

Electronic Supplementary Information

Mechanism of cationic ring-opening polymerisation of ϵ -caprolactone using metallocene/borate catalytic systems: a DFT and NCI study on chain initiation, propagation and termination

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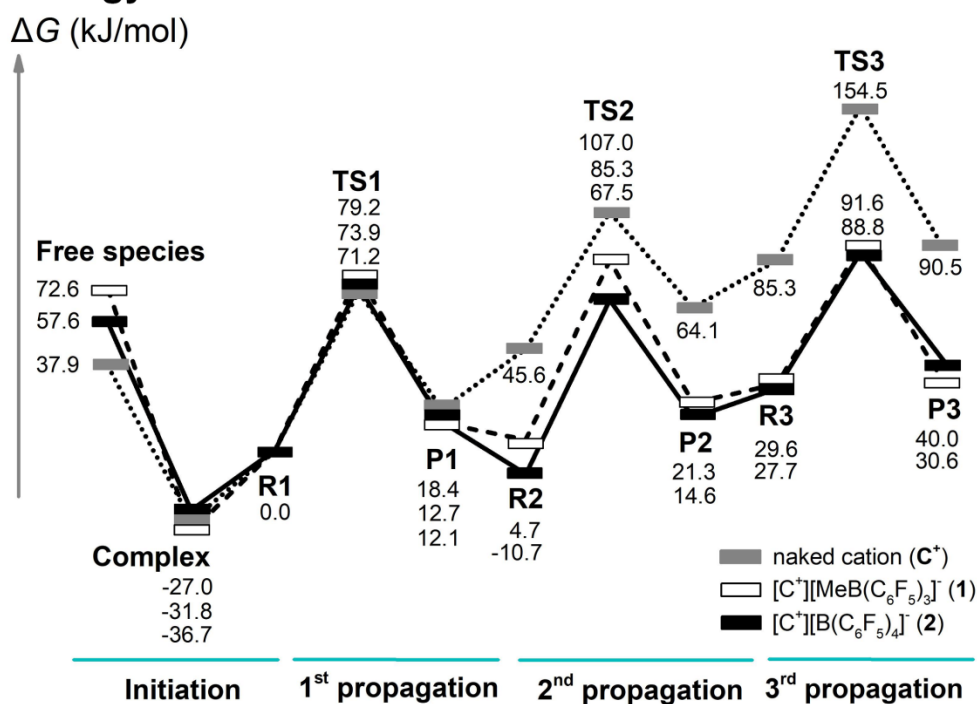
I. Energy profiles from different energy correction schemes

Table S1. Results of energy correction scheme II based on the suggested procedure of Gupta et al.¹ Corrections in thermodynamic energies (zero-point energy: ZPE, enthalpy: H, and Gibbs free energy, G) for the reactants of steps (**Complex**→**R1**, **P1**→**R2**, and **P2**→**R3**) calculated using B3LYP and B3LYP-D3(BJ) functional methods for systems **C⁺**, **1** and **2**.^a

Systems	B3LYP			B3LYP-D3(BJ)		
	ΔZPE	ΔH	ΔG	ΔZPE	ΔH	ΔG
Complex → R1						
2	-31.7	-24.2	-35.6 (-63.7) ^b	-78.3	-70.8	-82.2
1	-32.4	-29.1	-26.6 (-53.8) ^b	-63.5	-60.1	-57.7
C⁺	-20.7	-21.2	-12.4 (-41.0) ^b	-29.9	-30.5	-21.6
P1 → R2						
2	-34.8	-29.3	-34.1 (-58.6) ^b	-71.0	-65.5	-70.3
1	-34.1	-33.4	-18.8 (-56.5) ^b	-65.3	-64.6	-50.1
C⁺	-24.0	-22.6	-20.2 (-59.8) ^b	-36.0	-34.5	-32.2
P2 → R3						
2	-31.9	-28.6	-23.9 (-50.1) ^b	-57.0	-53.8	-49.0
1	-32.4	-26.7	-33.2 (-57.0) ^b	-65.2	-59.5	-66.0
C⁺	-24.5	-20.7	-26.6 (-48.3) ^b	-36.4	-32.5	-38.5

^a Values were obtained based on the toluene-optimised geometries at the B3LYP(SMD, toluene)/LANL2DZ+6-31G(d) and B3LYP-D3(BJ)(SMD, toluene)/LANL2DZ+6-31G(d) levels of theory. ^b Values in parenthesis were ΔG obtained from the gas-phase optimised geometries at the B3LYP/LANL2DZ+6-31G(d) level of theory

a) Energy correction I



b) Energy correction II

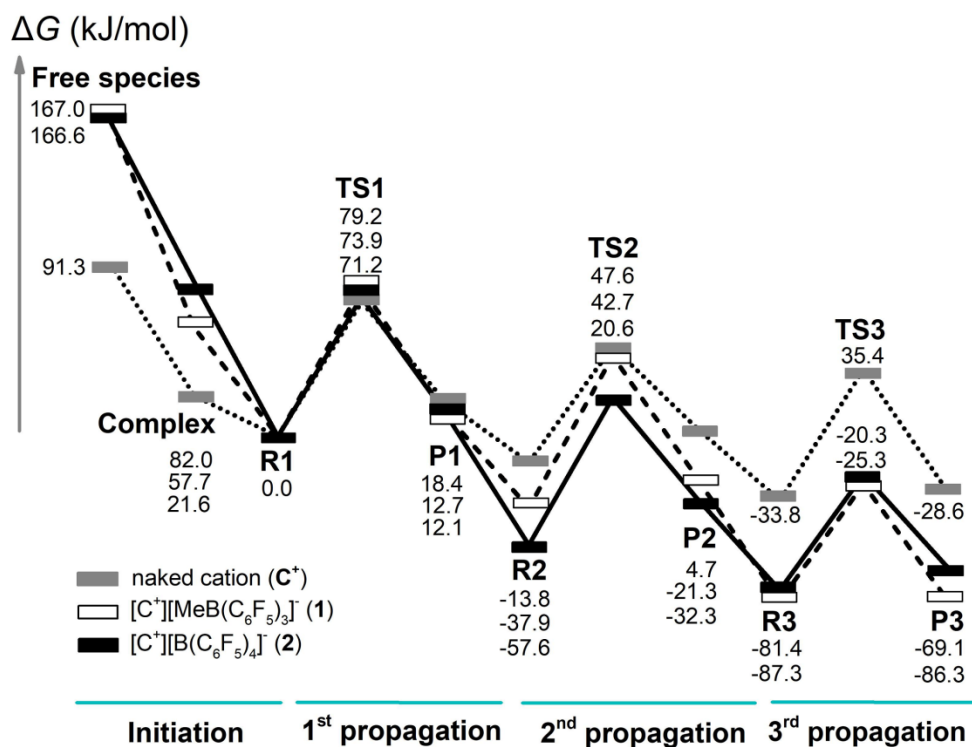


Figure S1. Gibbs free energy profiles resulting from the two energetic correction schemes I (a) and II (b). All energies were obtained at the B3LYP-D3(BJ)(SMD, toluene)/LANL2DZ, 6-31G(d) level of theory and were relative to the energy of **R1** (set to 0.0).

II. A benchmark for the chosen method in reaction barrier prediction

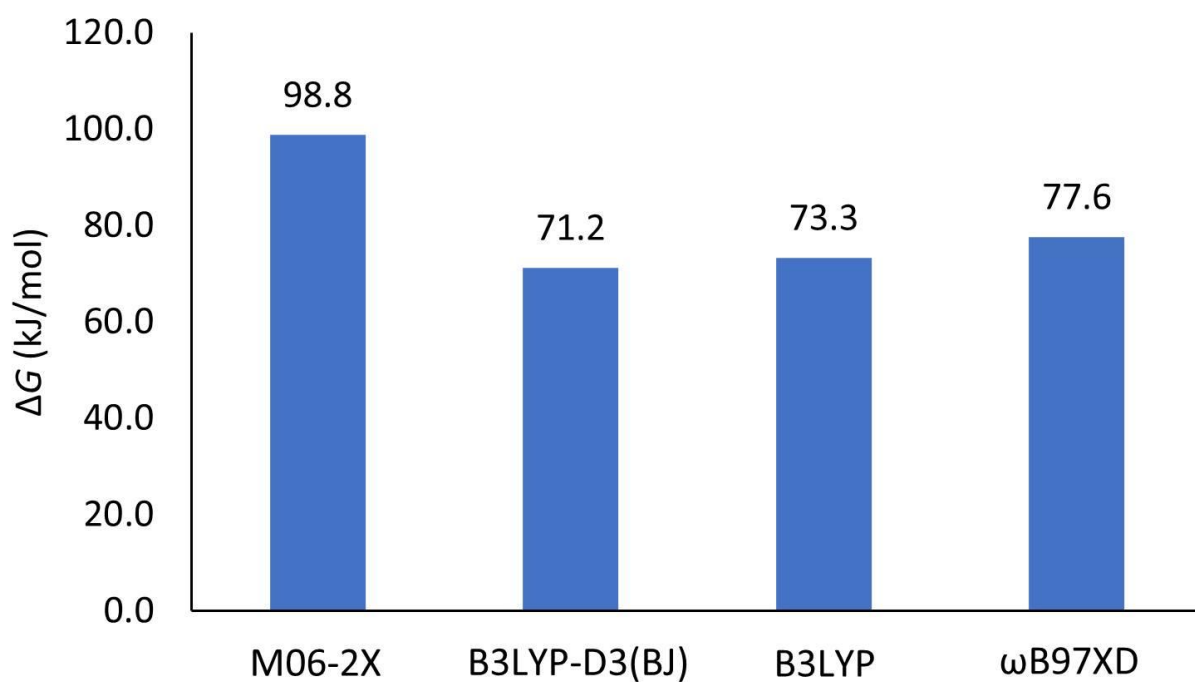


Figure S2. Bar chart showing the values of computed reaction barriers ($\Delta G^{\ddagger}_{Ea1}$) for the 1st propagation, as obtained in toluene using different DFT/LANL2DZ+6-31G(d) methods (DFT = M06-2X, B3LYP-D3(BJ), B3LYP, and ω B97XD) based on the naked model (C^+).

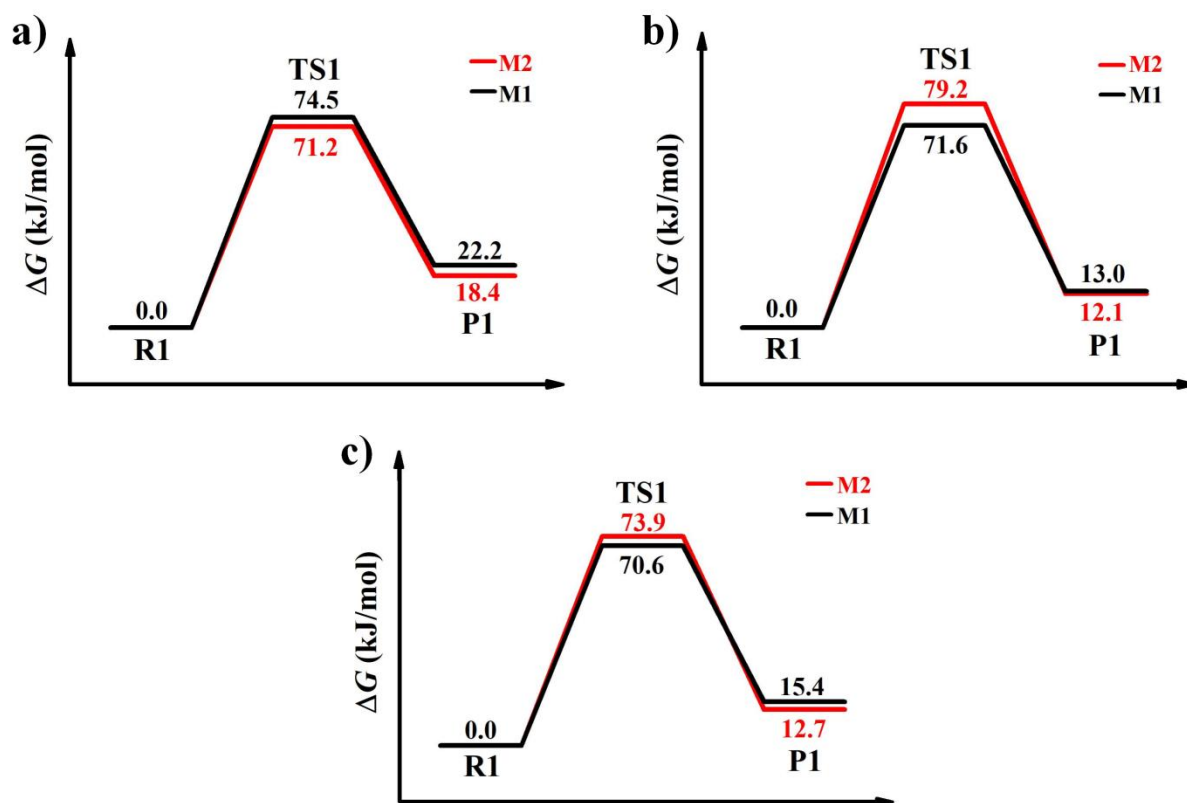


Figure S3. Comparison of solution-phase Gibbs energy profiles (kJ/mol) on the 1st propagation step (R1, TS1 and P1) for the C^+ (a), **1** (b), and **2** (c) systems, as obtained at the B3LYP-D3(BJ)(SMD, toluene)/LANL2DZ, 6-311++G(d,p) (labelled as **M1**) and the B3LYP-D3(BJ)(SMD, toluene)/LANL2DZ, 6-31G(d) levels (labelled as **M2**). Solution Gibbs energies are obtained using single-point energy calculation with SMD model (toluene, $\epsilon = 2.3741$).

III. Conformational analysis of CL monomer and counteranions

A conformational analysis was conducted to obtain the most stable configurations for the ion-pair model systems, as in a previous study of Sc complexes.² In particular, different arrangements of CL monomer around the Zr center were tested (Figure S4). The effect of the conformation of the counteranions ($[\text{MeB}(\text{C}_6\text{F}_5)_3]^-$ and $[\text{B}(\text{C}_6\text{F}_5)_4]^-$) were evaluated (Figures S5 and S6).

In Figure S4, two possible conformations, i.e., *front* and *side* conformers in Figure S4(a), could be envisioned after the insertion of CL monomer into the metal center of zirconocene catalyst (see also Scheme 2). Our relaxed potential energy scan shown in Figure S4(b) suggested that the **Complex** structure is more stable in their *side* conformations, similar to the case of trimethylene carbonate polymerization reported by our group.³ In particular, the *side* conformer is 3.5 kJ/mol more stable than its *front* conformer, and the energy barriers via $\text{TS}_{\text{side/front}}$ between the two conformers are calculated to be ~9, 12, and 22 kJ/mol for E, H, and G, respectively (Figure S4(c)). Thus, there is a significant entropic effect (~10 kJ/mol) for the interchange between the two conformations.

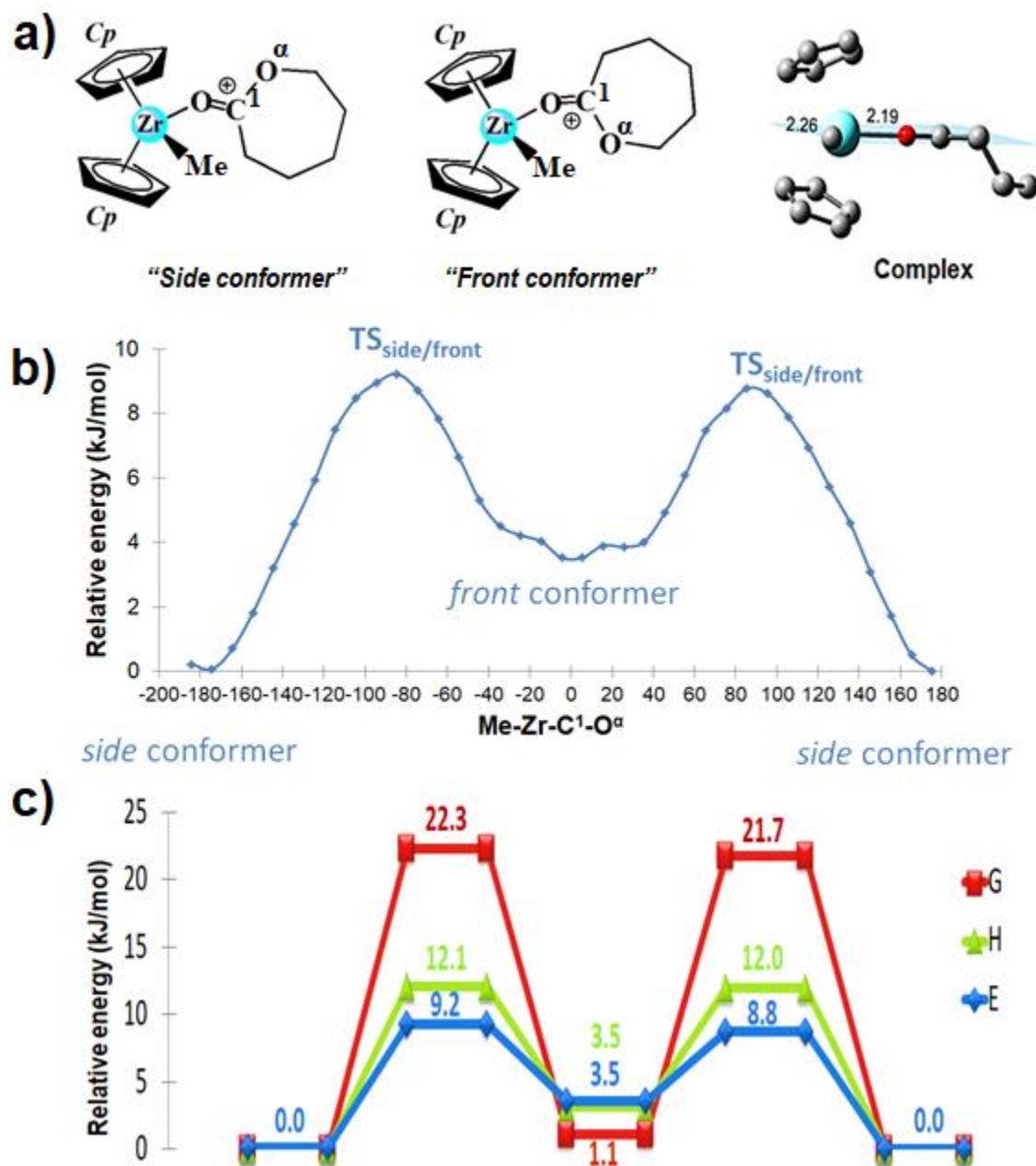


Figure S4. Relaxed potential energy scan as a function of the dihedral angle, Me-Zr-C¹-O^α, for **Complex** structure in different thermodynamic values in unit of kJ/mol (Gibbs free energy; G, enthalpy; H, and energy; E).

Zirconocene/cocatalyst models. To model the $[\text{Cp}_2\text{ZrMe}^+][\text{A}^-]$ system ($\text{A}^- = [\text{MeB}(\text{C}_6\text{F}_5)_3]^-$ and $[\text{B}(\text{C}_6\text{F}_5)_4]^-$), we first obtain the most stable geometry of the $[\text{Cp}_2\text{ZrMe-CL}]^+$ structure from the conformational analysis, i.e., the *side* conformer of CL coordination, as in our previous study on the CROP of trimethylene carbonate.³ Beginning with this *side* conformation (**Complex**, Scheme 3), we added the counteranion and placed it freely in various positions around the metal center of the catalyst and found that, after the geometry optimization without restraints (at B3LYP/LANL2DZ+6-31G(d) level), three different stable positions of the anion (see positions 1-3 in Figures S5-S6) were located. We then optimised the remaining species (**R1**, **TS1** and **P1**) following the positions 1-3. Free energies of the species (i.e., **Complex** \rightarrow **P1**) were generated using an energy correction scheme where the complex was treated in the vicinity of each other and all energies were relative to the energy of reactant **R1**. The results in Figures S5-S6 clearly indicate that, among different positions of cocatalyst, “position 1” where the anion locating close to the ring cleavage site yields the most preferred pathway, with relatively stable complexes (+12.1 and +12.7 kJ/mol) and the lowest Gibbs energy barriers (79.2 and 73.9 kJ/mol) in both **1** and **2** systems, respectively.

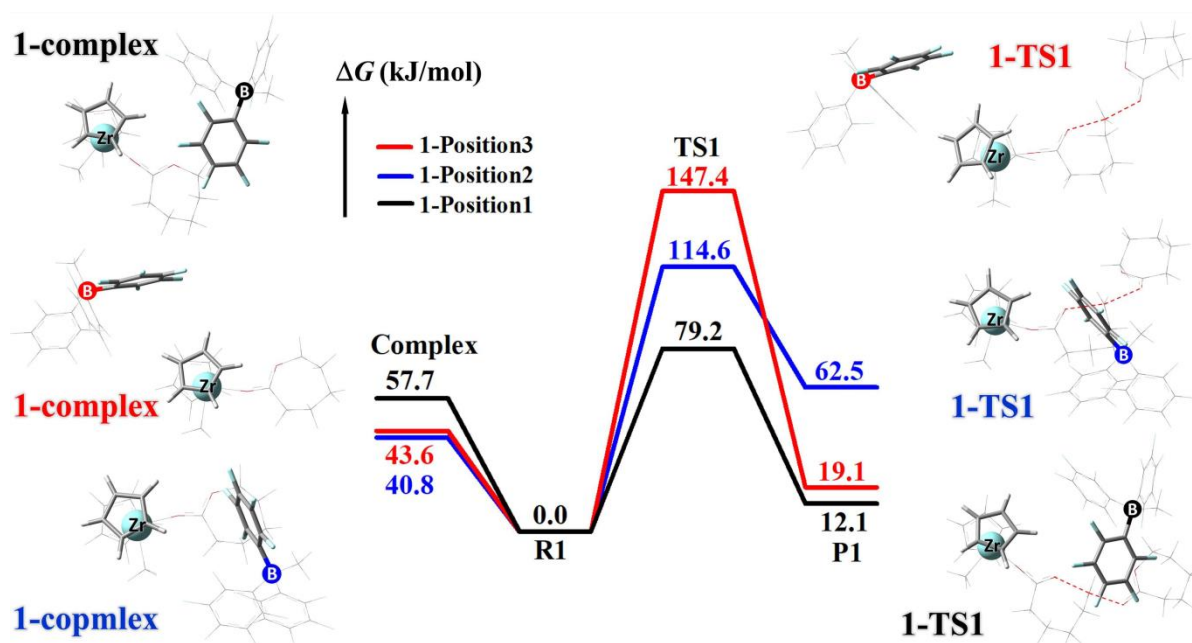


Figure S5. Relative Gibbs energies of the catalytic species (**Complex** \rightarrow **P1**) where the $[\text{MeB}(\text{C}_6\text{F}_5)_3]^-$ (**1**) counteranion was stably located in three different positions (1-3) around the catalytic Zr centre. Note that positions 1-2 corresponds to the terms “*side_up*” and “*side_down*” discussed in the main text, respectively. Since the relative barrier for position 3 is obviously high compared to the other conformations (positions 1 and 2), we thus discard this possibility and excluded it from the main text.

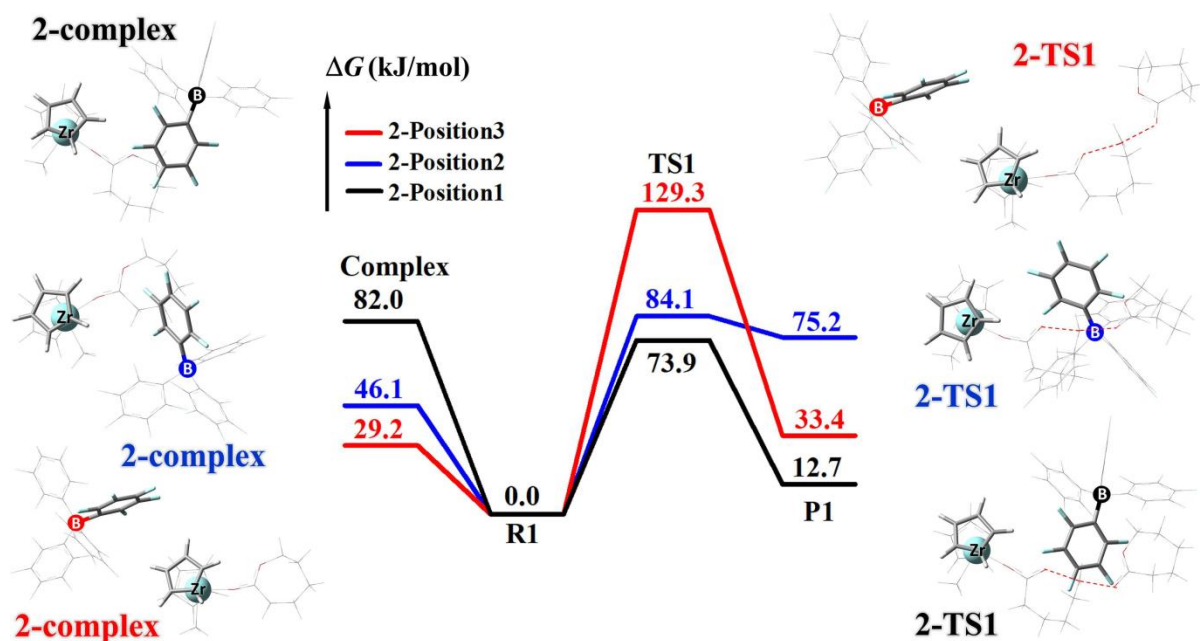
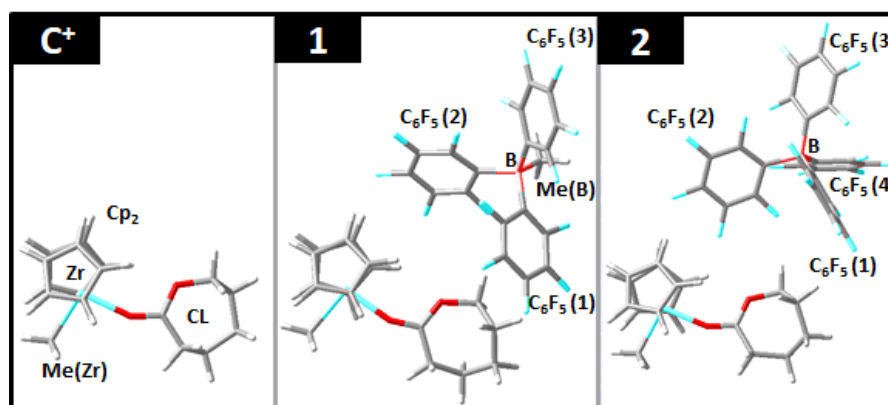


Figure S6. Relative Gibbs energies of the catalytic species (**Complex** \rightarrow **P1**) where the $[B(C_6F_5)_4]^-$ (**2**) counteranion was stably located in three different positions (1-3) around the catalytic Zr centre. Note that positions 1-2 corresponds to the terms “*side_up* and *side_down*” discussed in the main text, respectively. Since the relative barrier for position 3 is obviously high compared to the other conformations (positions 1 and 2), we thus discard this possibility and excluded it from the main text.

IV. Charge analysis of ligands, monomer (CL), functional groups in the Free species, Complex, R1 and TS1 structure

Table S2. Charge analysis (Hirshfeld, Mulliken, NBO; in unit of e) of ligands, monomer (CL), functional groups for the anion cocatalysts, $\text{MeB}(\text{C}_6\text{F}_5)_3^-$ and $\text{B}(\text{C}_6\text{F}_5)_4^-$ in isolated species.^a Figures below represent the **Complex** species, which are used to indicate the atomic definitions used for charge analysis.



Atom	$\text{MeB}(\text{C}_6\text{F}_5)_3^-$			Atom	$\text{B}(\text{C}_6\text{F}_5)_4^-$		
	Hirshfeld	Mulliken	NBO		Hirshfeld	Mulliken	NBO
B	0.032	0.400	0.394	B	0.039	0.407	0.382
C_6F_5	-0.281	-0.377	-0.378	C_6F_5	-0.260	-0.352	-0.346
C_6F_5	-0.288	-0.377	-0.384	C_6F_5	-0.260	-0.351	-0.345
C_6F_5	-0.278	-0.364	-0.376	C_6F_5	-0.260	-0.352	-0.346
Me(B)	-0.186	-0.282	-0.256	C_6F_5	-0.260	-0.352	-0.346

^a A total charge is -1 for each anion cocatalyst, as obtained with the gas-phase calculations at the B3LYP/LANL2DZ+6-31G(d) level of theory

Table S3. Charge analysis (Hirshfeld, Mulliken, NBO; in unit of e) of ligands, monomer (CL), functional groups in the intermediates (**Complex, R1, TS1**) for different catalytic systems [naked cation, C^+ , $[C^+][MeB(C_6F_5)_3]^-$ (**1**), and $[C^+][B(C_6F_5)_4]^-$ (**2**)]. Values were computed with the gas-phase calculations at the B3LYP/LANL2DZ+6-31G(d) level of theory

Atom/ Group	C^+ -Complex			Atom/ Group	1-Complex			Atom/ Group	2-Complex		
	Hirshfeld	Mulliken	NBO		Hirshfeld	Mulliken	NBO		Hirshfeld	Mulliken	NBO
Cp ₂	0.230	0.107	-0.252	Cp ₂	0.141	0.031	-0.283	Cp ₂	0.139	0.026	-0.291
Zr	0.509	0.800	1.293	Zr	0.508	0.803	1.305	Zr	0.507	0.803	1.307
Me(Zr)	-0.158	-0.173	-0.343	Me(Zr)	-0.185	-0.202	-0.368	Me(Zr)	-0.183	-0.197	-0.366
CL	0.417	0.266	0.302	CL	0.380	0.231	0.298	CL	0.385	0.226	0.296
				B	0.033	0.391	0.401	B	0.039	0.403	0.391
				C ₆ F ₅ (1)	-0.253	-0.354	-0.379	C ₆ F ₅ (1)	-0.241	-0.338	-0.344
				C ₆ F ₅ (2)	-0.201	-0.313	-0.365	C ₆ F ₅ (2)	-0.175	-0.281	-0.327
				C ₆ F ₅ (3)	-0.251	-0.328	-0.362	C ₆ F ₅ (3)	-0.230	-0.312	-0.328
				Me(B)	-0.174	-0.259	-0.247	C ₆ F ₅ (4)	-0.244	-0.330	-0.337

Atom/ Group	C^+ -R1			Atom/ Group	1-R1			Atom/ Group	2-R1		
	Hirshfeld	Mulliken	NBO		Hirshfeld	Mulliken	NBO		Hirshfeld	Mulliken	NBO
Cp ₂	0.207	0.079	-0.274	Cp ₂	0.129	0.013	-0.296	Cp ₂	0.126	0.008	-0.304
Zr	0.510	0.812	1.303	Zr	0.510	0.809	1.309	Zr	0.509	0.810	1.312
Me(Zr)	-0.161	-0.179	-0.347	Me(Zr)	-0.186	-0.204	-0.368	Me(Zr)	-0.184	-0.199	-0.367
CL-1	0.358	0.242	0.303	CL-1	0.308	0.204	0.294	CL-1	0.309	0.198	0.291
CL-2	0.085	0.045	0.016	CL-2	0.023	-0.007	-0.003	CL-2	-0.002	-0.024	-0.006
				B	0.032	0.395	0.402	B	0.039	0.403	0.391
				C ₆ F ₅ (1)	-0.247	-0.323	-0.359	C ₆ F ₅ (1)	-0.200	-0.305	-0.333
				C ₆ F ₅ (2)	-0.209	-0.315	-0.365	C ₆ F ₅ (2)	-0.167	-0.271	-0.321
				C ₆ F ₅ (3)	-0.186	-0.300	-0.359	C ₆ F ₅ (3)	-0.226	-0.308	-0.325
				Me(B)	-0.186	-0.204	-0.368	C ₆ F ₅ (4)	-0.208	-0.313	-0.338

Atom/ Group	C^+ -TS1			Atom/ Group	1-TS1			Atom/ Group	2-TS1		
	Hirshfeld	Mulliken	NBO		Hirshfeld	Mulliken	NBO		Hirshfeld	Mulliken	NBO
Cp ₂	0.116	-0.028	-0.352	Cp ₂	0.048	-0.084	-0.366	Cp ₂	0.050	-0.083	-0.368
Zr	0.509	0.835	1.328	Zr	0.508	0.826	1.327	Zr	0.508	0.829	1.331
Me(Zr)	-0.177	-0.197	-0.361	Me(Zr)	-0.200	-0.218	-0.379	Me(Zr)	-0.197	-0.215	-0.378
CL-1	0.188	0.135	0.132	CL-1	0.184	0.133	0.153	CL-1	0.185	0.126	0.151
CL-2	0.362	0.254	0.253	CL-2	0.256	0.174	0.208	CL-2	0.219	0.152	0.199
				B	0.032	0.401	0.402	B	0.039	0.405	0.391
				C ₆ F ₅ (1)	-0.215	-0.326	-0.369	C ₆ F ₅ (1)	-0.204	-0.311	-0.335
				C ₆ F ₅ (2)	-0.188	-0.297	-0.357	C ₆ F ₅ (2)	-0.168	-0.270	-0.323
				C ₆ F ₅ (3)	-0.246	-0.325	-0.359	C ₆ F ₅ (3)	-0.224	-0.307	-0.324
				Me(B)	-0.181	-0.284	-0.260	C ₆ F ₅ (4)	-0.212	-0.326	-0.344

V. Effect of metal: Hf vs Zr

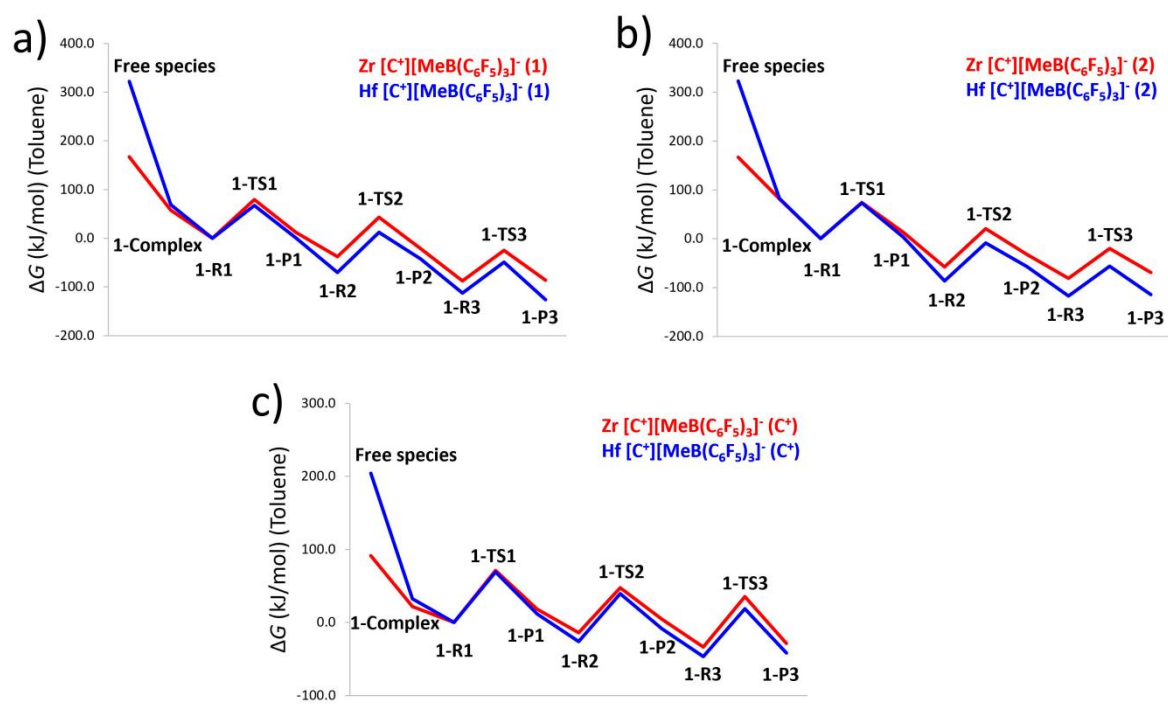


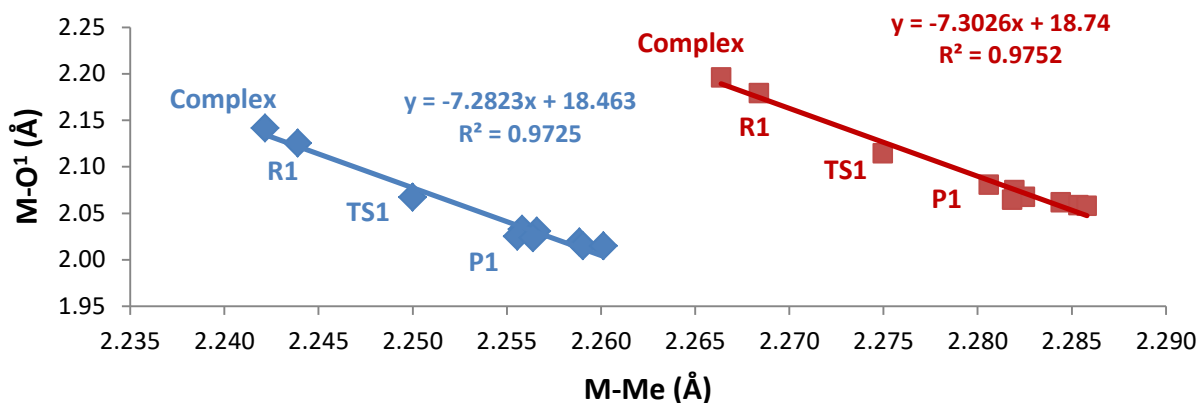
Figure S7. Gibbs free energy profiles in toluene for zirconocene and hafnocene catalyzed the chain initiation and propagation for the three different systems (C⁺, 1 and 2).

Table S4. Mulliken and Hirshfeld charges (q , in unit of e) on the central metals of catalyst (M = Zr, Hf) and cocatalyst (B) as well as important distances in Å (M-O, M-B, B-C $^{\alpha}$) for zirconocene and hafnocene systems. Values are taken from the gas-phase optimised geometries at the B3LYP/LANL2DZ+6-31G(d) level of theory.

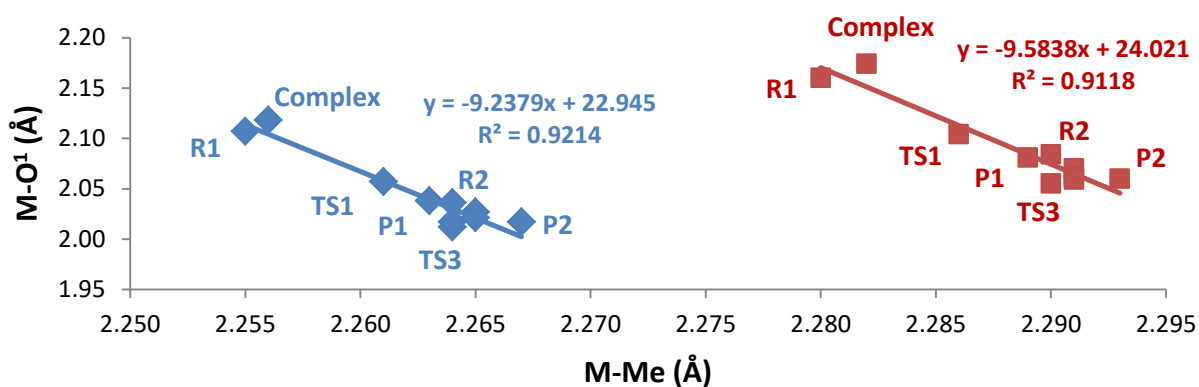
	Mulliken		Hirshfeld		Distances			
	$qM(\text{Zr/Hf})$	$qB(\text{Zr/Hf})$	$qM(\text{Zr/Hf})$	$qB(\text{Zr/Hf})$	Zr-Me/Hf-Me	Zr-O/Hf-O	Zr-B/Hf-B	Zr(B-C $^{\alpha}$)/Hf(B-C $^{\alpha}$)
	B(C₆F₅)₄ (2)							
Cation	0.824/0.805	n/a	0.659/0.623	n/a	2.242/2.210	n/a	n/a	n/a
Complex	0.792/0.771	0.398/0.397	0.507/0.457	0.038/0.038	2.278/2.253	2.175/2.121	7.345/7.365	5.836/5.833
R1	0.810/0.787	0.403/0.403	0.509/0.458	0.038/0.038	2.279/2.254	2.163/2.111	9.018/9.023	6.033/6.032
TS1	0.829/0.810	0.405/0.405	0.508/0.456	0.038/0.038	2.285/2.259	2.105/2.060	9.012/9.012	6.261/6.254
P1	0.826/0.810	0.395/0.395	0.506/0.455	0.039/0.039	2.288/2.262	2.081/2.037	9.273/9.273	5.999/6.003
R2	0.817/0.805	0.403/0.405	0.503/0.455	0.039/0.039	2.289/2.261	2.084/2.038	7.818/8.245	5.293/6.512
TS2	0.822/0.802	0.403/0.402	0.504/0.453	0.038/0.038	2.285/2.264	2.105/2.032	9.012/7.876	6.261/5.739
P2	0.838/0.818	0.399/0.398	0.506/0.455	0.038/0.038	2.290/2.264	2.059/2.016	8.710/8.710	5.408/5.895
R3	0.838/0.820	0.397/0.396	0.506/0.455	0.038/0.038	2.290/2.264	2.057/2.015	8.840/8.850	5.407/5.558
TS3	0.846/0.828	0.402/0.402	0.505/0.454	0.039/0.039	2.292/2.266	2.051/2.010	8.912/8.914	5.812/5.810
P3	0.838/0.825	0.394/0.394	0.509/0.458	0.040/0.040	2.291/2.264	2.060/2.017	9.332/9.347	5.744/5.747
	MeB(C₆F₅)₃ (1)							
Cation	0.824/0.805	n/a	0.659/0.623	n/a	2.242/2.210	n/a	n/a	n/a
Complex	0.785/0.768	0.384/0.383	0.508/0.458	0.032/0.033	2.282/2.256	2.174/2.118	7.371/7.376	5.712/5.710
R1	0.809/0.789	0.394/0.394	0.509/0.458	0.032/0.033	2.280/2.255	2.160/2.107	8.571/8.626	5.951/5.951
TS1	0.826/0.809	0.400/0.400	0.508/0.456	0.032/0.032	2.286/2.261	2.104/2.057	8.614/8.604	6.152/6.126
P1	0.823/0.808	0.402/0.402	0.506/0.455	0.032/0.033	2.289/2.263	2.081/2.038	9.056/9.053	5.708/5.709
R2	0.820/0.804	0.399/0.399	0.504/0.454	0.032/0.032	2.290/2.264	2.084/2.036	7.876/8.070	5.225/5.201
TS2	0.830/0.810	0.401/0.401	0.504/0.454	0.032/0.032	2.291/2.265	2.070/2.027	8.096/8.124	5.292/5.308
P2	0.832/0.811	0.395/0.395	0.503/0.452	0.032/0.033	2.293/2.267	2.060/2.017	8.376/8.381	5.314/5.317
R3	0.833/0.814	0.395/0.395	0.504/0.453	0.032/0.033	2.291/2.265	2.062/2.021	8.475/8.480	5.695/5.692
TS3	0.834/0.854	0.397/0.396	0.505/0.459	0.031/0.032	2.290/2.280	2.055/2.012	8.999/9.172	4.950/4.937
P3	0.835/0.818	0.388/0.387	0.505/0.455	0.030/0.031	2.291/2.264	2.059/2.017	8.956/8.955	5.909/5.914

n/a means the data is not available

a) system C⁺



b) system 1



c) system 2

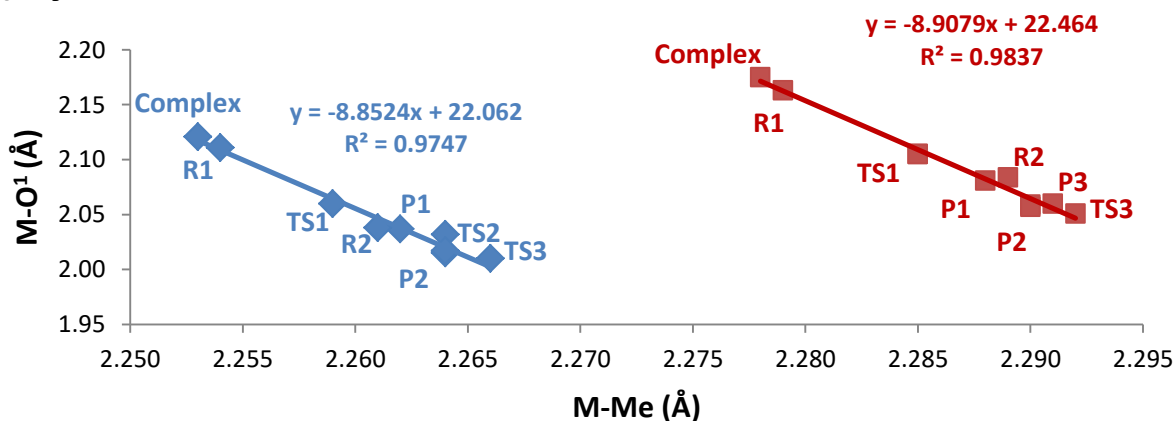


Figure S8. Correlations between the two bond lengths, metal to a carbonyl oxygen atom of CL monomer (M-O¹) and metal to Me group of catalyst (M-Me) where M = Hf (blue) and Zr (red) for the three catalytic systems (C⁺, 1 and 2).

