

Electronic supplementary information for

The Chameleon-Like Nature of the Elusive Cobalt-Oxygen Intermediates in C-H Bond Activation Reaction

Anran Zhou^{a,b}, Xuanyu Cao^{a,b}, Huanhuan Chen^{a,b}, Dongru Sun^{a,b}, Yufen Zhao^{a,b}, Wonwoo Nam^{c*}
and Yong Wang^{a,b*}

a. Institute of Drug Discovery Technology, Ningbo University, Ningbo 315211, China.

b. Qian Xuesen Collaborative Research Center of Astrochemistry and Space Life Sciences, Ningbo University, Ningbo 315211, China.

c. Department of Chemistry and Nano Science, Ewha Womans University, Seoul 03760, Korea.

*Corresponding authors: yong@nbu.edu.cn, wwnam@ewha.ac.kr

Table of Contents

Full citation for reference 13	3
Part I: Complexes $[\text{Co}(\text{O})(\text{TAML})]^{2-}$ binding with redox-inactive scandium ions in multiple coordination states.....	4
Part II: C-H bond activation of 1,4-cyclohexadiene (CHD) mediated by complex $[\text{Co}(\text{O})(\text{TAML})]^{2-}$ binding with multiple coordinated redox-inactive scandium ions ..	8
2.1 CHD oxidation by 1	8
2.2 CHD oxidation by 1-Sc^{3+}	10
2.3 HAT by $1\text{-Sc}(\text{OTf})_3$	12
2.4 HAT by 1-Sc	14
2.5 HAT by protonated 1, 1-H, $[\text{Co}(\text{OH})(\text{TAML})]^{1-}$	16
Part III: C-H bond activation of substrates with normal C-H bond mediated by 1.....	18
3.1 HAT of toluene by 1.....	18
Part IV: C-H bond activation of substrates with acidic C-H bond mediated by complex 1	20
4.1 C-H bond activation of acetonitrile by 1	20
4.2 C-H bond activation of phenylacetylene by 1	22
Part V: Cartesian coordinates	24

Full citation for reference 13

M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Milliam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, O. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, D. J. Fox, Gaussian 09, revision C.01; Gaussian, Inc.: Wallingford CT, 2009.

Part I: Complexes [Co(O)(TAML)]²⁻ binding with redox-inactive scandium ions in multiple coordination states

Table S1. Various SCRF energies of eight Co(O)(TAML) complexes calculated at the UMN12L/B2//B1 computational level

	OPT/B1+ZPE/B1		SOLV/B2+ZPE/B1		Free Energy, G/B1	
	E^a	ΔE	E	ΔE	G	ΔG
(a) [Co(O)(TAML)] ²⁻ , 1						
Doublet	-1474.545009	0.0	-1474.848569	0.0	-1474.597935	0.0
Quartet	-1474.522379	14.2	-1474.830440	11.4	-1474.578074	12.5
(b) {Sc-[Co(O)(TAML)]} ¹⁺ , 1-Sc ³⁺						
Doublet	-1520.429794	0.0	-1520.727472	0.0	-1520.481628	0.0
Quartet	-1520.420899	5.6	-1520.717578	6.2	-1520.473372	5.2
(c) {(OTf)Sc-[Co(O)(TAML)]} ⁰ , 1-Sc(OTf) ²⁺						
Doublet	-2481.593561	0.0	-2482.097953	0.0	-2481.655537	0.0
Quartet	-2481.580793	8.0	-2482.084551	8.4	-2481.644857	6.7
(d) {(OTf) ₂ Sc-[Co(O)(TAML)]} ¹⁻ , 1-Sc(OTf)₂ ⁺						
Doublet	-3442.750274	0.0	-3443.463883	0.0	-3442.821741	0.0
Quartet	-3442.733630	10.4	-3443.445215	11.7	-3442.807639	8.8
(e) {(OTf) ₃ Sc-[Co(O)(TAML)]} ²⁻ , 1-Sc(OTf)₃						
Doublet	-4403.898083	0.0	-4404.824439	0.0	-4403.977122	0.0
Quartet	-4403.886454	7.3	-4404.809454	9.4	-4403.967888	5.8
(f) {(OTf) ₄ Sc-[Co(O)(TAML)]} ³⁻ , 1-Sc(OTf)₄ ⁻						
Doublet	-5365.044993	0.0	-5366.187086	0.0	-5365.131983	0.0
Quartet	-5365.022898	13.9	-5366.159877	17.1	-5365.107208	15.5
(g) {(OH)(OTf) ₃ Sc-[Co(O)(TAML)]} ⁴⁻ , 1-Sc						
Doublet	-5440.915792	0.0	-5442.087173	0.0	-5441.000635	0.0
Quartet	-5440.889746	16.3	-5442.058931	17.7	-5440.980036	12.9
(h) [Co(OH)(TAML)] ¹⁻ , 1-H						
Doublet	-1475.040371	0.0	-1475.339103	0.0	-1475.095078	0.0
Quartet	-1475.016516	15.0	-1475.317474	13.6	-1475.072634	14.1

