
7	0.802417000	-0.000047000	1.471593000
13	2.212392000	-0.000001000	-0.019126000
6	3.169120000	1.722062000	-0.134240000
6	3.169274000	-1.721964000	-0.134376000
1	3.941495000	1.807677000	0.641013000
1	2.509819000	-2.591261000	-0.028471000
1	3.941866000	-1.807435000	0.640674000
1	3.684484000	1.826280000	-1.097914000
1	2.509529000	2.591283000	-0.028559000
1	3.684392000	-1.826173000	-1.098183000
1	-3.942058000	-1.807414000	-0.640343000
1	-2.509843000	2.591251000	0.028335000
1	-3.684407000	1.826219000	1.098098000
1	-3.683710000	-1.826609000	1.098381000
1	0.666704000	-0.000066000	2.480964000
1	-0.666707000	0.000029000	-2.480974000