VI. Effect of solvent on the HOMO-LUMO energies

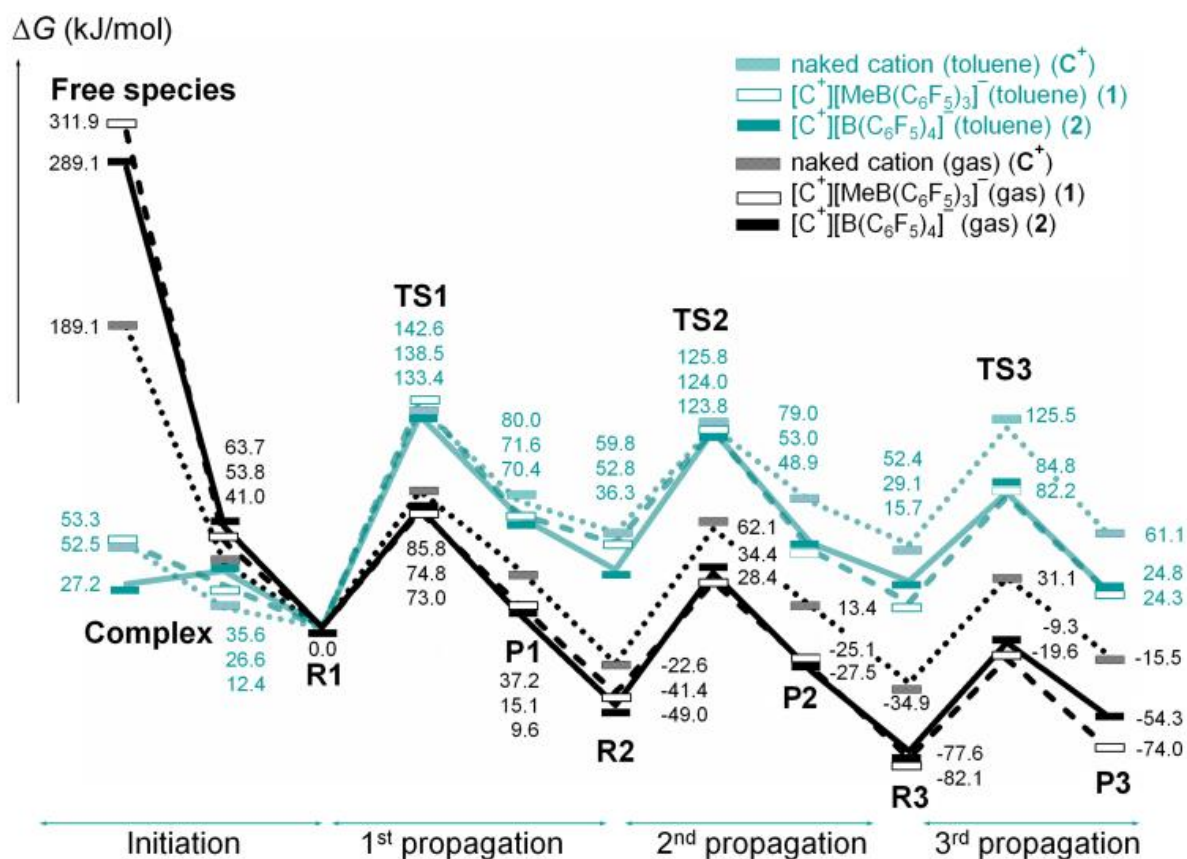


Figure S9. Calculated Gibbs free energy profiles in gas-phase (black) and toluene solution (cyan) for the chain initiation and propagation mechanism for the three catalytic systems (C^+ , **1**, and **2**). All energies were relative to the energy of **R1** (set to 0.0). Values of gas-phase energies were computed at the B3LYP/LANL2DZ+6-31G(d) level, while the solution energies at the B3LYP(SMD, toluene)/LANL2DZ+6-31G(d) level.

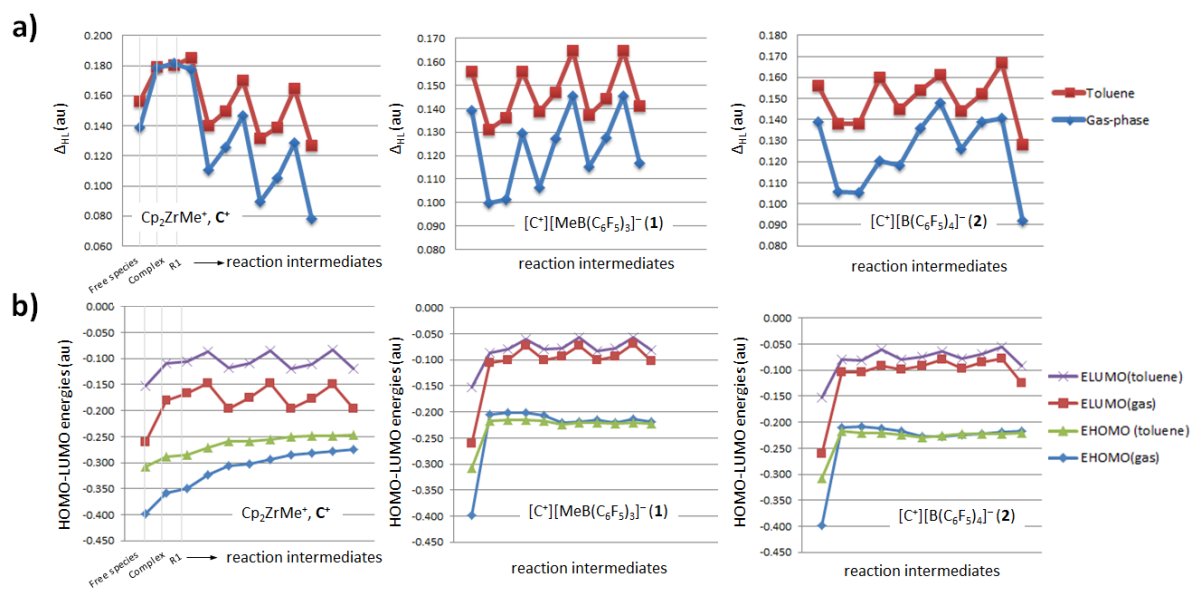


Figure S10. Effect of solvent toluene on the HOMO and LUMO energies and their differences (labeled as EHOMO and ELUMO, and Δ_{HL}) in comparison with the energies in gas-phase for the three catalytic systems (C^+ , **1** and **2**).

Table S5. Comparison of Mulliken charge (q , in unit of e) on Zr and B atoms in gas-phase and in toluene for the three catalytic systems (C^+ , **1** and **2**). HOMO and LUMO energies, E_{HOMO} and E_{LUMO} in units of au, and energy gap, Δ_{HL} , were also included.

Systems	Gas-phase		Toluene		Gas-phase			Toluene		
	q_{Zr}	q_{B}	q_{Zr}	q_{B}	E_{HOMO}	E_{LUMO}	Δ_{HL}	E_{HOMO}	E_{LUMO}	Δ_{HL}
2										
Cation	0.824	-	1.022	-	-0.399	-0.260	0.139	-0.308	-0.152	0.156
Complex	0.792	0.398	0.840	0.394	-0.210	-0.104	0.105	-0.218	-0.080	0.138
R1	0.810	0.403	0.863	0.400	-0.209	-0.104	0.105	-0.220	-0.082	0.138
TS1	0.829	0.405	0.877	0.396	-0.213	-0.092	0.120	-0.221	-0.061	0.160
P1	0.826	0.395	0.875	0.393	-0.218	-0.099	0.118	-0.224	-0.079	0.145
R2	0.817	0.403	0.859	0.398	-0.227	-0.091	0.136	-0.229	-0.075	0.154
TS2	0.822	0.403	0.864	0.399	-0.227	-0.079	0.148	-0.225	-0.064	0.161
P2	0.838	0.399	0.873	0.393	-0.224	-0.098	0.126	-0.222	-0.078	0.144
R3	0.838	0.397	0.876	0.394	-0.223	-0.084	0.139	-0.222	-0.070	0.152
TS3	0.846	0.402	0.880	0.398	-0.219	-0.078	0.141	-0.222	-0.055	0.167
P3	0.838	0.394	0.883	0.385	-0.217	-0.125	0.092	-0.220	-0.092	0.128
1										
Cation	0.824	-	1.022	-	-0.399	-0.260	0.139	-0.308	-0.152	0.156
Complex	0.785	0.384	0.855	0.383	-0.205	-0.106	0.100	-0.217	-0.086	0.131
R1	0.809	0.395	0.864	0.394	-0.201	-0.100	0.101	-0.216	-0.079	0.136
TS1	0.826	0.401	0.879	0.399	-0.202	-0.073	0.129	-0.216	-0.060	0.156
P1	0.823	0.402	0.867	0.400	-0.206	-0.100	0.106	-0.218	-0.079	0.139
R2	0.820	0.399	0.859	0.397	-0.220	-0.093	0.127	-0.224	-0.077	0.147
TS2	0.830	0.402	0.862	0.398	-0.218	-0.073	0.145	-0.221	-0.056	0.165
P2	0.832	0.395	0.875	0.394	-0.216	-0.101	0.115	-0.221	-0.083	0.137
R3	0.833	0.396	0.872	0.395	-0.220	-0.093	0.128	-0.223	-0.078	0.144
TS3	0.835	0.397	0.872	0.394	-0.214	-0.069	0.145	-0.221	-0.056	0.165
P3	0.835	0.388	0.867	0.382	-0.219	-0.102	0.117	-0.222	-0.081	0.141
C⁺										
Cation	0.824	-	1.022	-	-0.399	-0.260	0.139	-0.308	-0.152	0.156
Complex	0.800	-	0.885	-	-0.359	-0.180	0.179	-0.289	-0.110	0.179
R1	0.812	-	0.879	-	-0.349	-0.167	0.182	-0.286	-0.106	0.180
TS1	0.835	-	0.897	-	-0.324	-0.147	0.177	-0.272	-0.087	0.185
P1	0.841	-	0.898	-	-0.306	-0.196	0.111	-0.258	-0.119	0.140
R2	0.842	-	0.893	-	-0.302	-0.176	0.126	-0.259	-0.109	0.149
TS2	0.848	-	0.910	-	-0.294	-0.148	0.146	-0.256	-0.086	0.170
P2	0.849	-	0.889	-	-0.285	-0.196	0.089	-0.251	-0.119	0.132
R3	0.856	-	0.889	-	-0.282	-0.177	0.105	-0.249	-0.110	0.139
TS3	0.857	-	0.882	-	-0.279	-0.150	0.129	-0.248	-0.083	0.165
P3	0.854	-	0.895	-	-0.274	-0.196	0.078	-0.246	-0.119	0.127

VII. Observed planes on the stationary points for the naked model

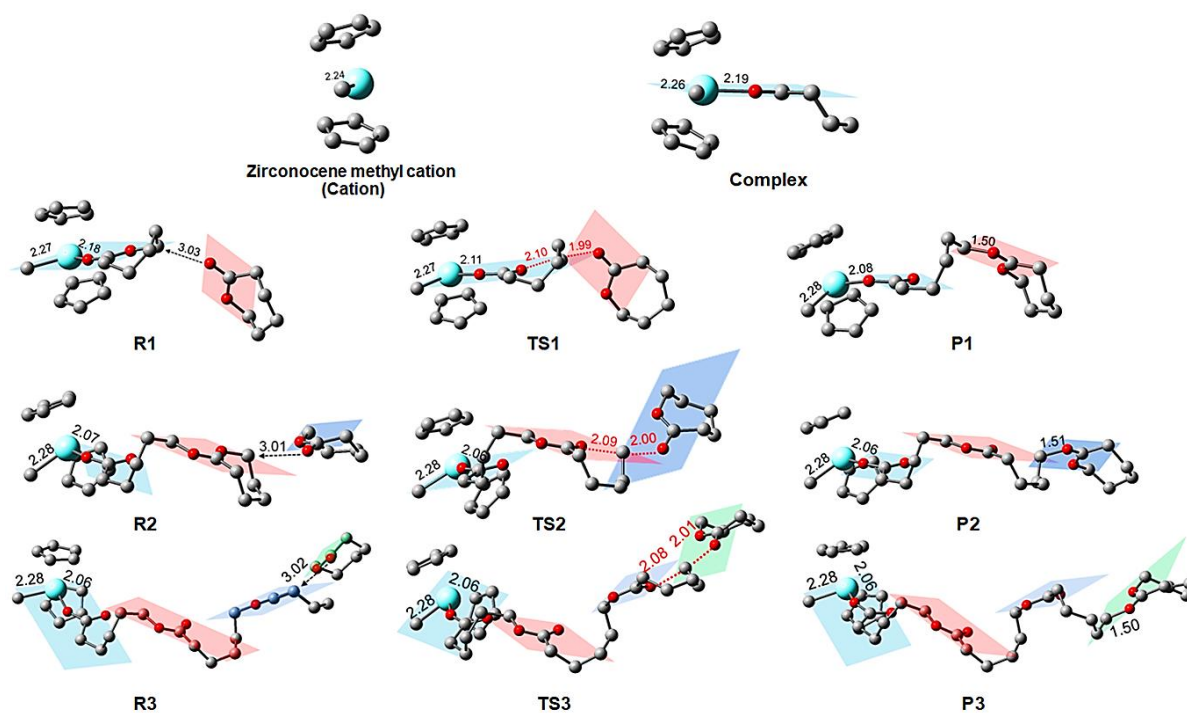


Figure S11. Observed planes on the stationary points in the initiation and chain propagation for the naked model (C^+). R^n , TS^n , and P^n ($n = 1-3$) denote reactant, transition state and product for the first, second and third propagation, respectively.

VIII. Additional data from NCI analysis

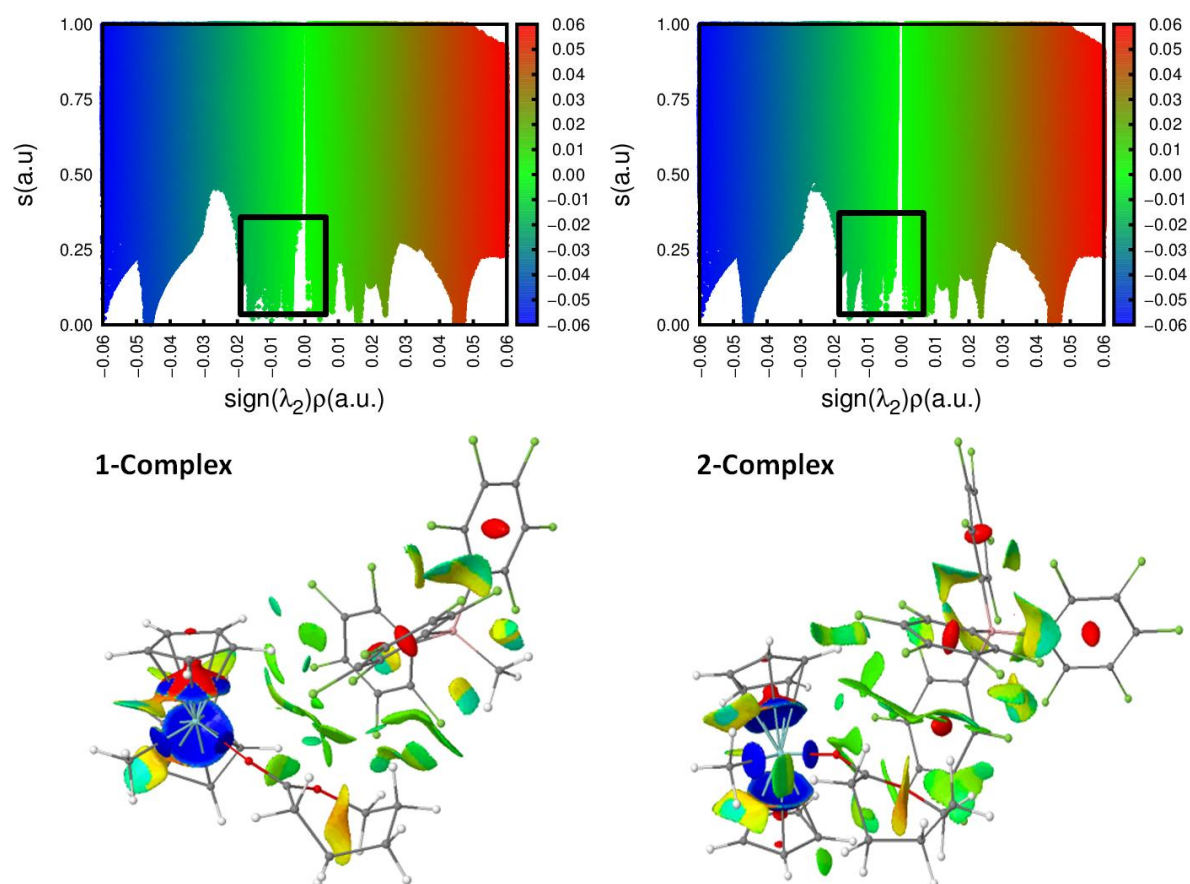


Figure S12. NCI analysis of Complex species. 2D (upper panel) and 3D (lower panel) isosurfaces of the **Complex** structures resulting from the initiation step of the zirconocene/borate systems **1** and **2**. Toluene-optimised geometries were used as inputs for this NCI analysis using promolecular density. The gradient 2D isosurfaces ($s = 1.0$ a.u.) are colored on a BGR scale according to the sign $(\lambda_2)\rho$ over the range -0.06 to 0.06 a.u., whereas the 3D representations are visualised with the cutoff, $s = 0.3$ a.u. (atom color code: light gray, C; dark blue, N; white, H; red, O; pink, B; green, F; cyan, Zr).

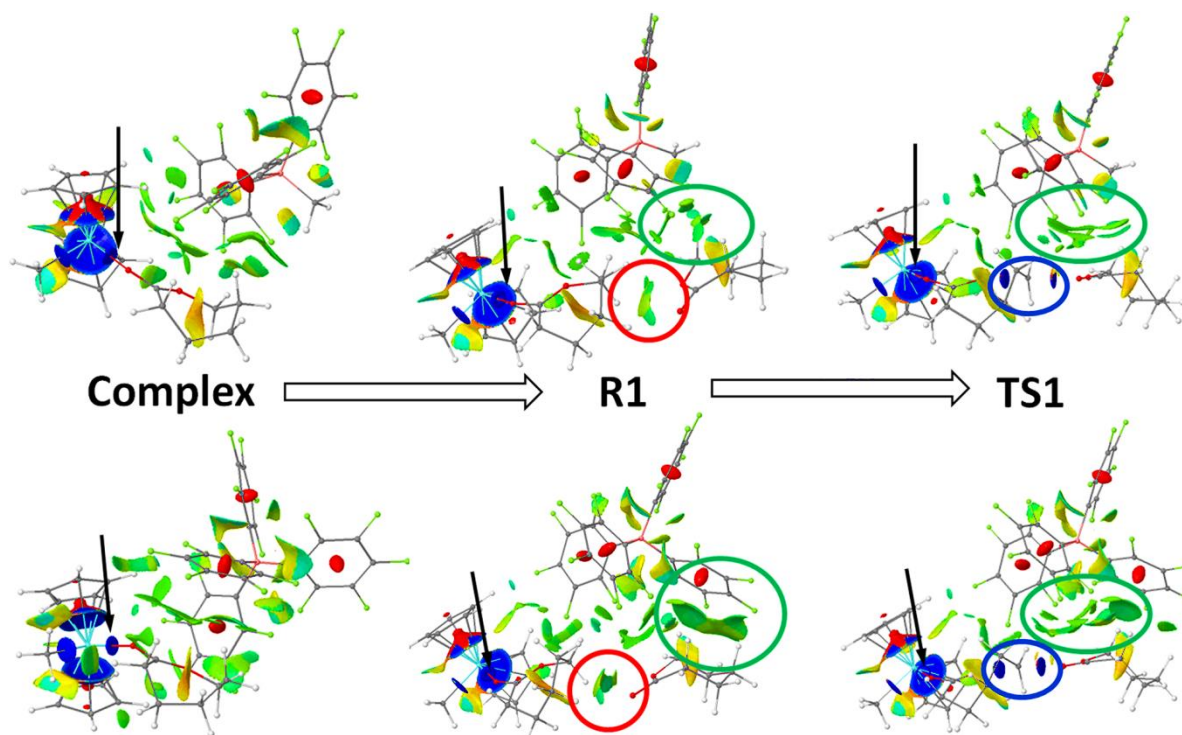


Figure S13. Evolution of 3D isosurfaces ($s = 0.3$ a.u.) of selected structures (**Complex**, **R1**, and **TS1**) along the reaction pathway. Black arrows indicate the attractive Zr-O interactions, in blue, with the intensity gradually decreasing from thin isosurfaces at **Complex** into donut-shaped isosurfaces at **TS1**. Red and green circles indicates van der Waals regions corresponding to the interacting sites of CL monomer to the C^α atom and the $-C_6F_5$ ring of counteranion, respectively. Blue circles indicate the appearance of two attractive forces near the C^α position.

Transition state comparison (TS3 vs. TS3^{ter}). The results in Figures S14-S15 indicate a marked difference between the two transition states (TS3 and TS3^{ter}). There are two blue-green peaks at low density gradient near $\text{sign}(\lambda_2)\rho = -0.03$ and -0.02 a.u., which are not present at 1-TS3 (see blue arrows). However, in case of $[\text{B}(\text{C}_6\text{F}_5)_4]^-$, intensity of the blue and disk-shaped isosurfaces between a methanol molecule and the $-\text{C}_6\text{F}_5$ rings is disappeared at -0.03 scale in the 2D NCI plot (see Fig. S15(b) below), which is the indication of weaker attractive interactions compared to the case of $[\text{MeB}(\text{C}_6\text{F}_5)_3]^-$. These results could explain the favourable termination over the third propagation in the $[\text{MeB}(\text{C}_6\text{F}_5)_3]^-$ system (Table 2). A slight difference at the vdW contact is found between the two distinct molecule (CL and CH_3OH) and the $-\text{C}_6\text{F}_5$ rings (see peaks near $\text{sign}(\lambda_2)\rho = 0.02$ a.u., Fig. S15).

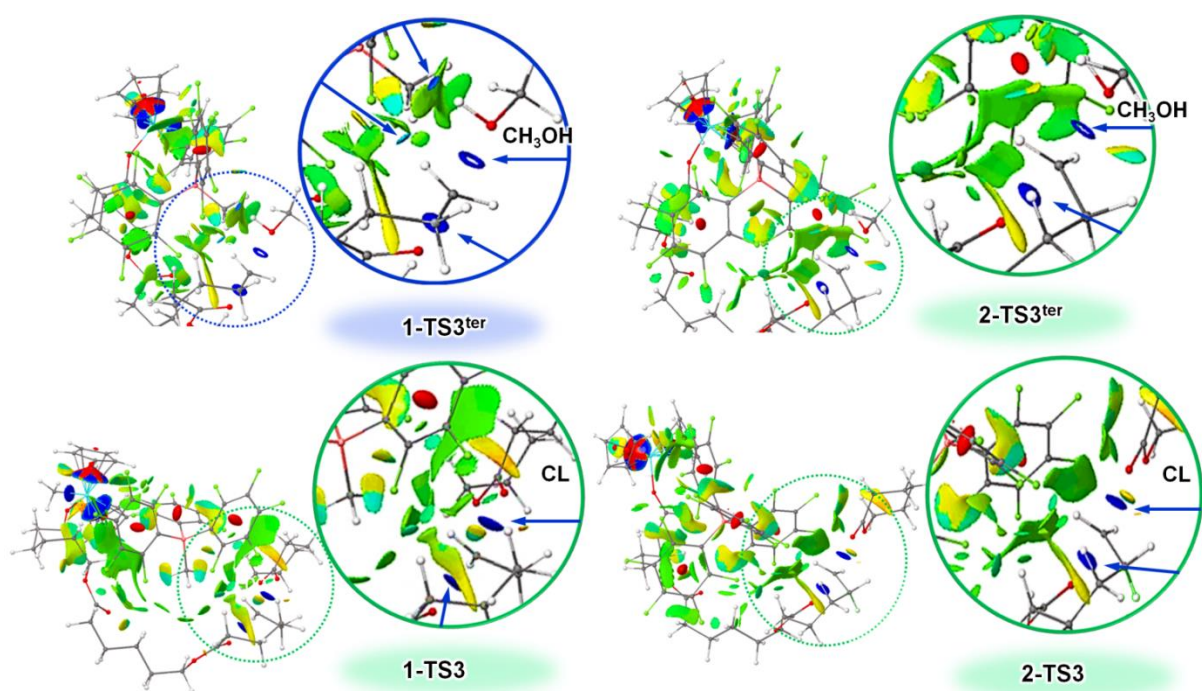


Figure S14. Comparison of 3D NCI isosurfaces between two transition states (TS3 and TS3^{ter}) in the 1st termination and the 3rd propagation for zirconocene/borate systems **1** and **2**. Circle lines and images indicate bond-breaking and forming regions with distinct interaction types and strengths. Blue circles indicate more attractive interactions compared to the corresponding interactions at the same region (see blue arrows). The greater the intensity of the 3D isosurface, the stronger the interacting forces present.

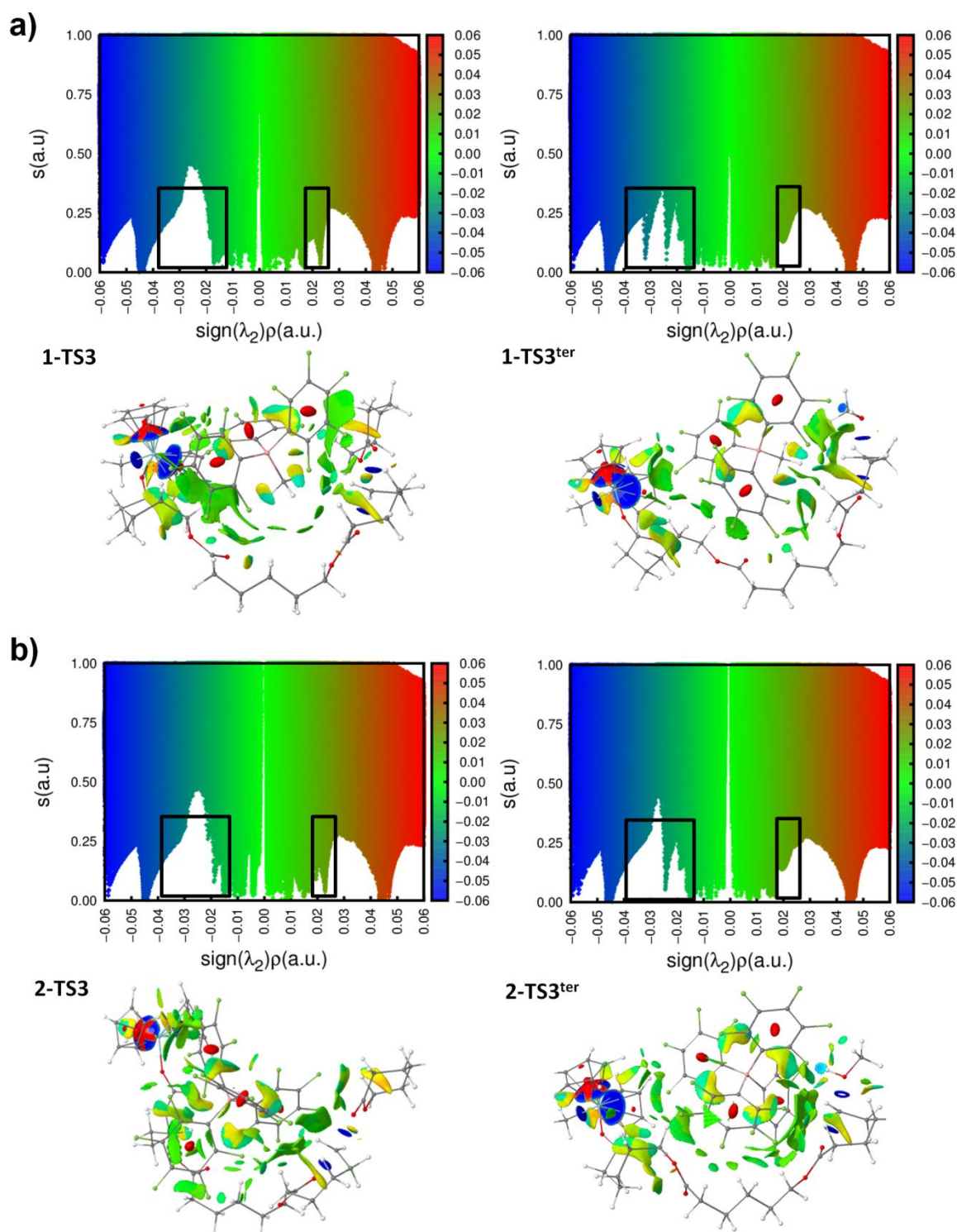


Figure S15. Comparison of 2D and 3D NCI plots between two computed transition states in the 3rd propagation and the 1st termination (TS3 vs. TS3^{ter}) for zirconocene/borate systems **1** (a) and **2** (b). Toluene-optimised geometries were used as inputs for this NCI analysis using promolecular density. Rectangular lines indicate two marked differences on the RDG plots between TS3 and TS3^{ter} of both reaction steps: the large one indicates the absence and presence of one or two spikes at -0.04 to -0.03 a.u. and -0.03 to -0.02 a.u. at low gradients, while small rectangular lines indicating a lack of weak interactions formed by the counteranion and an incoming CL monomer.

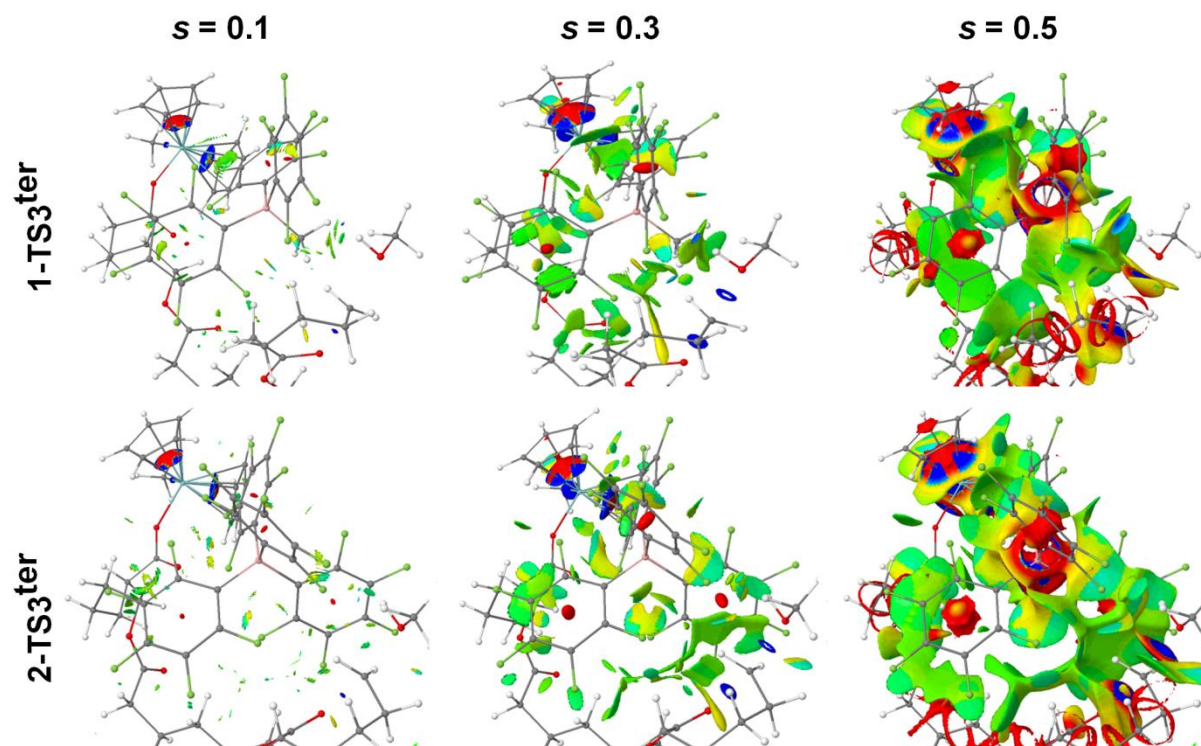


Figure S16. 3D isosurfaces of **1-TS3^{ter}** (upper panel) and **2-TS3^{ter}** (lower panel) using different cutoff ($s = 0.1, 0.3$ and 0.5).

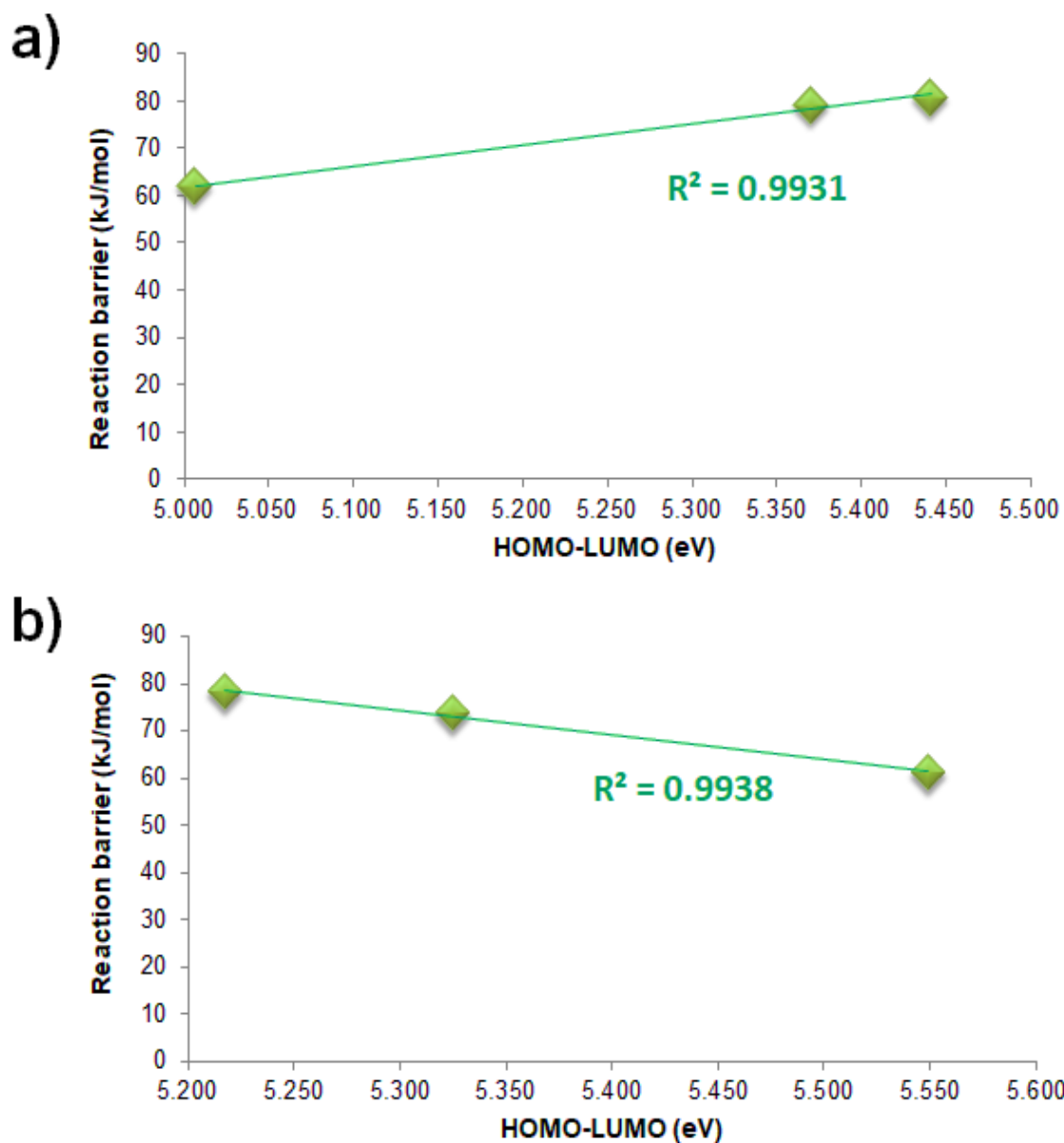


Figure S17. Linear correlation between the HOMO-LUMO energy gaps (eV) and reaction barriers (kJ/mol) calculated for the cocatalyst systems, **1** (a) and **2** (b). The HOMO-LUMO gaps were obtained as the difference between the HOMO energy of the CL monomer (-7.000 eV) and the LUMO energies of the transition states of the zirconocene/borate systems (**1** and **2**).

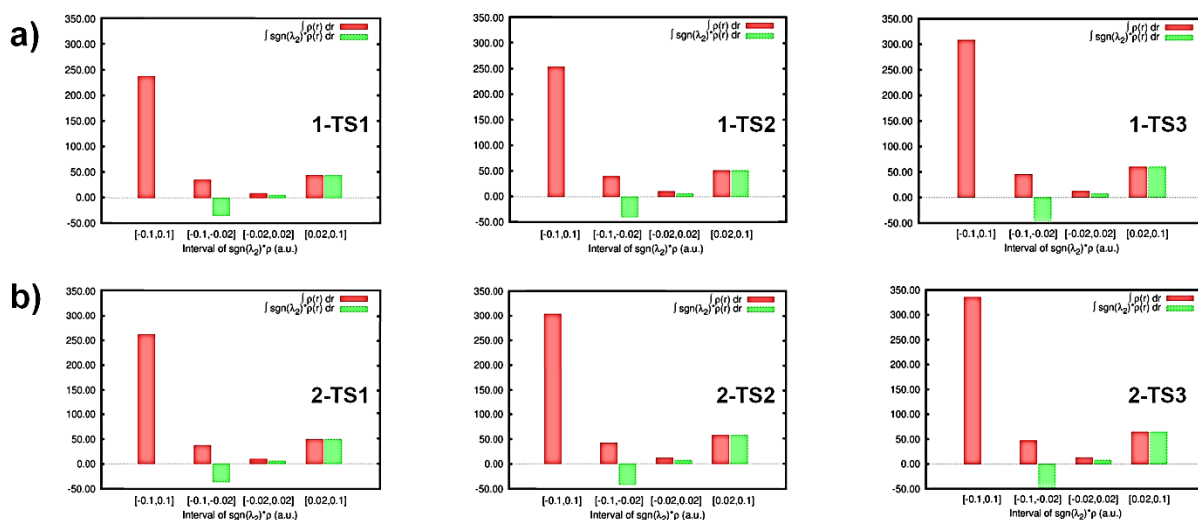


Figure S18. Bar charts showing volume integrals of electron density ($\int \rho(r) dr$ in red and $\int \text{sgn}(\lambda_2) \rho(r) dr$ in green) from 2D-RDG isosurfaces in different $\text{sgn}(\lambda_2) \rho(r)$ intervals for transition states (**TS1**, **TS2** and **TS3**) in the zirconocene/borate systems, **1** (a) and **2** (b). The plots provide a quantitative estimate of the interaction strength, based on integration over the NCI regions. If we look at the total density in the [-0.1, 0.1] range, we recognise the increment for the $\int \rho(r) dr$ values from **TS1** to **TS3** in both **1** and **2**. Other ranges [-0.1, -0.02] and [0.02, 0.1] related to the attractive and repulsive interactions, respectively, also show the same trend, with the former being significantly increased (shown in green bar).

IX. References

1. J. Kumawat and V. K. Gupta, *ACS Catal.*, 2020, **10**, 1704-1715.
2. J. Chen, A. Motta, J. Zhang, Y. Gao and T. J. Marks, *ACS Catal.*, 2019, **9**, 8810-8818.
3. J. Jitonnom and W. Meelua, *J. Organomet. Chem.*, 2017, **841**, 48-56.

X. XYZ coordinates for all optimized species

A. Optimized species shown in Figure 1

C⁻-Complex_front

C	-0.0060900	-0.2595240	-0.6937290
C	-0.3389680	-0.2506070	0.6853800
C	1.4002790	-0.0816660	-0.8103420
C	1.9418340	0.1077100	0.4942070
C	2.9825540	0.1734970	0.7419230
C	0.8645700	-0.1008220	1.4232060
C	1.4071610	-4.0171250	2.2405150
C	2.2473460	-2.8981560	2.4792410
C	1.8818470	-4.6787820	1.0780510
C	3.2565100	-2.8794360	1.4699140
C	4.3019730	-3.9858530	0.6141270
Zr	1.0571240	-2.3665190	0.3116840
C	-1.0305590	-3.1526210	0.7136880
H	-1.4404370	-2.9381160	1.7082770
H	-1.7199360	-2.7206850	-0.0283400
H	-1.0296360	-4.2434490	0.5889750
H	1.9629840	-0.0348960	-1.7347590
H	-0.7066680	-0.3568560	-1.5138390
H	-1.3328820	-0.3398560	1.1010740
H	0.5580050	-4.3154650	2.8397270
H	1.4519240	-5.5686660	0.6302500
H	3.6279730	-4.2465210	-0.2511760
H	4.0718840	-2.1724350	1.3960150
H	2.1712220	-2.2124170	3.3128970
H	0.9435170	-0.0227660	2.4998570
H	-1.1539910	-4.7456820	-3.7796430
H	-0.5042920	-6.0826160	-4.1737270
H	-1.2042490	-4.0411480	-4.6163530
H	-2.1548870	-4.8697590	-3.3668980
C	1.8814420	-3.7615150	-0.4008600
C	0.7137250	-5.9827070	-0.5032850
C	-0.3042420	-6.6588290	-3.2607840
H	-1.3161610	-6.6340990	-4.7193230
H	1.8912990	-5.2337100	-4.4167010
H	1.0387340	-3.2773000	-4.8636720
H	2.5057120	-3.2028300	-3.8809660
H	0.4480090	-5.4902560	-5.9991370
H	1.0420500	-6.9940000	-5.3174900
H	2.2549800	-5.7685180	-3.5296930
H	2.7255870	-5.2116370	-5.1254220
O	-0.4456720	-4.0875550	-2.6705310
O	0.7745900	-3.6243750	-2.7768880
O	1.2642300	-3.0736160	-1.7697550

C⁻-RI_front

C	0.3892620	0.3606300	0.0761320
C	0.4232470	0.3415790	1.4947050
C	1.6853880	0.0225120	-0.4014040
C	2.5143810	-0.2287020	0.7182890
C	3.5646380	-0.4873550	0.6878830
C	1.7303810	-0.0395090	1.8948640
C	1.0214250	-3.9812780	2.4458710
C	2.2557550	-3.2815770	2.4004750
C	0.8349620	-4.6193360	1.1919960
C	2.8416470	-3.5023110	1.1186530
C	1.9651440	-4.3353010	0.3801800
C	-1.2370470	-2.1061170	1.7974370
H	-1.2154860	-1.8614790	2.8665350
H	-1.9001860	-1.3786970	1.3094290
H	-1.1891290	-3.1036840	1.6942490
H	1.9830460	-0.0461370	-1.4450760
C	-0.6977760	-3.0279580	-3.4854600
C	-1.3326800	-4.1619130	-4.2991600
H	-1.1155500	-2.0540730	-3.7827120
H	0.3770790	-2.9556450	-3.6787230
C	-2.9578020	-4.4037350	-1.8895800
C	-2.8652930	-4.0467420	-4.4253940
H	-1.0641020	-5.1270280	-3.8555850
O	-0.8853970	-4.1543460	-5.2958210
C	-3.5633640	-3.7084550	-3.0962160
C	-3.6315690	-4.3880980	-1.0334900
H	-2.6755430	-5.4364290	-2.0940260
C	-3.2593800	-4.9970300	-4.7971750
H	-3.1190640	-3.2799000	-5.1673460
H	-4.6083980	-4.0287870	-3.1477640
H	-3.5812200	-2.6262530	-2.9083020
O	-1.7640980	-3.7149660	-1.3272720
O	-0.8217600	-3.1000180	-1.9793830
O	0.0495450	-2.5117750	-1.2921730
H	-0.4689190	0.6089590	-0.5356070
H	-0.3997990	0.5767730	1.5476200
H	0.3433440	-4.0227210	3.2871380
H	-0.0187630	-5.2210350	0.9073780
H	2.1280020	-4.6842830	-0.6323330
H	3.8053580	-3.1356420	0.7851380
H	2.7001520	-2.7218050	3.2131250
H	2.0841530	-0.1195220	2.9147790
C	-3.7684460	-1.0276770	-2.2529490
C	-3.7058570	-1.8995860	-3.5355940
H	-4.6830040	-1.0277480	-1.6829370
H	-2.9157030	-1.0298980	-1.6096110
C	-5.8402390	-8.6049240	-3.6184510
C	-5.0196240	-10.9539820	-4.3271330

H	-2.8898470	-10.5079370	-4.1575250
H	-3.4184470	-11.9206240	-3.2535120
C	-5.5570890	-9.5896820	-4.7769690
H	-6.3610490	-9.1298540	-2.8059150
H	-6.4952130	-7.7999000	-3.9582030
H	-5.7835870	-11.4486290	-3.7099820
H	-4.8793160	-11.5910770	-5.2084560
H	-4.8646960	-9.1220050	-5.4891050
H	-6.4966420	-9.7428780	-5.3197200
O	-3.6420250	-8.6462950	-2.4705620
C	-4.6003370	-7.9172760	-3.0776520
O	-4.4178800	-6.7179480	-3.1857180
Zr	0.7689750	-2.0848250	0.7383880

C⁻-TS1_front

C	1.0494010	0.2859600	-0.5545380
C	0.8026100	0.3148980	0.8465890
C	2.3046880	-0.3322470	0.7667080
C	2.8252630	-0.7226440	0.4942520
C	3.7799860	-1.2020520	0.6700150
C	1.9000490	-0.3010090	1.4950600
O	-0.3909970	-3.6407360	1.9589940
C	0.8197450	-3.1743450	2.5281100
C	-0.0649900	-4.5054350	0.8808720
C	1.9019540	-3.7671770	1.8114890
C	1.3495400	-4.5984110	0.8061800
Zr	-1.5247900	-2.1722350	0.1831200
C	-1.4252550	-1.6611310	-0.1748740
C	-2.1769960	-2.2065560	0.4015950
H	-1.6999760	-0.6031550	-0.1798950
H	-1.4971840	-2.0285000	-1.2597000
C	2.7649260	-0.5224820	-1.7271690
C	1.6374680	-3.9327950	-3.8781950
C	1.2242980	-5.0787780	-4.8109790
H	1.7068530	-2.9821580	-4.4264640
H	2.6439860	-4.1056440	-3.4806350
C	-1.7114930	-4.9786570	-4.0011910
C	0.0847650	-4.7533380	-5.7924090
H	0.9670820	-5.9561010	-4.2038230
H	2.1008090	-5.3746020	-5.3995790
H	-1.1852850	-4.1750500	-5.1504220
H	-2.4540370	-4.5630010	-3.3372880
H	-1.2945190	-5.9328700	-3.7240680
H	-0.1743290	-5.6646280	-6.3462470
H	0.4421480	-4.0331870	-6.5387960
H	-1.9799130	-4.0898820	-5.8995790
H	-1.0192310	-3.1556340	-4.7859940
O	-0.4030720	-4.1936500	-2.5490900
C	0.7393630	-3.6940460	-2.6700460
C	1.2484340	-2.9236370	-1.7693480
H	0.3918210	0.6748200	-1.3214130
H	-0.0693270	0.7348620	1.3014660
H	-1.3863800	-3.3791600	2.2893830
H	-0.7680690	-4.9961600	0.2231320
H	1.9127700	-5.1776250	0.0856250
C	2.9551470	-3.6342640	2.0231920
H	0.9676750	-2.5228950	-3.3875890
C	2.0308720	-0.4060350	2.5637330
H	-1.1282380	-8.4458040	-2.7299490
C	-3.8842200	-9.7818310	-3.4211660
H	-5.1933960	-8.2029290	-2.6543550
C	-3.7002700	-8.4343450	-1.7272140
H	-4.8563500	-7.5353290	-5.3963560
H	-4.7326080	-10.0209160	-6.6779380
H	-2.8127740	-9.8689720	-4.6447440
C	-4.1086810	-10.5642110	-2.6853400
C	-4.5287260	-8.9943680	-5.1994960
H	-5.7999390	-7.5047510	-4.8343650
H	-4.9819680	-6.9110610	-6.2830650
H	-5.7942450	-10.0309380	-4.3932770
H	-4.5119580	-11.0204230	-5.0691620
H	-3.5020440	-9.0428030	-6.1851500
H	-5.1831910	-9.2504960	-6.6393740
O	-3.4420580	-7.3236740	-3.7498770
C	-3.7729190	-6.8808270	-4.5755090
O	-3.1488030	-5.9106190	-5.0307550