a. Absolute energies are in a.u. units and relative ones are in kcal mol⁻¹ units.

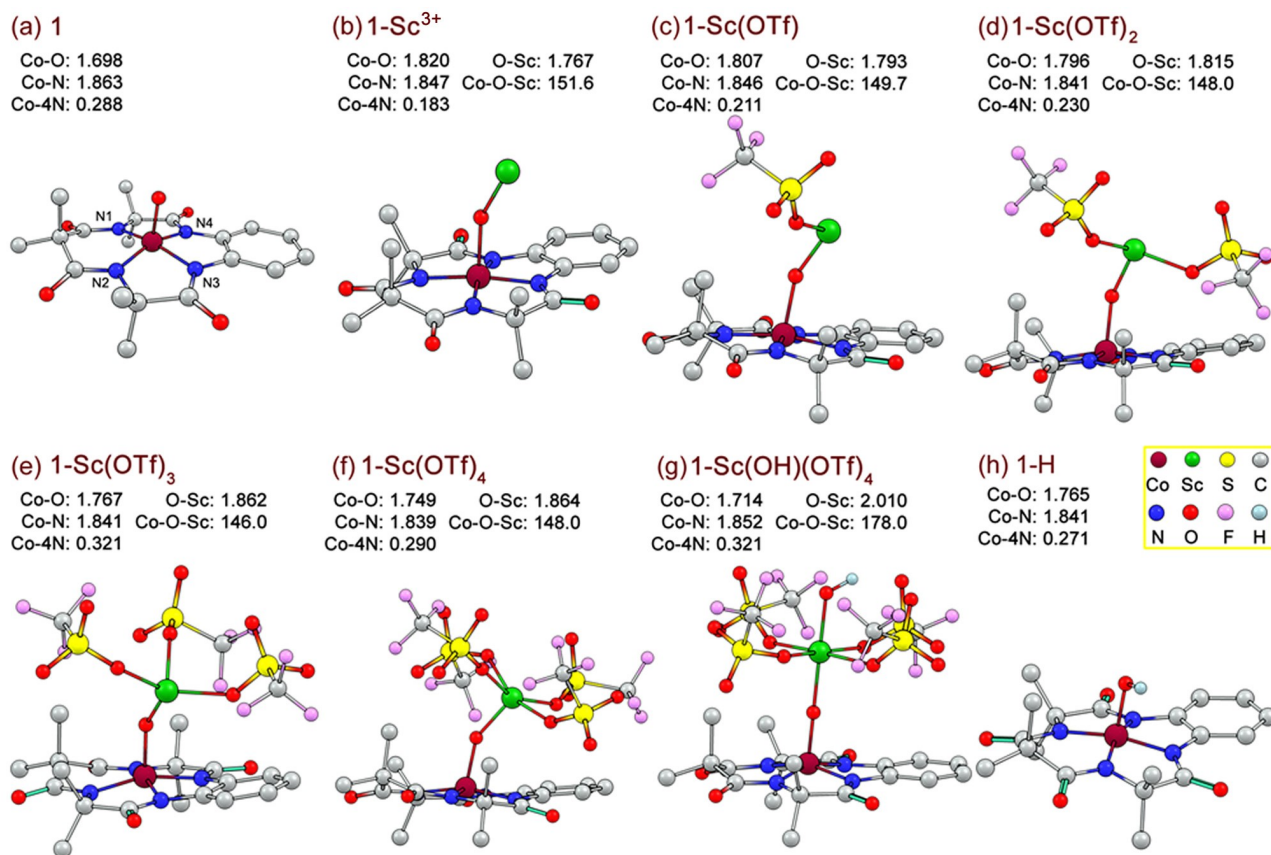


Figure S1. Molecular geometries of eight Co(O)(TAML) complexes on the ground doublet spin state. Calculations were performed at the UMN12L/B1 level. Lengths are in Å unit and angles are in degree (°) unit. Co-N denotes the average of four Co-N distance and Co-4N denotes the deviation of Co atom from the 4N plane (N1-N2-N3-N4). Hydrogen atoms in the TAML ligand are omitted for clarity and atomic color codes are shown on the bottom-right side.

Table S2. Mulliken atomic spin densities and charges of eight Co(O)(TAML) complexes calculated at the UMN12L/B1 computational level

		Charge						Spin			
(a) [Co(O)(TAML)] ²⁻ , 1											
	Co	O	TAML			Co	O	TAML			
Doublet	0.93	-0.62	-2.31			0.24	0.70	0.06			
Quartet	0.95	-0.56	-2.39			1.74	1.19	0.07			
(b) {Sc-[Co(O)(TAML)]} ¹⁺ , 1-Sc³⁺											
	Co	O	TAML	Sc		Co	O	TAML	Sc		
Doublet	1.16	-0.82	-1.46	2.12		0.09	0.00	0.91	0.00		
Quartet	1.09	-0.79	-1.35	2.05		1.85	0.07	1.06	0.01		
(c) {(OTf)Sc-[Co(O)(TAML)]} ⁰ , 1-Sc(OTf)²⁺											