I-Complex_front

C	-0.1425230	0.0112670	-0.0119990
C	-0.2021620	-0.2327260	1.3849130
C	1.1549160	0.5009090	-0.3221120
C	1.9066320	0.5380490	0.8771370
H	2.9309650	0.8718110	0.9465740
C	1.0678480	0.0787350	1.9350300
C	2.5257410	-3.5881660	2.0745860
C	3.2061490	-2.3518270	2.2350280
H	2.9309650	-4.0929170	0.7841900
C	3.9414760	-2.0936180	1.0409130
C	3.7191150	-3.1783060	0.1546400
Zr	1.4803610	-1.9320310	0.4350590
C	-0.2915890	-3.1880930	1.1296690
C	-0.5005970	-3.1673910	2.2063910
H	-1.1980370	-2.8450680	0.6120360
O	-0.1068920	-4.2320350	0.8462280
H	1.5267560	0.7617480	-1.3044120
C	0.4222000	-1.9632330	-3.8855130
O	-0.2026910	-2.6080840	-5.2047300
H	-0.1068920	-1.1350720	-3.6161040
H	1.4071440	-1.5053570	-3.9986710
C	-0.9822660	-4.6568310	-3.3997170
C	-0.2026910	-2.9782680	-5.2660320
H	0.5996970	-3.4840160	-5.4176770
O	0.2113010	-1.8927600	-6.0014120
C	-2.0123960	-3.7247630	-4.0151570
H	-1.4393500	-5.3997180	-2.7478450
H	-0.3694790	-5.1756370	-4.1333450
H	-1.6728050	-3.6146940	-6.1408660
H	-2.1141610	-2.0735660	-5.4092850
H	-2.8743790	-4.3408860	-4.2856400
H	-2.3560580	-3.0282280	-3.2377040
O	-0.0633380	-3.9674730	-2.4582900
C	0.5120480	-2.8153880	-2.6399540
H	1.1777190	-2.3707320	-1.6702730
H	-0.9526430	-0.1381390	-0.7151080
H	-1.0605790	-0.5957280	1.9325650
O	1.8889680	-4.0645010	2.8074580
C	2.8056990	-5.0170600	0.3501030
H	4.1677430	-3.2992490	-0.8215810
H	4.6013830	-1.2558700	0.8566680
C	3.2030280	-1.7348270	3.1239110
H	1.3359170	0.0222410	2.9821220
C	-2.9163444	-12.6347555	-10.3718571
H	-5.15235736	-12.7598245	-10.98708171
C	-3.62921764	-13.32941795	-10.83496171
H	-6.87987664	-12.85615495	-9.30311571
C	-3.60905664	-11.40025095	-12.88172771
C	-1.50419464	-12.85528795	-12.51843071
H	-0.92832964	-11.90896295	-10.63825771
H	-1.05923764	-13.66226995	-10.56812771
H	-2.12714664	-11.65529195	-13.24319171
H	-4.15797264	-12.35216695	-12.87385971
H	-4.07680864	-10.75860895	-13.63197571

C⁻-PI_front

C	0.3737370	0.1624040	-0.1482370
C	0.0888330	0.0472830	1.2402130
C	1.7683480	-0.0006770	-0.3269500
C	2.3499270	-0.2475730	0.9429430
C	3.4040840	-0.3906260	1.1429100
C	1.3078370	-0.2044960	1.1918650
C	0.5467460	-4.3285470	2.02

H	1.17488300	-10.31135100	-5.02749200	H	1.52254200	-10.21768500	-5.34091600	H	1.74832400	-10.15970900	-5.19971000	C	-1.01596000	-12.40912100	-12.55330100
C	1.016697400	-8.30437300	-7.70255600	C	-0.41110600	-8.46300700	-7.68688800	C	0.30093400	-8.05064800	-7.60401500	H	-3.09149200	-13.06989900	-12.63530900
H	-1.92385200	-9.00124800	-7.33322400	H	-2.20571000	-9.10335400	-6.61982100	H	-1.69976800	-8.69240200	-7.01618800	H	-2.81154000	-11.49734200	-13.39066700
H	-1.84196000	-7.40769900	-8.99134000	H	-2.40071100	-7.57627100	-7.49489300	H	-1.63896400	-7.03586000	-7.63850300	H	-1.06123600	-14.51430900	-12.08662300
H	0.19977200	-10.41901300	-7.28320600	H	-0.15633300	-10.53238600	-7.12730700	H	0.36100500	-10.18340800	-7.25436600	H	0.48848300	-13.74515900	-11.77833300
H	1.76708000	-9.62447900	-7.31388800	H	1.30069300	-9.76711100	-7.74700600	H	1.93223000	-9.44651500	-7.52736500	H	-0.47879500	-11.50523400	-12.24225600
H	0.69027300	-7.39799900	-7.50175100	H	0.18827500	-7.54704300	-7.76115500	H	0.93421600	-7.17015400	-7.46151900	H	-0.72034000	-12.60563800	-13.59032000
H	0.16185300	-8.47774100	-8.78370200	H	-0.70915400	-8.72621200	-8.70770300	H	0.17080500	-8.18139700	-8.68341900	O	-2.92842700	-11.95854300	-10.09690600
O	-1.21872000	-7.94239100	-4.86674200	O	-0.77343300	-7.84612200	-4.62561700	O	-0.65121300	-7.83802900	-4.59051300	C	-2.99989800	-11.36729500	-11.31086600
C	-1.56681300	-7.32721800	-6.01923800	C	-1.44115800	-7.35335600	-5.64699300	C	-1.09556200	-7.21883200	-5.62990500	O	-3.41585400	-10.22636200	-11.36227100
O	-2.00977100	-6.19796800	-5.94797000	O	-1.83734800	-6.17919000	-5.57592700	O	-1.59588300	-6.05814600	-5.45929900	B	5.88818700	-3.15809100	-4.86785500
B	5.73642600	-3.11910000	-4.86851200	B	5.76540300	-3.12041300	-4.86654200	B	5.74738300	-3.24383500	-4.85918100	C	7.46187400	-3.66495400	-4.85964900
F	7.29690000	-3.74127800	-4.68758500	F	7.29988000	-3.72622300	-4.70885400	F	7.28123700	-3.85910600	-4.74174000	C	7.89214200	-4.99168300	-4.92361400
C	7.62763700	-5.09729600	-4.70326400	C	7.64756300	-5.07750400	-4.74915900	C	7.61512300	-5.21299600	-4.80195900	C	8.49272500	-2.72451900	-4.95467100
C	8.41055100	-2.89365000	-4.69149400	C	8.40349800	-2.86525100	-4.70892300	C	8.39230400	-3.00850500	-4.76742900	C	9.23182800	-5.36531300	-5.03702600
C	8.93565300	-5.58434300	-4.69320000	C	8.96134200	-5.54885300	-4.75785800	C	8.92310200	-5.69713300	-4.84733000	C	9.84045700	-3.04803000	-5.06671700
C	9.73181000	-3.32804300	-4.67940300	C	9.72994300	-3.28395500	-4.71476900	C	9.71425900	-3.44008500	-4.80999700	C	10.21603400	-4.38777600	-5.10818300
O	10.00314400	-4.69343400	-4.67956000	O	10.01526200	-4.64569300	-4.73865100	O	9.98597800	-4.80416200	-4.84906300	C	4.80883100	-3.26028000	-3.66878800
C	4.59102500	-4.23952400	-4.49449300	C	4.61094600	-4.27306700	-4.50510200	C	4.59317600	-4.37334100	-4.43571900	C	5.03683000	-5.01081800	-3.16952500
C	4.54745500	-4.81483300	-3.22033300	C	4.56388600	-4.84373400	-3.22841000	C	4.62716800	-4.97382300	-3.17020800	C	3.57349000	-4.60582600	-4.95772800
C	3.52732000	-4.61938400	-5.31616000	C	3.58654600	-4.70559900	-5.34943100	C	3.68189100	-4.72941800	-5.19975500	C	4.13439400	-5.90784800	-2.59174300
C	3.56403000	-5.69030000	-2.77182200	C	3.60945000	-5.75893100	-2.79611100	C	3.66845600	-5.85780100	-2.68195700	C	2.65020200	-5.50169800	-4.41866000
C	2.51722800	-5.49303600	-4.90722600	C	2.61375800	-5.62677300	-4.95897400	C	2.49839100	-5.60432900	-4.74332800	C	2.91956600	-6.14780800	-3.22232800
C	2.52464300	-6.02952900	-3.62906300	C	2.61431300	-6.15659400	-3.67879800	C	2.57883300	-6.17059700	-3.48343600	C	5.56059400	-1.95416900	-3.76021600
C	5.42929400	-1.87183700	-3.79837300	C	5.41522800	-1.89271000	-3.77868700	C	5.42839800	-2.00136300	-3.78036300	C	4.37286500	-1.22058200	-3.85021000
C	4.28272800	-1.09344600	-3.98633900	C	4.26769600	-1.11097000	-3.95228400	C	4.27972300	-1.21533900	-3.93662700	C	6.30559200	-1.68422500	-2.60643200
C	6.12993800	-1.55070600	-2.62774600	C	6.12258800	-1.58791900	-2.60805700	C	6.16239900	-1.69114700	-2.62810900	C	3.96495100	-0.26770900	-2.92632600
C	3.87559600	-0.06262300	-3.14390500	C	3.87552000	-0.08429500	-3.09698200	C	3.91199000	-0.17535600	-3.08951900	C	5.92076600	-0.75264700	-1.63827900
C	5.75679100	-0.52968700	-1.75116700	C	5.75703900	-0.57910000	-1.714499800	C	5.82602300	-0.66576500	-1.74294800	C	4.74611600	-0.03336300	-1.80042500
C	4.62223600	0.22648400	-2.01120100	C	4.62487000	0.18454900	-1.96134300	C	4.69725000	0.10683400	-1.97745000	F	11.50838300	-4.72781100	-5.21820900
F	11.26613400	-5.14015700	-4.67099600	F	11.28681900	-5.07707700	-4.74833800	F	11.25278100	-5.24793300	-4.89478000	F	10.77675000	-2.08843300	-5.14018600
F	10.74753700	-2.44744800	-4.67180000	F	10.73543700	-2.39149200	-4.70250800	F	10.72842600	-2.55727800	-4.82074300	F	8.19490900	-1.40547700	-4.93838600
F	8.23435600	-1.55085300	-4.70202900	F	8.21216800	-1.52508200	-4.69813200	F	8.21419300	-1.66698000	-4.75133400	F	7.01142500	-1.60572100	-4.87850000
F	6.66467500	-6.05157800	-4.74329700	F	6.69699400	-6.04480600	-4.79828900	F	6.65317000	-6.17072200	-4.83716000	F	9.57531400	-6.63460500	-5.08295700
F	9.17164500	-6.90858000	-4.70381400	F	9.21293900	-6.87047100	-4.79263000	F	9.16094200	-7.02135900	-4.89872100	F	3.16828800	-6.99306000	-6.08959700
F	3.38888100	-4.14571700	-6.61087000	F	3.45848600	-4.24711700	-6.61083900	F	3.27216900	-4.24329500	-6.44064700	F	1.46395300	-5.72051400	-5.04279600
F	1.47932200	-5.78334800	-5.73345100	F	1.61644400	-5.98339500	-5.81841800	F	1.40696600	-5.88263600	-5.52831600	F	2.00623200	-6.96633000	-2.66230000
F	1.53025700	-6.84543400	-3.22595900	F	1.65627000	-7.02651200	-3.29658000	F	1.60936700	-7.00211600	-3.04246400	F	4.40013400	-6.49649100	-1.41426900
F	3.58373300	-6.18014100	-1.51500900	F	3.61989100	-6.23984300	-1.53799100	F	3.75850200	-6.38148800	-1.44772200	F	6.15930300	-4.78927600	-6.22647900
F	5.50217700	-4.50187400	-2.31213800	F	5.48773300	-4.49395000	-2.30570000	F	5.63924200	-4.69211900	-2.32605900	F	3.51983500	-1.43291500	-4.88243900
F	3.43069200	-1.34759000	-5.01506000	F	3.41278700	-1.34845200	-4.98059600	F	3.40311000	-1.45923300	-4.94455700	F	2.79470000	-0.39962800	-3.07555000
F	2.72635700	0.61367000	-3.38280500	F	2.73590700	0.61194600	-3.32621700	F	2.77540700	0.52529300	-3.29752100	F	4.34263200	-0.84224200	-0.85636900
F	4.22713500	1.19215900	-1.15546200	F	4.23687000	1.13985800	-1.09231100	F	4.34587200	1.08389000	-1.11763100	F	6.64609000	-0.57813000	-0.51930900
F	6.45469900	-0.30289500	-0.61543300	F	6.45430600	-0.36922800	-0.58131000	F	6.44893700	-0.44620000	-0.62862500	F	5.49825600	-2.33479700	-2.34123900
F	7.21376100	-2.24865700	-2.24723400	F	7.21094500	-2.29014500	-2.24609900	F	7.25352600	-2.39821300	-2.28301500	C	5.62529100	-3.64966600	-7.45243900
C	5.73322900	-2.58027300	-6.41932300	C	5.70493200	-2.56216700	-6.41010300	C	5.64814200	-2.71409900	-6.41125700	C	5.72484200	-1.37033200	-6.91141300
H	6.52727800	-1.83800500	-6.56957800	H	6.47212000	-1.79001900	-6.55015000	H	6.43619700	-1.97213200	-6.59387500	C	5.56793500	-3.35897100	-8.81119900
H	5.93033500	-3.39942800	-7.12314500	H	5.92828500	-3.36243500	-7.12777700	H	5.81965500	-3.53528000	-7.12048600	C	5.67036500	-1.02964400	-8.26381800
H	4.79246600	-2.11620600	-6.72337100	H	4.74722300	-2.12621800	-6.70290900	H	4.69685700	-2.24982300	-6.67890300	C	5.59053900	-2.03024000	-9.22375400

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C	-0.18835500	0.08502400	0.07185300	C	-0.25780200	-0.16973500	1.46627800	C	-0.12653300	0.52637400	-0.23249300	C	1.87614700	0.52881800	0.96992400
C	2.91187000	0.82428700	1.06164600	H	3.21668700	0.78472900	1.11409000	H	3.21668700	0.78472900	1.11409000	H	3.21668700	0.78472900	1.11409000
C	1.02004300	0.09480000	2.02207000	C	2.17306400	-3.73728900	1.66132900	C	2.17306400	-3.73728900	1.66132900	C	2.17306400	-3.73728900	1.66132900
C	2.43321100	-3.63864000	2.07898000	C	3.02485800	-2.65297900	1.99648000	C	3.02485800	-2.65297900	1.99648000	C	3.02485800	-2.65297900	1.99648000
C	3.12696100	-2.41436200	2.25954300	C	2.31128700	-3.99121400	0.27133000	C	2.31128700	-3.99121400	0.27133000	C	2.31128700	-3.99121400	0.27133000
C	2.71844600	-4.11395200	0.77055700	C	3.70155400	-2.24276600	0.81195700	C	3.70155400	-2.24276600	0.81195700	C	3.70155400	-2.24276600	0.81195700
C	3.84274100	-2.13167700	1.05965700	C	3.26215700	-3.07612900	-0.24760200	C	3.26215700	-3.07612900	-0.24760200	C	3.26215700	-3.07612900	-0.24760200
Zr	1.36151600	-1.93238600	0.48970900	Zr	1.23378800	-1.66687000	0.46523000	Zr	1.23378800	-1.66687000	0.46523000	Zr	1.23378800	-1.66687000	0.46523000
C	-0.41157600	-3.13333500	1.24225200	C	-0.61644900	-2.70184700	1.33541800	C	-0.61644900	-2.70184700	1.33541800	C	-0.61644900	-2.70184700	1.33541800
H	-0.56729600	-3.07993100	2.37927000	H	-0.65609300	-2.76270200	2.40988100	H	-0.65609300	-2.76270200	2.40988100	H	-0.65609300	-2.76270200	2.40988100
H	-1.33097300	-2.77861000	1.08535200	H	-1.51403700	-2.16538100	0.99868400	H	-1.51403700	-2.16538100	0.99868400	H	-1.51403700	-2.16538100	0.99868

H	-1.16472300	-9.40644200	-3.50202700	H	2.83051800	-2.86091300	2.75956400	H	-0.98638600	-0.19887700	2.32350100	O	0.20534600	-1.98793200	-2.16033700
H	-1.03744900	-8.02072800	-7.17607600	H	1.30375300	-0.65797300	3.22549500	H	1.44159400	-4.39376900	2.24025400	O	0.42566900	-3.09275600	-1.51520400
C	0.90435900	-9.49664100	-6.32029600	C	-0.06530900	-8.95314900	-4.16475700	H	1.65951700	-4.78989200	-0.42250100	O	0.59325100	-2.98890500	-0.27341700
H	1.07018100	-8.53016100	-4.36880700	C	0.92327500	-9.25201100	-5.28540400	H	3.46820000	-3.05699300	-1.37219800	H	-2.45385400	-7.64014600	-13.51874400
H	0.87678300	-10.27679800	-4.31024900	H	-0.85384300	-9.70993800	-4.08466100	H	4.36274400	-1.56405400	0.67082800	H	-2.09539100	-2.55869800	3.39664500
C	0.48334600	-8.30363700	-7.18816200	H	0.44468900	-8.87112000	-3.20700200	H	3.08932800	-2.37337200	2.91056800	H	2.69840500	-2.59687400	3.99657200
H	-1.59218600	-8.96440500	-7.27017000	C	-1.87455100	-8.33261300	-6.35371700	H	1.55050400	-0.16331300	3.21550300	H	3.46622400	-3.47036400	1.57253300
H	-1.31223400	-7.39185800	-8.02552800	C	0.28667800	-9.73470800	-6.59585600	C	0.03700800	-9.10958500	-4.69397400	H	3.17855000	-1.44058900	-0.91751900
H	0.43870700	-10.40882500	-6.72148400	H	1.53074500	-8.35508400	-5.44738700	H	1.29590600	-9.12948500	-5.54571200	H	2.21689100	0.68089400	1.16026200
H	1.98778900	-9.63967500	-6.41319400	H	1.60420100	-10.02688700	-4.91162900	H	-0.71894900	-9.82826500	-5.02675800	H	1.92028100	-0.03066000	3.74804500
H	1.02051100	-7.39975000	-8.87711700	C	-0.67583600	-8.73433600	-7.24916000	H	0.26458900	-9.28114800	-3.64356600	H	-0.77420600	-0.28861700	3.98731600
H	0.77900200	-8.50015400	-8.22581800	H	-2.30293300	-9.22491600	-5.87842800	C	-1.06183600	-7.69450700	-7.06544300	C	-2.74029000	5.22368000	-11.14997900
O	-1.42911200	-7.85305900	-4.73176700	C	-2.65785100	-7.86276000	-6.95166700	H	1.07078100	-9.15208400	-7.06359000	C	-3.61534700	4.16529200	-11.80123000
C	-1.50059200	-7.26181100	-9.95747700	H	-0.25115800	-10.67558000	-6.40816200	H	1.92898400	-8.28789400	-5.25197100	H	-2.73583600	6.15893500	-11.72473800
O	-1.91654800	-6.12087800	-5.99713200	H	1.08318000	-9.97359700	-7.30993800	H	1.83544700	-10.03887500	-5.25085600	H	-3.10788700	5.44560900	-10.14775400
B	5.88818700	-3.15809100	-4.86785500	H	-0.13665200	-7.82972300	-7.55789700	C	0.36746500	-7.91175600	-7.62661300	C	-0.97232600	4.17655100	-13.36631100
C	7.46187400	-3.66495400	-4.85964900	H	-1.08704400	-9.17659500	-8.16326400	H	-1.61452000	-8.64479000	-7.08094500	C	-3.47185600	4.05511000	-13.32430300
C	7.89214200	-4.99168300	-4.92361400	O	-0.69648600	-7.63962600	-4.29408800	H	-1.61328700	-6.97687400	-7.67605800	H	-3.38722200	3.19947400	-11.32010000
C	8.49272500	-2.72451900	-4.95467100	C	-1.49649200	-7.32782300	-5.29318000	H	0.49373200	-10.04920800	-7.33181300	H	-4.65558700	3.38790000	-11.54311700
C	9.23182800	-5.36531300	-5.03702600	O	-1.92625100	-6.16586700	-5.36020700	H	2.04395200	-9.25349500	-7.55626000	C	-2.05825000	3.70756100	-13.80880400
C	0.84045700	-3.04840300	-5.06671700	B	5.99326500	-3.10775200	-4.84027500	H	0.96633000	-7.01333400	-7.44832500	H	-1.33596600	5.74206100	-13.51872200
C	10.21603400	-4.38776700	-5.10818200	C	7.57411800	-3.59893200	-4.82207200	H	0.26309500	-8.01618500	-8.71152400	H	-0.07226200	4.59288800	-13.97260400
C	4.80883100	-4.32620800	-4.36878800	C	8.02314600	-4.91705400	-4.87347800	O	-0.62806200	-7.78655700	-4.63354400	H	-3.77812400	5.01107800	-13.77640200
C	5.03063800	-5.01081800	-3.16695200	C	8.59513600	-2.64373700	-4.86614800	C	-1.08362200	-7.16796600	-5.66451500	H	-4.17246100	3.30002000	-13.70087600
C	-1.54593900	-4.60582600	-4.95727800	C	9.36933000	-5.27074300	-5.02321000	O	-1.61654100	-6.02288000	-5.48614300	H	-1.78221400	2.70329000	-13.46473100
C	4.13439400	-5.90784800	-2.59174300	C	9.94876600	-2.94762300	-4.96296000	B	5.80545200	-3.27342800	-4.89002500	H	-2.05059700	3.67409800	-14.90429300
C	1.62050200	-5.50169800	-4.41866000	C	10.34236800	-4.28000900	-5.04194400	C	7.35038400	-3.85894700	-4.78045200	H	-1.37473500	4.79474800	-11.91997400
C	2.91956600	-6.14780800	-3.22232800	C	4.92277900	-4.31175200	-4.41405600	C	7.72055400	-5.20489100	-4.77246100	O	-0.51682400	4.53446600	-11.92848000
C	5.56059400	-1.95416900	-3.76021600	C	5.12931000	-5.04662500	-3.32900300	C	8.43006500	-2.97222100	-4.85595000	O	0.59966000	4.14383300	-11.64236100
C	4.37286500	-1.22058200	-3.85021000	C	3.71856300	-4.60355400	-5.05756200	B	9.04460800	-5.64450700	-4.79974600	B	-5.46467800	-4.00002000	-2.37661000
C	6.30559200	-1.68425200	-2.60643200	C	4.25547800	-6.01288200	-2.74592300	C	9.74653000	-3.36225700	-4.88327100	C	-4.75699000	-5.03660400	-1.27566300
C	3.96495100	-0.26770900	-2.92392600	C	2.82567900	-5.57375300	-4.60702700	C	10.07743200	-4.71798100	-4.85409900	C	-5.38270200	-6.13328500	-0.97421500
C	9.09276600	-0.75264700	-1.68327900	C	3.08280100	-6.27816600	-3.44216600	C	4.64830300	-4.38711300	-4.45051800	C	-3.41362200	-4.90445500	-0.91923200
C	4.74611600	-0.03336300	-1.80042500	C	5.63474800	-1.95035000	-3.69827500	C	4.74774100	-5.04201200	-3.21572600	C	-4.74543600	-7.00544600	-0.14286300
F	11.50838300	-4.72781100	-5.21820900	C	4.44709800	-1.21589400	-3.78694700	C	6.46578200	-4.65682900	-5.14031900	F	-2.74289700	-5.07310700	-0.02941300
F	10.77675000	-2.08843300	-5.14018600	C	6.35842000	-1.71885700	-2.52351000	C	3.79491200	-5.91957400	-2.70420200	C	-3.41215000	-6.80528500	0.54695700
F	8.19490900	-1.40547700	-4.93838600	C	4.02564500	-0.28854300	-2.84040300	C	2.49872000	-5.53875300	-4.66826800	F	-5.27382100	-2.40841100	-1.94846300
F	7.01142500	-6.01572100	-4.87850000	C	5.95749900	-0.81823200	-1.53390900	C	2.64655500	-6.16922400	-3.44539500	C	-5.51438200	-1.37841900	-2.86587500
F	9.57531400	-6.66346500	-5.08295700	C	4.78813800	-0.09058400	-1.69676600	C	5.46950900	-2.03752700	-3.82810500	C	-5.05513400	-1.94275700	-0.65049000
F	3.16828800	-3.99300600	-6.08975900	F	11.64108100	-4.60073300	-5.13869900	C	4.30017700	-1.28416500	-3.98279000	C	-5.47562700	-0.02293600	-2.55726100
F	1.46395300	-5.72051400	-5.04279600	F	6.01347600	-1.97455800	-4.98708900	C	6.18347600	-1.74533900	-2.66170400	C	-5.00732100	-5.91519700	-0.28857900
F	2.00623300	-6.96637100	-2.66203000	F	8.28170700	-1.32977300	-4.81344300	C	3.88643500	-0.28736900	-3.10609800	C	-5.21398800	0.38166800	-1.25298900
F	4.40013400	-6.49649100	-1.41426900	F	7.15576400	-5.95415800	-4.93284200	C	5.79722900	-0.76262200	-1.74766800	F	-2.78219300	-7.62010300	1.40617200
F	6.15903300	-4.78927600	-2.46647900	F	9.72985200	-6.56296000	-5.10730100	C	4.64663600	-0.02238600	-1.97421700	F	-1.44431900	-5.49679900	-0.29738400
F	3.31893500	-1.43291500	-4.88243800	F	3.32161900	-3.94450900	-6.16664400	F	11.35609700	-5.12242700	-4.88245700	F	-2.67108600	-3.86871200	-1.42373100
F	2.79470000	0.39666800	-3.07555000	F	1.67891000	-5.82187800	-5.29911200	F	10.74874100	-2.45017500	-4.94374200	F	-6.67609000	-6.41662500	-0.90791900
F	4.34263200	0.84224200	-0.85636900	F	2.20224200	-7.19448800	-2.98478600	F	8.19765000	-1.64203800	-4.90797200	F	-5.41413600	-0.03522600	0.75582900
F	6.64609900	-0.57813000	-0.51930000	F	4.51577800	-6.66803300	-1.60425500	F	6.79243500	-6.18867600	-4.74088200	F	-5.79127200	-1.67120000	-4.15941900
F	7.44983500	-2.33479700	-2.34123900	F	6.22918000	-4.82589300	-2.49564900	F	3.32626100	-6.95925600	-4.78055300	F	-5.66966000	0.19566600	-3.51501200
F	5.68526700	-2.68489800	-6.44126000	F	3.61559500	-1.39563200	-4.84221900	F	9.16465000	-4.06801100	-6.31491300	F	-1.59255500	1.68566600	-0.93752500
F	5.62529100	-3.64966600	-7.45243900	F	2.86576800	0.38871100	-2.99482700	F	1.36728800	-5.76191700	-5.40333100	F	-4.75217600	-0.23719800	0.98357600
F	5.72428400	-1.37032300	-6.91141300	F	4.37443700	0.76193400	-0.73748500	F	1.68628600	-7.00211700	-2.98503400	F	-4.85386400	-2.80656800	-0.37832400
F	5.56793500	-3.35897100	-8.81119900	F	6.66632300	-0.67720400	-0.40023900	F	3.95186400	-6.49927600	-1.50402100	F	-4.70033800	-4.40705700	-3.81397700
F	0.60736500	-1.02964600	-8.26311800	F	7.49949800	-2.37819700	-2.26002100	F	5.81872400	-4.82511000	-2.42990500	C	-5.00042900	-5.61812500	-4.45511900
F	5.59053900	-2.03024000	-9.22735400	C	5.81999700	-2.58085600	-6.40228400	F	2.348100700	-1.51710100	-5.03626900	C	-3.70613000	-3.67961500	-4.46803100
F	4.49440000	-4.34183100	-7.24746900	C	5.79586700	-3.50855300	-7.44917500	F	7.40120900	0.39445700	-3.31612100	C	-4.43499400	-6.03749900	-5.65932000
F	5.61680300	-4.96151200	-7.12381400	C	5.85413400	-1.24992700	-6.82551000	F	4.24983800	0.90952200	-1.08578700	C	-3.11729800	-4.50787000	-5.63755400
F	5.69728900	0.25899200	-8.64340700	C	5.76443900	-3.17075100	-8.79775500	F	6.89855000	-0.55641000	-0.61780700	C	-3.48133600	-5.24813100	-6.28552500
F	5.53578600	-1.72258400	-10.52793900	C	5.82596200	-0.86231500	-8.16623600	F	7.29961000	-2.41956400	-2.33330600	F	-4.78781400	-7.20876100	-6.21221000
F	5.81423200	-0.32499100	-6.05997800	C	5.77952900	-1.82833800	-9.16285900	F	5.72227100	-2.82539400	-6.83971700	F	-5.87185900	-4.48669700	-3.92050800

O	0.59325100	-2.98890500	-0.27341700	H	0.76919600	-4.53285600	3.75839100	H	3.81455800	-3.41651800	1.83396300	H	2.31622600	0.66152300	1.21075700
H	-2.45385400	-2.64014600	0.73154400	H	2.77062100	0.02782500	2.47760600	H	3.48163400	-1.06046100	0.58658200	H	2.01271400	-0.04850500	3.79816700
H	-2.09539100	-2.55869800	3.39664500	H	2.42184800	-0.35824200	-0.16499900	H	2.23064900	0.61272200	2.28034300	H	-0.68332600	-0.27110500	4.05591300
H	2.69840500	-2.59687400	3.99675200	H	-0.18278500	-0.04488400	-0.718113500	H	1.78905300	-0.71925200	4.58692800	H	-2.79406000	5.20747400	-1.12751900
H	3.46622400	-3.47036400	1.57255300	H	-1.46504600	0.54315000	1.56814700	H	-0.91521000	-1.37433700	4.51750300	H	-3.68549200	4.14054900	-1.90476600
H	3.17855000	-1.44058900	-0.17519400	H	0.37008300	0.57939200	3.55817300	C	-3.79999000	0.37022100	-6.22575000	H	-3.27601800	6.12352100	-1.87877000
H	2.21689100	0.68098400	1.16026200	H	0.28458300	-2.16096100	4.92797100	H	-4.57826200	-0.67611800	-6.98376800	H	-3.16908900	5.46994300	-10.28539200
H	1.92081000	-0.03066000	3.74800400	C	-2.89166000	0.52953800	-6.02690900	H	-3.62116800	1.28941300	-6.79910600	C	-1.00743100	4.59946000	-13.44880200
H	-0.77420600	-0.28861700	3.98731600	C	-3.91280400	-0.26557900	-6.82934200	H	-4.23992000	0.60854200	-5.27040900	C	-3.52103900	3.98570200	-13.42129600
H	-3.09998600	1.12035300	-5.64492400	H	-2.56109000	1.43357600	-6.51382000	H	-1.65800100	-0.46487700	-8.12350300	H	-3.48894900	3.19460300	-11.38886800
H	-3.97504300	0.05296500	-6.29617500	H	-3.29774400	0.81158300	-5.05807700	H	-4.19191900	-0.86093400	-8.45681000	H	-4.72403000	4.40172400	-11.67229200
C	-3.09553200	2.05560800	-6.21968300	C	-1.01519600	-0.47072800	-8.02105200	H	-4.53294100	-1.61988400	-6.43172200	C	-2.10861800	3.58907000	-13.87045900
C	-3.46758300	1.34228200	-4.64269900	C	-3.58228200	-0.43420700	-8.31804200	H	-5.62311900	-0.34734800	-6.92077600	H	-1.34757700	5.61729700	-13.64165400
C	-1.33202200	0.61322400	-7.86125600	H	-4.05654500	-1.23454900	-6.33990800	H	-4.20957000	-1.38315500	-8.68907000	H	-0.10231800	4.62278000	-14.03809800
C	-3.83155200	-0.04781600	-7.81924800	H	-4.86738900	0.26629100	-6.73108000	H	-1.84978800	0.57497300	-8.42779400	H	-3.79684100	4.93270700	-13.90928700
H	-3.74691800	-0.90385300	-5.81504500	C	-2.26679500	-1.16931300	-8.60616300	H	-0.68230400	-0.75019300	-8.52189000	H	-4.23387200	3.23493800	-13.78383400
H	-5.01528300	0.28046300	-6.03806200	H	-1.06559900	0.60948700	-8.21595900	H	-4.31561800	0.09599400	-8.98511800	H	-1.85991800	2.59275800	-13.48489000
C	-2.41794600	-0.39576600	-8.30374900	H	-0.10775800	-0.85063800	-8.49469800	H	-4.89780000	-1.55954600	-8.92001000	H	-2.09014100	3.51434800	-14.96431000
H	-1.69566200	1.63873400	-8.01366700	H	-3.54646700	0.55817500	-8.79176800	H	-2.64755300	-2.38827300	-8.27523100	O	-1.44225200	4.75453700	-11.01214600
H	-0.43195800	0.48956100	-8.46754900	H	-4.40234500	-0.97605500	-8.80399600	H	-2.58603700	-1.46005000	-9.76639500	O	-0.57496000	4.44881400	-11.99595200
H	-1.17828000	0.90774300	-8.27134700	H	-2.31179500	-2.19824200	-8.23255100	O	0.53072000	-0.09743000	-5.80463600	O	0.53072000	4.04910900	-11.68493300
H	-4.53215700	-0.80332500	-8.19582100	H	-2.12401800	-1.23385000	-9.69078600	H	-1.52266300	-0.47068800	-6.62983000	B	-5.51227000	-3.90116800	-2.41360300
H	-2.14191000	-1.40003200	-7.95967600	O	-1.70311800	-0.24255300	-5.65700300	O	-0.38095900	-0.82679300	-6.16286300	C	-8.80798400	-4.97747300	-3.85630700
H	-2.41749300	-0.42922900	-9.39986800	O	-0.83535600	-0.69666100	-6.53830000	B	-5.43647500	-3.72793000	-2.38280200	C	-5.40048700	-6.15012300	-0.87444300
O	-1.43343100	0.69142100	-5.41491900	O	0.14838800	-1.32675500	-6.12310800	C	-4.80558900	-4.83939100	-1.31969000	C	-3.47914700	-4.82357400	-0.95510600
O	-0.87652000	0.43113900	-6.42342500	B	-5.46686000	-3.39236200	-2.29415000	C	-5.51296500	-5.87617800	-0.70570500	C	-4.57671600	-7.05773100	-0.02792900
O	0.23996400	0.04056000	-6.13706600	C	-5.06360700	-4.68114700	-1.13200100	C	-3.43961400	-4.84858000	-1.02681300	C	-2.80688600	-5.68827000	-0.10156400
B	-5.46467800	-4.00500200	-2.37961000	H	-5.96366200	-5.60811600	-0.78801700	C	-4.92380400	-6.82774100	0.13252400	C	-3.44780100	-6.82543200	3.01725800
C	-4.75699000	-5.03660400	-1.27566300	C	-3.72655800	-4.96683000	-1.02834600	C	-2.80968700	-5.76263200	-0.19598300	C	-7.16551300	-3.98892100	2.46751900
C	-5.38270200	-6.13382500	-0.67421500	H	-5.57875200	-6.71655000	-0.02712300	C	-3.56045200	-6.77438500	0.39382800	C	-7.90441000	-3.94788300	-1.28031800
C	-3.41362200	-4.90445500	-0.91923200	C	-3.29692400	-6.05042100	-0.27361100	C	-5.12028200	-2.16155400	-1.91407100	C	-7.94722300	-3.94402000	-3.62421900
C	-4.74543600	-7.00544600	0.21486300	C	-4.23419300	-6.94186600	0.23769100	C	-5.28445900	-1.09022200	-2.79552400	C	-9.29316100	-3.90873900	-1.22095500
C	-2.74289700	-5.73190700	-0.02941300	C	-4.79282500	-1.97209100	-1.74261100	C	-4.85975200	-1.75270200	-6.60271400	C	-9.34222000	-3.90755000	-3.61498600
C	-3.41215000	-6.80528500	0.54695700	C	-4.67425200	-0.83963400	-2.55474600	C	-5.15491300	0.24856900	-2.44843200	C	-10.02379600	-3.88781000	-2.40499300
C	-5.27382100	-2.40841100	-1.94846300	C	-4.47322300	-1.71828400	-0.40689300	C	-5.28718900	-0.42145400	-0.20184200	C	-5.28718900	-2.31119700	-1.97759000
C	-5.14382000	-1.37841900	-2.86587500	C	-4.21930500	0.40233400	-2.12269800	C	-4.86340200	0.59698200	-1.13519200	C	-5.54091300	-1.28638400	-2.89700900
C	-5.05134000	-1.94275700	-0.65049000	C	-0.41582700	-0.49264200	0.07472900	F	-2.97905000	-0.67524200	1.19889500	C	-5.00798500	-1.84841000	-0.69039300
C	-5.47652700	-0.02293600	-2.55726100	C	-3.86962100	0.58220900	-0.78946100	C	-4.18281600	-5.67370400	0.05282300	C	-5.46509000	0.06968200	-2.60003000
C	-5.00973100	-0.59519700	-0.28887900	F	-3.84317200	-7.99482600	0.97025700	F	-2.63407100	-3.87528300	-1.54397800	C	-4.92604000	-0.96857000	-0.34381100
C	-5.21398800	0.38166800	-1.25298900	F	-1.97981300	-6.24434200	-0.01423100	F	-6.84118700	-6.01762300	-0.87868800	C	-5.14795100	0.47503700	-1.30804000
F	-2.78219300	-7.62010300	1.40617200	F	-2.74607600	-4.13602400	-1.48123300	F	-5.66734800	-7.79638500	0.69151600	F	-2.81299800	-7.67518900	-1.19028500
F	-1.44431900	-5.49679900	0.29738400	F	-7.29111700	-5.48062200	-0.97203200	F	-5.57802400	-1.31837900	-4.10870200	F	-1.52965100	-5.42564400	0.28063700
F	-2.67108600	-3.86872200	-1.42391700	F	-6.50028200	-7.56539300	0.45501700	F	-5.28989400	1.22052900	-3.38615300	F	-2.75195500	-3.75882800	-1.83551000
F	-6.67600900	-6.41662500	-0.90719100	F	-5.00329900	-0.90658600	-0.37159600	F	-4.72592000	1.88474600	-0.78251100	F	-6.66077300	-6.47992500	-1.20323700
F	-5.41413600	-8.03522600	0.75582900	F	-4.10027900	1.43491600	-2.98780500	F	-4.44688600	-0.11804300	1.07647500	F	-5.39870000	-8.15499700	0.40238900
F	-5.79127200	-1.67120000	-4.15941900	F	-3.40220000	1.76046100	0.34573300	F	-4.71757800	-2.65658100	0.39247600	F	-7.38278800	-3.92890600	-4.85135000
F	-5.66966000	0.91096800	-3.51501200	F	-3.68871500	-0.34633600	1.37931500	C	-4.69941600	-4.14946400	-3.82984100	F	-10.02919200	-3.87095600	-4.76888100
F	-5.15925500	1.68566600	-0.93752500	F	-4.59190900	-2.68465200	0.53726800	C	-5.09568300	-5.30928300	-4.51276900	F	-11.36348400	-3.84630900	-2.37669200
F	-4.75217600	-0.23719800	0.98357600	C	-4.88813500	-3.87294800	-3.79065600	C	-3.62888900	-3.49587200	-4.44085300	F	-9.93145000	-3.88240300	-0.03490400
F	-4.85386400	-2.80656800	0.37832400	C	-5.56863500	-4.84851900	-4.53465600	C	-4.54562900	-5.74983800	-5.71879600	F	-7.25912100	-3.93491700	-0.09152000
C	-4.70033800	-4.40705700	-3.81397700	C	-3.69578800	-3.46603900	-4.39030400	C	-3.04065500	-3.90792400	-5.63239800	F	-5.87045400	-1.59171500	-4.17232800
C	-5.00042900	-5.61812500	-4.45511200	C	-5.15570400	-5.32818700	-5.77924500	C	-3.50509500	-5.03279500	-6.29660600	F	-5.67365200	0.99966800	-3.55598600
C	-3.70613000	-3.67961500	-4.46803100	C	-3.23740800	-3.92416800	-5.62218600	F	-5.00540400	-6.85695100	-6.32081300	F	-5.06598900	1.77808000	-1.00369700
C	-4.43499400	-6.03749900	-5.69939200	C	-3.97490500	-4.85500400	-6.33898000	F	-6.05648000	-6.10370900	-0.10409300	C	-6.15527200	-0.13496100	0.91369200
C	-3.11729800	-4.05078700	-5.67375400	F	-5.87993300	-6.24784900	-6.43473800	F	-2.00189400	-3.20303100	-6.16956500	C	-4.77280600	-2.70796800	3.02882100
C	-3.48133600	-5.24183100	-6.28555200	F	-6.69222700	-5.41661300	-4.05550000	F	-2.95769300	-5.40609600	-7.46552900	C	-4.78211700	-4.31764700	-3.84836700
F	-4.78781400	-7.20876100	-6.21221000	F	-2.06191900	-3.46766200	-6.13356800	F	-3.06900500	-2.38332900	-3.89491300	C	-5.11817300	-5.52290400	-4.47904900
F	-5.87185900	-6.48676900	-3.90305800	F	-3.54879400	-5.28691700	-7.53637400	C	-7.07243700	-3.75354300	-2.53517500	C	-3.74332100	-3.63555400	-4.47695500
F	-2.16276200	-3.26713300	-6.23618100	F	-2.86725500	-2.57666200	-3.77664300	C	-7.55772500	-3.49259800	-1.58573400	C	-4.52812100	-5.09132300	-5.65017200
F	-2.91342400	-5.62168000	-7.43995100	F	-7.06892100	-3.03557900	-2.36207600	H	-7.38976700	-2.99958300	-3.26878800	C	-3.12929100	-4.55774500	-5.65422300
F	-3.21685800	-2.													