	Co	O	TAML	ScX		Co	O	TAML	ScX		
Doublet	1.16	-0.83	-1.50	1.18		0.14	0.01	0.85	0.00		
Quartet	1.11	-0.81	-1.41	1.12		1.84	0.09	1.05	0.01		
(d) {(OTf) ₂ Sc-[Co(O)(TAML)]} ¹⁻ , 1-Sc(OTf)₂⁺											
	Co	O	TAML	ScX		Co	O	TAML	ScX		
Doublet	1.16	-0.84	-1.57	0.25		0.24	0.02	0.74	0.00		
Quartet	1.09	-0.82	-1.42	0.16		1.84	0.10	1.04	0.02		
(e) {(OTf) ₃ Sc-[Co(O)(TAML)]} ²⁻ , 1-Sc(OTf)₃											
	Co	O	TAML	ScX		Co	O	TAML	ScX		
Doublet	1.20	-0.83	-1.73	-0.64		0.71	0.03	0.26	0.00		
Quartet	1.09	-0.80	-1.46	-0.82		1.84	0.12	1.02	0.02		
(f) {(OTf) ₄ Sc-[Co(O)(TAML)]} ³⁻ , 1-Sc(OTf)₄⁻											
	Co	O	TAML	ScX		Co	O	TAML	ScX		
Doublet	1.18	-0.82	-1.79	-1.57		0.72	0.05	0.23	0.00		
Quartet	1.05	-0.80	-1.52	-1.73		1.82	0.15	1.01	0.02		
(g) {(OH)(OTf) ₄ Sc-[Co(O)(TAML)]} ⁴⁻ , 1-Sc											
	Co	O	TAML	ScX		Co	O	TAML	ScX		
Doublet	1.29	-0.83	-2.05	-2.41		0.73	0.18	0.08	0.01		
Quartet	1.05	-0.55	-2.29	-2.21		1.83	1.05	0.10	0.01		
(h) [Co(OH)(TAML)] ¹⁻ , 1-H											
	Co	OH	TAML			Co	OH	TAML			
Doublet	1.11	-0.32	-1.79			0.72	0.05	0.23			
Quartet	0.98	-0.46	-1.52			1.76	0.26	0.98			