H	-13.56409100	-2.08831400	-2.12632000	H	-11.87413100	1.73748900	-10.12190900	H	-9.73781100	4.70307000	-12.35251300	O	-6.14223800	10.07681400	-0.02634200
				C	-11.00423600	1.86879200	-10.77962800	O	-7.72491200	4.25304600	-9.66430300	C	-5.40141000	10.96588000	2.63598600
				Zr	-9.10735500	1.42848200	-9.59020700	C	-7.42946300	4.56416600	-8.41235100	H	-5.60634400	12.80450200	1.46577400
				H	-11.16848100	1.25147100	-11.67212000	H	-7.95637300	5.93757000	-8.00614600	H	-7.12008300	12.15038700	2.02666400
C⁻P2 in gas-phase				O	-10.98205500	2.91836300	-11.10334600	O	-6.80778800	3.82450400	-7.66067800	C	-3.86325300	10.98212300	2.54409900
C	0.18072700	0.11643800	0.41269900	H	-9.35504900	2.86315600	-8.12669100	H	-7.60885100	6.40119800	-6.58354500	H	-5.78164100	9.94152700	2.55078100
C	0.86367300	0.33611600	1.75286000	C	-8.90741800	3.29975700	-6.96508400	H	-7.61568900	6.66480400	-8.75541200	H	-5.66920500	11.31012000	3.64292900
H	0.87534100	-0.15947600	-0.38609800	C	-9.77260700	4.41024100	-6.37557900	H	-9.04659600	5.89140200	-8.13278600	C	-3.22393400	10.31415000	1.31331900
H	-0.61081600	-0.62936300	0.47159300	O	-7.91402600	2.84149100	-6.41060600	H	-6.23856100	7.08619400	-6.41600400	H	-3.45917000	10.49849300	3.44204300
C	1.47239700	2.67887500	-0.28158300	H	-10.75892400	3.95896900	-6.20036900	H	-7.70246400	5.55097400	-5.89803600	H	-2.14246300	10.50381500	1.33333400
C	2.16257400	1.14851100	1.69312200	H	-8.23084800	6.19453700	-5.26725100	H	-6.21263100	7.56886100	-5.43104100	H	-3.45006000	8.81381100	1.20909100
H	1.43088800	0.78578100	2.44813100	H	-8.85011000	4.27450600	-4.43057400	H	-6.16251500	7.89892600	-7.15191800	H	-2.96689900	8.39489900	0.32372700
H	1.08366000	-0.66356000	2.14816100	H	-10.11678000	5.48159600	-4.55367900	C	-4.85132400	5.12448900	-5.48118200	H	-4.51588600	8.56668000	1.15622100
C	2.01270500	2.58216200	1.17061400	C	-6.82893900	5.80604000	-5.77304900	H	-4.09621800	6.84215100	-6.51671500	O	-2.87458200	8.19148900	2.39084500
H	1.99515800	1.95489800	-0.92249600	H	-8.11585700	6.71477700	-4.30811000	H	-4.93769900	5.68721200	-7.51585000	C	-2.99314000	6.86046000	2.49756700
H	1.64504000	3.67348200	-0.06718500	H	-8.65206500	6.93416400	-5.96220400	H	-3.94457000	4.52796800	-5.62573700	C	-2.34334100	6.36264000	3.77906600
H	2.89292200	0.61380800	1.06641400	C	-6.03799600	4.90980500	-4.83344200	H	-5.70312000	4.44354600	-5.47463800	O	-3.54007500	10.57382000	1.66764400
H	1.37303600	3.17374400	1.83755600	H	-6.25397900	6.72251700	-5.95688900	H	-4.75781400	5.78890800	-4.18757300	C	-2.27802700	4.92867700	4.18559600
C	0.00272600	2.41888600	-0.38151200	H	-6.89574000	5.27725800	-6.73009800	C	-4.76519100	5.00511400	-3.10564900	H	-1.25438000	6.46507500	3.64515900
O	-0.72735800	3.37280600	-0.80797300	H	-5.04920800	4.67288700	-5.23901000	H	-4.56267500	5.83818600	-1.83893100	H	-2.61579800	7.06955600	5.45708100
H	-14.33206100	1.61520900	-2.97351300	H	-5.85079800	5.63615000	-3.58069800	C	-4.97106500	5.11746700	-5.40404200	H	-1.09831100	10.15525500	1.18922400
H	-14.29404600	1.51414200	-4.06648200	O	-5.21116600	5.00407200	-4.25961900	H	-3.52822600	6.20701100	-1.77349700	H	-1.86676800	3.76888500	3.64528500
Zr	-12.13257700	1.14228800	-4.70554400	C	-5.07200000	5.89197800	-1.36985800	H	-5.17726000	6.73282000	-1.98435800	H	-2.67365900	4.87875400	5.28014000
H	-15.01358300	0.73584400	-4.35059000	O	-4.77872700	3.86523800	-2.68557500	C	-2.31776300	2.93535400	-1.34655400	H	-2.01251600	3.40515300	2.15172800
H	-14.68392000	2.46017200	-4.50546000	H	-5.13893900	5.15797700	-0.01425700	H	-3.90001700	4.30110700	0.21279200	H	-1.22551200	5.23360700	1.25311300
O	-10.33248300	2.88858700	-3.96487100	H	-4.12253400	6.44052300	-1.46231800	H	-5.83836800	4.47687600	-0.74174200	H	-1.26679400	3.83504000	1.05989300
H	1.29720900	3.07106100	1.17046000	C	-5.85714600	6.65176600	-1.42059900	H	-5.31967600	5.89204400	0.15384600	H	-0.80916000	3.96068500	3.87626800
O	-0.57006600	1.31073700	-0.05348300	H	-2.32079000	3.36589200	-1.17482300	C	-3.49726000	2.93448600	-0.38428500	H	-2.14153600	2.80658000	4.22917300
C	0.00272600	2.41888600	-0.38151200	C	-3.84522600	4.54652200	0.56340500	H	-2.44631200	3.67183000	-2.15175800	H	-3.04050600	3.58919000	1.82177600
O	-0.72735800	3.37280600	-0.80797300	H	-5.91605200	4.38448700	-0.05716400	H	-2.12564900	1.96540100	-1.76730800	H	-1.82269900	3.23007000	2.01682800
H	-14.33206100	1.61520900	-2.97351300	H	-5.48807300	5.89362900	0.70011100	H	-4.30047300	4.92066000	0.36492100	H	-8.31235400	9.37622900	-1.06014400
H	-14.29404600	1.51414200	-4.06648200	C	-3.34505400	3.22403200	-0.06198000	H	-3.00876000	4.11420500	1.21679500	H	-8.99297800	9.96856900	-1.65729800
Zr	-12.13257700	1.14228800	-4.70554400	H	-2.60064400	4.10033200	-1.92280400	H	-3.38734000	2.50681600	-0.93878900	C	-9.98225800	10.58588600	-1.16769200
H	-15.01358300	0.73584400	-4.35059000	H	-2.00818100	2.41715000	-1.65444200	H	-4.25927400	2.23206200	0.42450000	H	-8.97925900	10.06887300	-3.07019000
H	-14.68392000	2.46017200	-4.50546000	H	-4.03954400	4.35146900	1.62477000	H	-7.63854100	1.55201800	-8.17448900	H	-10.60439400	11.48928500	-0.22787600
O	-10.33248300	2.88858700	-3.96487100	H	-4.18271300	2.67476100	-0.50310400	H	-9.54521000	1.59870600	-9.33585800	H	-10.21949700	11.00383100	-1.25857000
H	1.29720900	3.07106100	1.17046000	C	-2.92049400	2.57504300	0.17484900	C	-7.71804400	0.45695000	-10.11936600	C	-9.83471000	10.00661000	-3.45693200
O	-0.57006600	1.31073700	-0.05348300	H	-8.91329700	0.25263700	-6.61872900	H	-9.89357200	1.03332500	-10.59074600	H	-11.40565700	12.21397900	-2.23232700
C	0.00272600	2.41888600	-0.38151200	C	-9.21107900	-0.17109900	-7.56890200	H	-10.18664400	2.21206000	-8.71612100	H	-10.24497400	11.27335500	-4.47138500
H	-14.33206100	1.61520900	-2.97351300	H	-10.51683200	-0.16083100	-8.12308700	H	-6.73241700	0.01552400	-10.19037600	H	-6.73829400	12.15230200	-4.36820800
H	-14.29404600	1.51414200	-4.06648200	H	-8.33873800	-0.75841000	-8.51855300	C	-8.76271200	0.33415700	-11.08231900	C	-7.73645800	13.12780200	-4.87299000
Zr	-12.13257700	1.14228800	-4.70554400	H	-10.45920400	0.76466500	-9.40732100	H	-8.74135200	1.12594800	-11.08762500	H	-5.87341300	12.69232400	-3.38379800
H	-15.01358300	0.73584400	-4.35059000	H	-11.40309400	0.24829200	-7.65449400	H	-10.81912000	0.22293700	-12.00908700	H	-6.63912500	11.18296900	-4.83905400
H	-14.68392000	2.46017200	-4.50546000	C	-7.27717000	-0.92234400	-7.86764500	C	-5.83202600	2.25298500	-12.18863300	C	-7.48662200	14.26254600	-3.84558900
O	-10.33248300	2.88858700	-3.96487100	H	-9.11234000	-1.12895800	-9.65740400	H	-6.82876000	2.00315500	-13.17709400	H	-8.52848800	13.03169700	-5.38862300
H	1.29720900	3.07106100	1.17046000	H	-11.29394800	-0.91361100	-10.07828200	C	-5.79148400	3.65095900	-11.95569400	C	-6.34222200	15.98839700	-3.05637000
O	-0.57006600	1.31073700	-0.05348300	H	-8.74318400	-1.62934500	-10.54335100	H	-5.19185300	1.51322600	-11.72587900	H	-5.02899100	12.18558200	-2.83452200
C	0.00272600	2.41888600	-0.38151200	C	-6.67732800	1.40990700	-10.38529500	C	-7.40837500	3.24494800	-13.53683100	H	-8.06684700	15.17469700	-3.90912000
H	-14.33206100	1.61520900	-2.97351300	H	-7.46272500	1.07295500	-11.52589100	H	-7.08062600	1.03786800	-13.59638300	H	-5.91166100	14.64806700	-2.30806000
H	-14.29404600	1.51414200	-4.06648200	C	-6.94739300	2.76063900	-10.05318100	C	-6.71367400	4.26179400	-12.77354400	O	2.01379100	11.61835300	0.91057000
Zr	-12.13257700	1.14228800	-4.70554400	H	-5.97537900	0.76044400	-8.97920700	H	-5.15331500	4.15647300	-11.24258100	C	2.00747000	-2.19803500	-0.22763300
H	-15.01358300	0.73584400	-4.35059000	C	-8.21816300	2.21595800	-11.88945700	H	-8.19690700	3.39444100	-14.26246400	H	1.04542400	-1.91963000	-1.03259400
H	-14.68392000	2.46017200	-4.50546000	H	-7.45952000	1.02115100	-12.04309500	C	-7.00942200	5.31792200	-12.80240700	C	3.10834400	-3.17088400	-0.50589400
O	-10.33248300	2.88858700	-3.96487100	C	-7.90858500	3.25447400	-10.97182000	O	1.83591500	-1.73369900	1.08858000	C	0.93100400	-2.50543800	-2.39771200
H	1.29720900	3.07106100	1.17046000	H	-6.53166000	3.29814800	-9.21070700	C	1.82877600	-2.73812800	0.36033500	C	2.60113200	-4.62044900	-1.72954800
O	-0.57006600	1.31073700	-0.05348300	H	-8.91154900	2.28408400	-12.71612500	O	0.99055200	-2.75736000	-0.66124400	C	6.65391300	-1.62045000	-1.39569000
C	0.00272600	2.41888600	-0.38151200	H	-8.34312600	4.24614400	-10.96595400	C	2.73762400	-3.90231400	0.66679500	C	3.79407500	-3.12350700	0.34237400
H	-14.33206100	1.61520900	-2.97351300	C	3.51369600	-0.27726900	4.07452200	C	0.90325400	-3.88267800	-1.59627400	C	0.69829400	-4.00775800	-2.37475300
H	-14.29404600	1.51414200	-4.06648200	C	3.50188100	-1.48527900	0.25964300	C	1.97408500	-5.19280200	1.05577800	H	1.83064700	-2.21467600	-2.94794300
Zr	-12.13257700	1.14228800	-4.70554400	C	2.29487100	-0.09802200	0.21804100	H	3.37922400	-4.09642700	-0.20352000	H	0.07628200	-1.96709900	-2.79651100
H	-15.01358300	0.73584400	-4.35059000	C</											

C	-8.19379800	6.20350400	-5.29523800	H	-3.57187200	6.21496900	-1.80292600	C	-9.14253900	9.77899500	-2.65646700	F	3.24089200	0.28393900	-4.26912000
H	-8.82599400	4.29515500	-4.44157900	H	-5.22792200	6.73155900	-1.98356300	C	-10.53501200	11.56192700	-2.24616600	F	4.12295600	1.28516500	-1.88513300
H	-10.08567700	5.50788100	-4.58038600	C	-2.31512100	2.99026300	-1.41330200	H	-10.13971100	11.60949900	-0.04838700	F	6.47714400	0.37820400	-0.83373900
C	-6.79301600	5.80221600	-5.79166800	C	-3.89894900	4.29645600	-1.77791600	H	-8.60866100	8.98447500	-3.16127300	F	7.96681700	-1.37568800	-2.14689200
H	-8.07961700	6.73361800	-4.34139500	H	-5.85143800	4.45853700	-0.74875100	C	-10.02428200	10.71982500	-3.26538400				
H	-8.60837500	6.93784600	-5.99969700	H	-5.33490400	5.87288200	-1.48806000	C	-11.23099900	12.37808700	-2.38323800				
C	-6.01008900	4.91133200	-4.83963000	C	-3.48381500	2.94256900	-0.43944400	H	-10.28438800	10.76250400	-4.31514400				
H	-6.21121700	6.71349000	-5.88270900	H	-2.45791400	3.72141200	-2.20429700	C	-6.69045000	11.13894400	-4.43378500				
H	-6.85793500	5.26363900	-6.74324200	H	-2.11526800	2.01202300	-1.85284500	C	-7.55219200	12.14416800	-4.96156300				
H	-5.02073800	4.66485300	-5.23798300	H	-3.01060100	4.92640800	-0.32831200	C	-5.72705600	11.77743900	-3.61356800				
H	-6.53251300	3.97809800	-4.62711700	H	-4.28748500	4.09265200	-1.18347200	C	-6.74430700	10.07872200	-4.64362800				
O	-5.82407100	5.65045600	-3.59358000	H	-4.32467100	2.50989600	-0.99082400	C	-7.11913900	13.39773200	-4.46128500				
C	-5.19590100	5.02635500	-2.59768600	H	-3.22791700	2.23231200	-0.35805000	H	-8.37437000	11.98328600	-5.64684600				
C	-5.05824100	5.92786400	-1.38122800	H	-8.97414700	1.91511500	-7.96528700	C	-5.99926600	13.16930800	-3.61873200				
O	-4.77068900	3.88320500	-2.66921500	C	-9.22019200	1.54081900	-8.95032600	H	-4.95071400	11.28170900	-3.04505200				
C	-5.15307300	5.21174400	-0.01780500	C	-10.27125600	1.99656500	-9.78669000	H	-7.56647200	14.35788000	-4.67809800				
H	-4.09201000	4.64036300	-1.46835200	C	-8.48582200	0.56317800	-9.66605800	H	-5.45706900	13.92463700	-3.06407700				
H	-5.83091200	6.69875300	-1.45096200	C	-10.20510900	1.28234300	-11.01256900	O	1.93673800	-1.16085900	-0.51328300				
C	-2.35133300	3.35510100	-1.11752500	H	-10.99293800	2.76505700	-9.53958100	C	1.59557200	-1.18517300	-1.95475000	Zr	1.29691100	-2.25398400	0.35030100
C	-3.87507900	4.59128300	-0.58426000	H	-7.62985100	0.01625400	-9.29322300	C	2.45868000	-1.60583900	-2.46568000	C	-0.47514500	-3.00421400	1.57474200
H	-5.93966300	4.44797000	-0.06109200	C	-9.09835800	0.39949800	-10.94309900	H	0.73248500	-1.84545600	-2.03847000	H	-0.55671300	-2.59108000	2.58804200
H	-5.50183100	5.96087600	-0.70280500	H	-10.87634000	1.39723800	-11.85247300	H	1.36282300	-0.17233300	-2.28905100	H	-1.40820400	-2.76771500	1.04622200
C	-3.86030000	3.25082200	-0.01087200	H	-8.79356600	-0.29949100	-11.71134600	H	-10.40386600	-0.66779100	-0.35644200	H	-0.40386600	-0.49630900	1.66892800
H	-2.62037900	4.06725000	-1.89031900	C	-5.75643800	1.69499900	-11.15029300					H	1.21923300	-5.38625200	-2.36717300
H	-2.10890100	2.39131100	-1.56435600	C	-6.36828300	1.57182400	-12.43188100					H	0.02352500	-0.50097500	-2.98398900
H	-3.06291500	5.33216800	-0.56554200	C	-5.51779500	3.07094900	-10.91090100					H	-0.34975600	-5.06175800	-4.47320500
H	-4.08484000	4.41617500	-1.64677300	H	-5.49476100	0.88079700	-10.48744700					H	0.50066900	-5.95192100	-2.67451900
H	-4.22651800	2.70366100	-0.44975900	C	-6.50699200	2.87316900	-12.97645500					H	-0.86195900	-4.90377200	-2.34996600
H	-2.97768000	2.61119500	-0.78237300	H	-6.64923600	0.64630300	-12.91754900					C	2.18874000	-3.67452000	-4.71099300
H	-8.87678900	0.25158800	-6.59626000	C	-5.99366200	3.79995200	-12.03084000					H	0.75125100	-5.65935500	-5.39667600
C	-9.19033500	-0.17825100	-7.53898400	H	-5.09770300	3.48965200	-10.00560700					H	-0.61319400	-4.05733000	-4.87122500
C	-10.50216200	-0.15696000	-8.07870300	C	-6.93533100	3.11796800	-13.93856900					H	-1.26567300	-5.65493500	-4.56699300
C	-8.33629200	-0.78576900	-8.48249400	H	-5.98226500	4.87712900	-12.13971900					C	2.15499600	-5.12078400	-5.03397700
C	-10.46685800	-0.77367000	-9.35746100	O	1.79751900	-1.76393000	0.84918500					C	3.18846000	-3.21086400	-4.78257100
H	-11.37795200	0.26765100	-7.60414700	C	-3.20414800	-2.54720300	-0.35221100					H	1.51635700	-3.04906600	-3.53534300
H	-7.27548300	-0.96208000	-8.37199600	H	2.54718900	-1.95427200	-1.11551600					H	0.52430100	-5.43468400	-6.40531100
C	-9.12708100	-1.15683600	-9.61923800	H	2.62533800	-3.42515800	-0.08358600					H	0.75797400	-6.75143900	-5.25449100
H	-11.31058000	-0.91886000	-10.01755500	H	1.05393600	-2.86140800	-0.71023300	Zr	2.17966700	-2.44017300	0.29723100	H	2.80159800	-5.27447000	-5.91062100
H	-8.77447200	-1.67049800	-10.50431400	H	2.65226800	-1.51445200	1.24543100					H	6.24273600	-6.67619800	-4.21189200
C	-6.65980900	1.36300300	-10.36847000									O	1.84933500	-3.32424900	-3.29805800
C	-7.44560000	1.01096800	-11.50427500									C	0.95459300	-3.89461100	-2.54866500
C	-6.92588500	2.71954100	-10.05742100									O	0.86645300	-3.50145200	-1.35959800
H	-5.95973700	0.71945700	-9.85241500	C ⁺ -P3 termination	C	0.86891500	-0.59945100	0.44440700				H	1.00472000	-4.80802500	1.32625300
H	-8.19757900	2.15046400	-11.88557100	C	1.48697400	-0.46545300	1.81296500					H	1.88505400	-10.52376000	-1.97027000
H	-4.44745500	0.05239800	-10.00695400	H	0.57218100	0.36756200	0.03668500					H	1.32833400	-5.01156400	-3.28972600
H	-7.88517800	3.20212000	-10.98388800	H	0.07632300	-1.34433000	0.37395600					C	0.57131900	-5.13146600	-4.61886200
H	-6.50858000	3.26873600	-9.22330000	C	2.28766100	2.87534200	2.72387800					H	2.24916300	-5.60955700	-3.30603500
H	-8.89037700	2.20808100	-11.87367200	C	2.74176100	0.44771600	1.85320200					H	1.76321100	-5.42889400	-2.46759300
H	-8.31675600	4.19530500	-10.99353900	H	0.68344800	-0.03018200	2.14605800					C	1.64591800	-2.45782600	-5.01470300
O	3.37616500	-0.44977300	0.44259600	H	1.70317700	-1.45393200	2.23320600					C	1.42611400	-4.87677400	-5.86494500
C	3.54830000	-1.62484900	-0.35468900	C	2.77143600	1.44666500	3.03865700					C	1.29617200	-4.45953300	-4.60287500
H	2.62736000	-1.75447000	-0.92846600	H	2.95674800	3.32622900	1.97649100					C	0.15723900	-6.14453600	-4.66611400
H	4.38465900	-1.52536200	-1.05881600	H	2.36279300	3.49791000	3.61918000					C	2.28291300	-3.59891900	-5.78388100
H	3.70722500	-2.51999500	0.26165800	H	2.82094400	1.03347400	0.92370600					C	2.14500800	-1.51380600	-5.21530700
H	4.19231400	-0.32447800	0.95345900	H	3.63451800	-0.18777600	1.99094600					H	0.75463800	-4.81587200	-6.73443600
				H	2.19479700	1.03181700	3.87471300					H	2.08627600	-5.73166700	-6.05060300
				H	3.80086300	1.53527700	3.40077100					C	2.50263200	-3.22633000	-6.79101200
				O	0.41411200	2.22667500	1.32265000					H	4.40174300	-6.60491000	-9.00942800
				C	0.87975000	2.98888500	2.16119600					C	3.32628300	-3.79652100	-5.33869700
				C	0.23834700	4.04242900	2.65493500					O	1.81328100	-2.56180300	-3.54497600
				H	-9.47862500	14.14493300	-1.21115700					H	1.72386300	-3.63301600	-2.81038300
				H	-8.93340200	14.12166600	-2.16433200					O	1.99151600	-3.49858400	-1.59278500
				Zr	-8.00653000	12.05242200	-2.43593800					H	-0.43659200	-1.33434800	-1.24901700
				H	-9.62980900	14.43934600	-2.95083700					H	-0.06275000	-1.26585300	1.43469000
				H	-8.12937100	14.86814400	-2.11115400					C	2.98238000	-3.95023600	3.01977900
				O	-6.83261200	12.05203900	-0.74201500					H	3.67324300	-5.26297900	0.76832400
				C	-6.28902500	11.31444400	-2.01100900					C	5.02354300	-3.56340300	-0.80827300
				C	-5.93989600	12.12068800	1.45866400					H	5.14528900	-1.18216200	0.43074600
				H	-6.10385500	10.10825700	0.10386800					C	3.88093500	-1.41957800	2.80663300
				H	-5.30408500	11.33219400	0.61443700					H	1.61673900	-0.07317500	2.37486000
				H	-5.30303200	12.96093600	1.14997300					H	7.35688800	-2.58169800	-4.94844400
				H	-6.87844800	12.58580200	1.78862700					C	5.71919800	-1.99815600	-6.47563300
				C	-3.77009900	11.19858900	2.57265400					H	8.02045800	-1.02318400	-6.44794600
				H	-5.77533200	10.34436600	0.67310700					H	8.14129100	-2.65850400	-7.09124200

F	7.86157100	-4.58689900	-7.27209200	C	12.40647200	0.55421000	-2.91039800	H	6.78845100	0.57076400	-9.30715300	C	3.98923300	-2.38741500	-4.32309600
F	7.69164900	-5.59939600	-4.72226600	C	8.11423000	-2.04231100	-3.90090100	H	4.01140700	-0.20120800	-9.17157200	C	3.07500400	-4.79841800	-4.35242000
F	8.01555000	-4.03498200	-2.61804900	C	8.23189100	-3.41347400	-3.63766200	H	5.28424300	-0.99539900	-10.08049300	H	1.28587000	-3.58372000	-0.40580300
F	5.86160900	-2.43890400	-2.16353800	C	8.10149000	-1.74285300	-5.26672000	O	4.04959300	-0.52059100	-6.37665500	H	0.98732700	-5.28750300	-4.35804700
F	4.91929500	-3.27519200	0.17182300	C	8.27303600	-4.40153600	-4.62250500	C	4.41019500	-1.61380400	-6.77612300	C	4.15137900	-3.82302800	-3.84598700
F	6.25658200	-2.72352800	2.50195700	C	8.13956600	-2.69269900	-6.28367800	O	4.44933600	-2.71340700	-6.01262200	H	4.15824000	-1.73287100	-3.83615700
F	8.67538500	-1.42507400	2.38045800	C	8.21739400	-4.04148100	-5.96347500	C	8.45184400	-0.50291700	-3.14766100	H	2.99182300	-1.99705700	-4.12786000
F	7.62348600	-0.64329800	0.05850700	C	7.62305900	-1.35865200	-1.24365900	C	7.26758700	0.53961800	-3.62862500	H	3.04887500	-4.74508400	-5.44858700
F	7.38757900	3.87241200	-4.46105100	C	6.49014400	-2.16301000	-1.08638600	H	7.32979000	1.48997600	-3.07837000	H	3.39159300	-5.82238000	-4.10643100
C	7.68487700	5.32430200	-4.81603800	C	8.14151200	-0.88271300	-0.03751500	H	7.28740000	0.77795100	-4.69284600	H	5.13828100	-4.17979700	-4.16644000
H	8.18755600	3.40402000	-3.88596800	C	5.93334000	-2.50317000	0.14032000	H	6.27720000	0.11920400	-3.41228900	O	4.17788100	-3.79957700	-2.87139000
H	6.46077300	3.78632100	-3.89299200	C	7.61453400	-1.18711900	1.01938600	C	9.99584200	0.09675800	-3.33060000	O	1.95385300	-2.51588200	-1.85303000
C	4.92226600	3.28960600	-6.48530500	C	6.49705100	-2.00562700	1.30865700	C	11.09253200	-0.50136400	-2.69761000	C	1.77764700	-3.64810200	-1.41101600
C	9.11317600	5.58013800	-5.31639200	F	13.68756500	0.94273000	-2.97764900	C	10.35847000	1.13149400	-4.19073400	O	1.81735300	-3.97316600	-0.12279200
H	6.94394800	5.66894600	-5.55014200	F	11.69383600	2.53290000	-4.02931800	C	12.41555500	-0.09604200	-2.85620100	H	0.55182300	-1.63229600	0.38803000
H	7.51487200	5.91349900	-3.90554900	F	9.17518800	1.78819500	-3.92376500	C	11.66432300	1.57880200	-4.38169100	H	0.85586600	-1.84468600	3.05865100
C	9.48549900	4.82931200	-6.60063900	F	10.45981900	-2.22660200	-1.69788700	C	12.71118000	0.96288500	-3.71170700	H	1.78058700	-5.47256200	4.32475200
H	9.89956700	2.95412900	-5.55540800	F	13.01211500	-1.44694100	-1.81189600	C	8.47711800	-1.89790900	-4.06143500	H	2.69043300	-6.46442500	1.99391200
H	9.95910800	2.82335000	-7.31401300	F	8.07188700	-0.44756000	-5.70020400	C	8.66818100	-3.19288200	-3.56360600	H	4.51593700	-4.76434900	1.01508800
H	9.82227700	5.30164100	-4.52451100	F	8.08916900	-2.31633200	-7.58236500	C	8.37729000	-1.85337800	-5.45554900	H	4.72606200	-2.68931200	2.71562100
H	9.24292600	6.65610100	-5.48428100	F	8.24888500	-4.97105800	-6.92878100	C	6.88863900	-4.34221400	-4.35412500	H	3.03993500	-3.18995000	4.78176100
H	8.85221000	5.16178100	-7.43445700	F	8.36910100	-5.69746300	-4.28768400	C	8.38133700	-2.97113900	-6.28535400	H	1.48636400	-1.20008600	4.21095800
H	10.11400600	5.08914200	-6.87514300	F	8.51289500	-3.87182000	-2.37406500	C	8.53327900	-4.23558200	-5.73157400	H	5.18240000	-3.08292800	-8.16667500
O	7.10984600	3.03947400	-5.63255300	F	5.84810600	-2.65605500	-2.17302600	C	8.05099800	-0.76720400	-1.55544900	C	5.38503300	-2.41983500	-8.78610600
C	8.02644600	2.71816500	-6.53050400	F	4.83715000	-3.28961300	0.20530700	C	6.96908300	-1.58696500	-1.21427000	H	6.13926200	3.54930200	-7.08590600
O	7.69807900	1.94254800	-7.44057100	F	5.94862300	-2.29221600	2.50898100	H	8.56693900	-0.06276100	-0.46869900	H	6.11444000	-4.47130600	-6.80961600
C	7.26134500	0.29827200	-2.92351500	F	8.16623000	-0.68334300	2.53566000	C	6.46678300	-1.73020000	0.07400500	C	4.05834500	-1.28105200	-7.84166400
H	6.23475700	-0.07730300	-2.85751900	F	9.20514300	-0.04521200	-0.02237400	C	8.09406300	-0.15788500	0.84006700	C	5.95549000	1.05257600	-8.09924800
H	7.36930200	1.07016500	-2.15356500	C	8.67852900	4.61708400	-4.70267100	H	7.03200300	-1.00711200	1.11755200	H	4.35494200	2.79348300	-8.69746900
H	7.35860500	0.79480200	-3.89644700	C	9.31892600	5.75761600	-5.47813000	F	13.97403400	1.37560500	-3.88409700	H	5.96748000	2.34245000	-9.86101900
				C	9.39765900	3.99045900	-4.17543300	F	11.91525100	2.61260300	-4.522542300	H	4.16727000	0.06678400	-8.56949100
				H	7.92446400	4.97101200	-4.00061800	F	9.42213100	1.81187100	-4.91951400	H	5.44703000	-1.74641600	-7.90933800
				C	8.95471100	2.95076600	-6.83291500	F	10.89186900	-1.53623700	-1.85917300	H	3.75887800	-1.98999800	-8.30456100
				C	10.58014000	5.36837100	-6.26280100	H	13.40897400	-0.71144900	-2.19807300	H	5.39438300	1.18587700	-7.02790200
				H	8.56681000	6.21480400	-6.13483300	F	8.28609900	-0.66145600	-6.10886000	H	6.49134100	1.06263100	-8.27299400
				H	9.58185900	6.52096800	-4.73465300	H	8.25549300	-2.83356400	-7.62027500	H	3.42864900	0.52010900	-8.41847400
				C	10.35446600	4.31950200	-7.35961200	F	8.34417200	-5.32660300	-6.50999500	H	4.52302700	-0.11316900	-9.64817500
				H	10.43022200	2.66032000	-9.94651100	H	8.85980600	-5.55143200	-3.79696400	C	3.70639100	-1.07008400	-5.81021200
				H	9.98019600	2.17014700	-7.58566800	F	8.84181100	-3.40840500	-2.24368200	C	4.09472800	-1.17827100	-6.38636900
				H	11.33359000	4.98931000	-5.55950500	C	6.32343400	-2.29519000	-2.16816200	C	4.24983900	-2.36305800	-5.57365000
				H	11.00407800	6.26995500	-6.71968000	F	5.41985500	-2.54549600	0.31610400	H	8.42116500	-2.96297600	-3.30719000
				H	9.66331800	4.69953100	-8.12335900	C	6.53734500	-1.07747000	2.36860800	C	7.53716300	0.96898900	-3.94597300
				H	11.30380200	4.12894200	-7.87098900	F	8.64308100	0.57865500	1.82556800	H	7.61136000	1.86280800	-3.31134400
				O	7.87793200	3.71624000	-5.56679000	C	9.57938300	0.83547200	-0.63927300	H	7.82884300	1.25779000	-4.95761000
Zr	11.99937000	-3.32038000	1.32421100	C	8.40814000	2.95075700	-6.453736900	C	8.94023000	4.81848200	-5.11908500	H	6.47118000	0.71057600	-3.99168800
H	-1.06254000	-3.60119800	1.57547400	O	7.64494200	2.16958600	-7.11491900	C	9.49110500	6.07427200	-5.76658600	C	10.04980100	0.12216300	-3.20447300
H	-1.45765800	-3.36241600	2.57177000					H	9.71591000	4.11274700	-4.82912300	C	10.89583400	-0.11615000	-2.11341700
H	-1.58838300	-2.96529600	0.84987000					H	8.31135600	5.02686400	-4.25912800	C	10.72427600	0.65771900	-4.30355000
H	-1.31943100	-4.64639400	1.35686800					C	9.76349500	3.54125700	-7.65981100	C	12.26014900	0.18084100	-2.09632000
H	2.88925400	-1.17514700	-0.23682000					C	10.61950700	5.82424500	-6.77643900	C	12.07969100	0.96809100	-4.34075600
C	0.82079900	-0.92813700	0.48003600					H	8.66991800	6.64856100	-6.21645100	C	12.86495800	0.73150700	-3.22046800
C	3.02111700	-0.94947300	1.80088400					H	9.88319400	6.66684600	-4.93307300	C	14.91968600	-1.65495900	-4.21898200
C	2.22745500	-1.10471500	0.55499900					H	10.22123800	4.98257600	-7.99647100	C	9.06186000	-2.80631200	-3.74773300
C	2.57956800	-1.25359600	1.91932900					H	10.45030800	3.08622000	-6.93486800	C	7.90053700	1.08776100	-5.50727900
H	3.57854700	-1.40759400	2.30464900					H	9.75862900	2.91282200	-8.55298400	C	9.18881500	-3.99506600	-4.46658900
C	1.38546300	-1.16362600	2.06186000					H	11.45033100	5.32974200	-6.25628400	C	8.09008000	-2.92626000	-6.27183600
C	1.00056300	-5.21005600	3.09113800					C	8.65955800	-4.06473100	-5.75060600	C	8.63597500	-1.49207800	-1.44923800
C	2.02331500	-4.33903000	3.54288900					H	7.86262000	0.50061900	-0.82795200	C	7.86262000	0.50061900	-0.82795200
C	1.45371300	-5.83406500	1.89727200					H	6.14551600	-1.53031600	-0.23617200	C	7.20684500	0.51431200	0.39513800
C	3.11045200	-4.42240300	2.62639700					H	6.33237700	-0.52240500	0.69987000	C	6.33237700	-0.52240500	0.69987000
C	2.75779300	-5.35665600	1.61919900					H	14.17278100	1.02814300	-3.32635500	H	14.17278100	1.02814300	-3.32635500
Zr	11.99937000	-3.32038000	1.32421100					H	12.63070600	1.50893000	-5.54044000	H	12.63070600	1.50893000	-5.54044000
H	-1.06254000	-3.60119800	1.57547400					H	10.04882800	0.93249000	-5.46809000	H	10.04882800	0.93249000	-5.46809000
H	-1.45765800	-3.36241600	2.57177000					H	10.42480800	-0.65287600	-0.97077100	H	10.42480800	-0.65287600	-0.97077100
H	-1.58838300	-2.96529600	0.84987000					H	12.99787100	-0.06106700	-0.99845700	H	12.99787100	-0.06106700	-0.99845700
H	-1.31943100	-4.64639400	1.35686800					F	7.23595300	-0.7					

C	10.97811800	5.02921600	0.14945400	F	7.62936600	-4.38670600	-6.88352600	O	4.01889000	-0.52747700	-6.33498600	H	-1.02566800	-2.92112100	3.02007800
H	10.30256000	2.99257900	-0.26514000	F	7.50231800	-4.83620100	-4.17960600	O	4.37609000	-1.62384000	-6.73059300	H	2.27549600	-6.26589600	3.88397500
H	11.77544700	3.44330700	-1.12245100	F	8.00362300	-2.88940100	-2.45737800	O	4.37007400	-2.72789100	-5.97473900	H	3.28629200	-6.07690280	1.44083900
H	9.49745600	4.50986000	1.62862600	F	5.98613100	-1.16016400	-2.49814500	B	8.54252900	-0.45089400	-3.32278100	H	4.70756700	-4.61654400	0.66933000
H	9.97413200	6.20166200	1.65407800	F	4.82192200	-1.31229000	-0.11130300	H	7.44299100	0.62478400	-3.91780300	H	4.57279900	-2.78449400	2.61936500
H	1.28984700	5.90368900	-0.43399200	F	6.06681000	-0.22324200	2.09674900	H	4.74807200	1.57137200	-3.35898000	H	3.06323300	-3.79926200	4.61711900
H	11.80637100	4.79597800	-0.82774100	F	8.46356600	1.01804400	1.82168800	H	7.56803300	0.85880800	-4.97616100	H	1.21183700	-1.98909100	4.18598100
O	8.77342800	4.53850100	-2.00958900	F	9.68356700	1.10444700	-0.51294300	C	6.42772700	0.22611400	-3.79236600	C	6.43113800	3.67600600	-8.12689300
O	10.02818700	4.11953700	-2.04851600	C	9.87067900	5.66153100	-4.54197000	C	10.12494400	0.07568700	-3.42175800	C	5.20676200	2.61415400	-8.60687300
C	10.57658800	4.02201200	-3.15538200	C	10.81403800	6.07855400	-5.65125100	C	11.15410300	-0.54639400	-2.70106600	H	6.36488400	3.64149500	-7.06823900
				C	10.07043300	3.15015400	-7.32386900	C	10.57563800	1.12372500	-4.21453900	H	6.62079300	4.28400100	-8.70730600
				C	11.69295200	4.95714900	-6.25244000	C	12.48785600	-0.14381200	-2.71884200	C	3.58271000	-0.82874000	-7.67535100
				H	10.18157500	6.52210700	-6.42740300	C	11.88807000	1.58789400	-4.24416600	C	4.95521100	1.31787400	-7.82595800
				H	11.45329800	6.88175500	-5.26321000	C	12.86437200	0.95116100	-3.49321800	H	4.34772500	3.29268500	-8.51072400
				H	11.16273900	4.22544700	-7.50438700	C	8.53863800	-1.88590600	-4.17122000	H	5.31606500	2.39814200	-9.67829900
				H	10.20305100	2.61728000	-6.37349300	C	8.65920200	-3.16192400	-3.60561500	C	3.70591400	0.56439100	-8.30120400
				H	10.15507900	2.38736600	-8.10342200	C	8.64219800	-1.90792700	-5.56733700	H	4.47406900	-1.43377100	-7.87898000
				H	11.94880700	4.22404300	-5.47846900	C	8.64583000	-4.34912100	-4.33803400	H	2.73679300	-1.37315100	-8.11728300
				H	12.64412200	5.42038100	-6.54262300	C	8.42949100	-3.06587000	-6.34016400	H	4.85160000	1.54593200	-6.75844200
				H	10.83068600	4.96454600	-8.24511400	C	8.51942200	-4.30580300	-5.72186400	H	5.83155100	0.66751900	-7.92116200
				H	12.02577300	3.71776400	-7.95201600	C	8.05207900	-0.60253300	-1.74353600	H	2.80798100	3.79926200	4.61711900
				O	8.29104700	4.76558700	-6.93735200	C	6.92949900	-1.36675200	-1.40990900	H	3.73698700	0.44952300	-9.39358500
				O	8.64747300	3.67133100	-7.34664700	C	5.93674200	0.16324200	-0.68105000	O	5.94778600	0.16927700	-5.55223200
				O	7.80631600	2.76736300	-7.84642300	C	8.35978800	-1.41443000	-0.14309800	C	3.35571700	-0.79350900	-6.17103500
Zr	1.83558100	-3.33796300	1.61634700	C	8.18393000	4.13430800	-1.10032500	C	10.0016900	0.15564400	0.60769100	O	6.65419500	-1.97960700	-5.61703400
C	-0.01416000	-4.45926000	2.37220100	C	8.45811000	4.82212500	0.22729000	C	6.89955000	-0.64565800	0.88027400	B	8.43893900	0.51775100	-2.66457400
H	-0.30792300	-4.24012800	3.404717800	H	8.45047400	3.07759500	-1.09336100	F	14.13251800	1.38459700	-3.50829100	H	8.72652500	2.01727800	-3.05038800
H	-0.86829500	-4.21398700	1.72619400	H	7.14915900	4.24385400	-1.42096400	H	12.20761800	2.69076300	-4.98148400	H	8.02259200	2.70169200	-2.20472800
H	0.16680400	-5.53989500	2.29225500	H	11.11985700	4.12939000	-1.32436900	H	9.71933800	1.81909800	-5.02678400	H	8.33066200	2.47403900	-3.93259900
C	2.21085000	-0.96960900	-0.46468400	C	9.79261300	4.43184000	0.87965200	F	10.86961700	-1.59101300	-1.90396300	H	6.79239800	1.98978900	-3.24211900
C	1.37410000	-5.24827000	-2.34480200	H	8.37566200	5.90942000	0.09632700	F	13.41011900	-0.78248000	-1.98570900	O	10.08701000	0.59235000	-3.24510700
C	1.56236600	-5.13090600	-3.86611400	H	7.63738700	4.52920000	0.89430300	H	8.42268900	-0.75029400	-6.28458200	O	10.76646900	0.50746700	-1.23289400
C	1.20216300	-6.02310200	-1.91701700	C	12.03549800	4.81269700	0.06378700	F	9.28995200	-2.98920500	-7.68146000	O	10.94180300	1.21403300	-3.25081700
C	3.45233300	-5.56392500	-2.11770000	H	10.86868100	3.06488800	-1.22580900	H	8.49437100	-5.43407000	-6.44387000	C	12.33501000	0.23921800	-1.00140900
C	3.76807000	-2.79302500	-4.41562300	H	12.12511200	4.19039400	-1.74500100	F	7.83188500	-5.53532300	-3.71866500	C	12.30017700	1.42613900	-3.50945800
C	3.02151200	-5.26012700	-4.34665600	H	9.79112100	3.34903700	1.05869400	F	8.78597600	-3.31949700	-2.27307100	C	12.91951300	0.93963200	-1.91036000
H	1.12755800	-4.18141400	-1.19272600	H	9.85834200	4.91200900	-0.83627600	F	6.30837700	-2.11357900	-2.35292300	C	6.33367500	-0.59772800	-3.88945100
H	0.97961800	-5.92541900	-3.34975100	H	11.10214200	5.90219400	-0.05501700	C	5.27704200	-2.18415300	0.09547200	C	8.72197800	-1.92315400	-3.65844600
C	3.99868300	-4.18443900	-4.84811000	H	11.93150500	4.50754400	0.61434600	F	6.34870200	-0.66285800	2.11238600	C	7.97504500	-0.32453100	-5.12522900
H	4.32480700	-2.03716900	-3.85879000	O	8.91422900	4.75848300	-2.23224100	H	8.52717400	0.92344900	1.57825200	C	8.74651000	-2.90225000	-4.62864100
H	2.71602100	-2.50308000	-4.04486300	C	10.19583800	4.70845600	-0.23410300	F	6.34824200	1.01116200	-0.85511500	C	7.99459600	-1.30395000	-6.22387400
H	3.03374000	-5.25767800	-5.44449100	O	10.71971900	5.22849000	-3.38671500	C	8.77354800	4.67494300	-4.93876600	C	8.37890400	-2.60596100	-5.93459200
H	3.40135000	-6.24546600	-4.0081500	H	9.25329200	6.48720600	-4.18103200	C	9.37653600	5.96634000	-5.46169600	C	7.55492800	0.09995300	-1.32272400
H	5.02637000	-4.49068200	-0.6803100	H	9.23600800	4.81738500	-4.80176700	H	9.50582400	3.91229800	-4.69752000	C	6.50359400	-0.81815800	-1.29604000
H	3.94335100	-4.10362300	-2.74962500					H	8.13170600	4.84201500	-0.07562000	H	7.20327000	0.80234800	-0.12340700
O	1.50753900	-2.84561200	-2.08005100					C	9.56538600	3.61913000	-7.58488600	C	5.70261100	-1.05098900	-0.17137300
O	1.58560300	-3.95034700	-1.56655800					C	10.49093100	5.77770700	-6.49955700	C	6.95239900	0.60866400	1.01973400
O	1.83585200	-4.15358800	-0.27458800	C	0.92157100	-0.60099700	0.42833000	C	9.79884800	6.46335500	-4.58228100	F	5.93035700	-0.33355900	0.99367700
O	-0.31958000	-1.73058900	-0.12199700	C	0.52457300	-0.47519700	1.78470000	F	10.06607000	5.07128200	-7.79107900	F	13.01772500	2.14617000	-3.97646900
H	-0.84171600	-1.76242400	2.53115200	C	2.82174300	-0.38176100	1.69753300	C	10.23946700	3.08269400	-6.90449300	F	10.46876900	1.68438400	-4.45050900
H	2.04836000	-5.28379500	4.20907100	H	3.86079600	-0.30316200	1.98770100	H	9.54424900	3.07030900	-8.52875300	O	10.11756600	-0.62525300	-0.29051100
H	0.93630200	-6.36403100	1.90865300	C	1.69810600	-0.35437400	2.57356800	H	11.30836900	5.20919000	-6.03762200	C	12.70504100	0.26536300	0.10064600
H	4.66374000	-4.63752200	0.78857300	C	2.08097500	-4.27971200	3.64092600	F	7.59451100	0.90081600	-5.61989900	F	7.66038900	-0.97411600	-7.49272100
H	4.83688000	-2.47841000	2.38137900	C	2.95916100	-3.18420500	3.83513900	H	10.92774000	6.76014000	-6.75797600	F	8.40705200	-3.53893700	-6.89626200
H	3.21527100	-2.87536800	4.49953600	C	2.54435900	-5.01742000	2.51800700	F	9.29079300	5.65391300	-8.31403600	F	9.12911200	-4.17061500	-4.32779100
H	1.39890200	-1.02184500	3.81921700	C	3.96603600	-3.24221600	2.82921600	H	10.91729400	5.01348100	-8.47118400	C	8.74075200	-1.96323200	-4.12448600
C	6.39871600	3.11920700	-7.88647000	C	3.71206000	-4.38382700	2.02700100	C	8.80862100	4.06678400	-5.90728400	F	6.17995200	-1.54650500	-2.38554800
C	5.64018400	2.01898500	-8.61173200	Zr	1.78710400	-2.71171300	1.59071500	C	10.10320700	3.52088200	-7.00414500	C	9.10302700	-2.29296200	-2.41736200
H	6.05709400	3.23191500	-6.85176500	O	-0.35796700	-3.31239900	1.213674800	H	7.32473100	2.86226000	-7.68000700	C	6.17995200	-1.54650500	-2.38554800
H	6.29359700	4.08751700	-8.38569600	H	-0.69269900	-2.97251400	3.12351600	O	11.12132100	4.82987900	-3.03341600	F	4.70902900	-1.96323200	-4.12448600
C	4.68848800	-1.72183400	-7.86192000	H	-1.04956500	-2.90246600	1.38784400	O	10.95557100	4.38059700	-1.68651700	F	5.17534300	-0.54140000	2.09305000
C	5.67523800	0.65516700	-7.90859200	H	-0.44379600	-4.40703400	2.11278100	H	11.90470000	4.39117500	-1.13366900	F	7.18241200	1.31599400	2.13746000
H	4.59810400	2.35888800	-8.69733800	H	2.93201600	-0.64759700	-0.52162200	H	10.27127600	5.08289400	-1.20355000	F			

H	-0.48133900	-5.36141700	1.99259400	H	9.90877900	5.06685400	-1.83370300	C	1.49066200	0.29047000	1.15788500	C	0.36665000	-0.41010900	-0.33962900
H	2.57503000	-1.13412600	-0.22809000	H	11.26623680	5.41251800	-1.59751300	C	1.28675200	-3.48702300	2.50610600	C	0.14507800	-0.23846900	1.05254300
C	1.77122700	-5.19104100	-2.38620500	H	10.55641600	6.73737500	-2.09619500	C	2.41393600	-2.63433500	2.37182600	C	1.76704000	-0.37550600	-0.57308700
C	2.15753600	-4.98678200	-3.85795500	H	11.38753700	4.43926800	-3.61485500	C	1.30115600	-4.40072700	1.42056800	C	2.16257000	-0.20945900	0.67459200
H	2.42983200	-5.92100600	-1.89986800					C	3.13574000	-3.03159100	1.20796600	H	3.48428300	-0.14256300	0.82484700
H	0.75998800	-5.61878400	-2.31909300					C	2.44879900	-4.12695500	0.62976000	C	1.41108000	-0.12621000	1.68279200
C	3.97764000	-2.34866800	-4.40252000					Zr	0.93204100	-2.06119700	0.40357800	C	1.60555000	-0.09735000	2.81240700
C	3.67224100	-4.88621500	-4.12642300					C	1.15674000	-2.19609600	1.30511400	C	2.46832000	-2.07902000	3.02240800
H	1.63546200	-4.10262600	-4.24064600					H	-1.27774400	-1.74746800	2.29895800	C	2.08666100	-4.79992200	1.68831700
H	1.77522200	-5.84324300	-4.42856800					H	-1.36797900	-1.69566700	0.63074800	C	3.49573100	-3.01855300	2.03520300
C	4.38383600	-3.60692900	-3.64886000					H	-1.44615100	-3.25254900	1.38352000	C	3.25910500	-4.15133200	1.21820300
H	4.45298400	-1.46146200	-3.97805700					H	2.01559000	-0.34719300	-2.07770300	Zr	1.32680600	-2.50513500	0.79354200
H	2.89771600	-2.18719600	-4.39455000					H	-0.39008000	-4.45558500	-3.17769800	C	-0.81458800	-3.06013000	1.36702900
H	3.84166100	-4.98366800	-5.26334400					C	-0.38349400	-4.72465700	-4.68747000	H	-1.13883200	-2.73133500	2.36251400
H	4.16546300	-5.75353800	-3.66455800					H	-0.25822000	-5.39662600	-6.21252700	H	-1.50768600	-6.25252500	0.63415600
H	5.46592800	-3.74537600	-3.75446200					H	3.85623300	-4.50219900	0.00944500	H	-0.92023700	-4.15274300	1.32871800
O	1.19993500	-3.41929100	-2.58560200					C	4.41028600	-2.39739800	0.75175400	C	2.26315900	-0.51214500	-1.52443500
O	1.66609900	-2.80235800	-1.99926200					C	4.41962800	-3.25316800	-0.37602400	C	0.81629000	-4.58599200	-3.10443800
C	1.73815800	-3.92710600	-1.53105100					Zr	1.96897000	-2.77279100	0.16593200	C	0.46227400	-4.48555100	-4.63561200
O	1.76557900	-4.19495800	-0.22710500					C	0.55723200	-4.32554900	1.05404400	H	1.17737700	-5.56989800	-2.77125600
H	-0.06777500	-1.42459300	-0.70802600					H	0.54361600	-4.38759800	2.14935600	H	-0.21104700	-5.16435000	-2.87053900
H	-0.76750100	-1.47041100	2.53367700					H	-0.46847700	-4.11440000	0.72311800	C	3.45389300	-2.98155400	-4.63399900
H	1.16166800	-5.38454300	4.29359800					H	0.84526200	-5.31455900	0.67212000	C	2.11401500	-5.01570100	5.30729200
H	1.96286700	-6.68618600	2.07772100					H	0.93605000	-0.30881700	-1.63707300	H	0.67329900	-3.44106200	-4.97278200
H	4.12981600	-5.42874000	1.11018500					C	0.81223900	-4.20750000	-3.97313400	H	-0.01752000	-5.01649400	-5.02690400
H	4.66994700	-3.33863000	2.70690300					C	-0.05017900	-3.74187600	-5.15617200	C	3.42742700	-4.47373400	-4.74200800
H	2.83623000	-3.31471100	4.66993100					H	1.46474200	-4.83342600	-4.31587300	H	4.27951600	-2.47385700	-4.15459700
H	1.47833100	-1.22273600	3.99051900					H	0.23649800	-4.82769500	-3.17836600	H	2.67221300	-2.35901100	-5.03555200
C	6.27445400	2.94846900	-0.95084900					C	1.74577000	-1.41489000	-4.93360600	H	2.06661100	-4.81346500	-6.38133500
C	5.43791600	1.76137500	-9.50397700					C	0.76798000	-3.30537900	-6.38170400	H	2.13658700	-6.12371200	-5.12128200
H	5.98292400	3.29532900	-8.05465900					H	-0.71116700	-2.92924300	-4.82647200	H	4.27301500	-4.83130000	-5.36324600
H	6.19680400	3.79530100	-9.74142700					H	-0.71383400	-4.56754700	-5.43389600	H	3.63793600	-4.87772000	-3.74565000
C	4.62935000	-1.79410700	-8.02879800					H	1.98882000	-2.43865000	-0.62721400	O	2.50880300	-2.82027600	-2.83753700
C	5.47961000	0.57488500	-8.53184000					H	2.54449000	-0.67857200	-4.89227300	C	1.61476100	-3.53836300	-2.33752200
H	4.40410100	2.11794000	-9.61431000					H	0.78273900	-0.90494800	-5.03069100	H	1.30292900	-3.44821600	-1.08911700
C	5.76965100	1.44793300	-10.50323100					H	0.10715900	-2.76208900	-7.06803800	H	-0.40189800	-0.54331500	-1.09103700
C	4.55959400	-0.57701400	-8.95855500					H	1.11864300	-4.19107100	-6.92402000	H	-0.81706800	-2.02782000	1.54927000
H	6.05215400	-2.17861500	-7.94048800					H	2.30975800	-1.87471900	-6.91168400	H	3.73661000	-4.32845900	3.60412900
H	4.53791200	-2.62236400	-8.44268100					H	2.85329900	-3.05137300	-5.75768200	H	1.63401100	-5.68574800	1.26092300
H	5.17601000	0.91669400	-7.53482000					O	1.77741500	-1.94231900	-3.54943500	H	3.85838500	-4.45372100	0.36853500
H	6.51191300	0.21549200	-8.44808300					C	1.41395700	-3.11590500	-3.12133000	H	1.31924900	-2.32518600	1.87327000
H	3.52336000	-0.21924600	-8.99476000					O	1.58930500	-3.34144600	-1.89952000	H	1.58307500	-0.24635700	2.73897600
H	4.84202500	-0.90203500	-9.97420000					H	-1.02304000	-1.61865800	-0.31374200	C	6.11817500	0.28585600	-5.87432500
O	3.41909500	-0.54751600	-6.32731200					H	-0.28752500	-1.81817800	2.26369900	H	5.89269300	1.28160100	-6.97870000
C	4.08716000	-1.51524800	-6.64007000					C	3.07848800	-5.21434500	1.97643800	H	7.09371400	-0.22195200	-5.94058100
O	4.43135800	-2.49363800	-5.77849300					H	3.74110300	-5.37060200	-0.62644300	H	6.03241000	0.70662300	-4.88514400
B	8.59886500	0.29504000	-2.58454500					H	4.79208300	-2.99923500	-1.36020600	C	5.90215900	-1.72208500	-7.98701600
C	7.66164200	1.63395100	-2.79708700					H	4.78045300	-1.38177200	0.78297700	C	6.19386300	0.581264900	-8.37612900
H	7.78453000	2.34659200	-1.96857300					H	3.71306100	-2.75076900	2.85101900	H	4.83750600	1.08262600	-6.96936900
H	7.83873800	2.17594800	-3.73050000					H	2.11708500	-0.63550900	2.53589500	H	6.47973000	2.16773300	-7.60485100
H	6.60492200	1.34021500	-2.79873600					H	7.48966500	-2.41396700	-4.66599000	C	5.63796200	-0.47442100	-8.86524600
C	10.23752700	0.60046100	-2.55564000					C	9.12996500	-2.59426100	-4.68301100	H	6.96196800	-1.77749900	-7.70968200
H	11.15964600	-0.42598000	-2.27995000					C	8.82004100	-3.80425700	-4.77270200	H	5.66792000	-2.63627100	-8.53398700
C	10.84903100	1.80279300	-2.84323100					C	9.94508700	-1.46135100	-4.77139900	H	7.40832700	0.66823300	-3.88380500
C	12.54478400	-0.27601400	-2.31910800					C	11.20656800	-3.89343700	-4.90450400	H	6.11499400	1.61359500	-9.09770300
C	12.22270000	2.00444100	-2.91070000					H	11.32877700	-1.50011000	-4.90140000	H	4.55475600	-0.31883000	-8.96053900
C	13.09746400	0.96413400	-2.64174100					H	11.96907800	-2.73416400	-4.96817500	H	6.00412400	-0.70530900	-9.87007200
C	8.846390200	-0.72734700	-3.89526900					C	6.66149400	-3.79477200	-4.23295400	O	5.10225000	-0.79248700	-5.83963400
C	8.26065000	-2.10149000	-3.86375600					C	6.97910800	-4.44817100	-3.03464400	C	5.08056000	-1.77596500	-6.72125300
C	8.66170000	-0.23395800	-5.18925200					C	5.12526700	-4.28683500	-4.85240400	C	4.32787000	-2.73359600	-6.50125900
C	8.04684400	-2.89491800	-5.00094000					C	6.23370200	-5.48709000	-2.48313300	H	9.44521500	-2.02034000	-3.08912200
C	8.53813200	-0.98878400	-6.35100500					C	4.73208700	-5.32001500	-4.33416300	C	11.05147800	-2.13989100	-2.70966100
C	8.20450500	-2.33380400	-6.26086100					C	5.08533700	-5.92206400	-3.13637100	C	11.90898600	-3.18647900	-3.05450600
C	8.05013900	-0.33591200	-1.15504400					C	6.93430200	-1.37248000	-3.48545200	C	11.69565700	-1.04472300	-2.12367100
C	6.78038200	-0.91830800	-1.07817000					C	5.59842600	-0.95944900	-3.49416100	C	13.28239900	-3.17402900	-2.80426800
C	8.66432300	-0.16969000	0.08762000					C	7.63780200	-0.98216800	-2.34108600	C	13.05797600	-0.98657200	-2.18420000
C	6.18503000	-1.34705600	1.01026600					C	4.99546400	-0.21437900	-2.48816100	C	13.86363600	-2.06798200	-1.95040000
C	8.10020600	-0.56218100	1.30347800					C	7.07501700	-0.23427200	-1.30266800	C	8.75205900	-3.45818900	-3.55698700
C	6.84560500	-1.15575800	1.31007900					C	5.74506100	0.15244500	-1.37738800	C	8.44732300	-4.12230000	-2.71168700
F	14.42239000	1.14174000	-2.69666200					C	13.30205600	-2.80232600	-5.09050700	C	7.92864300	-3.66769900	-4.66117300
F	12.69888900	3.25339800	-3.23760300					F	12.04760300	-0.36745600	-4.96746000	C	8.22390000	-5.97858900	-2.94545700
F	10.12200800	2.93976000	-												

C	5.78150700	0.08387900	-9.38502200	C	4.11394500	-3.78245300	-3.96380700	C	7.14985800	9.23426300	-0.59296900	F	7.76055400	-4.59433300	-4.28476200
H	4.16484400	1.30541400	-8.55759500	H	4.54854800	-1.68995700	-4.37029300	H	6.48238900	9.54308000	-2.64624900	F	7.62108200	-2.89669400	-2.27209500
C	5.41949300	2.24274300	-9.35788600	H	2.91955700	-2.18030300	-4.85067000	C	5.18506500	9.35592700	-1.47289800	F	5.47454500	-1.11684700	-2.21779000
H	4.77352200	-1.08378900	-9.53509400	C	3.43718800	-5.10845000	-5.51310800	C	5.88499500	8.75047000	-0.83841200	F	4.20240200	-1.86930700	0.01768700
H	5.85188900	-2.56400600	-8.34577900	H	3.57049700	-5.87118400	-3.94133200	H	8.09064500	6.67045100	-0.40634400	F	5.33205700	-1.42135300	2.47108000
H	4.23578400	-3.04730800	-8.75827400	H	5.16528100	-4.09329400	-3.99533700	H	9.74127000	6.90940800	-0.97770700	F	7.80550100	-0.24661400	2.61801000
H	6.67501200	-0.27331800	-8.86087400	H	3.89653800	-3.51911100	-2.92438200	F	6.75991600	8.73848800	0.30793700	F	9.10662100	0.46705800	0.41825600
H	4.62595600	0.35860800	-1.03884300	H	1.55928000	-2.65615100	-2.30375900	H	7.16747000	10.30820700	-0.36889300	C	8.56417300	5.02094300	-5.26221000
H	3.75191300	-0.68990600	-9.60001600	C	1.36176700	-3.78801100	-1.89051600	H	9.03861700	9.31021100	-1.66766600	C	9.63415000	5.81041100	-6.14649600
H	4.96946800	-1.57835300	-10.49424000	O	2.18942000	-4.10203200	-0.60670400	H	9.18784500	8.97707000	0.04885700	H	8.71899300	4.32768600	-4.70561000
O	3.92090400	-0.65900400	-6.79797700	H	-0.48973300	-1.27756200	-0.44320600	O	7.08572500	7.01773300	-2.98485200	H	7.58301000	5.68327900	-5.23101500
C	4.32029500	-1.77291300	-7.09217900	H	-1.39776600	-1.42318000	2.09652800	C	8.34816600	6.83065100	-2.53241000	C	8.59756800	2.66649100	-7.116470800
O	4.36797200	-2.80422000	-6.24269300	H	0.25145300	-5.47761800	3.81512400	O	9.16008100	6.35943600	-3.30456600	H	10.81263900	4.86895400	-6.45296200
B	8.32827100	-0.49650300	-2.47806500	H	1.12724100	-6.72478600	1.59695100	C	3.41257400	-5.54221100	0.82293300	H	9.16013400	6.16315600	-7.07012100
C	9.96162200	-0.19581100	-2.50776500	H	3.39533100	-3.55523500	2.54725000	C	2.00025000	-3.51931200	4.41086300	H	10.01468200	6.70553100	-5.64289700
C	10.86301900	-1.20495600	-2.14562900	H	0.72950800	-1.34766500	3.73793400	C	0.46713900	-2.14333400	2.40014300	C	10.56632400	3.80826200	-7.53947200
C	10.58254700	0.93465700	-3.03484600	H	5.74702300	1.66586200	-7.46077000	C	1.05098700	-1.37536600	0.84983500	H	9.78842200	2.34776400	-6.13499300
C	12.24673700	-1.09921200	-2.25654600	C	5.19668300	1.26378700	-8.41438100	H	1.73498500	-1.56285700	2.07686000	H	9.75183700	1.78986000	-7.99774400
C	11.95901300	1.08560100	-3.18493900	C	5.62238000	0.89536300	-6.70285800	H	2.78465100	-1.37133100	2.25018800	H	11.13939100	4.37844500	-5.52672300
C	12.80644100	0.06223600	-2.78347500	H	5.33662700	2.60648500	-7.09518000	C	0.97581000	-2.03918300	3.03677100	H	11.65309400	5.49150100	-6.78312600
C	8.15571600	-1.50133900	-3.79308200	C	4.93833800	-2.27672200	-8.37054200	C	1.88970200	-6.01433900	2.56533200	H	10.23774900	4.29325700	-8.46881300
C	7.93859300	-2.88243700	-3.77139200	C	5.78993100	-0.03225200	-9.43177800	C	2.52605000	-4.90640400	3.15396100	F	11.53077800	3.33991900	-7.76726300
C	8.33993100	-0.99469300	-5.07844700	H	4.11867000	1.15067000	-8.65945900	C	2.36081700	-6.14618400	1.23224400	O	7.63688500	4.04294300	-6.71125900
C	7.83655000	-3.66891600	-4.92233700	H	5.33136000	2.10570500	-9.50522200	C	3.43747400	-4.35642500	2.18465700	C	8.14033200	3.04272300	-7.24460200
C	8.32945400	-1.73342700	-6.25017300	H	4.84390000	-1.25653500	-9.51291700	C	3.20267200	-5.12967600	1.00231800	C	7.14787800	2.21129200	-7.96414900
C	7.99884100	-3.09360100	-6.17563000	H	5.97861300	-2.58481900	-8.20333400	Zr	1.07349700	-3.90436900	1.30159400	C	7.09952000	1.496562700	-2.80610100
C	8.32620300	-1.15106800	-1.06620300	H	4.40998700	-3.19835900	-8.64766600	C	-0.85104300	-5.06192100	1.75953600	C	7.20624600	2.63899200	-2.00313200
C	6.47324200	-1.68415500	-1.02628900	H	6.70680000	-0.31604000	-8.90226200	C	-1.09386200	-5.17631600	2.82430200	C	6.08413200	1.57031500	-3.76210000
C	8.39425000	-1.08904400	0.17997400	H	6.10913300	0.20833400	-10.45228100	H	-1.69936200	-4.55795200	1.27667400	C	6.41091500	3.70626400	-2.14961500
C	5.86259800	-2.16591600	0.12343400	H	3.80510900	-0.91994600	-9.61671500	H	-0.76806300	-6.06832200	1.32699800	C	5.27530300	2.69344300	-3.95387900
F	7.80896400	-1.53708900	1.36706300	H	5.07993700	-1.80276000	-10.43438600	H	1.50258400	-1.09092100	-0.09128400	C	5.43953400	3.80697200	-3.14280800
C	6.52961400	-2.07609200	1.33891100	H	3.87488200	-0.72315600	-6.82823800	C	4.05724200	-4.24921400	-3.06412000	F	4.35458800	2.71211400	-4.93521400
F	14.13382200	0.18218600	-2.91538600	H	4.36110200	-1.82040600	-7.04159600	C	1.04134900	-4.02271000	-4.46756600	F	4.82660100	0.54158000	-4.59172400
F	12.46009700	2.21030600	-3.73538000	O	4.45318700	-2.79331200	-6.12784700	O	0.38942000	-5.31660900	-2.82179100	F	4.67928700	4.90662500	-3.31093900
F	9.85734700	1.99791100	-3.49974400	C	8.17857700	-0.05289900	-2.46003200	H	-0.597565100	-3.87235100	-3.02811600	F	6.58801600	4.40636200	-1.34136200
F	10.39457300	-2.37706400	-1.67494400	B	8.17857700	-0.05289900	-2.46003200	H	4.22867900	-3.42984100	-4.21541800	C	8.12908200	2.69825900	-1.02107500
F	13.07473400	-2.10761400	-1.87833600	C	10.71154100	-0.66569100	-1.98554100	C	5.19743600	-4.94484800	-4.83407800	F	5.98705300	7.66292900	-2.64284100
F	8.59131100	0.33771900	-5.24036500	C	10.40538300	1.40897200	-3.02021900	C	4.21669300	-4.57521400	-4.21541800	C	6.23715500	9.13540500	-2.34586800
F	8.45224000	-1.13957800	-7.45199200	C	12.09475900	-0.52737100	-2.02525500	H	0.24406600	-4.20121600	-5.20083900	C	5.86067000	7.06878400	-1.74464500
F	7.87907200	-3.82292500	-7.29567900	C	11.78313300	1.58768000	-3.12869500	H	1.33251200	-2.97321100	-4.57521400	C	5.13792500	7.53013200	-3.31250500
F	7.55158300	-4.97590400	-4.82186000	C	12.64060200	0.61497900	-3.26201300	H	0.24406600	-4.20121600	-5.20083900	C	6.85858000	7.29179800	-1.50845100
F	7.78591700	-3.55035200	-2.61451600	C	8.09061000	-1.13560000	-3.71947900	H	3.57539100	-2.58009300	-4.02211900	F	7.19307200	9.40215300	-1.17535900
F	5.73434200	-1.75039200	-2.15889900	C	7.91973700	-2.51966500	-3.62684200	H	2.44767600	-4.80736700	-5.89934100	H	6.59431600	9.62386300	-3.26237200
F	4.62395800	-2.69779900	0.07433400	C	8.31937400	-0.69474200	-5.02277000	H	1.89401900	-5.99044900	-4.73153300	H	5.26105700	9.85314800	-2.11852300
F	5.93301800	-2.49343800	2.47217800	C	7.90491100	-3.37420100	-4.73258700	H	4.21809400	-5.56818700	-4.29945200	H	8.00924200	6.81043200	-0.76263800
F	8.46627600	-1.43832100	2.53189000	C	8.33532400	-1.50168200	-6.15074800	H	3.20964400	-4.88261900	-2.95469400	H	9.67213300	9.23579900	-1.33393700
F	8.09318900	4.29371900	-9.89917600	C	8.10650200	-2.86517700	-6.00840000	O	1.88106000	-2.54043800	-2.10418100	H	7.62575900	10.48461700	-1.01696200
C	8.94532700	5.34696000	-5.67435400	C	7.57612800	-0.63744200	-1.03185700	C	1.19073200	-3.53292000	-1.93222300	H	9.10093900	9.29851400	-2.21495400
H	8.65332200	3.65800900	-4.30268600	C	6.29871300	-1.20518200	-1.00553400	O	0.97589800	-4.07830900	-0.74024500	H	9.20593200	6.08877900	-4.47650600
H	7.25048500	4.73846700	-4.46203600	C	8.15170600	-0.47308400	0.23101300	O	1.07918100	-1.74197400	0.28927800	O	7.07369000	7.03397400	-3.39212200
C	9.49331400	2.48899400	-6.88838300	C	5.65155400	-1.62128400	0.15020900	H	-1.18645400	-2.47709400	2.86137300	C	8.26379000	6.78721300	-2.87119900
C	10.29344900	4.84436400	-6.22047100	C	7.53063000	-0.85783600	-4.42211200	H	1.15105100	-6.64266300	3.04365300	O	9.07867500	6.14991100	-3.55355500
H	8.35948000	5.83226600	-6.46341800	C	6.26761600	-1.43307700	1.38113400	H	2.02687200	-6.87979800	0.50949100				
C	10.13578300	6.11655000	-4.91419200	F	13.96901900	0.76535300	-2.72293500	H	4.09648500	-3.51178600	2.32636100				
C	9.16889200	3.80276100	-7.33937600	F	12.27990400	2.66803100	-3.72836200	H	2.41949700	-4.55293800	4.16889400				
H	9.89151400	2.19016300	-5.90676800	F	9.66284100	2.41351700	-3.56776100	H	1.00268700	-2.25614000	4.07721900				
H	8.62322900	1.66905400	-7.56771000	O	10.25405900	-1.81952500	-1.45800400	H	5.92716700	2.44996800	-0.85519400				
H	10.87963300	4.41259800	-5.39744400	C	7.57612800	-0.63744200	-1.03185700	C	5.34091200	1.24957500	-8.74164000				
H	10.86323600	5.70222100	-6.59545800	C	8.54795700	-0.97346700	-7.37750100	H	5.58452400	2.59061300	-7.04371700				
H	9.63811400	4.22215100	-8.20418500	F	8.53561800	0.63331800	-5.24792400	H	5.82758200	3.37707000	-8.61890800				
H	11.17022100	3.53391400	-7.71971200	F	7.66558700	-4.68414000	-4.56857700	C	4.88663100	-2.53819800	-7.78831800				
F	7.39725900	3.39135500	-5.94028600	F	7.73075700	-3.12554300	-2.44092000	C							

C	4.10936700	-2.23316300	-7.70216300	C	0.73045300	-3.51542500	3.09636100	O	6.71490100	3.34475800	-5.85663100	F	12.54845700	2.97086700	-2.79726400
C	4.79582200	0.23179600	-7.89552600	C	1.87688900	-2.73453600	3.38407100	C	7.44647400	2.68519700	-6.68085800	F	9.91379900	2.92566200	-3.05254400
H	4.24027000	1.79133900	-8.49115300	C	1.13231400	-4.58895500	2.25475900	C	6.86227200	1.87238800	-7.47788100	F	9.84518900	-1.46843800	-1.20459300
H	4.73062700	1.53324500	-9.64073100	C	2.98932200	-3.32098200	2.71449800	C	7.20383400	0.76392600	-2.49995700	F	12.49753600	-1.38117100	-0.94196600
C	3.95762100	-0.91701100	-8.47367400	C	2.52525500	-4.47522900	2.03286500	F	7.34071900	1.77448500	-1.53996600	F	8.73013600	1.33044200	-5.07009700
H	4.58925000	-2.53802600	-7.61085200	Zr	1.46153300	-2.42987000	0.85626900	C	6.07238200	0.90261000	-3.30409900	F	8.87036600	-0.20702200	-2.24634900
H	3.60732000	-3.04877400	-8.24205300	C	-0.82371400	-2.29292600	0.81294500	C	6.46881600	2.84869800	-1.41166200	F	8.35879800	-2.89745800	-7.08909100
H	4.58982900	0.32360200	-6.82203200	H	-1.27778400	-1.68753300	1.60822300	C	5.16927500	1.96427200	-3.21230900	F	7.71066300	-3.99642300	-6.65798400
H	5.86435000	0.00583400	-7.99905400	H	-1.13421600	-1.86447600	-0.14970500	C	5.37059900	2.95180100	-2.25811200	F	7.52994200	-2.50077000	-2.49369000
H	4.23474700	-0.63299800	-8.46211900	H	-1.24148000	-3.30599100	0.88531000	F	4.45717300	2.06260800	-4.07143600	F	5.43215900	-0.69592700	-2.37506100
O	4.64160700	-1.35993200	-5.97448700	C	1.67755200	-5.11516200	-2.67992400	F	5.78850200	0.00744800	-4.27932200	F	3.98546100	-1.52997200	-0.47527300
C	4.37788600	-2.17091800	-6.31769800	C	2.00221200	-5.24428800	-1.17656400	F	6.71020200	3.82422100	-0.50383200	F	7.45503400	-0.21155200	-2.65187400
C	3.94443300	-3.15185500	-5.52349900	H	-2.32893400	-5.75393200	-2.06940400	F	8.38461400	1.75502700	-0.68809600	F	8.92515600	0.59113200	0.59316100
B	7.79448000	0.38158400	-2.51474600	H	0.65692600	-5.47054300	-2.47961400	H	7.63439900	5.99620200	-2.20169700	C	8.59355500	4.87627100	-5.13079300
C	9.43698700	0.37718400	-2.25998000	C	4.22339000	-2.98887800	-4.89988000	C	6.59552400	6.85881400	-1.74497000	C	9.19502100	5.80431100	-6.14239000
C	10.07637800	-0.76047100	-1.75168000	C	3.49487200	-5.43433800	-4.50961000	H	5.65298200	6.31848900	-1.59106100	H	9.00861500	3.90057700	-4.92570500
C	10.32048100	1.37785800	-2.65412500	H	1.59860500	-4.36939800	-4.69834300	H	6.88814300	7.37239500	-0.81209600	H	7.62993000	5.10099800	-4.69965600
C	11.55476400	-0.88571000	-1.60500000	H	1.46463000	-6.11556100	-4.57223000	H	4.64453600	7.61609700	-2.51940500	C	9.23656200	2.93810000	-7.77842100
C	11.70542500	1.30206100	-2.53092800	C	4.44128800	-4.28296100	-1.13025100	H	7.72895200	5.29722800	-1.53552100	C	10.33095100	5.20164300	-6.98844100
C	12.28635000	0.16052400	-1.99733500	C	4.84437900	-2.18373700	-4.50383000	C	4.84437900	-2.18373700	-4.50383000	C	8.38275000	6.17193000	-6.24634900
C	7.68172500	-0.57037400	-3.86875500	C	3.18474400	-2.65828600	-4.87261400	H	9.55516300	6.69108700	-5.60735900	H	9.55516300	6.69108700	-5.60735900
C	7.35435500	-1.92933400	-5.88245600	H	3.59106900	-5.62452000	-5.58678000	C	9.90772300	4.28018300	-8.14710600	C	9.90772300	4.28018300	-8.14710600
C	8.06955800	-0.07239600	-5.11637100	H	3.84833500	-6.34686100	-4.00879300	C	-0.55340900	-1.96577400	0.63775500	H	9.75603500	2.45617200	-6.94224200
C	7.36471500	-2.71884600	-5.03331100	H	5.47765400	-4.61143400	-4.27836300	C	-0.77812100	-2.19785100	0.20270600	H	9.28992100	2.25495400	-6.62041400
C	8.08876100	-0.81692200	-6.28874600	C	4.35094100	-4.03099500	-3.06551700	C	0.79752400	-1.56470600	0.46692700	H	11.03021900	4.66493600	-6.33209700
C	7.72423300	-2.15735500	-6.25044700	O	1.84086900	-2.70210400	-2.81381000	C	1.41790300	-1.57258800	1.74092300	H	10.90130000	6.03134800	-7.42325800
C	6.92393800	-0.16420600	-1.21316100	C	1.73499000	-3.69766400	-2.11387400	C	2.44883000	-1.31663000	1.94205600	H	9.25880000	4.83629900	-8.83665000
C	5.59133300	-0.55833400	-1.37027600	O	1.61991500	-3.67198900	-2.78954000	C	0.84219400	-1.96400000	2.70368400	H	10.81244400	4.03684500	-8.71616200
C	7.35639600	-0.13440100	0.11545700	H	1.03661000	-0.51150800	-1.66543200	C	1.66534200	-5.82825200	3.29169500	O	7.36300100	3.89867600	-6.52312700
C	4.76287200	-0.95012300	-0.32451700	H	-0.05069100	0.42867900	0.62787500	C	2.33263900	-4.62850400	2.66178000	C	7.78482400	3.07949900	-7.38741200
C	6.55764200	-0.50284100	1.19946400	H	-0.27405200	-3.32817600	3.45071200	C	2.14721100	-6.24267900	1.64615700	O	6.97503800	2.31393800	-8.08678200
C	5.25028100	-0.91216700	0.97625500	H	0.48165200	-5.34700100	1.83770200	C	3.23320500	-4.30060700	1.23100700	C	7.23683700	1.94513100	-2.61796000
C	13.61710100	0.06509000	-1.86888200	C	3.12664800	-5.12319400	1.40887600	C	3.12413900	-5.30918700	1.22015100	C	7.38561600	3.03820400	-1.75517200
F	12.48536000	2.33390400	-2.93344000	H	4.01554900	-2.98273200	-4.87591000	Zr	0.88153900	-4.01609400	1.23931100	C	6.13411000	2.11158000	-3.55562900
F	9.86248000	2.53226700	-3.21064000	H	1.90561100	-1.85496100	-4.01425800	H	-1.03616100	-5.17667200	1.71189800	C	6.62869200	4.20609700	-1.91933700
F	9.32441000	-1.82558000	-1.37204200	H	1.83349600	0.29826800	2.54289100	H	-1.36299900	-5.14413900	2.75955000	C	5.41965900	3.25687100	-3.65076500
F	11.99358400	-2.00373300	-1.09572400	C	5.40509300	1.53615000	-7.35167900	C	-0.85599000	-4.78073600	1.09639200	C	5.62430400	4.31831800	-2.77854100
F	8.45556200	1.22538100	-5.23864700	C	4.91007600	1.07293700	-8.70636200	H	-0.89080000	-6.23149700	1.44171400	F	4.46520300	3.34344000	-4.95927000
F	8.43000100	-0.25027000	-7.46370200	H	5.35787400	0.75641300	-6.59208700	H	1.29138100	-1.37391300	-4.07629100	F	9.52840500	1.15479700	-4.46455700
F	7.69495300	-2.88744600	-7.36715000	H	4.88905600	2.42838600	-6.99703800	C	0.73631500	-4.93223500	-3.09170000	F	4.88704000	5.42854500	-2.85997000
F	7.02377400	-0.401502400	-4.97499900	C	4.94294800	-2.54056300	-8.52749100	C	1.34358400	-4.70350700	-4.84238000	F	6.86037800	5.20110700	-0.96816500
F	6.09919200	-2.57262800	-2.75359200	C	5.64593500	-0.15007800	-9.31846000	H	0.84064800	-5.97681600	-2.77178000	F	8.33059300	3.00736000	-4.78691900
F	5.03599300	-0.56947000	-2.60218700	H	3.85340500	0.83619100	-8.54420500	H	-0.34715800	-4.74578700	-3.12052900	O	9.36183300	5.58810200	-3.44317100
F	3.49925400	-1.35319800	-0.55566900	H	4.94059600	1.92349400	-9.39895200	C	4.36686500	-3.55045000	-4.19330900	H	10.77358000	8.59365900	-3.88178000
F	4.46184200	-1.27044200	2.01137600	C	4.78028000	-1.41536600	-9.55902700	C	2.67450700	-5.43417300	-4.74724800	H	10.92555700	6.28967600	-3.20294600
F	7.03819200	-0.45425700	2.45216000	H	5.99346300	-2.84758100	-8.44272200	H	1.46007800	-3.62958200	-4.65985500	H	11.36913300	4.93117400	-3.38601900
F	8.60344700	0.26933000	0.43583900	H	4.40543500	-3.43942300	-8.85699800	H	0.62206300	-5.06342500	-5.22941500	H	11.04218700	6.00456600	-4.05474800
O	10.67939600	5.19843300	-3.68279100	H	6.50948000	-0.41557300	-8.70051600	C	3.90018100	-4.97978000	-3.93529400	H	9.14350600	4.82828500	-2.83168200
C	10.15972800	5.38223700	-5.18583400	H	6.06941700	0.16324900	-10.27932700	H	5.21812500	-3.30796200	-3.55401600				
C	8.92049000	3.20115300	-7.96424500	C	3.72169800	-1.13751500	-9.62905600	H	3.57415400	-2.82253800	-4.03015100				
C	10.00415600	4.10976400	-5.83801100	H	5.04752300	-1.84142700	-10.53346900	C	5.12526700	-5.34137600	-5.81537500				
H	9.98124800	6.21581800	-5.39727200	C	3.95417800	-1.12397200	-6.82152600	C	5.25734600	-6.50952600	-4.56883600				
H	11.55230900	5.63924300	-5.60957900	C	4.44433100	-2.19548100	-7.13569900	C	4.73655300	-5.65905000	-4.14716200				
C	9.86886700	4.24457200	-7.36280300	O	4.61704600	-3.21671700	-6.28913500	C	3.70057300	-5.06114300	-2.85943400				
H	9.14524700	2.18851400	-7.10707700	B	8.28631100	-0.49860400	-2.49954000	C	1.92368000	-3.01643100	-2.19885900				
H	9.01450400	3.16728300	-9.05689600	C	9.86492400	0.01385800	-2.57612600	C	1.27866000	-4.03161800	-1.98531700				
H	9.01928900	3.91134700	-5.40700400	C	10.90201700	-0.89311200	-2.32411700	O	0.95792100	-4.45098200	-0.76721700				
H	10.63165100	3.23499400	-5.59170500	C	10.31105200	1.24729800	-3.04711300	H	-1.28416100	-2.08586400	-0.15253000				
H	9.48585600	5.24240300	-7.60990300	C	12.25417100	-0.60448900	-2.48431800	H	-1.71069200	-2.50794400	2.47166000				
H	10.85620100	4.15436100	-7.83351300	H	11.64921400	1.58182700	-3.24289900	H	0.91512900	-6.33592000	3.50790500				
H	7.07858300	4.43655600	-6.96719300	C	12.63673000	0.65098100	-2.95059400	C	1.12523600	-7.11047700	1.09202000				
C	7.46448000	3.49328000	-7.63426100	C	8.19371000	-1.46278300	-3.85113800	C	3.66282700	-5.33545600	0.28169000				
C	6.60089000	2.58387700	-8.18717900	C	8.14562700	-2.8									

H	5.04883700	-2.26819100	-7.58890000
H	3.42892800	-2.59136900	-8.17089500
H	4.77950100	0.52625900	-6.55090000
H	5.96422600	0.21477200	-7.82139400
H	2.93771400	-0.11326000	-8.18618100
H	4.18488600	-0.59400000	-9.34183900
O	2.74421400	-0.97211600	-5.74985600
C	3.47456200	-1.84053900	-6.18422800
C	3.88061700	-2.90875800	-5.48089300
B	7.93063200	0.33597000	-2.38133100
C	9.58403800	0.32284600	-2.21214700
C	10.24205900	-0.87412900	-1.90322600
C	10.45113600	1.37423500	-2.50456000
C	11.62532500	-1.02253900	-1.86158700
C	11.84099200	1.27370100	-2.49244600
C	12.43991100	0.06576200	-2.16282000
C	7.74555700	-0.53726400	-3.78791500
C	7.37322200	-1.88430100	-3.86552700
C	8.11900700	0.00318900	-5.01962500
C	7.33745200	-2.61727200	-5.05407800
C	8.09930900	-0.68326400	-6.22535400
C	7.69365900	-2.01115100	-6.25049900
C	7.10691500	-0.30541700	-1.09736200
C	5.74439000	-0.58950200	-1.23071900
C	7.60373800	-0.47516600	0.19695500
C	4.93571500	-1.05014800	-0.19898600
C	6.82720000	-0.91972000	1.26941000
C	5.48362700	-1.20548700	1.06919200
F	13.77406300	-0.05377300	-2.14555900
F	12.60449300	2.33933900	-2.81642700
F	9.98586900	2.60270400	-2.85562000
F	9.51939600	-1.98064400	-1.63639800
F	12.18120900	-2.02206600	-1.54999900
F	8.52846900	1.30453200	-5.10037300
F	8.43312900	-0.06261000	-7.38269200
F	7.61684100	-2.67840200	-7.41218500
F	6.95316900	-3.90083400	-5.05161000
F	7.00720600	-2.57449100	-2.76909100
F	5.14238600	-0.42243000	-2.43238500
F	3.63757600	-1.33726300	-0.41063400
F	4.71771300	-1.63093800	2.09495300
F	7.36484400	-1.06230900	2.48993800
F	8.89043800	-0.20763300	0.49349500
F	9.95373700	5.58047100	-4.19252300
C	11.15678100	4.86688000	-4.79446000
C	9.31883800	3.11323400	-7.71287500
C	10.79826500	3.65248800	-5.06828600
H	11.77048600	5.58154100	-5.63778700
H	11.75737500	4.52254100	-3.94576300
O	4.42813500	3.99972600	-7.13196000
H	9.48255800	2.05139600	-7.49316800
H	9.27510900	3.18373500	-8.80754000
H	9.98854300	3.10183600	-5.18284700
H	11.66479400	2.95993600	-5.67341400
H	10.14224000	5.05315500	-7.22691700
H	11.30840800	3.88992400	-7.27256300
O	7.60567200	4.31207300	-6.38577800
C	7.92649400	3.41786500	-7.23494800
O	6.99106800	2.73018400	-7.78577200
C	7.29981300	1.87403600	-2.44665100
C	7.61903200	2.78314800	-1.42887700
C	6.37216000	2.36365000	-3.36572600
C	7.13785400	4.08712000	-1.35792500
C	5.86381700	3.66274500	-3.33911600
C	6.25252400	4.53504200	-2.33325500
F	5.01449400	4.08761100	-4.29799900
F	5.92058700	1.60093400	-4.39148600
F	5.81158600	5.80774600	-2.32615900
F	7.52286900	4.91591200	-0.37494000
F	8.44759900	2.42011200	-0.45405900
O	9.02778000	5.99433500	-5.23822700
H	10.26511000	6.48548100	-3.65881900
H	9.41724300	4.92829900	-3.49401800
C	8.05739500	6.96326800	-4.78948200
H	7.41794400	7.18031900	-5.65631300
H	7.45047500	6.58008800	-3.97161000
H	8.57596800	7.87594100	-4.48814500
H	8.34244600	4.93279600	-5.92698400
C. Optimized structures in toluene			
CL in toluene			
C	0.00002300	0.00471000	-0.00073300
C	0.00164400	-0.00008600	1.52647000
H	1.02021000	0.00084500	-0.40548800
H	-0.50862200	-0.88496000	-0.38018100
C	0.90551400	2.72236500	0.26592000
C	0.99872800	0.97257200	2.16853100
H	-1.02077000	0.20484700	1.87110700
H	0.24190100	-1.02122800	1.85095800
C	0.80386200	2.44340300	-1.78232300
C	1.76375000	2.18086100	-0.15619800
H	1.07513000	3.78708400	0.05095900
H	-2.01818000	0.66698500	1.89031900
H	0.93741800	0.87894600	3.26010700
H	-0.16347100	2.80945700	2.15219500
H	1.57204100	3.04290600	2.28523300
O	-0.75667100	1.08865300	-0.58241700
C	-0.36583700	2.38227500	-0.50753600
O	-1.04223100	3.22169400	-1.05021400
A⁻ = [MeB(C₆F₅)₂]⁻ in toluene			
B	-0.03031200	0.06803900	-0.02351500
C	-0.03846200	0.03736500	1.65154400
C	1.08021900	-0.01034500	2.48938300
C	-1.25170700	-0.02101600	2.34789800
H	1.01771000	-0.05038300	3.88155900
H	-1.36516200	-0.06341500	3.73557700
C	-0.21664300	-0.07293500	4.51528300
C	1.44792300	0.49024500	-0.66462300
C	2.07241700	-0.12515800	-1.75123200
C	2.09941600	1.65487400	-0.24166300
C	3.24514100	0.33788400	-2.34984400
C	3.26860300	2.15626100	-0.80257700
C	3.85318500	1.48879300	-1.87232900
C	-0.47184700	-1.48324100	-0.43863300
C	-1.63953300	-1.85603500	-1.10547000
C	0.31996200	-2.56797800	-0.04580700
C	-2.00183700	-3.18039200	-1.35936600
C	0.00343500	-3.90163400	-0.27543500
C	-1.17686300	-4.21355300	-0.94103600
F	-0.29979100	-0.11444900	5.85750100
F	2.14536300	-0.08088700	4.61940300
F	2.33911100	-0.03212600	1.98295700
F	-2.57547600	-0.10820600	4.32756700
F	-2.40387100	-0.06694400	1.68017800
F	1.55270000	-1.23956700	-2.32237200
F	3.78682100	-0.31954700	-3.39480400
F	4.98245700	1.95502600	-2.43686600
F	3.83822800	3.28141800	-0.32637600
F	1.95903700	2.37938900	0.78752600
F	1.49301000	-2.34284200	0.59339400
F	0.82272400	-4.89161800	0.13113100
F	-1.51104400	-5.49560800	-1.17590000
F	-3.14855500	-3.46502300	-2.00868600
F	-2.51618100	-0.93399000	-1.56682500
F	-1.04172300	1.24053600	-0.58296800
H	-1.04163500	1.28551800	-1.68095900
H	-2.08317200	1.13395900	-0.26967300
H	-0.70135200	2.22438300	-0.23133500
A⁻ = [B(C₆F₅)₂]⁻ in toluene			
B	2.35510000	-4.33901800	0.66098100
C	2.49691100	-4.25383300	2.31520100
C	3.48315300	-5.00183400	2.96717100
C	1.81451000	-3.37141100	3.155227400
C	3.75752800	-4.92715000	4.32777300
C	2.05569900	-3.26016700	4.52512300
C	3.03357400	-4.04357400	5.11981100
C	3.73527400	-3.54697900	1.07935200
C	4.90784900	-4.14401400	-0.28788500
C	3.84785600	-2.16685600	0.37932300
C	6.07792400	-3.43935700	-0.57323600
C	4.99020300	-1.42276500	0.10880700
C	6.12206800	-2.06695100	-0.37683300
C	2.22965500	-5.89127600	0.07981200
C	-2.36553400	-6.13245800	-1.29134700
C	1.83212400	-7.01254500	0.81125400
C	2.17176500	-7.36905800	-1.89573500
C	1.62508000	-8.27274700	0.24907900
C	1.79813400	-8.45659100	-1.11489400
F	3.28131300	-3.94644600	6.43741900
F	4.71837100	-5.69044900	4.88222900
F	4.24695600	-5.86664700	2.25897100
F	1.35213900	-2.38987300	5.27412700
F	0.85785000	-2.54373600	2.67979800
F	4.98469100	-5.47760200	-0.49173600
F	7.16873600	-4.08258600	-1.03130700
F	7.24129700	-1.37204200	-0.64378700
F	5.01482000	-0.09248300	0.31635800
F	2.79525800	-1.47204500	0.86943900
F	1.60685800	-6.94095700	2.14189800
F	1.24974000	-9.31121800	1.02002800
F	1.60223700	-9.66308200	-1.67429600
F	2.33485600	-7.52351700	-3.22347900
F	2.70135000	-5.11740700	-2.12097200
F	0.95370400	-3.66476900	0.07251400
F	-0.27966000	-4.07486800	0.59008000
C	0.84520000	-2.80843700	-1.02493600
C	-1.51449200	-3.65459700	0.11017200
C	-0.37072100	-2.35798900	-1.54050700
C	-1.56213000	-2.78297900	-0.97148700
F	-0.39701400	-1.52166000	-2.59565500
F	1.93916900	-2.35439300	-1.67569900
F	-0.31530700	-4.94224700	1.62833500
F	-2.65887200	-4.08787300	0.67220100
F	-2.74237500	-2.36302700	-1.45912000
Cp₂ZrMe⁺ in toluene			
C	0.14012000	0.04888000	-0.24688500
C	-0.15447200	0.14366800	1.13642300
C	1.55744400	-0.00742100	-0.40068100
C	2.13663700	0.04569800	0.88870500
C	3.19478600	0.04529300	1.11458000
H	1.07979700	0.11650300	1.84296500
H	1.10713000	-4.14271900	2.40547000
C	2.04211500	-3.14477900	2.79762100
H	1.51711100	-4.64600300	1.14461800
C	3.05130600	-3.06539300	1.79448300
C	2.72724900	-3.99018100	0.77467400
Zr	0.83644500	-2.18565900	0.78293200
C	-1.30671500	-2.64609300	1.33359000
H	-1.57546200	-2.45648100	2.38125100
H	-1.99057000	-2.05565500	0.70851200
H	-0.49840200	-3.71266200	1.14131000
H	2.09438500	-0.05204200	-1.34130700
H	-0.58937900	0.05293600	-1.04931000
H	-1.13902300	0.22399500	1.57675300
H	0.24787400	-4.47206500	2.97273500
H	1.02149900	-5.42584900	0.57764000
H	3.30067900	-4.16680500	-0.12901600
H	3.91784000	-2.41682700	1.81636500
H	2.03091900	-2.59490000	3.73058600
H	1.19810100	0.19686300	2.91690100
C⁺-Complex in toluene			
C	2.42583800	2.61998800	0.35744700
C	3.83791000	2.74047600	0.31909400
C	1.98458400	2.17919200	-0.92167200
C	3.12364300	2.00991800	-1.74387900
C	3.12175900	1.69385700	-2.77935300
C	4.27536400	2.34865000	-0.97279900
C	5.12978600	-1.61195100	0.06047800
C	5.09540500	-1.04813700	-1.24266300
C	3.89876600	-2.28196600	0.27927100
C	3.84096900	-1.37992500	-1.83301200
C	3.10979500	-2.15013100	-0.89519400
C	4.25875700	0.39322000	2.16716800
H	5.31161200	0.70444000	2.17758000
C	3.69590400	1.13055100	2.75671500
C	4.19698500	-0.57274400	2.68631700
C	0.95774900	2.00118700	-1.21676600