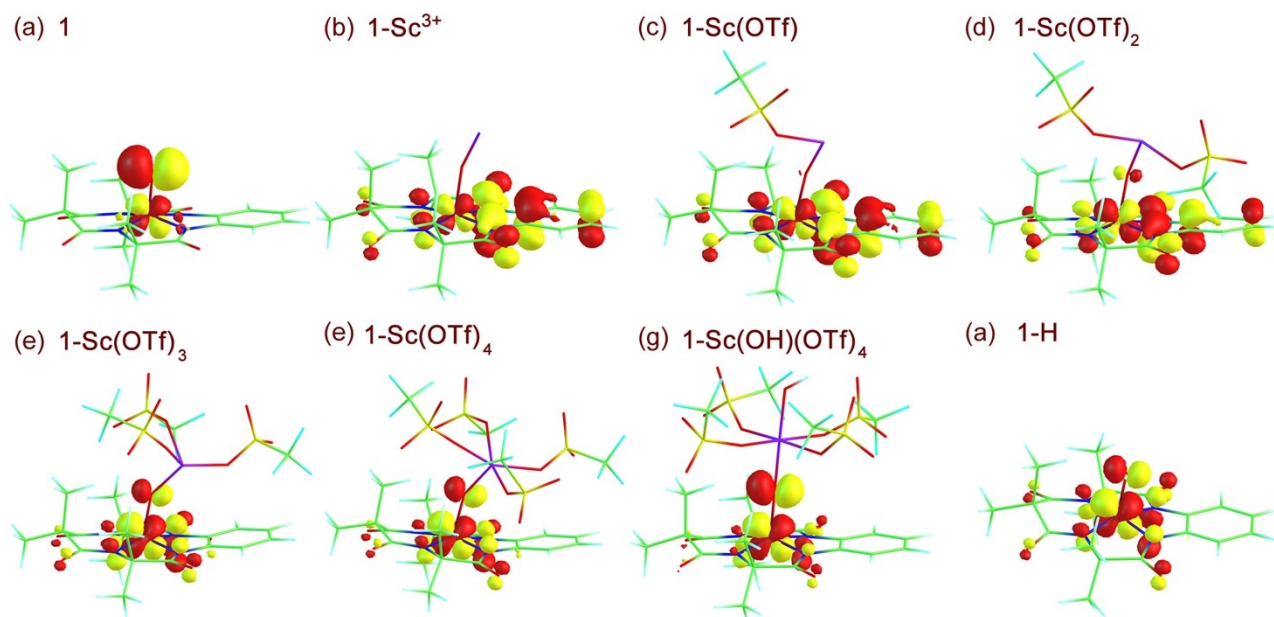


Figure S2. Singly occupied natural orbitals of eight Co(O)(TAML) complexes on the ground doublet spin state. Calculations were performed at the UMN12L/B1 level.

Part II: C-H bond activation of 1,4-cyclohexadiene (CHD) mediated by complex $[\text{Co}(\text{O})(\text{TAML})]^{2-}$ binding with multiple coordinated redox-inactive scandium ions

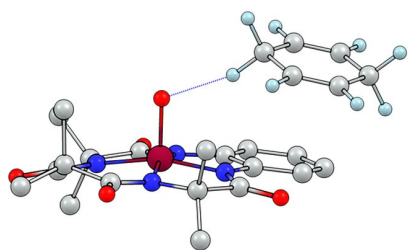
2.1 CHD oxidation by 1

Table S3. Various SCRF energies of hydrogen atom transfer of CHD by **1**. Calculations were done at the UMN12L/B2//B1 computational level

	OPT/B1+ZPE/B1		SOLV/B2+ZPE/B1		Free Energy, G/B1	
	E^a	ΔE	E	ΔE	G	ΔG
^2RC	-1707.606219	0.0	-1707.951945	0.0	-1707.663297	0.0
^4RC	-1707.582632	14.8	-1707.933113	11.8	-1707.640827	14.1
^2TS	-1707.597683	5.4	-1707.943199	5.5	-1707.658636	2.9
^4TS	-1707.576706	18.5	-1707.927014	15.6	-1707.637763	16.0
^2PC	-1707.649468	-27.1	-1707.995490	-27.3	-1707.705579	-26.5
^4PC	-1707.633244	-17.0	-1707.985538	-21.1	-1707.689876	-16.7