H	-0.85634600	-2.91396100	-3.23578700	C	-9.70200500	-1.92142000	-4.27029200	C	0.34073200	0.22314400	0.42799000	H	-10.92832300	2.76889200	-11.08365700
C	3.60160900	-2.71607700	-5.34541000	C	-11.09949000	-1.77544500	-4.07071700	C	1.05243400	0.48247400	1.74293500	O	-9.21134700	2.95979800	-8.20003100
H	1.44290800	-4.10982900	-5.58085000	C	-9.47921800	-3.17098200	-4.90076500	H	1.01666800	-0.06806700	-0.38069400	H	-8.78564700	3.41288800	-7.03507100
C	0.74841800	-2.08317400	-5.14835000	C	-11.74164900	-2.94485800	-4.55661200	H	-0.44562300	-0.52435500	0.52466700	O	-9.63953800	4.55323300	-6.49072800
H	-0.50867700	-3.24930500	-5.51137800	H	-11.59317600	-0.91869500	-3.62883700	H	1.59658500	2.72727900	-0.37081000	O	-7.81743300	2.94388800	-6.44525100
C	2.89871100	-4.03232700	-5.08920400	H	-8.51645700	-3.57971400	-5.18083300	C	2.34805500	1.29586700	1.62583500	C	-9.16611600	5.18926700	-5.17483800
H	4.63330300	-2.71556900	-4.98740300	C	-10.74294700	-3.80662700	-5.07621500	H	0.34767800	0.94876500	2.44356600	H	-9.74317000	5.30732600	-7.28222000
C	3.06474700	-1.86378700	-4.93129700	H	-12.80513000	-3.14188200	-4.53572800	H	1.28603000	-0.50673700	2.15643400	H	-10.64749000	4.13491400	-6.36232400
H	1.43375800	-3.98472700	-6.67163700	H	-10.90782800	-4.78679600	-5.50609400	C	2.17604500	2.71305900	1.06736400	C	-8.12236800	6.31527400	-5.30629100
H	1.08619200	-5.13138200	-5.39610400	C	-9.18013200	-2.89330000	-8.33748200	H	2.09914000	2.03483600	-1.01216200	C	-8.79978100	4.40019900	-4.50808400
C	3.48099900	-4.84467000	-5.54144000	C	-10.44701300	-3.53185500	-8.46836000	H	1.75478000	3.75861700	-0.81236700	H	-10.04567900	5.62218600	-4.68171100
H	2.95054600	-4.18118400	-4.00427900	C	-9.31805100	-1.55773900	-8.79166800	H	3.05880000	0.74582800	0.99394800	C	-6.70801200	9.91754100	-5.76321700
C	2.01528300	-1.86104300	-2.88207800	H	-8.26904000	-3.35252300	-7.97502100	H	2.80787300	1.36699100	2.61760800	H	-8.03865600	6.81953300	-4.33545800
O	1.09887700	-2.59174700	-2.51204900	C	-11.36036000	-2.58992000	-9.00275900	H	1.55067900	3.19456000	1.73426700	H	-8.50897700	7.06935900	-6.00611500
O	0.82959300	-2.83419800	-1.24829000	H	-10.66530000	-4.56531100	-8.22963600	H	3.15331600	3.20426700	1.02591000	C	-9.56440000	4.98597900	-4.81812000
H	-0.99457400	-0.15783500	-0.81602500	C	-10.66489100	-1.36597100	-9.19133500	O	-0.42927400	1.40427200	-0.04946000	H	-6.11358900	6.82979100	-5.90583700
H	-1.38974700	-0.22174400	1.84577800	H	-8.53728200	-0.80759600	-8.80356000	C	0.12873700	2.50349300	-0.41877500	H	-6.74289800	5.41119800	-6.73484500
H	0.61504700	-4.55660400	2.92970300	H	-12.40353900	-2.76878400	-9.22630000	O	-0.62544200	3.44471800	-0.84552000	H	-4.96648800	4.74835300	-5.16999100
H	1.50557600	-5.39192100	-0.59491100	H	-10.40559000	-2.76878400	-9.22630000	H	-14.48238300	2.00094900	-3.32451800	H	-6.50084800	4.05402100	-5.45594300
H	3.57657100	-3.82670200	-1.18624000	H	-11.09219300	-0.44399400	-9.56530000	C	-14.33627600	1.84926200	-4.40290300	O	-5.80848400	4.67590100	-3.53864300
H	3.95965200	-2.01376300	1.83088700	H	-11.09219300	-0.44399400	-9.56530000	Zr	-12.19251100	1.14339000	-4.79717900	C	-5.29821300	5.96571600	-2.52476500
H	2.12056900	-2.45894100	3.75493700	H	-15.13448900	1.18168800	-4.75386200	H	-15.13448900	1.18168800	-4.75386200	H	-5.17873400	5.81063700	-1.26866100
H	1.00028500	0.06986400	3.04792400	C	-0.48362300	1.36864300	-2.63374700	H	-14.47860500	2.82111000	-4.89652500	O	-4.96283800	3.79655000	-2.62229900
C	5.33607400	0.64530500	-6.98803700	C	-0.36834100	-0.00732800	-1.99100800	H	-11.32484800	2.83914600	-4.00077600	H	-5.26227500	5.03090000	0.06007400
C	4.38751800	1.57910900	-7.72933500	O	0.47540300	1.73833800	-3.01087900	C	-10.40174100	3.37675700	-3.22201700	H	-4.23264900	6.36891700	-1.33263800
H	6.20758400	0.35988800	-7.57909000	H	-1.19863300	1.36031800	-3.45725800	O	-10.86232700	4.67331600	-2.56208200	H	-5.96701800	6.56910000	-1.30746800
H	5.66961100	1.08270200	-0.604396100	O	0.92943400	2.27242000	-0.26236600	O	-9.30278500	2.86969300	-3.03116700	C	-2.38422900	3.39914900	-1.12485600
C	4.23103300	-1.37773500	-8.82702700	C	0.84104600	-0.18650600	-1.06345600	C	-9.77733100	5.48313100	-1.83730400	C	-3.96874600	4.43565500	0.64991900
C	4.02924900	1.18366200	-0.81200400	H	-1.30639000	-0.22648400	-1.14607500	H	-11.37643100	5.28074900	-3.31751700	H	-6.01902300	4.24343000	-0.02867700
H	3.46236000	1.68093900	-7.14732700	O	-0.29887700	-0.73308400	-2.81126300	H	-11.64607500	4.37610000	-1.85060300	H	-5.64749000	3.77319400	0.80731500
H	4.86728700	2.56581800	-7.71678100	C	0.89247300	0.77505400	0.12949800	C	-8.91454000	6.47146800	-2.71963500	C	-3.40240500	5.16665900	-0.02166300
C	3.40518300	-0.17549400	-9.35513300	H	1.63482900	2.42756900	-1.08691900	H	-9.09585100	4.79027400	-1.33028100	H	-2.68813700	4.15605700	-1.84146400
C	5.27698300	-1.28444500	-1.91074000	H	1.26576400	2.87938900	0.58015000	H	-10.23699800	6.06885700	-1.04734700	H	-2.21177800	2.48039000	-1.65026500
H	3.84112500	-2.31876900	-9.21853500	H	1.76071600	-0.06687400	-1.65339500	H	-8.08556300	5.86694600	-3.80668000	H	-3.19433800	5.21419700	0.69830500
H	5.03153500	1.18525900	-9.75162300	H	0.84831400	-1.21620300	0.68747000	H	-8.37544500	7.10469400	-2.06851000	H	-4.19253900	4.18001700	1.69271400
H	3.45693300	1.95460700	-9.63170600	H	0.04511900	0.59872700	0.80483300	H	-9.70755200	7.14648600	-3.20840000	H	-4.21183500	2.58925000	-0.48044000
H	2.41785600	-0.17730500	-8.87720400	H	1.79838800	0.57138800	0.71060500	H	-6.91398100	5.04921200	-3.28547400	H	-2.94568000	2.51374900	0.73361600
C	3.23621800	-0.36104500	-10.42057200	O	-1.05192200	2.38035800	-1.73698600	H	-7.69589500	6.67707600	-4.43715400	H	-8.65528500	0.43755600	-6.48859000
O	4.95670500	-0.60140600	-6.527188400	C	-0.42186600	2.80915400	-0.65685000	H	-8.66311400	5.21006400	-4.46840700	C	-9.01472800	-0.05461150	-7.38282600
C	4.21287400	-1.48405500	-7.33899500	O	-0.98901100	3.65866400	0.04632400	H	-6.32633100	4.62630700	-4.10646400	H	-10.35049000	-0.05328800	-7.86154500
C	3.67497900	-2.52770400	-6.83184300	H	-13.31229600	2.19557500	-5.44638100	O	-6.04979200	5.94051400	-2.52084000	C	-8.21398200	4.07472900	-8.32509100
				H	-12.44729100	1.59433300	-5.75910700	O	-4.96755300	5.39544700	-1.95532300	H	-11.19843500	0.41677700	-8.78222000
				Zr	-11.41628400	0.72849300	-3.90581400	C	-3.78580600	4.22849800	-2.64441000	H	-7.14931800	-0.92650600	-8.24463300
				H	-12.80860000	0.83548300	-6.48546400	C	-4.15033500	4.62750500	-1.19939900	H	-9.06100200	-1.18883200	-9.38308500
				H	-11.75397000	2.26153500	-6.28976800	O	-4.68615700	4.21092700	-2.04994100	H	-11.25845400	-0.94695200	-9.69758200
				O	-11.09554400	2.56577300	-3.01131500	C	-3.18778100	6.09791400	0.29570300	H	-8.76251200	-1.77030300	-10.24450000
				C	-10.32131200	3.44201000	-2.39961500	C	-1.87781600	6.53581100	-1.71756000	C	-6.58617200	1.73136300	-10.39950100
				H	-10.87235600	4.86476500	-2.45811300	C	-0.62647300	7.38933200	-1.28052200	C	-6.92264100	0.83632700	-10.46088100
				C	-9.29642700	3.13913900	-1.79766800	C	-2.11842000	3.29319500	-0.94494600	C	-7.37391100	2.74531600	-10.45686900
				O	-9.91947900	5.97281100	-1.98554200	C	-2.69778900	5.23176200	0.67782600	C	-6.92264100	0.83632700	-10.45686900
				H	-11.23638000	5.05419500	-3.47577600	H	-4.82541100	5.65423900	0.71938600	H	-5.83875900	0.83705000	-9.82689700
				H	-11.77298000	4.85348200	-1.82838100	H	-3.78580400	7.05919400	0.80684000	H	-8.20483800	1.87296500	-11.95522300
				C	-8.99155700	6.54906800	-3.07170300	C	-2.37471500	3.72179200	0.35613500	H	-7.33347900	-0.17899700	-11.83414000
				H	-9.33767300	5.60048300	-1.13430900	H	-2.76660300	3.93649300	-1.178365500	C	-7.93118000	3.04798000	-11.20025600
				H	-10.52428700	6.80432500	-1.60322000	H	-2.32367900	2.25456600	-1.20262100	H	-6.51012100	3.42066100	-9.51983000
				H	-7.96741800	5.58571900	-3.69539400	H	-1.78927100	5.66541300	0.23684900	H	-8.92276400	1.78754900	-11.27597000
				H	-8.45518500	7.41011100	-2.65287000	H	-2.57387200	5.33358000	1.76264500	H	-8.41752200	4.00780400	-11.32495100
				H	-9.61295900	6.94846800	-3.88473700	H	-3.81843800	3.39952800	0.28322600	C	3.55144200	-2.18883200	0.21709700
				C	-6.90582400	5.05406800	-2.74848800	H	-2.33355200	3.13773100	1.17323500	C	3.50259800	-1.49037900	0.07735300
				H	-7.46915600	6.08455300	-4.53682800	H	-10.02578200	0.46758000	-2.54389700	O	2.28067800	-2.06587600	0.01490800
				O	-8.47364000	4.70819500	-4.11599900	C	-10.91572800	-0.04170500	-2.88973300	C	4.74235800	-2.35874600	-0.00094900
				H	-6.22599600	4.36274600	-3.25365400	C	-12.23429000	1.16435100	-2.40826200	C	2.10025300	-3.49415100	-1.89929000
				H	-7.33594200	4.55136900	-1.88135500	C	-10.93281000	-0.95868600	-3.96900200	C	4.89568600	-3.32938800	1.19318000
				H	-10.25762000	6.19735500	-2.27573000	C	-11.31808100	-0.64378300	-3.17214				

O	-6.8077880	3.8245040	-7.6606780	C	-3.6148730	10.6897770	2.3768020	O	3.6211920	-1.5687030	-0.6494550	H	5.1150430	-1.2438120	-10.2843090
C	-7.6088510	6.4011980	-6.5835450	H	-5.6569450	9.9588240	2.6237000	H	5.6891650	-1.9588210	1.7818480	H	3.9464710	-0.3349520	-11.2325840
H	-7.6165890	6.6648040	-8.7554120	C	-5.2641390	11.4055130	3.5339930	H	7.8699600	-0.8279940	0.6790200	H	2.1770410	-2.0046840	-10.7451230
H	-9.0465960	5.8914020	-8.1327860	C	-3.1715010	9.8197710	1.1872580	H	6.1232360	1.2633270	-3.4468570	H	3.5929700	-2.7561140	-11.4623640
C	-6.2385610	7.0861940	-6.4160040	H	-3.2213260	10.2375780	3.2959170	H	3.8057090	-0.0965110	-3.6185130	O	2.6974310	-1.8002750	-7.4953380
H	-7.2072460	5.5509740	-5.8980360	H	-3.1241440	11.6694040	2.2883090	H	2.1336500	0.8602780	-1.7462070	C	2.4409480	-2.9195290	-8.2063900
C	-4.9865230	6.2008400	-6.5481260	C	-3.6241040	8.3684100	1.2544550	H	3.4029680	2.8246200	-0.4171360	O	1.4942690	-3.6021020	-7.8576510
H	-6.1263120	7.1269400	-6.2760030	H	-2.7054200	9.8443930	1.1213760	H	5.8867700	3.0537350	-1.4427210	H	8.0556360	-2.2746510	-5.0610220
C	-4.8725150	7.5688610	-5.4310410	H	-3.5513660	10.2291970	0.2440130	H	7.4699530	1.8309380	0.5846180	C	7.8979660	-1.2513240	-6.3399970
H	-6.1625150	7.8989260	-7.1519180	H	-3.2914910	7.8093840	0.3727710	H	-2.3959880	0.8406480	0.1822190	H	8.4507220	-0.3229070	-6.1473960
C	-4.8513240	5.1244890	-5.6118200	H	-4.7090390	8.2796850	1.1784000	C	-3.2739180	-0.3294470	0.9413360	H	8.3167320	-1.6779260	-7.2610110
H	-0.0962180	6.8421510	-6.4517150	O	-3.0199860	7.7639590	2.4324950	H	-3.4533900	-0.1381070	2.0031610	H	6.8659040	-0.9612450	-6.5604530
H	-4.9736990	5.6872100	-7.5158500	C	-3.4841080	6.5585120	2.8076420	H	-4.2590780	-0.4172620	0.4630380	C	9.6930500	-2.5115190	-4.9156610
H	-3.9445700	4.5279680	-5.6257370	C	-2.8550080	6.1241340	4.1209180	H	-3.0178410	-1.3208880	0.8688740	C	10.3808810	-3.6827170	-5.2410390
H	-5.7031200	4.4435460	-5.4746380	O	-4.3219620	5.9330210	2.1861760	C	-3.2757980	2.2577630	0.1573730	O	10.5400590	-1.4416690	-4.6013940
O	-4.7578140	5.7889080	-4.1875730	C	-3.0439950	6.4607210	4.4671500	C	-3.5185590	3.0734050	-0.9514980	C	11.7713840	-3.8041120	-5.2335300
C	-4.6751910	5.0051140	-3.1056490	H	-1.7977110	6.4141450	4.1251050	C	-3.8169520	2.7613560	1.3456270	C	11.9283270	-1.5122650	-4.5777120
C	-4.5627500	5.8381860	-1.8389310	C	-3.3308220	6.7443170	4.8939860	C	-4.2783210	4.2409420	-0.9150180	C	12.5559880	-2.7111470	-4.8970170
O	-4.6730630	3.7868700	-3.1481240	H	-1.2774270	4.3421390	1.4485180	C	-4.5766770	3.9258880	1.4346250	C	7.2288610	-0.3710750	-5.2234820
C	-4.9710650	5.1174670	-0.5400420	C	-2.0622120	3.6406560	3.8264260	C	-4.8177350	4.6731380	0.2894350	C	7.2267780	-4.6368690	-4.1741070
H	-3.5282260	6.2070110	-1.7349700	H	-0.4724810	4.3520460	4.2196300	C	-2.1026160	0.1996490	-1.3293650	C	6.4154630	-0.0774520	-6.2943890
H	-5.1772600	6.7328200	-1.9843580	C	-2.9463900	4.5415540	5.5553170	O	-0.9004370	-0.3624530	-1.7563810	C	6.4800780	-5.8096410	-4.1571330
C	-2.3117760	2.9535540	-1.3465540	C	-2.1661440	3.4386700	2.2985070	C	-3.1483250	0.0015090	-2.2420310	C	5.6420460	-5.2383390	-6.5226870
C	-3.9000170	4.3011070	0.2127920	H	-1.4232810	5.4023600	1.6609800	C	-0.1766450	-1.0176610	-2.9723920	C	5.6944120	-6.1123440	-5.2460430
H	-5.8383680	4.4768760	-0.7417420	H	-1.4489120	4.1669810	0.3841460	C	-3.0178410	-0.6412480	-3.4692440	C	7.3418320	-11.7448800	-3.7135110
H	-5.3196760	5.8920440	0.1538460	H	-1.0320410	3.9181020	4.0904800	C	-1.7631300	-1.1601690	-3.8458080	C	5.9964680	-1.1890150	-3.7660080
C	-3.4972060	2.9344860	-0.3842850	H	-2.2422880	2.6711020	4.3089440	C	-0.9663370	1.2360600	0.9464270	C	7.9338010	-1.3445450	-2.4666260
H	-2.4463120	3.6718300	-2.1517580	H	-3.1995810	3.5955980	1.9692340	C	-0.3839200	0.5287110	1.9992530	C	5.3078910	-0.5745460	-2.7240000
H	-2.1256490	1.9654010	-1.7673080	H	-1.9127220	2.4024160	2.0437030	C	-0.2244530	2.3564440	0.5483400	C	7.2917840	-0.1718200	-1.3973780
H	-3.0047390	4.9206600	0.3649210	H	-8.5722140	9.4585740	-0.7611490	C	-0.1335990	0.8888430	2.6158790	C	5.9710930	-0.3176440	-1.5327500
H	-4.3008680	4.1142050	1.1267950	C	-9.1915990	10.1130470	-1.3601980	C	0.9858990	2.7696990	1.1533260	C	13.8959590	-2.8060930	-4.8850400
H	-4.3387340	2.5068160	-0.9387890	C	-9.9237030	11.2339610	-0.8910140	C	1.4922380	2.0215860	2.1936100	C	12.6688820	-0.4359760	-4.2534330
H	-3.2592740	2.2320620	0.4245000	C	-9.3418650	10.0533870	-2.7633580	F	-5.5454570	5.8003320	0.3489230	F	10.0155360	-0.2332120	-4.2821740
H	-7.6385410	1.5520180	-8.1744890	C	-10.5491330	11.8550940	-2.0057120	F	-5.0682800	4.3374370	2.6182980	F	9.7213490	-4.8006770	-5.6103380
C	-8.2074580	1.2284230	-9.0361990	H	-9.9914080	11.5625900	1.1388600	F	-12.3565200	2.1282590	2.5244910	F	12.3565200	-4.9724900	-5.1556680
C	-9.5445210	1.5987060	-9.3358580	H	-8.9092100	9.3063190	-3.4219370	F	-2.9920620	2.7768030	-2.1616940	C	6.3104280	-3.2997330	-7.4037900
C	-7.7180440	0.4569500	-1.1193660	C	-10.1891370	11.1284740	-3.1680740	F	-4.4791690	4.9654780	-2.0318980	F	4.8272350	-5.4969060	-7.3691030
C	-9.8935770	1.0333250	-10.5907460	H	-11.1851100	12.7294840	-1.9723590	F	-4.3900500	0.4470720	-1.9526100	F	4.8994450	-2.7149540	-5.2408940
H	-10.1866640	2.2120660	-8.8761210	H	-10.5136350	11.3421100	-4.1789550	F	-0.4276270	-0.7786570	-4.2899720	F	6.5178110	-6.6444730	-3.1017010
C	-6.7324170	0.0155240	-10.1903760	C	-6.8241100	11.5287490	-4.5072860	F	-1.6319890	-1.7949890	-5.0187270	F	7.9906640	-4.4086830	-3.0816140
C	-8.7627120	0.3341570	-11.0823190	C	-7.6075030	12.6776140	-4.8177330	F	4.0924260	-1.5374580	-3.2924630	F	5.2465790	-1.4359800	-4.8751630
H	-10.8493520	1.1259480	-11.0876250	C	-5.7845050	11.9317880	-3.6320420	F	0.2204670	-0.3338010	-0.9676490	F	4.0037130	-0.2423330	-2.8500200
H	-8.7141200	-0.2229370	-12.0098700	H	-6.9832880	10.5272950	-4.8866300	F	0.9363630	-0.6172100	2.4694420	F	5.3265330	-2.7698900	-5.0228810
C	-5.8320260	2.2529880	-12.1886330	C	-7.0473870	13.7856160	-4.1326060	F	1.3537140	0.1147850	3.5837850	F	7.9320860	-0.5139440	-0.2339660
C	-6.8287600	2.0031550	-13.1770940	H	-8.4640730	12.7038360	-5.4798600	F	2.6674820	2.3659370	2.7557420	F	9.1953000	-1.7420810	-2.2054400
C	-5.7914840	3.6509590	-11.9556940	H	-5.9272030	13.3230200	-3.3931090	F	1.6276480	3.8527260	0.7055540				
H	-5.1918530	1.5132260	-11.7258790	F	-5.0321140	11.2848240	-3.1983270	F	-0.6226430	3.0945550	-0.5094140				
C	-7.4083730	3.2449480	-13.5368310	H	-7.4092910	14.8042270	-4.1670970								
H	-7.0806260	1.0378680	-13.5963830	H	-5.2996880	13.9244300	-2.7471540								
C	-6.7736160	4.2617940	-12.7735440	O	2.0483410	-1.3192570	0.7747600								
H	-5.1533150	4.1564730	-11.2425810	C	2.0338380	-1.8885980	-0.3716440								
H	-8.1960970	3.3944410	-11.4262430	O	1.0510150	-1.6220690	-1.1559860								
H	-7.0094220	5.3179220	-12.8024070	C	3.1455010	-2.8434440	-0.6796730								
C	1.8287760	-1.7336990	1.0885800	O	0.9266440	-2.2064730	-2.5206350								
C	0.9905520	-2.7381280	0.3603350	C	2.6517890	-4.2910630	-0.8844890								
C	2.7376240	-3.9023140	0.6667950	H	3.6573180	-2.4808160	-1.5857000								
C	0.9032540	-3.8826780	-1.5962740	C	3.8534850	-2.7766920	-1.4932800								
C	1.9740850	-5.1928020	1.0557780	H	0.7143590	-3.7095850	-2.4967850								
C	3.3792240	-4.0964270	-2.0352000	H	1.8155720	-1.9008880	-3.0786580								
C	3.3824770	-3.5760530	1.4850310	H	0.8549300	-1.6742000	-2.9063040								
C	0.3536910	-5.1538010	-0.9608920	H	1.9727200	-4.5419640	-2.2374900								
H	1.8891330	-4.0330630	-2.0487910	H	1.9837680	-4.5653530	-0.0582040	Zr	0.7609670	-4.1777970	1.3913430				
H	0.2280740	-3.4968370	-2.3606080	H	3.5345920	-4.9319410	-0.7967990	C	3.7009830	-2.1689800	1.1644550	Zr	0.7857570	-0.2015720	0.6524980
C	1.3709660	-5.9514680	-1.1331800	H	0.0575470	-3.9452460	-1.7722120	O	3.5247870	-3.4485590	0.5837880	C	-1.3647370	-2.0416420	1.3528880
H	1.1975210	-4.9482510	1.7921610	H	0.3110300	-3.9682600	-3.4837980	H	-1.5805630	-2.2326120	3.3858550	H	-1.5805630	-2.1495690	2.3998920
H	2.6876840	-5.8458140	1.5691790	H	2.7027000	-4.3487250	-0.0397210	H	-2.0420520	-1.8041240	0.7260950	H	-1.6244340	-3.4598670	1.2091210
H	-0.5266660	-4.8911530	-0.3596610	H	1.7163130	-5.6037930	-2.3053040	H	1.7766770	-0.0123500	-1.5997410	H	1.7766770	-0.0123500	-1.5997410
H	-0.0118490	-5.7845740	-1.7808820					H	0.0866240	-5.0565990	-2.9172420	H	-0.5119200	-4.8224900	-3.2852070
H	2.1851140	-6.2826720	-0.7933390					H	-0.3160870	-5.0979300	-4.3981150	H	-1.5507040	-3.1038150	-2.812

H	3.19024100	0.80238900	-9.02734500	O	5.36012600	-1.05357500	-5.86881300	B	8.35095400	-0.85921600	-2.61016300	H	6.99525900	-0.12818800	-7.30936400
H	4.55366900	0.50843700	-10.09403100	C	5.22798800	-2.09601700	-6.60609300	C	9.94214800	-0.38005600	-2.61062700	H	6.06818500	1.04894100	-6.23910500
O	4.04962600	-0.04963200	-6.01378100	O	4.60456800	-3.09456100	-6.10332500	O	10.96131000	-1.33211700	-2.49314000	C	5.20171000	-2.25747800	-8.50105500
C	3.85933900	-0.88237100	-7.02415600	B	9.55509000	-1.98110900	-3.07828100	O	10.41306500	0.91499600	-2.81838400	C	5.44265300	0.12012000	-9.59990100
C	3.02361700	-1.78374400	-6.87902700	C	9.48724300	-0.66341100	-4.06248500	C	12.31973800	-1.04698400	-2.56721200	H	4.35943500	1.18072500	-8.02407500
B	7.34810700	-3.03396400	-4.28574700	H	9.92860000	0.20400300	-3.55426800	H	11.76322300	1.25386800	-2.91076500	H	5.73011600	2.00909400	-8.67035500
H	8.19673500	-1.73874400	-5.27919600	H	10.06635800	-0.81252300	-4.98492000	C	12.72878700	0.26625600	-2.78045200	C	4.66373000	-1.20119700	-9.48973300
H	8.29536300	-2.04158400	-4.25768600	H	8.47552400	-0.37142800	-4.35607200	C	8.20540000	-1.83727300	-3.67577800	H	6.29534000	-2.33285400	-8.57713300
H	7.28925600	-1.15842600	-5.46585100	C	11.17127200	-2.12955500	-2.72699100	C	8.14074000	-3.23240700	-3.99085100	H	4.80292600	-3.24446300	-8.74928200
H	8.93236000	-1.04987900	-4.84286700	C	12.04201300	-3.06902700	-3.28279900	C	8.33791000	-1.27141000	-5.24547200	H	6.49219800	-0.08835800	-9.84871700
C	9.50216400	-3.69132600	-4.16512700	C	11.82188500	-1.16020600	-1.95448700	C	8.03485200	-3.99457300	-5.15523900	H	5.03155400	0.67120400	-10.45433700
C	9.94440000	-4.84428500	-4.81725100	C	13.42196600	-3.07928800	-3.07543100	C	8.28685100	-1.99451800	-6.43295100	H	3.61053600	-0.99157100	-9.25958000
C	10.52850300	-2.99393600	-3.51715600	C	13.19120400	-1.12793200	-1.71575200	C	8.08659000	-3.37175900	-6.39459000	H	4.67009500	-1.66972100	-10.48065600
C	11.26590800	-5.29273200	-4.80861000	C	14.00543500	-2.10208100	-2.28256000	C	7.91993700	-1.64804300	-1.21038200	O	5.00584300	-0.88205800	-6.46669600
C	11.85774500	-3.39936200	-3.47705800	C	8.93054200	-3.37620600	-3.74211800	C	6.69437500	-2.31446600	-1.11796400	C	4.87688000	-1.98127600	-7.05402000
C	12.23469500	-4.56676800	-4.13147100	C	8.97419800	-4.57306600	-3.01570800	C	8.40640900	-1.59301000	0.00570200	O	4.43448400	-3.03814100	-6.40579200
C	6.85937000	-4.13691100	-4.82805900	C	8.25583600	-3.49104100	-4.95422400	C	6.20036900	-2.91247600	0.03318800	B	8.36015000	-1.05134100	-2.70054700
C	6.62266100	-5.30846800	-4.09967200	C	8.41130700	-5.77406300	-4.34553800	C	8.14690300	-2.16378000	1.19478400	C	9.90652700	-0.43853200	-2.70166500
C	6.02345300	-3.98861100	-5.93564200	C	6.76833600	-4.67117100	-5.42212300	C	6.93196400	-2.83350000	1.21165400	O	10.98060500	-1.20849100	-2.24038700
C	5.66394800	-6.26144300	-4.42971100	C	7.74591400	-5.82389200	-4.65457100	F	14.03385700	0.56830400	-2.86371100	C	10.29652600	0.78013000	-3.25277100
C	5.05059600	-4.91733800	-6.30536000	C	8.58231600	-1.74267400	-1.73528200	F	12.31135200	2.53126800	-3.13045500	C	12.31296800	-0.81299400	-2.89939700
C	4.86121000	-6.06059500	-5.54317400	C	7.24009500	-1.38375000	-1.90101500	F	9.56166500	1.96554000	-2.96387300	C	11.61639200	1.22219300	-3.33116900
C	7.34815600	-2.52972900	-2.81872300	C	8.94327000	-1.92230500	-0.39513200	F	10.63658100	-2.63004800	-2.28722700	C	12.63886800	4.20721200	-1.84536000
C	6.19690300	-1.73522500	-2.78886500	C	6.34304500	-1.16184400	-0.86046100	F	13.24016300	-0.20189600	-2.44042900	C	8.43611600	-2.32846400	-9.87542100
C	7.82547200	-2.85627000	-1.54421500	C	8.08707300	-1.69855300	0.68371300	F	8.49837000	0.06545500	-5.40648300	C	5.17396000	-3.61984400	-3.66435000
C	5.60716900	-1.23680200	-1.63112300	C	6.77750800	-1.30352100	0.44977600	F	8.30311000	-1.36130900	-7.62915000	C	8.49156500	-1.88627700	-5.22714400
C	7.27346400	-2.38018600	-0.35439100	F	15.33204900	-2.09141300	-2.07223200	F	7.95483000	-4.07401500	-7.53280800	C	8.57203600	-4.56773400	-4.68703400
C	6.16202500	-1.55068900	-0.39891200	F	13.73645100	-0.16338900	-0.95182600	F	8.14518200	-5.32509700	-5.08489100	C	8.53253300	-2.79403500	-6.28011200
F	13.51339100	-4.97850400	-4.11332800	F	11.10696800	-0.16282300	-1.37892400	F	7.80891300	-3.95089200	-2.85005000	C	8.56725500	-4.15580900	-6.01352200
F	12.78157500	-2.62744100	-2.82108400	F	11.58671200	-4.05185200	-4.09886100	F	8.18519400	-2.41497900	-2.20837900	F	7.88236400	-1.62347000	-1.12623100
F	10.25473300	-1.83565100	-2.86702700	F	14.19142400	-4.02443800	-3.64684800	F	5.00807800	-3.54969100	0.02079300	C	6.74120400	-4.23996000	-0.06628000
F	9.09215800	-5.61591500	-5.53561400	F	8.09607800	-2.42059700	-5.78832600	F	6.46300800	-3.38256100	2.34755500	C	8.39709000	-1.20470000	0.01252700
F	11.60895000	-6.41931600	-5.46102600	F	7.02702400	-4.69305500	-6.60711400	F	8.66716200	-2.06182200	2.32465800	C	6.17375100	-2.81006000	0.11112500
F	6.10340300	-2.89928100	-6.74272200	F	7.16527700	-6.95898100	-5.07613700	F	9.78821400	-0.94520300	0.11313900	F	7.85879400	-1.55611000	1.25117000
F	4.26299900	-4.69667000	-7.37970700	F	8.49224200	-6.87936000	-2.67414700	C	7.31333400	4.07709400	-4.48823200	C	6.73495900	-3.26748500	1.30212100
F	3.91265300	-6.95286200	-5.87518000	F	9.60354800	-4.60111700	-1.82146700	F	8.11735200	5.36842100	-4.61451100	F	13.91735200	0.82442000	-2.91212900
F	5.49538100	-7.36317700	-3.67196700	F	6.70447900	-1.26150800	-3.15006700	F	7.85153600	3.32178300	-3.90918000	F	11.90300700	2.01703400	-3.89165600
F	7.36566600	-5.56956600	-3.00086000	F	5.06033300	-0.82495700	-1.11105200	F	6.36275200	4.26979700	-3.98564800	F	9.38332700	1.64470400	-3.77631300
F	5.54466600	-1.41179600	-3.994155400	F	5.93422400	-1.08136200	1.48005700	C	9.25413200	3.02399600	-6.35478800	F	10.74331000	-2.42539400	-1.70207100
F	4.50000300	-0.46591300	-1.69322300	F	8.51328500	-1.87179200	1.94581200	C	9.59869300	5.16604100	-4.95861900	F	13.28872900	-1.60683400	-1.81514200
F	5.60709300	-1.08419500	0.74161000	F	10.17547100	-2.34984900	-0.05485600	H	7.62790700	6.01590700	-5.35512000	F	8.53231000	-0.57894800	-5.96197700
F	7.80033300	-2.72231100	0.83354500					H	8.04365400	5.88695100	-3.64938400	F	8.52330100	-2.35600400	-7.56285400
F	8.87718000	-3.68400100	-1.38318500					H	8.84802600	4.44899100	-6.29078300	F	8.60323500	-0.505111200	-7.01283700
								H	9.45998100	2.50066900	-5.41386400	F	8.62654600	-5.88016600	-4.40164400
								H	10.19628000	-0.04044100	0.47840800	F	8.54416300	-4.11925200	-2.47122400
								H	2.91213800	-0.90791600	-0.49463900	H	10.07460300	4.58552500	-4.15572600
								H	3.17692700	-0.72060000	0.88499000	H	10.08959900	6.14295900	-4.97714600
								H	4.11070700	-0.93129700	1.39018700	H	9.46271800	5.04749200	-7.12775300
								C	2.00301400	-0.18985800	1.49027200	F	10.92999600	4.56234300	-6.44560600
								C	0.63257000	-3.73632700	2.94837700	O	8.69651700	3.51048700	-5.75836300
								C	1.84781600	-3.08504400	3.27613400	F	7.76598300	2.97566900	-6.64206000
								C	0.93006100	-4.77975500	2.02844000	F	7.30659200	2.48193300	-7.65689300
								C	2.89677400	-3.71518300	2.54814800	H	7.26565900	0.37526900	-2.71156700
								C	2.32615500	-4.77191000	1.79217900	H	6.55613600	-0.01492800	-2.69367600
								Zr	1.41588300	-2.58062200	0.75154800	H	8.30320400	3.62511600	-4.05307100
								C	-0.86484900	-2.37331800	0.64093100	H	6.55612600	3.90659800	-5.05252600
								H	-1.32767900	-1.77844900	1.44031700	C	9.50967300	3.35894400	-6.64418100
								H	-1.13663400	-1.90581300	-0.31606000	O	9.07771400	5.72543000	-5.67464900
								H	-1.31987400	-3.37292100	0.66807500	H	6.90248800	5.67139800	-5.86664000
								H	3.59070800	-1.33236400	-1.22246200	H	7.48832200	0.67620100	-4.25903000
								C	1.39585400	-5.06182300	-2.96317000	C	9.48111000	4.88398300	-6.89257200
								C	1.74014200	-5.13128200	-4.45880600	C	10.01175200	3.13522700	-5.69168000
								H	1.95069700	-5.81254000	-2.38634200	H	10.07096000	2.85551300	-7.43167500
								H	0.33518300	-5.30601400	-2.81049100	C	8.91253800	5.56153900	-4.87337400
								C	4.20559200	-3.06504200	-4.85174100	H	9.13883800	6.78852300	-5.94132400
								C	3.21022600	-5.45746800	-4.78640800	H	8.82095900	5.10126300	-4.87313300
								H	1.43777200	-4.19002500	-4.93218300	H	10.49028800	5.17612300	-7.20388600
								H	1.12691600	-5.91614500	-4.91873800	O	7.22358100	3.05446300	-5.74453800
								C	4.27791900	-4.46968100	-4.28719700	C	8.14709800	2.71239900	-

H	3.3730900	-6.0694900	-4.0669110	H	-0.9646180	-3.2218950	2.9378120	C	8.3077000	4.2473050	-0.9883130	C	6.3964750	-0.5144370	0.8325150
H	4.5915330	-4.0187330	-3.8113260	H	-1.1654870	-3.1300200	1.1791300	C	8.4303370	4.8230950	0.4197840	F	14.2225430	0.8744280	-3.1579580
C	3.2846740	-3.9482830	-2.6519980	H	-0.7054030	-4.6655710	1.9433240	H	8.5367330	3.1775530	-1.0060100	F	12.6701260	1.4582310	-5.3481440
O	5.0170200	-3.3235420	-2.3005210	H	2.9111580	-1.1360830	-0.5667550	H	7.2942010	4.3839760	-1.3715000	F	10.0692800	0.9589490	-5.3395500
C	0.7702210	-4.4395190	-1.8695900	C	1.4545630	-5.2350430	-2.3024620	C	11.8370400	4.0757740	-0.8874850	F	10.4586160	-0.7589640	-0.8949500
O	0.9037300	-4.7301530	-0.8803840	C	1.7233600	-5.1545690	-3.8134410	C	6.6645710	4.3396140	1.1915980	F	13.0458950	-0.2407610	-0.9481600
H	-0.8367190	-1.9400680	-0.3221800	H	2.1322720	-5.9427420	-1.8102100	H	8.4121190	5.9194770	0.3516110	F	7.2252910	-0.7364800	-6.0018220
H	-1.4447080	-1.9873970	2.3112030	H	0.4413630	-5.6247060	-2.1246700	H	7.5276000	4.5289210	0.9712850	F	7.4549190	-2.9531720	-7.4319490
H	0.5375090	-6.0116000	3.9170350	C	3.7757620	-2.6774350	-4.2528840	C	11.0043010	4.6769610	0.5248760	F	8.6868800	-5.1718300	-6.4095780
H	6.4352000	-7.2323740	1.6355790	C	3.2117030	-5.1958800	-4.2114290	H	7.5276000	4.5289210	0.9712850	F	9.2726440	-5.0851200	-3.8746070
H	3.4124910	-5.9248880	0.6478860	H	1.2423270	-4.2516000	-4.2059490	H	12.2397310	4.0817890	-1.1665580	F	9.5536900	-2.8520220	-2.4180280
H	3.9785500	-3.8811290	2.2979970	H	1.2273030	-6.0049870	-4.2987950	H	9.9202600	3.2504030	1.3192630	F	6.5059100	-2.4495590	-2.2013810
H	2.2058800	-3.9387470	4.3319230	C	4.0926250	-4.0517040	-3.6831330	H	9.6492940	4.7730460	2.1997910	F	5.2748160	-2.4774680	0.1141260
H	8.0544100	-1.7627810	3.6902590	H	4.3011610	-1.8968580	-3.6970980	H	11.1436540	5.7658380	0.4771510	F	5.7572250	-0.5378280	2.0199330
C	6.5998400	3.1274000	-7.2478250	H	2.7095780	-2.4499220	-4.2278590	H	11.8158260	4.2897040	1.1520700	F	7.5308560	1.4872870	1.4227480
C	5.6043720	2.2786190	-8.0109640	H	3.2806910	-5.2168390	-5.3073120	O	9.1243150	4.9329320	-1.9735990	F	8.7918220	1.5329630	-0.9135560
H	6.4079030	3.1411440	-6.1724060	H	3.6380230	-6.1469440	-3.8623930	O	10.4725700	4.8372200	-1.9904740	C	9.7030960	4.4242020	-5.0158910
H	6.6613870	4.1504520	-7.6257060	H	5.1459890	-4.2764530	-3.8910060	C	10.0454700	-1.5669450	2.5897090	C	10.7026710	5.3002680	-5.7046390
C	4.0670330	-1.3108490	-7.6254490	H	4.0144950	-3.9782730	-2.5915510	H	8.7820710	3.3460950	-5.0240280	H	9.7820710	3.3460950	-5.0240280
C	5.4469860	0.8468010	-7.4809960	O	1.3780820	-2.8234290	-2.1146250	C	8.8525410	-0.9455240	2.0605060	C	8.8525410	-0.9455240	-4.5093940
C	6.4452060	2.8089030	-7.9315700	C	1.5096330	-3.9031850	-1.5558770	C	9.9981430	3.0185270	-7.9782490	C	9.9981430	3.0185270	-7.9782490
C	8.1761840	2.2763530	-9.0759300	O	1.6685390	-4.0507720	-0.2449310	C	11.6567460	4.5797500	-6.6704140	C	11.6567460	4.5797500	-6.6704140
C	4.3197290	0.0883580	-8.1961110	H	0.2498160	-1.0535580	-0.4277550	C	10.1560530	6.1051500	-6.2106720	C	10.1560530	6.1051500	-6.2106720
H	4.9832060	-1.9119210	-7.6065000	H	-0.4511700	-0.6814880	2.1563420	C	11.2885950	5.7883980	-4.9178850	C	11.2885950	5.7883980	-4.9178850
H	3.3609200	-1.8579800	-8.2655220	H	0.8422300	-4.8156630	4.2372440	C	12.0642000	4.4325240	0.0605060	C	12.0642000	4.4325240	0.0605060
H	5.2282760	0.8858470	-6.4070100	H	1.6870510	-6.2826650	2.1425060	C	10.2988090	2.2539800	-7.2702110	C	10.2988090	2.2539800	-7.2702110
H	6.3933770	0.3036970	-7.5954470	H	4.0243700	-5.2569670	1.2962740	H	9.9096930	2.5427140	-8.9578670	C	9.9096930	2.5427140	-8.9578670
H	3.3911480	0.6673740	-8.1249570	H	4.6258350	-3.1516090	2.8475940	C	12.0988160	3.7134300	-6.1631340	C	12.0988160	3.7134300	-6.1631340
H	4.5583960	-0.0056300	-8.2697700	H	2.6544660	-2.8740760	4.6753850	C	12.4864200	5.2640730	-6.8856240	C	12.4864200	5.2640730	-6.8856240
O	2.9346710	-0.3199600	-5.7160620	H	1.8099970	-0.5640320	3.6114410	C	10.6611440	5.0075350	-8.5539780	C	10.6611440	5.0075350	-8.5539780
C	3.4692510	-1.2862300	-6.2265280	C	6.2509380	3.2735970	-7.4461340	C	11.8963680	3.7588170	-8.6321520	C	11.8963680	3.7588170	-8.6321520
C	8.0592880	-2.4815990	-5.6294520	C	5.3823600	2.2704180	-8.1777690	C	8.3917340	4.2231680	-6.9562510	C	8.3917340	4.2231680	-6.9562510
B	3.8669300	-0.2131720	-2.7920110	H	6.2031320	3.1614700	-6.3612020	Zr	6.8293670	5.3383400	-7.5774460	C	6.8293670	5.3383400	-7.5774460
C	7.0503990	1.0284950	-3.1632600	H	6.0301600	4.3086360	-7.1946000	O	6.6707160	3.1061370	-8.3919030	C	6.6707160	3.1061370	-8.3919030
H	0.7213170	1.8052060	-2.3850950	C	4.5741980	-1.5363820	-7.7087640	H	-0.5369900	-4.4984120	3.3695920	C	8.0946760	4.6567100	-8.2761360
H	7.2491730	1.5253330	-4.1152420	H	5.5441470	0.8291110	-7.6784870	H	-0.4089500	-4.1676020	1.7042730	C	8.4451600	5.8324830	0.0343260
C	1.0149440	0.6637170	-3.2059460	H	4.3462710	2.5989390	-8.0181020	H	-1.0949110	-5.6227390	2.0737710	C	8.1153080	3.7065710	-0.3734100
C	9.6718620	0.2180560	-2.6619000	H	5.5703640	2.3469390	-9.2567910	H	1.9075660	-0.9321780	-0.1496450	H	7.0340890	4.8066160	-1.2510650
C	10.1118800	-0.6526050	-2.0945440	C	4.5800500	-0.1501120	-8.3636820	C	1.3620030	-4.8941590	-2.3713760	C	10.8952410	4.0667120	-2.0524980
C	10.2461430	1.3546460	-3.2258140	H	5.5843190	-1.9584800	-7.6551870	C	1.5821440	-4.6508930	-8.3274710	C	9.7031520	5.5823200	0.8762790
C	11.9829520	-0.4220230	-2.0595730	H	3.9823290	-2.2414550	-8.3087330	H	1.9415520	-5.7557200	-2.0163850	H	8.5517540	6.7399270	-0.5751580
C	11.6139640	1.6214980	-3.2350380	H	5.3564000	0.8161490	-6.5985200	C	3.0098000	-5.1531870	-2.1825840	H	7.5957380	6.0090250	0.7067940
C	12.4973370	0.7318830	-2.6431540	H	6.5774300	0.4898700	-7.8206590	C	3.9200370	-2.4234990	-4.2937520	C	10.9765660	5.3076550	0.0668710
C	8.1231420	-1.3597090	-0.4070950	H	3.5624400	0.2568870	-8.3300710	C	3.0282960	-4.8460260	-3.6698980	H	10.4375740	3.2251470	-0.3184670
C	8.0984790	-2.7491760	-3.8407700	H	4.8486980	-0.2573380	-4.9277950	H	1.2083430	-3.6474900	-1.1671790	H	11.8950050	7.3562300	-1.1617390
C	8.3128740	-0.9740000	-5.3363100	O	3.3044910	-0.5968800	-5.8646310	H	0.9472940	-5.3547680	-4.4261630	H	9.5163760	4.7288700	1.5432430
C	8.1933400	-3.6661900	-4.8878000	C	3.9692820	-1.5127930	-6.3126600	C	4.0873630	-3.8650930	-3.8370600	H	9.8763210	6.4500300	1.5239480
C	8.4528780	-1.8465430	-6.4144200	O	4.2473510	-2.6350380	-5.6314090	H	6.4236980	-1.7701460	-3.7723720	H	11.2475300	6.1874140	-0.5322490
C	8.3481200	-3.2154150	-6.1929280	B	8.4234310	-0.3578940	-3.1264830	H	2.9124130	-2.0446880	-4.1178140	H	11.8075460	5.1400790	0.7608700
C	7.4271400	-0.7819000	-1.3681420	C	6.2651280	0.7050330	-3.6195120	C	3.0266700	-4.7927240	-5.4664850	O	8.8370300	6.6184710	-2.1088570
C	6.2159860	-1.4805630	-1.3685560	H	7.2684420	1.6154660	-3.0014670	H	3.3468000	-5.8678240	-4.1175240	O	10.1224770	4.3094670	-2.1252480
C	7.8752870	-0.4475910	-0.0889620	H	7.3417070	1.0247780	-4.6591130	H	8.0029390	-4.2093720	-4.1452590	O	10.6969020	4.2590250	-3.2230650
C	5.5117570	-1.8482720	-0.2253760	C	6.2679730	0.2586970	-3.4972750	H	4.0955350	-3.8572530	-2.7415110				
C	7.2117700	-0.7912980	1.0898580	C	9.9849280	0.2148550	-3.2586880	O	1.8195460	-2.5679200	-1.8807190				
C	6.0203320	-1.4988060	1.0209350	H	11.0503990	-0.4084780	-2.5956950	C	1.6625330	-3.7058940	-1.4622150				
F	13.8171080	0.9734460	-2.6416710	C	10.3948470	1.2375050	-1.1123440	C	1.7130570	-4.0346790	-0.1772760				
F	12.0879890	2.7377520	-3.8442050	C	12.3879880	-0.0496700	-2.7329470	H	-0.5949600	-1.6418490	0.4656020				
F	9.8557200	2.3005120	-3.8539300	C	11.7206170	1.6292950	-4.2898470	H	-0.7794900	-1.8480410	3.1475800				
O	10.1967580	-1.8117400	-1.5411520	C	12.7336810	0.9844880	-3.5964310	H	1.7194600	-5.7662530	4.0992620				
O	12.8178540	-1.3034210	-1.4848980	C	8.4564320	-1.7373090	-4.0689100	H	2.6569200	-6.5387430	1.6974710				
F	8.4376940	0.3428860	-5.6668800	C	8.6619660	-3.0382450	-3.5939120	H	4.5195890	-4.7590920	0.9208790				
F	8.5751830	-1.3656450	-7.6670120	C	8.4341790	-1.6726740	-5.4613930	H	4.7218780	-2.8766550	2.8177500				
F	8.4410040	-0.4823930	-7.2130900	C	8.6952120	-4.1739940	-4.4018300	C	2.9858590	-3.4980460	4.7979630				
F	8.1140250	-4.9871130	-4.6456200	C	8.3499200	-2.7788670	-6.3068090	H	1.6271890	-1.2478010	4.1901200				
F	7.9776490	-3.3006300	-2.6150820	C	8.5263320	-4.0484830	-5.7750380	C	6.2676640	3.4940190	-8.0984550				
F	5.6395780	-1.8302060	-2.5451430	C	7.9760070	-0.6538470	-1.5519980	C	5.3561270	2.4569800	-8.7007650		</		