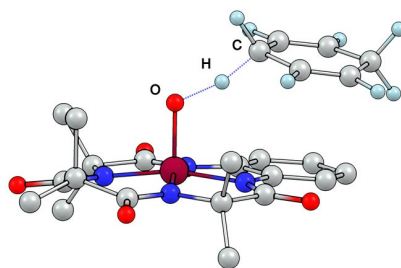
(a) $^2/4\text{RC}$

Co-O: 1.705/1.922
Co-N: 1.864/1.872
Co-4N: 0.292/0.320



(b) $^2/4\text{TS}$

Co-O: 1.758/1.925
Co-N: 1.862/1.874
Co-4N: 0.242/0.312
O-H: 1.332/1.348
H-C: 1.246/1.228
C-H-O: 162.5/160.0
Co-O-H: 112.7/108.1
 ν_{img} : 1441.8/1380.2



(c) $^2/4\text{PC}$

Co-O: 1.828/1.978
Co-N: 1.863/1.874
Co-4N: 0.215/0.327

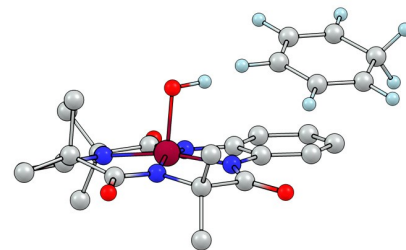
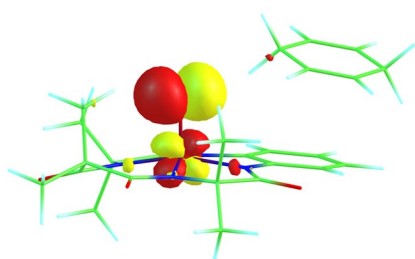


Figure S3. Molecular geometries of key intermediates in C-H bond activation of CHD by **1**. Values on the left side of slash are for the doublet spin state and the quartet spin state ones are presented on the right side of slash. Lengths are in Å unit and angles are in ° degree unit. Co-N denotes the average of four Co-N distance and Co-4N denotes the deviation of Co atom from the 4N plane (N1-N2-N3-N4). Hydrogen atoms in the TAML ligand are omitted for clarity. Calculations were done at the UMN12L/B1 level in solvent.

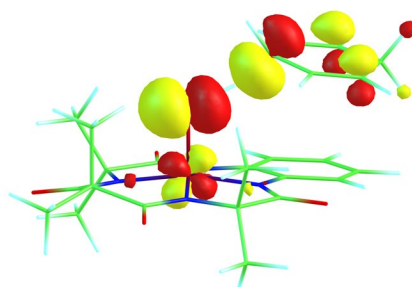
Table S4. Mulliken atomic spin densities and charges of key intermediates in C-H bond activation of CHD by **1**. Calculations were done at the UMN12L/B1 level in solvent.

	charge						spin				
	Co	O	TAML	H	sub		Co	O	TAML	H	Sub
2-RC	0.95	-0.60	-2.33	0.19	-0.22		0.18	0.75	0.06	-0.01	0.02
4-RC	0.94	-0.54	-2.36	0.14	-0.18		1.72	1.18	0.09	0.00	0.01
2-TS	0.91	-0.67	-2.36	0.31	-0.20		0.07	0.57	0.04	-0.07	0.38
4-TS	0.94	-0.67	-2.39	0.30	-0.18		1.75	0.87	0.07	-0.08	0.40
2-PC	0.86	-0.74	-2.40	0.31	-0.03		0.00	0.00	0.01	0.00	0.99
4-PC	0.90	-0.79	-2.37	0.29	-0.03		1.80	0.18	0.04	0.00	0.99

(a) ^2RC



(b) ^2TS



(c) ^2PC

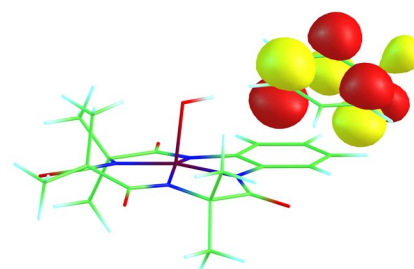


Figure S4. Singly occupied natural orbitals of key intermediates in C-H bond activation of CHD by **1**. Calculations were done at the UMN12L/B1 level in solvent.

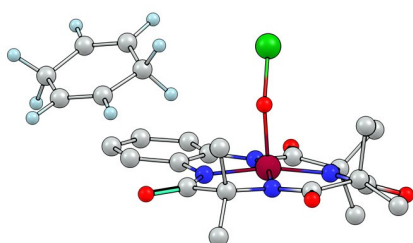
2.2 CHD oxidation by 1-Sc³⁺

Table S5. Various SCRF energies of C-H bond activation of CHD by 1-Sc³⁺. Calculations were done at the UMN12L/B2//B1 computational level

	OPT/B1+ZPE/B1		SOLV/B2+ZPE/B1		Free Energy, G/B1	
	E^a	ΔE	E	ΔE	G	ΔG
² RC	-1753.490075	0.0	-1753.827594	0.0	-1753.547444	0.0
⁴ RC	-1753.482811	4.6	-1753.819891	4.8	-1753.541008	4.0
² TS	-1753.456993	20.8	-1753.792854	21.8	-1753.518696	18.0
⁴ TS	-1753.461350	18.0	-1753.801031	16.7	-1753.524884	14.2
² PC	-1753.510930	-13.1	-1753.852008	-15.3	-1753.568654	-13.3
⁴ PC	-1753.510826	-13.0	-1753.851917	-15.3	-1753.569271	-13.7

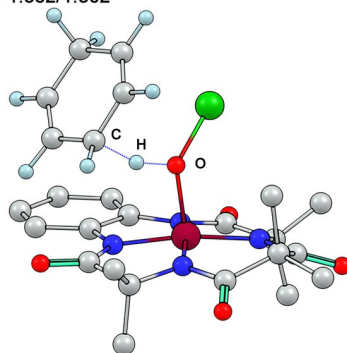
(a) ^{2/4}RC

Co-O: 1.822/2.102
Co-N: 1.847/1.856
Co-4N: 0.183/0.236



(b) ^{2/4}TS

Co-O: 1.875/2.349 C-H-O: 159.3/163.3
Co-N: 1.856/1.850 Co-O-H: 106.2/111.0
Co-4N: 0.211/0.198 ν_{img} : 1802.3/1576.1
O-H: 1.230/1.342
H-C: 1.382/1.302



(c) ^{2/4}PC

Co-O: 3.032/3.034
Co-N: 1.828/1.828
Co-4N: 0.015/0.014

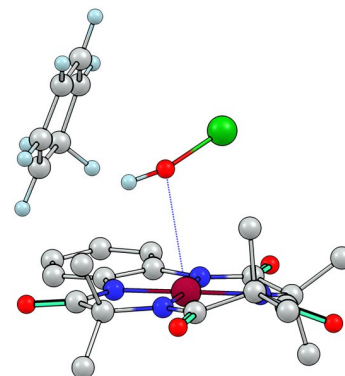
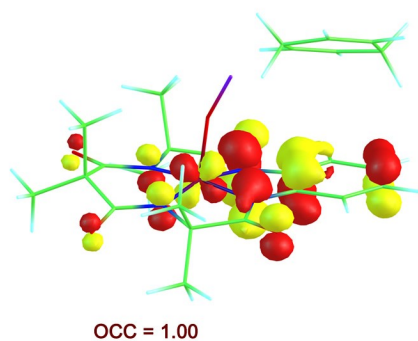


Figure S5. Molecular geometries of key intermediates in C-H bond activation of CHD by 1-Sc³⁺. Values on the left side of slash are for the doublet spin state and the quartet spin state ones are presented on the right side of slash. Lengths are in Å unit and angles are in ° degree unit. Co-N denotes the average of four Co-N distance and Co-4N denotes the deviation of Co atom from the 4N plane (N1-N2-N3-N4). Hydrogen atoms in the TAML ligand are omitted for clarity. Calculations were done at the UMN12L/B1 level in solvent.