H	4.65636200	2.45904500	-8.88468100	H	6.27160500	0.86589900	2.49144900	H	2.49689900	-4.61041500	-6.21157900	H	0.70014600	-3.44503000	-4.94629200
H	6.12508800	1.99566400	-9.73835400	H	4.08333100	1.06314500	-2.56707900	H	2.21900100	-6.00711000	-5.17124300	H	-0.05296900	-5.02009100	-5.00321400
C	4.80037500	-0.25813600	-8.64664000	C	3.52074900	3.30221000	1.38708200	C	4.46143100	-4.64562300	-4.94736800	C	3.40495300	-4.56747400	-4.67425400
H	5.74741200	-2.01622000	-7.76712400	C	3.58040700	4.69537400	0.73181600	H	3.69197600	-5.20710300	-3.47819800	H	4.30754900	-2.58095200	-4.13218500
H	4.18242000	-2.33604200	-8.48450600	H	2.83213800	3.29240000	2.23446900	H	2.76881800	-2.93467300	-2.56548900	H	2.71371600	-2.44117600	-0.53079800
H	5.33935000	0.96714700	-6.89534400	H	4.49794100	3.00576100	1.77547800	H	1.62585700	-3.47753000	-2.27223100	H	2.05467200	-4.93893700	-6.31752100
H	6.72070600	0.41336600	-7.88505100	C	1.30233400	3.46174900	-0.76320100	H	1.17769700	-3.24850800	-1.12097600	H	2.06318700	-6.19217200	-5.08513600
H	3.18164900	0.13891900	-8.73769700	C	2.21900000	5.40604700	0.66303400	H	-0.25543900	-0.19371000	-1.00630200	H	4.24724100	-4.92268300	-5.27629600
H	5.15972500	-0.44875400	-9.66688000	H	4.01189500	4.59851600	-0.27311100	H	-0.75081100	0.07278500	1.62495900	H	3.59441600	-4.94453800	-3.66282800
O	3.37412100	-0.56092600	-6.17738500	H	4.28773100	5.30644600	1.30174400	H	0.34168500	-4.10216300	3.43363100	O	2.51102700	-2.82787300	-2.82355100
C	4.06557400	-1.49334200	-6.54243200	C	1.04880400	4.46118600	0.35087300	H	1.07943300	-5.56275800	1.30039100	C	1.57422000	-3.49122900	-2.32759600
O	4.30863400	-2.57940900	-5.78834200	H	0.37975100	2.97856900	-1.08180800	H	3.94743800	-4.65609300	0.45597200	O	1.23926900	-3.34807000	-1.08866500
B	8.58794700	-0.22165000	-3.17805000	H	1.77716300	3.91700300	-1.63659100	H	4.20254200	-2.61996800	2.04592300	H	-0.29175100	-0.31941800	-1.07357200
C	7.65230500	0.99033000	-3.78794200	H	-2.27093900	6.19800400	-0.09368000	H	2.26734000	-2.27402200	3.89587300	H	-0.76099200	-0.00570200	1.55806700
H	7.63291900	1.87392800	-3.13511000	H	2.01351200	5.90234000	1.61884500	H	1.61248600	0.08831200	2.91736700	H	4.02395800	-4.14050700	3.42606600
H	8.06992600	1.33599000	-4.78347500	H	0.17984900	5.04852200	0.02804500	C	5.85794300	0.14407800	-6.19304800	H	1.20405200	-5.61891000	1.31870900
H	6.61110800	0.64555200	-3.86273300	H	0.71700100	3.93361700	1.25039500	C	5.92296900	1.08805700	-7.39086000	H	3.56926900	-4.66047900	0.45733000
C	10.12241490	0.09708700	-3.13962400	C	2.15228300	2.29164800	-0.43274500	H	6.78786900	-0.41322000	-6.05790300	H	4.23973200	-2.57455500	2.00963400
C	11.21766800	-0.87535100	-0.69218000	C	3.09738800	2.19350300	0.45606800	H	5.66676700	0.70462800	-5.27651500	H	2.29597200	-2.25200500	3.85505800
C	10.84633000	1.27494800	-3.54539000	C	3.67747200	1.08279700	0.51972400	C	5.77249500	-1.95146800	-8.17695500	H	1.61521300	0.07589400	2.82140900
C	12.12325200	-0.71949000	-2.66670200	O	6.17344900	2.35313200	-1.43761500	C	6.54029900	0.47795900	-8.65617000	C	6.03568100	0.21725200	-5.97169400
C	12.23325200	1.48912400	-3.52637800	H	8.14440400	0.56519800	-1.06254300	H	4.91027100	1.46358300	-7.59159100	C	5.64819000	1.17089700	-0.79203500
C	12.05763000	0.48152000	-3.08825200	H	6.86027200	-1.97549200	2.39912600	H	6.52428100	1.95555700	-7.09011100	H	7.05215500	-0.16681600	-6.07814800
C	8.44210300	-1.57923000	-4.13691400	H	4.45908000	-1.02138800	1.34195100	C	5.83046900	-0.77736700	-9.18026300	H	5.95187500	0.69519800	-4.99600500
C	8.25139700	-2.89272000	-3.69418400	H	2.64132100	-1.78040100	1.63159900	H	5.45743700	-2.08360400	-7.68844800	C	5.86460000	-0.34807600	-8.01888600
C	8.51777000	-1.47374000	-5.53053600	H	3.90140400	-3.15589100	-0.58525500	H	5.54574400	-2.88256800	-8.70123800	C	6.03963800	0.70048200	-8.89695900
C	8.06899800	-3.98629300	-4.53800800	H	6.52069500	-3.30541300	-0.80079700	H	7.29337300	0.23450500	-8.45865200	H	4.56635300	1.36358800	-7.03039000
C	8.34051000	-2.53684800	-6.41220600	H	7.28031700	-1.82525700	-1.95735700	H	6.54809000	1.23766300	-9.44823600	H	6.14453900	2.12584800	-6.88280600
C	8.10398500	-3.81025200	-5.91440400	H	-1.91388100	-1.21159900	0.07791400	H	6.58105900	-0.53014200	-9.50570700	C	5.44943400	-0.65269000	-8.91774400
C	7.98255400	-0.41111200	-1.63556500	C	-2.22421400	-2.74305900	0.62549500	H	6.36031400	-1.13122400	-10.07252600	H	6.93680300	-1.79123500	-7.79302100
C	6.74956900	-1.03029100	-1.39873700	C	-2.35809000	-3.12737500	1.96037000	O	4.74510200	-0.78531700	-6.24349400	H	5.68429100	-2.78965800	-8.52708500
C	8.50656600	0.20356600	-0.49769100	C	-2.54297100	-3.75033700	-0.29112600	C	4.69322000	-1.80991100	-7.12066100	H	7.13543800	0.64228600	-8.55883600
C	8.12252800	-1.09141100	-0.15953200	C	-2.74481100	-4.40659800	2.36230800	O	3.47123900	-2.57269000	-7.03726400	H	5.73214600	1.04210400	-9.22678400
C	7.91142600	0.18996800	0.76391000	C	-2.93018600	-5.03772400	0.06113200	H	9.47110100	-2.03606800	-3.05448500	H	4.35333100	-0.59472700	-8.96189600
C	6.70666700	-0.47498100	-0.93985100	C	-3.03189900	-5.37193100	1.40746800	C	11.10570100	-2.06254600	-2.77782100	H	5.78649000	-0.88726000	-9.93431000
F	14.39817800	0.66980100	-3.05672300	F	-1.26367100	-0.20185400	1.23109200	C	12.01022400	-2.98249500	-3.31293600	O	5.12541200	-0.91953700	-5.84616700
F	12.73831100	2.68535900	-3.88836000	C	-0.10080800	-0.58843000	1.90341500	H	11.71356300	-1.00577700	-2.09195800	C	5.10186600	-1.91087200	-6.71988700
F	10.11455000	2.35376600	-3.96256200	F	-1.64716500	1.11711900	1.48484000	C	13.39276900	-2.89706400	-3.14578100	O	4.38822800	-2.89291600	-6.46101000
F	10.66720400	-2.05596000	-2.22876000	C	0.64179500	0.23451600	2.74147400	C	13.08411500	-0.87956900	-1.89785100	B	9.54606100	-1.99977500	-3.09354300
F	13.30756200	-1.70550700	-2.22432900	C	-0.94415200	1.97549000	2.33139700	C	13.93717300	-1.83987800	-2.43060000	C	11.16205200	-2.10008000	-2.73400100
F	8.77812500	-0.28278700	-6.12702400	C	0.21628100	1.53994400	2.95310400	C	8.86364000	-3.48884800	-3.59072000	C	12.03822000	-3.10342200	-3.15292900
F	8.36277300	-2.33127200	-7.74465700	C	-0.72382700	-1.14101000	-1.08786200	C	9.12827000	-4.65650500	-2.86514700	C	11.79400200	-1.02802700	-2.09472700
F	7.91072100	-4.84624100	-6.74484100	C	0.50170800	0.05665300	-1.77547400	C	7.96712800	-3.67838300	-6.64219600	C	13.41488500	-3.07334800	-2.62350000
F	7.83034900	-5.20918100	-4.02848000	C	0.23086300	-2.12632000	-1.35517600	C	8.60214000	-5.90827100	-3.16658200	C	13.15932000	-0.95397900	-1.84644600
F	8.21462000	-3.18646100	-2.37534600	C	0.53741800	0.27297100	-2.67135000	C	7.41849500	-4.91235200	-4.98689400	C	13.98305500	-2.19924600	-2.62732600
F	6.07166900	-1.60604400	-2.41597600	C	1.29015800	-1.95415200	-2.24816900	C	7.72969000	-6.40021000	-4.24711500	C	8.88013900	-3.43539500	-3.59725900
F	4.94310900	-1.72884100	-0.01875800	C	1.44520000	-0.74870100	-2.91500400	C	8.54363900	-1.77820500	-1.69673600	C	9.02035800	-4.57614200	-2.79752500
F	6.10356000	-0.50548200	-2.14487800	F	-3.40486800	-6.60753900	1.77546700	C	7.17721200	-1.51517700	-1.83700100	C	8.03284900	-3.62103400	-4.68843400
F	8.48347600	0.84017500	1.79682900	F	-3.21217200	-5.95615400	-0.79863500	C	8.95923800	-1.90298900	-0.36863500	C	8.41501300	-5.80075900	-3.05888600
F	9.65650700	0.93977900	-0.56295800	F	-2.48126600	-3.48879800	-1.61744800	C	6.29615400	-1.34173600	-0.77812900	C	7.40586900	-4.27760000	-4.994430100
C	9.78948700	5.68661400	-4.54719300	F	-2.12016700	-2.25819900	2.96769700	C	8.11532700	-1.71897200	0.72918500	C	7.59133400	-5.92916500	-4.17209500
C	10.73796000	6.22443300	-5.59882600	F	-2.84509700	-4.70926900	3.66899500	C	6.77610400	-1.42440100	0.52233700	C	8.57828400	-1.946370400	-1.78910300
C	10.01747400	3.39117700	-7.38664000	F	-2.72203000	1.66845400	0.88737800	F	15.26466100	-1.74135100	-2.26097000	C	7.22907300	-1.32626100	-1.98781300
C	11.66413700	5.18754900	-6.27054700	F	-1.34371700	3.25049300	2.50111600	C	8.93901600	0.16009100	-1.21188100	C	8.93901500	-1.74316600	-0.44312100
C	10.10909600	6.71522900	-6.34898900	F	0.94636800	2.38815300	3.70520500	C	10.94871200	-0.01916500	-1.57042000	C	6.31414500	-1.09932200	-0.96720100
H	11.34210100	7.01073300	-5.12914200	F	1.78304900	-0.20174600	3.31242700	H	11.58955900	-0.430407900	-4.04957800	C	8.05879300	-1.57316700	0.61674500
H	11.14823200	4.48525200	-7.54305100	F	0.39572800	-1.83547200	1.71405600	C	7.42019500	-3.82836000	-3.68048200	C	6.73875600	-1.18518000	0.35257100
H	10.18341900	2.86880900	-6.42651800	F	-1.31347500	1.12085600	-1.55744700	C	15.50208600	-2.64375200	-5.41591600	C	5.30541400	-1.948360900	-2.04391000
H	10.19624500	2.62136300	-8.15437500	F	0.70640400	1.47277200	-3.26247900	F	6.59566500	-5.00572600	-6.01917600	F	13.68941400	0.10812900	-1.21463100
H	11.97135800	4.43065200	-5.53789800	F	2.48058400	-0.55504300	-3.75447000	C	7.15304400	-7.23239400	-4.54774300	H	11.05705800	-0.02877100	-1.67755000

C	0.87541900	-3.96643600	-4.83248900	H	-1.50545300	-2.40449000	1.43160300	C	5.16717100	1.90616400	-2.65183400	F	9.90331500	-1.31149300	0.31402700
C	0.36099200	-4.83159900	-2.88745100	H	-1.25293500	-2.39836200	-0.32145100	C	5.36947300	2.78926000	-1.60121200	C	7.17127800	4.13685800	-4.58808100
H	-0.71478900	-3.55513100	-3.41801500	H	-1.30975300	-3.93665800	0.56391500	F	4.10401600	2.06191900	-3.46676200	H	7.66558600	5.49410400	-5.07268300
C	3.96164900	-3.07153800	-4.54171200	H	3.44403100	-1.28551000	-0.98447800	C	5.75795300	0.05402500	-3.90895600	C	6.87914700	3.63839100	-3.93281200
C	1.23252800	-4.84279900	-5.00061400	C	1.56916500	-5.17615800	-3.00456200	F	4.51471500	3.79779400	-1.37928200	H	6.22568700	4.23728500	-4.05560400
C	1.05254200	-2.95384500	-5.21277400	C	1.89279200	-5.16144200	-4.50588000	F	6.69044000	3.44212200	0.24910500	C	9.18171400	3.10002100	-6.41060900
C	0.09085700	-4.39909300	-5.46255100	C	2.19635000	-5.89641300	-2.46406600	F	8.39705700	1.43421300	-0.19014000	C	9.13298800	5.52651700	-5.51857400
C	3.38246900	-4.43043000	-4.20294600	H	0.53614700	-5.51660400	-2.84705100	C	3.38358300	-5.32243800	-4.86061800	H	7.00104600	5.84399000	-5.29412300
H	4.78924600	-2.78871700	-3.88914100	C	4.13698300	-2.84855100	-4.85022300	C	1.48694900	-4.24143800	-4.94235900	H	7.53269000	6.19045600	-4.23475800
C	3.21272000	-2.27605100	-4.54467900	C	1.35572200	-5.99003700	-4.98413300	C	1.35572200	-5.99003700	-4.98413300	H	9.46818700	4.59318500	-6.68744300
H	2.38923100	-4.88604300	-6.06749900	H	4.34718500	-4.25133300	-4.32362300	C	2.88714400	-0.91823900	-0.52877900	H	9.54716500	2.81966800	-5.41631500
H	1.88366600	-5.87241900	-4.71083300	H	4.76416100	-2.11581000	-4.34044100	C	3.29833000	-0.74144100	0.83587300	H	9.70047500	2.47127900	-7.13679200
H	4.16575000	-5.18766600	-4.33343600	H	3.09767500	-5.22772000	-4.80921500	C	2.88714400	-0.91823900	-0.52877900	H	7.69552200	5.26513300	-4.66174100
C	3.16186500	-4.40638400	-3.12864200	H	3.48007800	-5.37458600	-5.95358700	C	4.18429000	-0.97467200	1.29040900	H	9.39644700	6.55398600	-5.79764900
O	1.62185400	-1.85057800	-3.00691200	H	3.72916700	-6.29438900	-4.48323200	C	2.09883200	-0.18968600	1.50449700	H	8.93149900	4.90422200	-7.59371400
C	1.05349200	-2.82553800	-2.52557200	H	5.38130500	-4.57271300	-4.52258600	C	0.61818300	-3.69193300	3.00272400	O	10.53620900	4.68025900	-6.91567500
O	0.97667900	-3.07674200	-1.23326000	H	4.26755400	-4.16815800	-3.23300400	C	1.86286900	-3.09282700	3.31764900	O	6.82252100	3.21974400	-5.67528800
H	0.03478100	0.08365900	-1.00229100	H	1.76464100	-2.76737000	-2.90467300	C	0.86194900	-4.74808800	2.08088600	O	7.72424900	1.94262000	-6.50552000
H	-0.52489800	0.25242500	-1.62970700	O	1.66621600	-3.82553900	-2.29726300	C	2.87706900	-3.76872700	2.58147300	O	7.33502800	4.72528700	-7.38787500
H	0.05632600	-4.27797100	-3.13655900	C	1.86621600	-3.82553900	-2.29726300	C	2.25458400	-4.79988000	1.83133300	C	7.39642200	0.34693900	-2.28703600
O	0.56837300	-5.54995500	0.82230900	C	1.56992500	-3.92565500	-0.98228800	Zr	1.41017400	-2.57565500	0.78261100	C	7.55431900	1.26119500	-3.12778200
C	3.05754200	-4.88942300	0.03991600	H	0.88695700	-0.79416500	-1.58835900	C	1.41017400	-2.57565500	0.78261100	C	6.27615000	0.59868600	-3.07728400
H	4.05959600	-3.19184200	1.85599500	H	-0.39853700	-0.10104100	0.68535900	H	-1.31128500	-1.70228200	1.47758000	C	6.71142800	0.23110200	-0.99510600
H	2.22440700	-1.281203100	3.77754300	H	-0.47492500	-4.23687200	-3.14517800	H	-1.31128500	-1.70228200	1.47758000	C	5.40844700	1.67280600	-2.88537300
H	1.76623300	-0.12814100	2.98864400	H	0.55541000	-5.94981900	1.34254800	C	6.25114000	2.55444000	-1.83742400	C	6.25114000	2.55444000	-1.83742400
C	6.06596600	0.06143700	-6.10840300	H	1.52323400	-2.67384800	0.40635500	H	-1.34320300	-3.31794300	0.71241300	C	9.39418100	1.88837000	-3.74196600
C	5.56641900	0.76354400	-7.35861300	H	3.79904300	-3.44565400	2.80314000	C	1.32978800	-1.34521700	-1.29380400	F	5.95970300	-0.19790400	-0.17990400
H	7.09320400	-0.29686600	-6.18759500	H	1.37930900	-0.21505300	2.70290800	C	1.38868500	-5.10888800	-2.89490000	F	4.82769700	3.62211100	-1.67184600
H	9.57106000	0.68745000	-5.22309100	H	4.70320500	0.72901500	-6.78831200	C	1.68937700	-5.16582100	-4.40042700	F	6.94354500	1.81843900	0.02434000
C	5.76094100	-2.37969600	-7.78572400	C	3.82927800	1.08688300	-7.97442000	H	2.03196900	-5.78287100	-2.32485000	F	8.59173500	1.12146200	-0.38092700
C	5.88187800	0.04808200	-8.67902800	H	5.76865900	0.77107900	-7.01917300	C	0.36129700	-5.44125800	-2.70182300				
H	4.48961900	0.95063200	-7.25685200	H	4.49211800	1.33619400	-5.91088200	C	3.96516200	-2.90300000	-4.96822400				
H	6.05143900	1.74824200	-7.36017900	C	5.20079000	-1.76237100	-8.31490300	C	3.17379800	-5.36037600	-4.76420700				
C	5.26034200	-1.34677600	-8.82352800	C	4.26245000	0.44827100	-9.30084900	H	1.28866200	-4.26366400	-4.87647600	C	0.20791900	-1.23133600	0.54297000
C	6.68197700	-2.32275200	-7.36346400	C	2.78259700	0.85504300	-7.73640900	H	1.13606300	-6.01146900	-4.82816100	C	-0.26382800	-1.35536000	1.87611200
C	5.51803400	-3.39836800	-8.09230000	H	3.89506700	2.17779500	-8.06867200	H	4.162545100	-2.15335000	-4.53168400	C	1.62595300	-1.21372300	0.57546100
H	6.97184500	-0.03253500	-8.97198600	H	4.23759700	-1.08614000	-9.32346500	C	4.62545100	-2.15335000	-4.53168400	C	0.20369300	-1.34659300	1.92576600
H	5.53075400	0.67406600	-9.50728800	C	6.17995600	-1.26584100	-8.34100900	C	3.93733500	-2.54359800	-4.90398100	C	3.05907200	-1.37692200	2.27746500
H	4.16468600	-1.28831600	-8.78470400	C	5.35940700	-2.81362300	-8.56246700	H	5.19510700	-6.31086100	-4.33136400	C	0.86485900	-1.43694100	2.73241600
O	5.51482600	-1.75059500	-9.80884500	H	3.21861400	-1.46101500	-9.16153400	H	4.07553300	-4.09779700	-3.23063100	C	0.98195000	-5.45607200	3.12188400
O	4.52317500	-3.16848900	-5.92374100	H	4.54150700	-1.43244900	-10.31687200	O	1.52051200	-2.68541200	-2.92370800	C	1.95970400	-4.50933200	3.51636600
B	6.95976000	-1.94076900	-3.08210700	C	4.41623600	-0.64115900	-6.26805900	H	1.47679600	-3.71115000	-2.26279700	C	4.23628800	-0.63003000	1.91403400
C	11.28473300	-1.85839600	-2.76940000	C	4.70697500	-1.71358900	-6.90671000	O	1.44694000	-3.74126700	-0.94195500	Zr	0.94830000	-5.96765000	1.57003800
C	12.26416900	-2.69557300	-3.30786300	C	4.54380200	-2.83004900	-6.29536200	H	0.99925500	0.52152600	-1.63418800	C	-1.26299300	-4.18800100	1.41450100
C	11.79781000	-0.78222600	-2.03801400	C	9.86148700	-0.16701000	-2.24575300	H	0.08237800	0.38531400	0.73827700	C	-1.74971300	-0.40406500	2.38897100
C	13.63289800	-2.51423000	-3.10757600	C	8.26806600	-0.62992100	-2.21253900	H	-0.34789500	-3.40322300	3.39603800	H	-1.83411300	-3.61085400	0.67308100
C	13.15105800	-0.56230300	-1.80962100	C	10.86510300	-1.13397000	-2.11895300	H	0.11202000	-5.39138500	1.63811800	H	-1.35412300	-5.25149100	1.15350500
C	10.82889000	-1.44155900	-2.35058600	C	10.34244200	1.10154800	-2.57727200	H	2.75614600	-5.48051700	1.15521000	H	2.26962200	-1.57024000	-0.29177900
C	9.16395200	-3.41772100	-3.66394200	C	12.22367500	-0.88154800	-2.27351000	C	3.93856700	-3.56303400	2.61263400	C	1.03212300	-4.91135300	-2.90484700
O	9.48995300	-4.58557900	-2.96313100	C	11.69249300	1.40066200	-2.75248500	C	2.10719900	-2.26539400	3.99096000	C	1.48493000	-6.89509000	-4.35435300
C	8.28703800	-3.63686800	-4.72268000	C	12.64565500	0.40407000	-2.59730300	C	2.04740900	0.07598100	2.55319200	H	1.51915900	-5.79369600	-2.47196100
O	9.02520900	-5.85524200	-3.29029800	H	8.15396100	-1.46964400	-3.64586300	C	5.68412600	0.76907400	-7.18816700	H	-0.04585600	-5.12971600	-2.87957500
C	7.78679000	-4.88463600	-5.08784100	C	8.11122100	-2.88848000	-3.79372900	C	6.49078300	1.11924400	-8.44148700	C	3.80603900	-2.44863000	-8.85604800
H	8.15722600	-6.01006600	-4.36669300	C	8.22217800	-0.78182800	-4.85995300	H	4.66483100	0.02523400	-7.17912200	C	2.99571800	-4.87195900	-4.60122900
H	6.89092900	-1.79846200	-1.73719900	C	8.07678700	-3.50872200	-5.02954800	C	5.40815000	1.21737000	-6.24493700	H	1.15173500	-3.69922500	-4.68625300
C	7.31138800	-1.63223500	-1.89043900	C	8.20531900	-1.38427700	-6.11113600	C	0.95828700	-2.20270700	-8.47965700	C	0.95828700	-2.20270700	-8.47965700
C	6.90976200	-1.97742900	-4.01201000	C	8.11574500	-2.76852800	-6.20210400	C	5.19121400	0.16635200	-9.62156000	C	3.92783600	-3.75603700	-4.09337800
C	3.69707300	-1.61267900	-0.84511200	C	8.54189800	-1.62724300	-0.31125900	H	4.438296500	1.19067400	-8.19905600	H	4.43652000	-1.66521800	-4.40232000
C	8.21268800	-1.94885000	0.67554600	C	8.54189800	-1.62724300	-0.31125900	C	5.25842200	2.13398100	-8.71846700	C	2.77925500	-2.02719400	-4.88232500
C	6.85632000	-1.76147600	0.45734000	C	6.60748500	-2.19777200	-0.87490800	C	4.15980000	-1.21597300	-9.53696300	C	3.16237600	-4.98949100	-5.67984800
F	15.39551700	-1.25044600	-2.15000400	C	8.54189800	-1.62724300	-0.31125900	H	6.15740600	-2.18					

C	7.81327200	-3.58039500	-4.91774100	C	5.82235200	-0.08597500	-9.51931600	C	2.64649600	-5.18569600	2.89347600	C	8.21752700	3.06692700	-7.26319700
C	8.35413200	-1.65313200	-6.21940000	H	4.16412700	1.13656000	-8.78190900	C	2.37178200	-6.11642100	0.81333100	O	7.50651100	2.23546200	-7.99871300
C	8.02715700	-3.00262700	-6.16115000	H	5.42404900	2.06083000	-9.58623200	C	3.46093800	-4.46365200	1.97739300	C	7.23017600	1.35477000	-2.79220300
C	7.74129100	-1.08298100	-1.03720900	C	4.87538800	-1.30956800	-9.56243000	C	3.29229800	-5.04301200	0.69393200	C	7.30904600	2.53310500	-2.04270400
C	6.42599700	-1.55783600	-1.01738000	H	5.99000400	-2.58411700	-8.18461400	Zr	1.02908500	-3.95073500	1.28368500	C	6.18956700	1.34998800	-3.72447000
C	8.34574800	-1.04035000	0.22149200	H	4.43781100	-3.22437300	-8.64920600	C	-0.86170900	-5.15763100	1.77481600	C	6.47466500	3.26945000	-2.21798900
C	5.76671200	-1.99083300	1.02536700	H	6.75483600	-0.36393900	-9.01285800	H	-1.00987100	-5.39727200	2.83637400	C	5.34295200	2.43719100	-3.94867400
C	7.71839800	-1.45297900	1.39863200	H	6.11061800	0.14072100	-10.55214900	H	-1.74856900	-4.60375500	1.43528800	C	5.48418500	3.91909000	-3.19168800
C	6.41574000	-1.92844100	1.35164700	H	3.83888100	-0.97491900	-9.62990400	H	-0.83238000	-6.10696800	1.22083200	F	4.40470400	2.38408600	-4.91291800
F	14.19572400	-0.02041000	-2.71527300	H	5.12292800	-1.88990200	-10.45970500	H	1.13471700	-1.01166200	0.05702300	F	5.94142300	0.26963500	-4.49323000
F	12.64380300	2.08888600	-3.54034900	O	3.75980900	-0.74611300	-6.92591700	C	0.07797400	-4.00563200	-3.05570500	F	4.68333700	4.65322000	-3.39317400
F	10.01477000	1.98742400	-3.38442900	C	4.33009700	-1.81136500	-7.08657400	C	0.65397100	-3.77384300	-4.46260000	F	6.63135200	0.26729900	-1.45886200
F	10.31567000	-2.42466100	-1.60104300	O	4.47318600	-2.73670500	-6.12782800	H	-0.02776200	-5.07434300	-2.83624300	F	8.24580800	2.65801200	-1.07656800
F	12.98011400	-2.27463200	-1.73782400	B	8.25134800	-0.08591500	-2.43871800	H	-0.93746900	-3.58554800	-3.00347700	C	5.88612800	7.58488700	-2.70911600
F	8.72192000	0.39836300	-5.18431200	C	9.87337700	0.25814400	-2.39704400	C	3.85720700	-3.24675600	-4.18809200	C	6.05540000	9.08477100	-2.50589100
F	8.57818700	-1.06206200	-7.41338400	C	10.77611100	-0.71285300	-1.94930700	C	1.81806100	-4.70554600	-4.84941200	H	5.74849500	7.04377500	-1.76974800
F	7.90570300	-3.72053300	-7.28885300	C	10.48751000	1.38989000	-2.93351100	H	0.95615600	-2.72599900	-4.55879100	C	5.03843000	7.36503700	-3.35785900
F	7.48059700	-4.87887900	-8.83711100	C	12.15934600	-0.57559600	-1.98682800	H	-0.15205900	-3.93216100	-5.19095200	C	8.56001900	7.41540600	-1.56517300
F	7.69957900	-3.47465800	-2.61017400	C	11.86807900	1.57029800	-3.00314300	C	3.11191900	-4.56880900	-4.02867700	C	7.00103500	9.47364200	-1.36211800
F	5.17026600	-1.60655900	-2.16523700	C	12.71505800	0.58269100	-2.52029200	H	4.67099000	-3.17482600	-3.46393800	H	6.37888300	9.53538500	-3.45429800
F	4.50139500	-2.45257300	0.05813700	C	8.17502300	-1.15430700	-3.71112800	H	3.20699000	-2.38122800	-4.07166400	H	5.05653600	9.48085200	-2.29648800
F	5.78440500	-2.31311100	2.47748100	C	7.99546500	-2.53734400	-3.63580100	H	2.05311600	-4.54389000	-5.91006300	C	8.43743000	9.95524000	-1.50668200
F	8.36072700	-1.37987400	2.57598900	C	8.41415800	-0.69768200	-5.00845900	H	3.79761400	-5.38183100	-4.30177100	H	7.92008100	8.95215600	-0.80396400
F	9.60113300	-0.57215400	0.38010800	C	7.97379600	-3.37842200	-4.75032000	H	2.89890900	-4.70035200	-2.96031400	F	9.58653300	7.10512600	-1.36015200
C	8.36152300	4.37067000	-5.18413200	C	8.42515000	-1.49323800	-6.14495600	H	2.08799000	-3.33644800	-1.92269300	H	6.58423400	9.10069100	-4.91580600
C	9.09933300	5.40431100	-6.01868000	C	8.18653400	-2.85621800	-6.01785200	H	1.50184400	-2.31152300	-2.07903000	H	7.02627100	10.56688300	-1.27905600
C	9.01740100	3.78095400	-4.54068400	C	7.64053600	-0.68782400	-1.01771500	C	0.85306100	-3.33644800	-1.92269300	H	8.91537000	9.39225500	-2.39370200
H	7.57329500	4.82267200	-4.58417800	C	6.36420200	-1.25875400	-1.00038000	O	0.72584600	-3.95090000	-0.75519900	H	9.02325200	9.29189300	-0.64418600
C	9.62268000	2.47703000	-7.03829100	C	8.20900400	-0.53829600	0.24979000	H	-1.32165500	-1.79589600	0.82489000	C	7.00219800	6.97462500	-3.43420100
C	10.39995000	4.91157400	-6.66784100	C	5.71425300	-1.697177100	0.14774400	H	1.15351900	-2.71755100	3.34925000	C	8.20699700	6.82955100	-2.90851200
H	8.41026500	5.81348700	-6.76821300	C	7.58630100	-0.94140300	1.43828500	H	1.28421400	-6.92981200	2.58740300	O	9.06297400	6.22457200	-3.57068400
H	9.33175700	6.22928500	-5.33331000	C	6.32692400	-1.52174600	1.38240100	H	2.01795700	-6.74361300	0.00445900				
C	10.22692600	3.75842600	-7.66370600	F	14.04638500	0.73654400	-2.57825800	H	3.76353000	-4.69834000	-0.21736800				
H	10.08805700	2.27918100	-6.06484700	F	12.38214900	2.68842000	-3.54887400	H	4.10612600	-3.62956900	2.21506600				
H	7.98599700	1.60340800	-7.66983500	F	9.75627300	2.40637100	-3.46338500	H	2.56269100	-4.99692300	3.95677600				
H	11.09580300	4.59848800	-7.69749900	F	10.30879600	-1.88011700	-1.45455200	H	4.40773600	-2.48786200	4.14738400				
H	10.87456000	5.75386100	-7.18403300	F	12.96121100	-1.55075000	-1.52753600	C	6.70046000	-2.48952000	-8.14014200				
H	9.61921500	4.07274300	-8.52174700	F	8.63716600	0.63018200	-5.21654800	C	5.44335700	1.27365500	-8.79751900				
H	11.20750700	3.47923700	-8.06281700	F	8.64014600	-0.95686700	-7.36588900	F	6.65372500	2.67319600	-7.14693900				
O	7.58710400	3.34109600	-6.01587700	F	8.14145100	-3.64093000	-7.10650300	H	5.95390800	3.39546000	-8.74347400				
C	8.14942600	2.57762900	-6.81986900	F	7.72005900	-4.68912100	-4.60184200	C	4.83783700	-2.45210100	-7.70502400				
O	7.39971200	1.81080500	-7.51361300	F	7.79898300	-3.15768000	-2.45551300	C	5.50837000	0.00990800	-7.93017400				
C	4.49766600	0.97015300	-2.55151000	F	5.67928200	-1.41215900	-2.15769900	H	4.39522800	-1.53358000	-9.00068600				
C	7.75050400	2.00545500	-1.64346100	F	4.49190800	-2.25711600	0.07658500	C	5.91905000	1.10116400	-9.77263600				
C	6.41898600	1.22068000	-3.39991400	F	5.69984100	-1.90388300	2.511233500	C	4.78010100	-1.18284200	-8.56293600				
C	7.04116100	3.20118400	-1.59780300	F	8.19228500	-0.76211800	2.61840800	H	5.86978100	-2.72949400	-7.46436300	Zr	0.96207100	-4.72754700	1.26373700
C	5.68478500	2.40691000	-3.40185300	F	9.42073900	0.03220700	0.41097400	H	4.41719300	-3.30094800	-8.26314600	C	-0.69963200	-6.22664100	1.76644600
C	5.99827700	3.40925900	-2.49463300	C	7.96158100	-4.58749300	-5.52252100	H	5.06806400	0.22877800	-6.94983700	H	-1.13371300	-6.13002000	2.77119300
F	4.69652200	2.59671000	-4.29522700	C	8.60208700	5.59849800	-6.46567400	H	6.35807000	-0.25383600	-7.75327400	H	-1.51858400	-6.12054300	1.04083800
F	6.02488400	0.30971400	-4.32474100	H	8.66286600	4.11886800	-4.83196100	H	7.12910200	-0.92255900	-8.73809000	H	-3.03338400	-7.24754700	1.67380600
F	5.32736100	4.57279900	-2.50267700	H	7.13630600	5.01860100	-4.96150800	H	5.22255200	-1.40621500	-9.54294400	H	9.03064100	-3.79022000	-0.90102500
F	7.36080800	4.15969300	-0.71173800	C	9.40463200	2.65482200	-7.18292900	C	3.07478300	-1.61159300	-6.26468800	C	1.60459900	-6.60779000	-2.71976400
F	8.75219500	1.87835500	-0.74661800	C	9.95085500	5.17400000	-7.05344300	C	4.03465200	-2.34260200	-6.41733900	C	2.14178100	-6.31609100	-4.13028300
				H	7.88337700	5.86495600	-7.24352400	O	4.50870600	-3.19195100	-5.48851000	C	2.33147000	-6.17315600	-2.12601300
				H	8.75053400	6.49179700	-5.84177800	B	3.23300000	0.08248600	-2.40988200	H	0.70911700	-7.24297700	-2.79161600
				C	9.90646800	3.91620500	-7.92974100	C	8.93163800	0.52637300	-2.31519500	C	3.34960100	-3.29758200	-4.19066300
				H	9.86258700	2.60180000	-6.18762100	H	10.76201100	-0.31234300	-1.69077900	C	3.61453200	-5.86623000	-4.18145500
				H	9.66138600	1.74077500	-7.72039200	C	10.41136500	1.62387100	-2.95124500	H	1.49161900	-5.57311800	-4.60586900
				H	10.66177200	5.01035000	-6.23223700	H	12.13240100	-0.07520600	-1.65416700	H	2.05283300	-7.23283300	-4.472732400
				H	10.34926500	6.00367400	-7.64917600	C	11.77650000	1.90202800	-2.94924000	C	3.95460800	-4.52074000	-3.51642700
				H	9.29202400	4.08416100	-8.82384600	H	12.64952400	1.04856100	-2.28987100	C	3.59523200	-2.38643000	-3.63737500
				H	10.91672000	3.68811200	-8.258543200	C	8.28571500	-1.11307600	-3.56042200	H	2.26292300	-3.86112600	-2.47533800
				C	7.27751700	3.48498200	-6.27059300	C	8.28047700	-2.48696000	-3.30356700	H	3.92895900	-5.81934400	-5.23177300
				C	7.92272800	2.64859300	-7.00029300	C	4.80592700	-0.79588400	-4.90643700	H	4.23298800	-6.64633900	-3.14691600
				C	7.25907600										

C	8.02125800	-0.06235400	-5.09746300
F	7.36980500	-2.72164300	-4.99468200
C	8.05907100	-0.81732100	-6.26304200
C	7.70283500	-2.16352400	-6.21483400
C	6.85101500	-0.13999700	-1.19983600
C	5.52329000	-0.54493700	-1.07066700
C	7.25505400	-0.07493200	0.13629600
C	4.67420000	-0.90555700	-0.33040600
C	6.43491800	-0.41055700	1.21373700
C	5.31196700	-0.82463100	0.97843100
F	13.55893200	0.00765900	-1.80282600
F	12.46924600	2.25983200	-2.93155000
F	9.84800100	2.49703600	-3.22199200
F	9.25831100	-1.80405100	-1.26763300
F	11.90111700	-2.01330600	-0.97678600
F	8.38123700	1.23986600	-5.23019100
F	8.39093100	-0.25542600	-7.44240600
F	7.70791000	-2.90409300	-7.33557900
F	7.05127500	-4.02505900	-4.92685700
F	6.98343600	-2.56591900	-2.71741500
F	4.98993700	-0.59766100	-2.61196400
F	3.41568300	-1.31819400	-0.57703900
F	4.32111600	-1.14311700	2.00809500
F	6.89130800	-0.32428100	2.47500900
F	8.49743900	0.33570300	0.47223900
C	10.74361300	5.24648800	-3.72911800
C	10.57394600	5.44293300	-5.22738100
C	8.84865900	3.27457700	-7.99282000
C	9.92290700	4.20340200	-5.86512000
H	9.93331800	6.31438900	-5.41317700
H	11.55050800	5.65027000	-5.68214900
C	9.78205800	4.33029000	-7.38931900
H	9.08621600	2.26549000	-7.63690100
H	8.93425100	3.24114700	-9.08516500
H	9.85556600	4.06241400	-5.42082900
H	10.03853000	3.30593300	-6.62212800
H	9.39374200	5.32444000	-7.62434700
H	10.77045100	4.24481800	-7.188855600
O	6.96042200	4.52781900	-7.08335300
O	7.38413300	3.54507400	-7.68937900
O	6.59805400	2.56897100	-8.17012800
C	7.11086800	1.92191300	-2.70427000
C	7.45735700	2.96470200	-1.83443400
C	6.10697000	2.25974800	-3.61339600
C	6.91450500	4.24293800	-1.89727000
C	5.52002200	3.52384700	-3.69631500
C	5.93341000	4.52866500	-2.83443900
F	4.56454100	3.77764300	-6.40535000
F	5.63820300	1.58643000	-4.50166600
F	5.40292100	5.76550600	-2.90833500
F	7.34099700	5.21722400	-1.05786800
F	8.38680200	2.77025500	-0.87104200
C	8.00563700	8.02582100	-3.21256000
C	8.05514000	9.36239600	-3.02946600
H	8.14283400	8.11047600	-1.23008500
H	7.12802000	7.43556600	-2.52515600
C	10.89571700	8.60735700	-2.00273600
C	9.07632800	10.36201000	-2.56509400
H	8.06772500	9.18608100	-4.11092400
H	1.01148900	9.79063300	-2.84277700
H	10.52282900	9.90362100	-2.76784700
H	10.50826200	8.62527300	-0.97546100
H	11.97880800	8.48433700	-1.94689100
H	8.91514500	10.58590100	-1.50103900
H	8.92900800	11.30524300	-3.10383200
H	10.74170400	9.76862400	-3.83477400
H	11.20128000	10.68336100	-2.40688300
O	9.09891000	7.12792400	-2.80649400
O	10.34786000	7.37738600	-2.64675700
C	11.19410000	6.52096000	-3.08377100
H	11.54484900	4.55562900	-3.47443500
H	9.82536500	4.94158300	-3.23239800

D. Hafnocene systems			
<i>Cr:HfMe^c</i>	0.19404700	-0.07032100	-0.22957000
C	-0.15096600	0.19603500	1.11849000
C	1.61656900	-0.18990100	-0.31097500
C	2.14638200	0.02759500	0.98890700
C	3.19509800	0.03827400	1.25483000
H	1.05663300	0.23160300	1.88201600
C	1.17580200	-1.14902400	2.42796800
C	2.18276600	-3.20294800	2.83924100
C	1.40947800	-4.53865100	1.13150900
C	3.05972900	-3.04550100	1.72831800
C	2.56972200	-3.84687200	0.66373000
Hf	0.81449700	-2.10781900	1.07846900
C	-1.31407900	-2.69428900	1.19382300
H	-1.65433300	-2.47553700	2.22656900
H	-1.91125200	-2.12821700	0.54204500
H	-1.59412100	-3.76226200	1.04349300
H	2.19357700	-0.34668400	-1.21470100
H	-0.50179700	-0.15704900	-1.05607000
H	-1.15253100	0.34463900	1.50057100
H	0.37317300	-4.50522200	3.10624800
H	0.81720400	-5.24707900	5.56494600
H	3.03113500	-3.96138400	-0.31093200
H	3.94683600	-2.42661300	1.70122800
H	2.30637800	-2.74899700	3.81569800
H	1.13492600	0.45452800	2.94008000

C ^c -Hf-Complex			
C	-0.25647600	-0.44424900	-0.64145900
C	-0.10084900	-0.17431200	0.74276000
C	1.03834900	-0.55021800	-1.21743600
C	1.99569100	-0.37377700	-0.18881600
H	3.07039800	-0.37392100	-0.31306400
C	1.28951400	-1.42521000	1.02923100
C	1.35347200	-0.40409600	2.34338300
C	2.29400800	-2.97633200	2.35657100
C	1.57860400	-4.80809900	1.17274300
C	3.12399300	-3.10741800	1.20424400
C	2.68151500	-4.23758000	0.47669100
Hf	0.80279100	-2.51645700	0.39390800
H	-1.20637100	-2.91417800	1.30623800
H	-1.33705800	-2.53142800	2.32754300
H	-2.00062100	-2.45937200	0.69819500
H	-1.39895100	-3.99531300	1.35059600
H	1.26134600	-0.74326600	-2.25916300
H	-1.19957700	-0.53794300	-1.16499800
H	-0.90156200	-0.02528100	1.45414200
H	0.59559700	-4.22937900	3.09084900
H	1.01884400	-5.68535600	0.87316100
H	3.10986100	-4.60009200	-0.44963500
H	3.96101700	-2.47205100	0.94715700
H	2.40395900	-2.23641200	3.13895000
H	1.73611000	0.07825500	1.98987200
C	2.22289900	-3.98093900	-4.42376700
C	1.39939200	-3.36865600	-5.55855000
H	2.23552200	-5.07505800	-4.46638000
H	3.25067700	-3.61886900	-4.44494200
C	-0.89929000	-4.74300700	-3.35982000
C	0.05060000	-0.05385500	-5.81900100
H	1.26856200	-2.29724500	-5.35650400
H	2.01446800	-3.43446700	-6.46466800
O	-9.22621000	-0.03705900	-4.63422400
O	0.07268400	-5.70151300	-3.63403900
H	-1.20748200	-4.95726200	-2.66898200
H	0.23165700	-5.09571400	-6.11807400
H	-0.43093000	-3.57017700	-6.67597000
H	-1.21352900	-3.00812400	-4.38608500
H	-1.84362500	-4.55520400	-4.90211700
O	1.77047600	-3.57252400	-3.99891000
C	0.61068800	-3.92380500	-2.59366300
O	3.50444300	-3.52995800	-1.43782900

C ^c -Hf-RI			
C	-0.26290100	0.06604500	0.21666200
C	-0.17015400	0.01686400	1.63061700
C	1.05622000	0.15170700	-0.30950600
C	1.96436300	0.13347200	0.77593100
H	3.04146900	0.20693700	0.70618900
C	1.20622900	0.03867300	1.98028900
C	6.87189000	-3.92477000	2.39629600
C	2.64714200	-2.87885700	2.39344400
H	1.69577100	-4.53010400	1.11280000
C	3.26231000	-2.84981800	1.10721900
C	2.68036600	-3.87675300	3.02455600
H	-1.04565900	-2.83268400	1.74693600
H	-1.12121000	-2.65786500	2.82873200
H	-1.90370200	-2.32237500	1.28691900
H	-1.18132400	-3.91224800	1.59398700
H	1.32397000	0.20980100	-1.35707400
C	-0.58822700	-3.50568600	-3.23590300
C	-0.65878400	-3.11061700	-4.71923200
H	-0.43867400	-4.59131300	-3.13159600
H	-1.52722100	-3.28959000	-2.71762400
C	1.24253100	-2.48535400	-4.23395000
C	0.41453300	-3.77940600	-5.59053100
H	-0.59867500	-2.01866400	-4.80735700
H	-1.65371500	-3.38222900	-5.08717300
C	1.81896200	-3.75111100	-4.96171500
H	3.21290200	-2.34473400	-4.06440000
H	1.77645200	-1.57472600	-4.75641200
H	0.45232200	-3.26657700	-6.55593400
H	1.13429400	-4.82094500	-5.78905400
H	2.56808900	-3.85675000	-5.75236800
H	1.97545900	-4.59355800	-4.27415700
O	1.62428000	-2.39931600	-2.83714100
C	0.48411200	-2.84737800	-2.39965600
O	0.27485100	-2.72569000	-1.16718100
H	-1.18009600	0.05246100	-0.35878100
H	-1.00064000	-0.03659500	2.30623000
H	1.05640000	-4.20866000	3.22745000
H	1.06694400	-5.35295000	0.96907200
H	2.93696600	-4.11103900	-0.70085400
H	4.06260800	-2.18988400	0.79718100
H	2.90594100	-2.25076100	3.23576200
H	1.60544200	0.04694700	2.98632000
C	2.46478300	1.88991800	-7.97144500
C	1.52295800	2.09659000	-9.15576100
C	3.51712900	1.96123500	-8.27270500
C	2.28532800	2.64429600	-7.20269000
C	3.05053600	-0.64147500	-9.22395600
H	1.92996000	1.35169300	-10.43428900
H	0.50954000	1.81224900	-8.84253100
H	1.49218900	3.17328800	-9.36607700
C	2.03132300	-0.17168000	-10.28806400
H	3.97870900	-0.06163000	-9.32003500
H	3.30641700	-1.69186400	-9.38074300
H	2.90093200	1.73914700	-10.77527600
H	1.21153800	1.58705300	-11.22857400
H	1.04604000	-0.60051900	-10.06091100

H	2.33603800	-0.59808600	-11.25043000
O	2.24675100	0.64546400	-7.26201800
C	2.53371600	-0.55691900	-7.79995900
C	2.34306800	-1.54541100	-7.11383000
Hf	0.86297100	-2.14222400	0.79013400

C ^c -Hf-TSI			
C	0.38587900	-0.11355900	-1.08162700
C	0.04963100	0.23750100	0.25252400
H	1.79588900	-0.25107400	-1.15963700
C	3.33268300	-0.01338500	0.13006600
H	0.78908800	-3.51162600	2.50470200
H	1.24961700	0.29247500	1.00592700
C	1.68445100	-2.44448200	2.77578000
H	3.19654300	-4.35911300	1.54327700
C	2.88549000	-2.64642000	1.99364700
C	2.67912100	-3.83015300	1.23702800
Hf	0.97999400	-2.13413000	0.36721000
C	-1.23598400	-2.47202200	0.56150800
H	-1.70573600	-2.02277200	1.44695200
C	5.25494900	-2.06423100	-0.31456200
H	-1.45154100	-3.54901400	0.60124600
H	5.26368100	-0.53718800	-

H	-10.66173500	-4.72668300	-5.37511100
C	-9.24254800	-3.01060500	-8.09467900
C	-10.54432900	-3.57423200	-8.22711200
C	-9.27760000	-1.68719000	-8.59937400
H	-8.36713800	-3.51355500	-7.70565400
C	-11.38641200	-2.59578600	-8.81427300
H	-10.83185700	-4.58346000	-9.96287400
C	-10.61346700	-1.42607900	-7.90295900
H	-8.46108800	-0.98860400	-8.62200500
H	-12.43491200	-2.71692500	-9.04831900
H	-10.97646300	-0.49389100	-9.44635700

C'-HF-TS2

O	-0.68595200	-0.28845400	0.33206200
C	-0.57145900	0.03112300	1.81762600
O	0.25867000	-0.64374200	-0.09329600
C	-1.45303800	-1.04063000	1.14572500
O	-0.90216600	2.13262700	-0.00154200
C	0.69163200	0.80835200	2.21353700
O	-1.47877800	0.56366000	2.13181900
C	-0.57995800	-0.92915100	2.34836700
O	0.84252400	2.18061000	1.54533600
H	1.57249700	1.32435800	-0.34752200
H	0.84252400	3.06832300	-0.39963100
H	1.57397400	0.19763900	1.97512200
H	0.69797800	0.94256300	3.00106500
H	0.03262000	2.85315700	1.85707300
H	1.77362100	2.64301200	1.88869900
O	-1.15800800	0.84286600	-0.47141100
O	-0.46444900	1.94171300	-0.64958800
C	-0.92919100	2.83875800	-1.35811700
H	-14.55799900	1.39595200	-0.96587400
H	-1.31186300	0.34370800	-0.76632300
H	-12.15637900	1.05995500	-0.12784500
H	-15.05119200	-0.02431300	-0.00415600
O	-14.47730600	-0.21245500	-1.69992800
H	-11.37026500	0.92311400	-1.83115000
O	-10.33432300	1.45301500	-2.44876400
C	-10.69593600	2.06007000	-3.80089100
O	-9.20258800	1.47334900	-1.97293500
C	-9.52491300	2.62174000	-0.62039700
H	-11.26037400	1.30995300	-4.37062900
H	-11.42213500	2.85583200	-3.58707900
C	-8.78962900	1.60921800	-5.51919900
H	-8.82236700	3.11820400	-3.94059800
H	-9.91919400	3.40604800	-5.27807700
C	-7.98688000	0.49707100	-4.82016200
H	-8.11070800	2.16207600	-6.18067300
H	-9.52433000	1.12829600	-6.17880800
C	-6.83359700	0.97815600	-3.95695900
H	-7.60018500	-0.19472000	-5.57935700
H	-8.63432700	-0.09258900	-4.16104200
H	-6.28166200	0.14719200	-3.50923100
H	-10.16435000	1.64692100	-3.16273200
O	-5.89777700	1.17202000	-4.82701800
C	-4.79339100	2.18563600	-4.30104100
C	-9.38327000	2.94917300	-5.28251200
O	-4.51301900	2.02077500	-3.10361400
C	-3.71415500	4.42677300	-4.88261900
H	-2.92717800	2.43407800	-5.37574400
C	-4.42412600	2.89730300	-6.22619300
H	-2.72841500	2.66498300	-2.26160000
C	-2.66805100	4.69700600	-3.78839400
H	-4.67540900	4.87284600	-4.95987600
C	-3.39387800	4.95713300	-5.78627700
C	-2.97538800	4.13486600	-2.39027000
H	-2.23467700	2.07878800	-2.98567100
H	-3.11814800	2.12890700	-1.37507100
H	-1.68547500	4.32861900	-4.11513200
H	-2.56438300	5.78413300	-3.69603400
H	-4.01226500	4.33618800	-2.09736600
H	-2.35182700	4.64618100	-1.64880700
H	-10.13008600	2.57499200	0.35712400
O	-10.97603900	2.18415600	0.90719800
C	-12.33315000	2.56187800	0.74223000
C	-10.92641300	1.13748300	1.86157200
C	-13.12342500	1.76626900	1.61361200
H	-12.70666500	3.31567100	0.06800700
H	-10.03065900	0.64440700	2.21514100
C	-12.25753900	0.88058300	2.30290000
H	-14.19767900	1.82102800	1.72417900
H	-12.55173400	0.16222600	3.05695500
C	-12.22024000	-2.13420600	0.97169400
C	-12.94262400	-2.27482200	-0.24165900
H	-10.85765300	-1.88577100	0.64475100
C	-12.63071100	-2.23412100	1.96884800
C	-12.03115200	-2.10188800	-1.31552900
H	-14.01206400	-2.46987600	-0.33306700
C	-10.74220200	-1.87346300	-0.76753500
H	-10.04720300	-1.75692700	1.34967400
H	-12.28057400	-2.12380600	-2.36867600
H	-9.83581700	-1.67823200	-1.32626900

C'-HF-P2

C	0.18324500	0.12398000	0.40872800
C	0.86845900	0.34085100	1.74817600
H	0.87668400	-0.14887700	-0.39213700
C	-0.60730900	-0.62291500	0.46704000
C	1.47060000	2.68968100	-0.28128300
C	2.16956900	1.15476000	1.68802900

H	0.14871100	0.78803700	2.44596600
H	1.09025200	-0.65960300	2.14048500
C	2.01406400	2.58962100	1.16955400
H	1.99277900	1.96796300	-0.92522100
H	1.64138600	3.68558100	-0.69455100
H	2.89606900	0.62241200	1.05854800
H	2.60546100	1.19205800	2.69213400
H	1.37528600	3.17889300	1.83934600
H	2.99292000	3.07940800	1.16851900
O	-0.56982500	1.31870400	-0.05270400
C	0.00103200	2.42836700	-0.37894800
O	-0.73105400	3.38254800	-0.80153000
H	-14.26893200	1.68086200	-2.93160500
C	-14.23786900	1.58185200	-4.02569800
HF	-12.13028300	1.13520200	-4.70468700
H	-14.98980300	0.82834700	-4.29782300
O	-14.57650800	2.53759900	-4.44983600
O	-11.31125500	2.84533800	-3.98460600
H	-10.34543500	3.46447700	-3.33712100
O	-10.1074000	4.77308000	-2.70630000
O	-9.20386000	3.03222900	-3.24484600
H	-9.72590000	5.60011300	-1.99964800
H	-11.32013200	5.36081200	-2.25146000
H	-8.93486500	6.57214700	-2.89631500
H	-9.04579400	4.91887100	-1.47517900
H	-10.21517700	6.20236000	-1.22041800
H	-8.00590800	5.95363300	-3.96519700
H	-8.33434000	7.22617300	-2.25152700
H	-9.64788300	7.23044200	-3.41143900
C	-6.84821200	5.13892800	-3.40126300
H	-7.60348300	6.75745600	-4.58653700
H	-8.56703600	5.28064700	-4.62038900
H	-6.22452800	4.72771700	-4.20079300
H	-7.19053900	4.31215500	-2.77842300
O	-6.01638200	6.03127000	-2.59576900
C	-4.94833500	5.49644100	-2.00780400
C	-4.16937300	6.52791000	-1.20790000
C	-4.63727000	4.31813200	-2.10834000
C	-3.94254500	6.16230300	0.07862300
H	-3.20174300	6.67747400	-1.70687700
H	-4.70513100	7.47833700	-1.26828400
C	-2.23079600	3.26299000	0.94748400
H	-2.75735600	5.24302300	0.64131400
H	-4.86711700	5.74693400	0.70033400
H	-3.77443700	7.10822200	0.86071600
C	-2.90895100	3.77427200	0.32594500
H	-2.44009800	3.89911000	-1.80103300
H	-2.44781000	2.22320200	-1.18933900
H	-1.83971600	5.63436100	1.79851100
H	-2.60540900	5.34248700	-1.72544400
H	-3.96502300	3.47443300	0.20308600
H	-2.57799900	3.12902800	-1.02625000
H	-9.70052900	0.66622100	-2.70342200
C	-10.59310000	0.05489800	-3.00956500
C	-11.82354900	0.03388100	-2.41065000
C	-10.57716500	-0.78275400	-1.15308300
C	-12.65094500	-0.84270900	-3.16350600
H	-12.12835800	0.59673500	-1.53741600
H	-9.74729900	-0.98680100	-4.81622900
C	-11.88367300	-1.34791400	-4.24180900
H	-13.68633000	-1.07477100	-2.95451100
H	-12.62242600	-2.06098800	-4.98267700
H	-11.24988400	0.62689500	-7.03881200
C	-12.61016300	0.20312700	-0.02625900
C	-11.23239900	2.03962800	-6.92608100
H	-10.38401300	-0.01312900	-7.14453200
C	-13.42572600	1.35656100	-6.90423900
H	-12.96176500	-0.81567200	-7.12510900
C	-12.57428000	2.48993000	-6.83105900
H	-14.30467900	2.66210500	-6.88508500
H	-10.50604400	1.37027500	-6.86548800
H	-12.89294700	3.51680100	-6.70628500

O	-7.88810800	2.81873700	-6.39961800
H	-9.26317500	5.03259200	-5.10473700
H	-9.91534600	5.11797700	-7.19252600
H	-10.74637900	3.92104000	-6.23936000
C	-8.24793100	6.17843300	-5.28172400
C	-8.86063200	4.25733400	-4.44254400
H	-10.13464700	5.45175500	-4.58951700
H	-6.84014800	5.80186400	-5.77703600
H	-8.14493900	6.69894800	-4.32181000
H	-8.67028000	6.91415200	-5.98011100
C	-6.04510800	4.91591900	-4.83031900
H	-6.27173300	6.72317300	-5.95988500
H	-6.89487700	5.27061800	-6.73350200
H	-5.05395200	4.68311100	-5.23251600
H	-6.55527800	3.97506000	-4.62164000
O	-5.86500800	5.65019900	-3.58132200
O	-5.22496200	5.02533300	-2.59208200
C	-5.08928100	5.92021000	-1.37067500
H	-4.78964200	3.88717500	-2.67508200
O	-5.15079300	5.19346000	-0.01097300
H	-4.14278400	6.47316700	-1.46724600
C	-5.87835700	6.67574900	-1.42452400
C	-2.33309700	3.39398900	-1.16648800
C	-3.85425100	4.58645200	0.56654000
H	-9.52724100	4.41894100	-0.04711400
C	-3.88764700	4.26058800	0.27658200
H	-5.91484600	4.36467400	-0.47462300
H	-5.34458800	5.81763100	0.32163600
C	-3.51688900	2.88295400	-0.31497800
H	-2.74541300	3.55612000	-2.24557300
H	-6.34032000	1.88714600	-1.82018800
H	-2.99639400	4.90314700	0.31295900
H	-4.17614800	4.09748600	1.34929700
H	-4.40966300	2.40334100	-0.73015000
H	-3.14551000	2.22722500	0.48252900
H	-10.72651800	2.12981300	-9.30898500
H	-10.40280300	2.05386400	-10.34015600
H	-10.48480700	3.07780500	-11.31878800
H	-9.78594500	0.92537400	-10.93634800
C	-9.93307600	2.57775900	-12.52695300
H	-10.88041100	0.470352700	-11.16527400
H	-9.59628400	-0.02460400	-10.45335700
O	-9.49419200	1.24964500	-12.29205400
H	-9.85523100	1.31732800	-13.46057500
C	-9.04638700	0.59014300	-13.02403700
C	-6.64480000	2.74695600	-10.04811100
C	-6.34486100	0.87968900	-11.43619900
C	-6.09468100	1.86458400	-9.37085000
H	-7.16745500	-0.07904700	-9.58399100
C	-5.62424000	0.28636100	-11.61204000
H	-6.59743100	0.17059700	-12.21365000
C	-5.48274600	2.70087300	-10.33817300
H	-6.20971900	2.08439300	-8.31783900
H	-5.25711100	1.47819400	-12.55801200
O	-5.00188800	3.65163700	-10.14524000

H	5.42358200	-1.43676800	-9.88770300	C	4.89860800	-1.99917500	-6.93357100	C	6.09860300	0.68146500	-7.22241600	H	2.98464300	-2.08598600	-4.67050100
O	5.33682600	-1.08329700	-5.76843000	O	4.51913000	-3.03307000	-6.27941000	C	5.27359100	1.05752000	-8.41479600	H	2.63505000	-4.87935600	-5.85641100
C	5.20879000	-2.11241700	-6.52507400	B	8.28654500	-0.78600100	-2.67236500	C	6.88502800	-0.05181500	-7.28974300	H	2.71723700	-5.92649000	-4.45189000
O	4.56087900	-3.11124900	-6.05215400	C	9.87082000	-0.29428500	-2.67414700	H	5.89188600	1.10191000	-6.25139000	H	4.71838400	-6.80816900	-4.44705700
B	9.50571000	-1.94728500	-3.09639100	C	10.89356800	-1.23336700	-2.49555700	C	5.10321700	-2.27830400	-8.48932000	H	3.76163200	-3.97934500	-3.14236500
C	9.49051400	-0.66158200	-4.12419600	C	10.33595200	0.99266500	-2.93383200	C	5.37172700	0.09075300	-9.60657400	O	1.75665800	-2.42054600	-2.28168800
H	9.08051000	0.19477700	-3.64686800	C	12.25183700	-0.94213300	-2.56653500	H	4.23369100	1.17791000	-8.08945400	C	1.36505900	-3.50984300	-1.89570300
C	10.46992000	-0.87375400	-5.04642200	C	11.68432200	1.33720300	-3.02783900	H	5.60927400	2.05162100	-8.72992500	C	2.19498200	-6.30608000	-0.61579400
H	8.48805800	-0.33128200	-4.41052600	C	12.65527400	0.36292100	-2.83975800	C	4.58383400	-1.22659500	-9.49077900	H	0.25748200	-0.82022800	-4.12246000
C	11.10769200	-2.16355900	-2.73703200	C	8.21700300	-1.84153400	-3.97414500	H	6.42944700	-0.12531900	-9.81006100	H	0.88376600	-6.40024000	2.09652400
C	11.91997000	-3.19009000	-3.22203200	C	8.08452400	-3.23513800	-3.92960100	H	4.67951200	-3.26040200	-8.71546300	H	0.01846400	-5.36811000	3.51684700
C	11.81144400	-1.18155500	-2.02921900	C	8.33192500	-1.34289900	-5.27659900	H	6.42944700	-0.12531900	-9.81006100	H	0.88376600	-6.40024000	2.09652400
C	13.29762400	-3.26594300	-3.00953400	C	7.97364100	-0.40505900	-5.05869500	H	4.99500800	0.61863600	-10.49112700	H	3.36304600	-5.57622400	0.73625400
C	13.80602000	-1.21238600	-1.78750000	C	8.25916100	-2.12084000	-6.42918200	C	3.52986200	-1.00564800	-9.27479800	H	4.03171500	-3.87827400	2.69200200
C	13.93644700	-2.27036500	-2.28320100	C	8.05105900	-3.49057100	-6.32724300	H	4.59600800	-1.70281700	-10.47829600	H	1.96013400	-3.74123200	4.42588900
C	8.81286300	-3.33533500	-3.70973800	C	7.83559900	-1.48374300	-2.13361200	O	4.88969000	-0.85199200	-6.52207200	H	1.30198100	-1.26390000	3.79466600
C	8.73902800	-4.48545300	-2.91124400	C	6.62077600	-2.16417800	-1.11796200	C	4.79949200	-1.97426900	-7.04134200	C	6.17922000	2.00367300	-6.81863200
C	8.18425000	-3.48042400	-4.94159400	C	8.48791500	-1.31185900	-0.00853400	O	4.42973800	-3.03214400	-6.35521100	C	5.48255400	1.59148600	-8.09527600
C	8.08589100	-5.66044500	-3.27240600	C	6.10623600	-2.67434200	0.06558700	B	8.32557700	-0.92067700	-2.69118900	H	6.14162200	-1.21959700	-6.06185000
C	7.53134300	-6.43297200	-5.36046200	F	7.99968900	-1.78032900	1.21479100	C	9.95229700	-0.47530700	-2.74027300	H	5.81956900	2.94883000	-6.41166100
C	7.46367100	-5.73642200	-4.51546000	C	6.79357800	-2.46621200	-2.12546100	C	10.95415200	-1.40375300	-2.43095100	C	4.75986000	-1.93214400	-8.34270000
C	5.95377000	-1.61635900	-1.76679800	F	13.95768700	0.66954200	-2.92402800	C	10.44997500	0.73803000	-3.20555600	C	6.03352000	0.29222600	-8.73052100
C	7.20220700	-1.25189200	-1.94968400	F	12.04490200	2.60517700	-3.38014500	C	12.31877700	-1.15938900	-2.55009300	H	4.44256600	1.44024400	-7.79119500
C	8.90396400	-1.72007400	-0.41837700	F	9.47731900	2.03018900	-3.13600600	H	11.80393500	1.03240200	-3.35835800	H	5.49681400	0.24216200	-8.81318600
C	6.30738900	-0.96169400	-0.92390600	F	10.57147100	-2.51987800	-2.23274900	C	12.75302500	0.07664900	-3.02454400	C	4.93726800	-6.68401000	-9.22417000
C	8.05208400	-1.42218600	0.64729900	F	13.17552400	-1.89859100	-2.38090000	C	8.24807800	-2.02746200	-3.94320400	H	5.69914300	-2.50079200	-8.30264100
C	6.74515800	-1.03016200	0.39130700	F	8.51866100	-0.01736400	-5.50372600	C	8.07903700	-3.41376500	-3.83987600	H	4.01677300	-2.61346600	-8.77619900
F	15.25999900	-2.32257200	-2.06820200	F	8.32907400	-1.54436500	-7.65519600	C	8.36644700	-1.58704400	-5.26493700	H	6.68057600	-0.22378200	-8.01350600
F	13.77988200	-0.23295700	-1.08869500	F	7.90726800	-4.24132200	-7.43264600	C	7.92372800	-4.26979800	-4.93419700	H	6.68637200	0.56183200	-9.56876100
F	11.15233800	-0.11107400	-1.52495300	F	7.74897400	-5.37029100	-4.92774000	C	8.25817200	-2.40644800	-6.38327400	H	3.97847700	-1.06357000	-9.31878700
F	11.40252800	-4.19749700	-3.96978300	F	8.00815700	-3.89405200	-2.75832500	C	8.00489300	-3.76344200	-6.22511200	H	5.18903500	-1.04291000	-10.20358400
F	14.01042300	-4.29053300	-3.50952100	F	5.83536000	-2.36542300	-2.21451800	F	7.88742500	-1.53803700	-1.22357500	O	4.17777000	-0.53335000	-6.43324100
F	8.14091900	-2.45592500	-5.85235500	F	4.92856700	-3.34036800	0.07402200	C	6.65642600	-2.18677100	-1.08626100	C	3.44780000	-1.64338000	-6.90757400
F	6.92857100	-4.68924800	-4.57347600	F	6.28156700	-2.90026200	2.24327100	C	6.13404800	-1.31317200	-0.00530700	O	4.20971200	-2.77997800	-6.21600800
F	6.77974500	-6.83395500	-4.88120600	F	8.67828900	-1.55937600	2.35909700	C	8.52706300	-2.62485500	0.11982400	H	8.08894800	-0.83201200	-2.54751800
F	8.03443500	-6.71024400	-2.43895400	F	9.65377200	-0.63743300	0.07164500	C	8.03047300	-1.70862100	1.23700400	C	6.95104300	0.131436600	-0.30723700
F	9.92015500	-4.48700000	-1.69633200	F	7.39488200	0.40363700	-4.82371700	C	6.81101300	-2.36869600	1.30137800	H	6.98406400	1.12013400	-3.25270200
F	6.66134100	-1.19785000	-3.20648500	C	8.24574700	5.29948700	-4.93764700	F	14.06191800	0.33409300	-3.16118100	H	7.03382800	0.78364000	-0.45386000
F	5.02331500	-0.63628600	-1.11600800	H	7.86971900	3.28592100	-4.18708400	F	12.18617500	2.23153800	-3.84470600	H	5.94734100	-0.12538500	-3.00119100
F	5.90127500	-0.75040200	1.40948800	H	6.41874000	4.27520000	-4.39547600	F	9.61529000	1.75371400	-3.57821000	C	9.65690400	-0.26689500	-2.77113500
F	8.47631100	-1.52542600	1.91527400	F	9.42386600	2.87602400	-6.53851000	F	10.64420000	-2.63044000	-1.98914400	C	7.101881700	-1.03443000	-2.27131800
F	10.12613500	-2.14574000	-0.05625100	F	9.73993900	5.04339500	-5.17658400	F	13.22078800	-2.09904600	-2.22599300	C	10.07488800	0.92018300	-3.36032000
				H	7.82563300	5.93459600	-5.72983600	F	8.62087000	-0.27607300	-5.54632500	C	12.05862700	-0.56569100	-3.22693000
				H	8.12543000	5.85349200	-3.99714300	F	8.32072600	-1.87761200	-7.63285600	C	11.39829500	1.34657100	-3.34508300
				C	10.05032300	4.28650800	-6.47363200	F	7.83938000	-4.55393800	-7.29658600	C	12.10193100	0.55420400	-2.91595800
				H	9.55855300	2.37260100	-5.57432700	F	7.68020200	-5.57668100	-4.74906200	C	8.11585500	-2.04030000	-3.89956900
				C	9.92326600	2.27146900	-7.29858600	F	8.02286500	-4.02224100	-2.64118200	C	8.23469000	-3.41137500	-3.63632500
				H	10.14549800	4.46810700	-4.33338000	F	5.87561200	-2.42034400	-2.17510400	C	8.09977500	-1.74120500	-5.26544300
				H	10.27016100	6.00404900	-5.18561900	F	6.90558800	-3.26468100	0.15741400	C	8.27362500	-4.39970500	-4.62099900
				H	9.73437300	4.87304800	-7.34739000	F	4.28043900	-2.72955500	2.48740600	C	13.55549000	-2.969134300	-6.28224000
				H	11.13686800	4.16792700	-6.55794500	F	8.70502700	-1.44017500	2.36637200	C	8.21442400	-4.00027600	-5.26190000
				C	7.04491100	3.43751800	-6.09884900	F	9.71098900	-0.65209700	0.04547900	C	7.62819400	-1.353700800	-1.94168200
				C	7.95395500	2.84778300	-6.90910900	C	7.37264300	3.88543400	-4.46154700	C	6.49573000	-2.16174300	-1.08573200
				C	7.53854300	2.30975200	-7.91969900	C	6.79804000	5.31129800	-4.80440000	C	8.14725300	-0.881490800	-0.03564000
				F	7.18710200	0.42469400	-2.87711800	H	8.16993900	3.37933700	-3.89165300	C	5.94016500	-2.50298300	0.14315500
				H	6.16730000	0.01799600	-2.86308000	H	6.44606700	3.77425600	-3.89286100	C	7.62138200	-1.18991000	1.22115500
				H	7.24426100	1.15311300	-2.05853300	C	9.39972500	3.27908500	-6.49411300	C	6.50413200	-0.00577900	1.31148900
				H	7.30114500	0.98199500	-3.81073400	C	9.10892000	5.56136500	-5.30531200	F	13.69156000	9.40221000	-2.98560700
								H	6.93996300	5.66775800	-5.53395300	H	11.69712500	2.53061600	-4.03883800
								H	7.51577800	5.89350700	-3.88834600	F	9.17845300	1.78709700	-3.92848000
								C	9.47319400	4.81918100	-6.59684300	F	10.46420300	-2.22299700	-1.69565400
								H	9.87548300	2.93336800	-5.56708100	F	13.01653700	-1.44486700	-1.81396400
								H	9.93263700	2.81567900	-7.32693300	F	8.06659000	-0.44607900	-5.69934500
								C	8.01815200	5.27076800	-4.51742000	F	8.08182200	-1.31540900	-7.58092700
								H	9.24696800	6.63780800	-5.46400700	F	8.24353900	-4.96985000	-6.92

C	-0.37728600	-3.14590300	2.00744300	O	7.52397000	2.75326700	-7.70483900	C	6.22777300	-0.48072700	0.59846700	C	5.66973000	0.65687800	-7.93067500
H	-0.74894500	-2.81496700	2.98758700	C	8.11513000	3.93604800	-0.77891600	F	14.19811200	1.04277800	-3.09365500	H	4.59676500	2.35738600	-8.73223600
H	-0.99290800	-2.64529100	1.24635300	C	8.25588000	4.46835200	0.64512000	F	12.72442400	1.49583600	-5.37170700	C	6.02949000	1.92895900	-9.66201300
H	-0.57839800	-4.22397600	1.93450400	H	8.42786900	2.89065400	-0.85100100	F	10.14295200	0.91728500	-5.45291100	C	4.73335300	-0.36461600	-8.59386100
H	3.27704900	-0.73857800	-0.34094900	H	7.07841900	4.00656600	-1.11486200	H	10.38453300	-0.61763200	-0.93626800	H	5.68125900	-2.16656200	-7.79543700
C	1.41103800	-4.59391500	-2.32114600	C	11.00468400	4.00031200	-0.80523400	F	12.95752100	-0.02218600	-0.89429600	H	4.08531300	-2.43652300	-8.45629200
C	1.59959800	-4.51096600	-3.84385400	C	9.56000600	4.06099600	1.34308900	F	7.27190800	-0.78448600	-6.13696300	H	5.35902900	0.79270100	-6.88803900
H	1.95682600	-5.44563500	-1.89538500	H	8.14427200	5.56100000	0.62098700	F	7.53459200	-3.02578700	-7.52031000	H	6.69579000	0.27242800	-7.91246400
C	0.35467200	-4.77780700	-2.07802700	H	7.40729200	4.07994900	1.22388400	F	8.82927400	-5.19475200	-6.46975900	H	3.71811200	0.04971200	-8.62930400
C	4.09685300	-2.54188300	-4.58935900	C	10.83557600	4.53558500	0.63467800	F	9.88276800	-0.53680300	-3.94453200	H	5.04686200	-0.53267500	-9.33020800
C	3.01224800	-4.86719700	-4.34724100	H	10.76513900	2.92985000	-0.83102500	F	9.65114500	-2.78113200	-2.52196900	O	3.45783100	-0.66910000	-6.06117900
H	1.31106900	-3.50834500	-4.17904500	H	12.04184000	4.11140900	-1.12926800	F	6.58912200	-2.51323200	-2.34989200	C	4.06284200	-1.63201200	-6.49038600
C	0.89517000	-5.20943700	-4.31366000	H	9.58200100	2.96662900	1.42850000	F	5.22909200	-2.51304000	-0.80864300	O	4.25718800	-2.76470700	-5.78980800
C	4.14818800	-3.91482500	-3.93632900	H	9.55488900	4.45318300	2.36785600	F	7.25801600	1.58411400	1.17863700	C	6.59818500	0.03988500	-3.17205200
H	4.83495600	-1.87034100	-4.14520100	H	10.88020600	5.63331200	0.62348400	F	8.63937400	1.60109200	-1.08407400	H	7.81377100	2.20655100	-3.10715100
H	3.26082800	-5.87796600	-3.99356300	O	10.88310780	4.72041700	-1.76803600	C	9.63236000	4.25563000	-4.95851300	H	8.03110200	1.64141000	-4.76127500
H	5.11342700	-4.37384500	-4.18493100	O	10.18232000	4.72640900	-1.85356300	C	10.16773210	5.20797300	-5.57197200	H	6.67977200	1.05554900	-3.79923100
H	4.15627000	-3.75780500	-2.85303000	O	10.68566600	5.32924900	-2.78337000	H	9.74776200	3.18519700	-5.02736200	C	10.24918600	0.24629700	-3.09112800
O	2.04244300	-2.26825400	-2.06738900					H	8.75120500	4.62121600	-4.45548700	H	11.07258400	-0.78139100	-2.61136500
C	1.80073800	-3.34205400	-1.54043300					C	10.06855200	3.02701000	-7.97711800	C	10.95830800	1.37431000	-4.34866800
O	1.82631400	-3.54912700	-0.32292400					H	11.63174700	4.56926600	-6.53438800	C	12.46238200	-0.17173100	-2.54142300
H	0.62051200	-0.507707100	-0.37761800					H	10.05282800	6.00914700	-0.66376000	C	12.34443900	1.50588500	-3.42224200
H	-0.24701700	-0.32227800	2.17021200					H	11.15785000	5.68264000	-4.74609700	C	13.11199900	4.05254400	-2.94691000
H	0.94422100	-4.56923200	1.12865300					H	10.36631400	2.22200300	-7.29407900	C	8.38857700	-1.27219000	-4.17621000
H	1.78454800	-5.91737900	4.19652100					H	10.02563200	2.59792800	-8.98109700	C	8.09674100	-2.58232700	-3.77677200
H	4.14603300	-4.84744400	1.19337200					H	12.0840100	3.69388400	-6.05380300	C	8.50422800	-1.12417300	-5.56083700
H	4.76413700	-2.88531100	2.87331200					H	12.44427900	5.29029000	-6.68496700	C	7.84983900	-3.63018900	-4.66194600
H	2.77969800	-2.68659200	4.70081500					H	10.69872700	5.05899500	-8.43531400	C	8.26013700	-2.14400500	-6.48079100
H	1.90670900	-0.34562500	3.77995200					H	11.96383100	3.84868500	-8.52158400	C	7.90990300	-3.40612700	-6.03095300
C	6.16158200	2.51789500	-7.13424400					H	8.38697900	4.11629300	-6.58959100	C	7.96017800	-0.14956300	-1.64389900
C	5.36115100	1.70184800	-8.12411900	HF	1.65494900	-3.44452500	1.93312800	C	8.67431000	3.46442000	-7.60471500	C	6.69167200	0.20728600	-1.44046900
H	6.32158300	1.98811300	-6.19243300	O	-0.17234200	-4.75023300	2.32897000	C	7.75907600	3.11349300	-8.48674300	C	8.49574700	0.41173600	-0.48518500
H	7.72794200	3.50045100	-6.93594300	H	-0.02636600	-5.60559900	2.99768700	C	7.97277200	4.66416100	-0.84091600	C	6.05082100	0.77358100	-2.08055000
H	4.87464700	-1.91506100	-8.17612600	H	-1.07918900	-4.23130800	2.65879700	C	8.45121200	5.76969900	0.09297600	C	7.88856600	0.04033800	-6.79826000
C	6.01631100	0.37080700	-8.53626900	H	-0.39925600	-5.17255500	1.35343700	H	7.94879900	3.68445400	-0.36005700	C	6.64992400	-0.21419700	0.91490700
H	4.42092600	1.48215100	-7.06627900	H	1.23627700	-1.00865800	-0.05265000	H	6.97742400	4.88314300	-1.22939900	F	14.44551000	0.55522800	-2.87355700
H	5.12039900	2.30913100	-9.602639100	H	1.42308300	-4.70200900	-2.23361000	C	10.767978100	3.83287500	-0.80155100	C	12.94132500	2.66861700	-3.77408900
C	4.99121800	-0.66905100	-9.06308900	H	1.58436100	-4.43963200	-3.73898000	C	9.67709900	5.40440900	0.94902000	F	10.30423400	4.93157800	-3.93888100
H	5.81941000	-2.42356500	-8.11043600	C	2.00702900	-5.57522000	-1.91480800	H	8.63875500	6.67583500	-0.49889000	C	8.86921300	0.06281600	-6.10967200
H	4.18333100	-2.64591300	-8.61647600	C	3.07895300	-4.95528000	-2.00071000	H	7.61297900	6.00488600	0.76102500	F	13.17987900	-1.74013200	-2.06872200
H	6.55431200	-0.04848100	-7.67948800	C	3.99057800	-2.31603300	-4.31307000	C	10.93722000	5.05253400	-0.13412500	F	8.86921300	0.06281600	-6.10967200
H	7.77999200	0.56624100	-9.29820200	C	2.99605800	-4.69209700	4.30364900	H	10.25359200	3.01764600	-0.28174200	F	8.71307400	-1.89433400	-7.80474600
H	4.00922100	-0.20283200	-9.16158600	H	1.25960000	-3.41561800	-3.95509000	H	11.74536400	3.45429500	-1.11285600	F	7.64422000	-3.38508300	-6.90314700
H	5.27551100	-1.00997900	-10.06825100	H	0.89188700	-5.10256700	-4.27376300	H	9.41958800	4.55279200	1.58600500	F	7.51704400	-4.84967900	-4.20109100
O	4.03812400	-0.51853100	-6.36634700	C	4.11268100	-3.75063200	-3.82148100	H	9.90823700	6.24112400	1.61122000	F	8.10988100	-2.91208800	-2.46959500
C	4.39771400	-1.61277600	-6.76377500	H	7.473780100	-1.67692100	-3.83752700	H	11.27046000	5.92123500	-0.44788600	F	5.99619500	-1.20403500	-2.48225400
O	4.43367400	-2.71122700	-5.99810700	H	3.00619600	-1.86926600	-4.11888800	H	11.76639200	4.81758600	0.83043800	F	4.84555200	-1.36157000	-0.09045400
B	8.40663700	-0.50312000	-3.15087400	H	2.94788200	-4.63767900	-5.39901900	C	8.74835200	4.56320600	-2.06533000	F	6.03019200	-0.25603000	-2.11028200
C	7.27544300	0.53989800	-3.62852500	H	3.28424700	-5.72601500	-4.06448100	C	10.02057300	4.13518600	-2.07673300	F	8.47456400	1.00524300	1.82131200
H	7.33799900	1.48928400	-3.07665800	H	5.038209500	-4.14238400	-4.15379100	O	10.58949800	4.02539300	-3.172077000	F	9.68262300	1.09849300	-0.51871400
H	7.29395300	0.78020700	-4.69229300	H	4.15610300	-3.71663600	-2.72813300					C	9.85678700	5.65419400	-4.54080500
H	6.28546600	0.11879800	-3.41164900	O	2.03542600	-2.41198500	-1.17911600					C	10.97937900	6.07537000	-5.65040700
C	10.00404000	0.09774200	-3.33674800	C	1.77903600	-3.53527000	-1.31728700					C	10.06026800	3.14781300	-7.32285700
C	11.10188700	-0.50002500	-2.70366800	C	1.17588300	-3.87084700	-0.03102500					H	11.68052400	4.95748400	-6.25221700
C	10.36483000	1.13357300	-4.19384300	H	-1.02661900	-1.90107100	1.10567200					H	10.16350300	6.51705900	-6.42598100
C	12.42430000	-0.09321200	-2.86265800	H	-0.59999000	-2.04564400	3.76106700					H	11.43456000	6.88057900	-5.62202600
C	11.66998600	1.58238000	-4.38584000	H	1.92862800	-5.53795400	4.38972300					H	11.52394000	4.22351800	-6.50371700
C	12.71804000	0.96680400	-3.71749300	H	2.65529400	-6.49480400	1.97943800					H	10.19013200	2.61875800	-6.36957000
C	8.48526400	-1.89657600	-4.06702000	H	4.37176800	-4.73621600	0.87516200					H	11.49009200	2.38232000	-8.09934100
C	8.67734400	-3.19220300	-3.57126900	H	4.68028600	-2.68933100	2.57215900					H	11.18390700	4.22490000	-5.84782700
C	8.38222000	-1.85026000	-5.46078600	H	3.18711600	-3.19900500	4.77084400					H	12.63001700	5.42362800	-6.54282100
C	8.69576000	-4.34057700	-4.36326100	H	1.90909700	-1.21413800	4.24395000					H	8.102091800	4.96129500	-5.24599900
C	8.38364600	-2.96702100	-6.29196300	C	6.35864100	3.47250700	-8.23984800					H	12.01634800	3.71571500	-7.94945500
C	6.97867800	-4.23217900	-5.74017000	C	5.46535600	2.40628500	-8.85024500					C	8.27771700	4.76615000	-6.93988000
C	8.06107900	-0.77115900	-1.5												

C	0.53029600	-4.32843000	0.95935600	C	2.16203200	-5.04673900	-4.65814300	H	-0.20970500	-4.47422300	-2.69105600	H	2.65092100	-0.45366900	-1.22827600
C	0.48653400	-4.40528300	2.05445300	H	3.27871500	-3.18246400	-4.43469600	C	3.56889900	-2.97940300	-4.60853800	C	0.38364500	-3.99767200	-3.32239600
H	-0.49374400	-4.12344700	0.61663600	H	1.71626500	-2.97754400	-5.24072000	C	2.10445600	-5.02358600	-5.27237500	C	0.84549400	-4.04606700	-4.78657000
H	0.81390600	-5.32182600	0.58401300	H	0.77428800	-5.55372900	-6.22821500	H	0.67387000	-3.42321300	-4.89884800	C	0.50158800	-4.96761300	-2.82611600
H	0.99065000	-0.29954000	-1.63874700	H	0.63941600	-6.58221300	-4.80100200	H	-0.02617300	-5.02033400	-4.98388500	H	-0.69228000	-3.77645000	-3.27906900
C	0.82304500	-4.19930400	-3.91104300	H	2.92029000	-5.32519100	-5.39509900	C	3.42355000	-4.47129200	-4.71547300	C	3.88018600	-2.94844300	-4.64546400
C	-0.04324900	-3.75108200	-5.10018600	H	2.46225500	-5.52367200	-3.71469900	C	4.69747200	-2.47440400	-4.14006400	C	2.14849800	-4.83056000	-5.03587300
H	1.65884100	-4.82908600	-4.24965500	O	1.74463000	-3.09625200	-3.14197400	H	2.29049000	-2.35327900	-5.01327800	H	0.93118700	-3.01757600	-5.53538800
C	0.25022900	-4.80983400	-3.20717100	C	0.64733200	-3.47266800	-2.57053200	H	2.05413000	-4.81203100	-6.34735000	H	0.05914600	-4.52227300	-5.38625100
H	1.75377900	-1.41861400	-4.91691700	O	0.43372400	-3.03019000	-1.41022800	H	2.12059400	-6.11610700	-5.17178500	C	3.40673000	-4.34547000	-4.29374600
C	0.77013200	-3.33013400	-6.33440700	H	-0.60108300	0.04224700	-1.44538000	H	4.26431300	-4.78359200	-5.34186600	H	4.69858800	-2.60382700	-4.01090500
H	-0.70494800	-2.93548800	-4.77955000	H	-0.75035500	0.53504400	1.19322600	H	3.63943000	-4.87707700	-3.72047500	H	3.08271900	-2.06859000	-4.648185400
C	-0.70599800	-4.58192000	-5.56412100	H	0.54573400	-3.54606500	3.22245900	O	2.52745400	-2.80681800	-2.81462100	H	2.35347000	-4.83833000	-6.11480500
C	1.19124400	-2.45669000	-2.22572800	H	0.62376300	-5.20052700	1.10711400	C	1.62563400	-3.51116000	-2.31190400	H	1.95982500	-5.87969200	-4.75536400
H	2.55376600	-0.68314900	-4.86613000	H	2.80752700	-4.58015800	-0.35445800	O	1.31615600	-3.40627700	-1.06270200	H	4.23246400	-5.04350800	-4.47703200
H	0.79073100	-0.90904000	-5.01422300	H	4.05698900	-2.53112600	0.84265500	H	-0.37736300	-0.55621200	-1.10750300	H	3.23787300	-3.47153000	-3.21014500
H	0.10558700	-2.79793500	-7.02573100	H	2.67012100	-1.89501100	3.06631000	H	-0.82197100	-0.23391800	1.52406500	O	1.59154000	-1.93317200	-2.97505600
H	1.20594000	-4.22272300	-6.86533900	H	1.74200300	0.43198400	2.20210000	H	0.71818000	-4.33806700	3.34839700	C	1.06575800	-2.92160400	-2.47715400
H	2.30685800	-1.90405800	-6.88109000	C	3.95979400	-0.96222900	-0.803830700	H	1.62957900	-5.66550800	1.19832100	O	1.01882600	-3.16468200	-1.18089300
H	1.85819800	-3.06463600	-5.72517900	C	3.59579400	-0.45208900	-9.46303700	H	3.85553300	-4.41570800	0.32824400	H	0.00852900	-0.07256900	-1.06355500
O	2.79068000	-1.92976500	-3.52517400	H	4.80172200	-1.36585400	-7.88584900	H	4.30644300	-2.30974300	1.92752700	H	-0.65792500	0.07013800	1.54694000
C	1.42547300	-3.09424500	-3.08112700	H	3.65158500	-0.15194000	-7.23092900	H	2.36405500	-2.25682400	3.80191500	O	0.29993900	-4.22096600	3.21663800
O	1.06125600	-3.30094900	-1.85395700	C	3.72877600	-3.59243400	-9.24488400	H	6.16333200	0.01482500	2.74669200	H	0.71656400	-5.62242900	1.07468700
H	-1.00029000	-1.61488600	-0.36558800	C	4.10357700	-1.39663500	-10.56128100	H	6.11680600	0.25381500	-5.87198400	H	3.10420400	-4.89799500	0.01578800
H	0.31392600	-1.84192500	2.22208400	H	2.52961600	-0.22688500	-9.60283800	C	5.89005100	1.27546300	-6.97682900	H	4.16141100	-3.03276200	1.64047600
H	3.03677300	-5.21646100	1.94487800	H	4.13481300	0.50033700	-9.54435800	H	7.09225900	-0.22681000	-5.93883100	H	2.42856700	-2.61850200	3.66304400
C	3.68996000	-5.55879100	-0.65905700	H	3.47781800	-2.79721100	-10.544484500	H	6.03231500	0.70349500	-4.88337100	H	1.58891600	-0.22931400	2.99197300
H	4.75253900	-2.98689700	-1.38019100	H	4.77214300	-3.47986100	-9.82834000	C	5.89786600	-1.72855500	-7.98147000	C	6.15195900	0.11527700	-6.05149600
H	4.76192300	-1.38795000	0.77537500	H	3.55629400	-4.65836800	-9.40827600	C	3.31462000	0.80446100	-8.37482700	C	5.93518600	0.85546500	-7.35889900
C	3.68665700	-2.76529400	2.83817600	H	5.19398800	-1.49060000	-10.47114000	H	4.43489300	1.58018600	-6.96704600	H	7.13767600	-0.33888800	-5.96744200
H	2.08944000	-0.67073000	2.55283300	H	3.91738700	-0.93423000	-11.53907000	H	6.47743000	2.16204500	-6.70577100	H	5.97604900	0.74961300	-5.18476900
H	7.91721600	-2.40817000	-4.66837900	H	2.39711700	-2.73435000	-10.73367400	C	5.63243800	-0.48331700	-8.85904800	C	5.82658400	-2.30425900	-7.80691500
C	9.13716100	-2.58993600	-6.09111100	H	3.89969500	-3.37791000	-11.37377600	C	6.95807500	-1.78463200	-7.70541000	C	6.38053700	0.09499600	-8.61579600
C	9.82594600	-3.80053600	-4.78199600	C	2.82054400	-1.94801600	-7.62056500	H	5.66199600	-2.64469200	-8.52701800	H	4.88329700	1.16119500	-7.43326200
C	9.95266800	-1.45761500	-7.83921300	C	2.81748300	-3.21326600	-8.09340300	H	4.03511500	1.60436000	-0.99657900	H	6.52478900	1.77745000	-7.27663000
C	11.21191100	-3.89038100	-4.91892900	O	2.04472700	-4.00058600	-7.57834400	H	6.14911800	1.60436000	-0.99657900	C	5.61542400	-1.20944900	-8.87512600
C	11.33580700	-1.49752500	-4.91917400	B	8.11852700	-2.25547600	-5.04628500	H	4.50982700	-0.32781400	-8.95485600	H	6.98308200	-2.41207700	-7.57285300
C	11.97495400	-2.73214400	-4.98691200	C	9.76227400	-2.13304600	-5.18342100	C	5.99702500	-0.71555900	-9.86613200	H	5.48345500	-3.27917400	-8.16018000
C	6.66847400	-3.78774600	-4.23211700	C	10.60680200	-3.06493600	-5.79068100	C	11.00276500	-0.79672800	-5.83452600	H	7.45627700	-0.11664200	-8.54756800
C	6.98796100	-4.44155200	-3.03447100	C	10.39685500	-0.94129500	-4.81706000	C	5.07770800	-1.78220900	-6.71465000	H	6.25172600	0.75215100	-8.94381900
C	5.51622300	-4.27675200	-4.84765500	C	11.97388700	-2.85803000	-6.98277500	O	4.32524100	-2.73876900	-6.49128300	H	4.54248700	-1.02076000	-8.993131600
C	6.24135000	-5.47812800	-2.49796100	C	11.75377600	-0.69054000	-4.98640700	C	9.44739200	-2.02038900	-3.08773500	H	5.95201100	-1.63693100	-8.85275700
C	4.73427800	-5.30690700	-4.32593900	C	12.55459200	-1.66356600	-5.67272300	C	11.05332000	-2.13840900	-2.71492500	O	5.17774700	-0.99756600	-5.81529800
C	5.08977600	-5.91005400	-3.12943300	C	7.53693900	-3.80226600	-5.22954000	C	11.91218300	-3.18407000	-3.06421500	C	5.13768400	-2.06464600	-6.50104700
C	6.94708400	-1.36626200	-3.48891500	C	8.06902000	-4.83624300	-4.44909600	C	11.70120900	-1.04288800	-2.13149100	O	4.42694900	-0.31417000	-6.70374600
C	5.61127100	-0.95336400	-3.48893300	C	6.43119800	-4.18716300	-5.98552300	C	13.28670900	-3.17053800	-2.80226900	B	9.58633900	-1.92624100	-3.08386800
C	7.65457500	-0.97693100	-2.34380200	C	7.59073100	-6.14341400	-4.44235200	C	13.06469700	-0.98370200	-1.86798600	C	12.11207400	-1.88782400	-2.81955700
C	5.01204700	-0.20978900	-2.47980100	C	5.91539100	-5.48173900	-6.01355300	C	13.86972700	-2.06425300	-2.21638400	C	12.14818100	-2.76126100	-3.38668200
C	7.09556200	-0.23117200	-1.30180300	C	6.49454200	-6.47335500	-5.23436200	C	8.75366200	-3.45938400	-3.55142700	C	11.78802100	-0.82560100	-2.11095500
C	5.76488100	0.15433200	-1.37035000	C	7.52771200	-1.88021900	-3.53537300	C	8.85425000	-4.57167800	-2.70573100	C	13.52833600	-2.62771700	-3.20546400
C	13.30737000	-2.80137800	-5.11886900	C	6.14794300	-1.75258200	-3.35285300	C	7.92501800	-3.67050600	-4.65138300	C	13.15553300	-0.65239900	-1.92657000
F	12.00516400	-0.36549400	-4.98945000	C	8.26505100	-1.79995700	-2.35023900	C	8.20378400	-5.79482700	-2.93545100	C	14.05834300	-1.56687700	-2.99010000
F	9.39048800	-0.22828100	-4.73965300	C	5.53751600	-1.52879200	-2.12770800	C	7.28404100	-4.87660700	-4.92893500	C	9.03018000	-3.46001300	-3.60829700
F	9.17158600	-4.98151200	-4.74453000	C	7.69606700	-1.55476900	-1.09620400	C	7.43031800	-5.95095800	-4.06335900	C	9.35297000	-4.56218400	-2.88399000
F	11.81281900	-5.08999000	-4.99055400	C	6.32102900	-1.41009900	-0.98794700	C	8.48028500	-1.59525500	-1.80064000	C	8.09831200	-3.63483400	-4.61468000
F	5.06897000	-3.73612400	-5.99255900	F	13.86588000	-1.44766500	-5.75497600	C	7.13053500	-1.29821600	-2.01127500	C	8.83402900	-5.82715400	-3.14701700
F	3.59636700	-5.68775900	-4.95958900	F	12.29454200	0.47583600	-4.59651800	C	8.44897300	-1.62176900	-0.45113600	C	7.53994300	-4.87490400	-4.91361800
F	4.93595800	-6.85588300	-2.57642600	F	9.67136200	0.05530800	-4.25920200	C	6.22136200	-0.99891300	-1.00448800	C	7.90838200	-5.98935600	-1.74688800
F	6.58181100	-0.60266800	-1.30291900	F	10.13589900	-4.24576500	-6.24453600	C	9.79347100	-1.31723300	0.59631000	C	8.64130600	-1.72728000	-1.79294700
F	8.05341800	-4.03873100	-2.31732300	F	12.73052400	-3.80262700	-5.65558400	C	6.67651000	-0.99382900	0.31480100	C	7.26424300	-1.53064300	-7.82672500
F															

Table with columns for category (Hf, C, H, etc.), numerical values, and labels (C, F, H, etc.). The table is divided into sections for '2-Hf-TS2', '2-Hf-P2', and '2-Hf-R3'.

Table with columns for numerical values and labels (C, F, H, etc.). This table continues the data from the first table, showing various numerical values and their corresponding categories.

Table of financial data with columns for stock codes, numerical values, and labels (e.g., H, C, O, HF, F). The table includes a central section labeled '2-HF-P3' and a bottom section labeled '2-HF-TS3'. The data is organized into multiple columns, alternating between labels and numerical values.