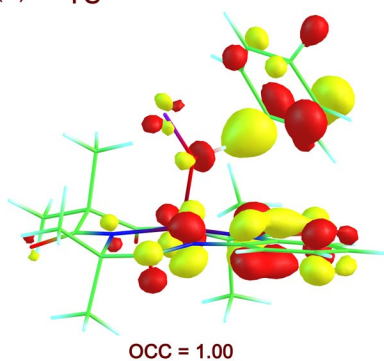
Table S6. Mulliken atomic spin and charges of key intermediates in C-H bond activation of CHD by **1-Sc**³⁺. Calculations were done at the UMN12L/B1 level in solvent.

	charge						spin					
	Co	O	TAML	H	sub	Sc	Co	O	TAML	H	Sub	Sc
2-RC	1.14	-0.82	-1.46	0.13	-0.11	2.11	0.10	0.00	0.89	0.00	0.01	0.00
4-RC	1.10	-0.79	-1.41	0.17	-0.11	2.03	1.87	0.07	1.00	0.00	0.06	0.01
2-TS	1.05	-0.87	-1.65	0.40	-0.02	2.09	0.03	0.03	0.56	0.01	0.33	0.04
4-TS	1.02	-0.81	-1.82	0.37	0.08	2.16	1.91	0.10	0.37	0.04	0.56	0.02
2-PC	0.91	-0.75	-1.87	0.39	0.07	2.25	1.77	0.00	0.22	-0.01	-0.97	-0.01
4-PC	0.91	-0.75	-1.87	0.39	0.07	2.25	1.77	0.00	0.23	0.01	0.97	0.01

(a) ²RC



(b) ²TS



(c) ²PC

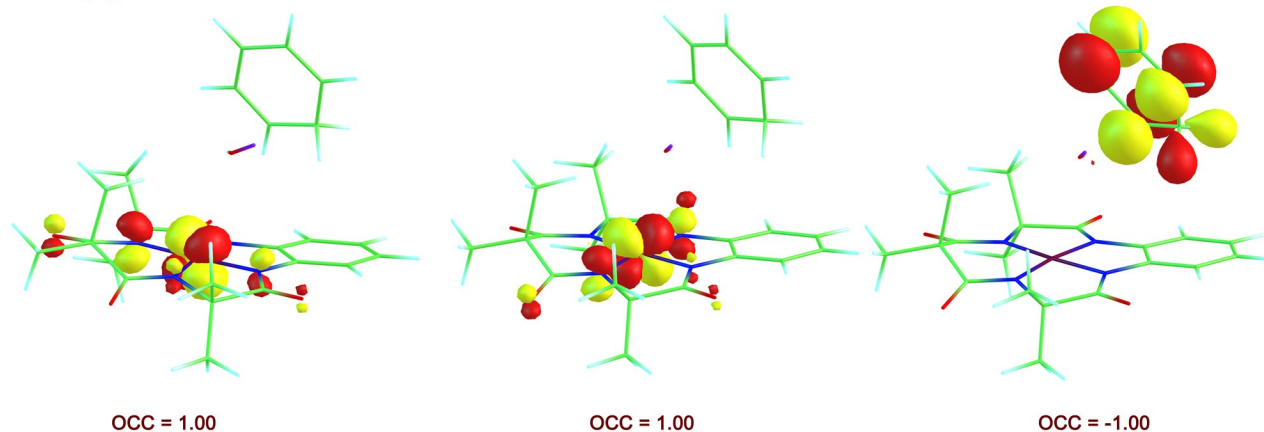


Figure S6. Singly occupied natural orbitals of key intermediates on the ground doublet spin state for C-H bond activation of CHD by **1-Sc**³⁺. Calculations were done at the UMN12L/B1 level in solvent.

2.3 HAT by 1-Sc(OTf)₃

Table S7. Various SCRF energies of C-H bond activation of CHD by 1-Sc(OTf)₃. Calculations were done at the UMN12L/B2//B1 computational level

	OPT/B1+ZPE/B1		SOLV/B2+ZPE/B1		Free Energy, G/B1	
	E^a	ΔE	E	ΔE	G	ΔG
² RC	-4636.911687	0.0	-4637.927515	0.0	-4636.993776	0.0
⁴ RC	-4636.895723	10.0	-4637.910172	10.9	-4636.981344	7.8
² TS	-4636.902013	6.1	-4637.917801	6.1	-4636.982453	7.1
⁴ TS	-4636.887239	15.3	-4637.896748	19.3	-4636.969457	15.3
² PC	-4636.945749	-21.4	-4637.961745	-21.5	-4637.027779	-21.3
⁴ PC	-4636.928758	-10.7	-4637.946747	-12.1	-4637.014863	-13.2

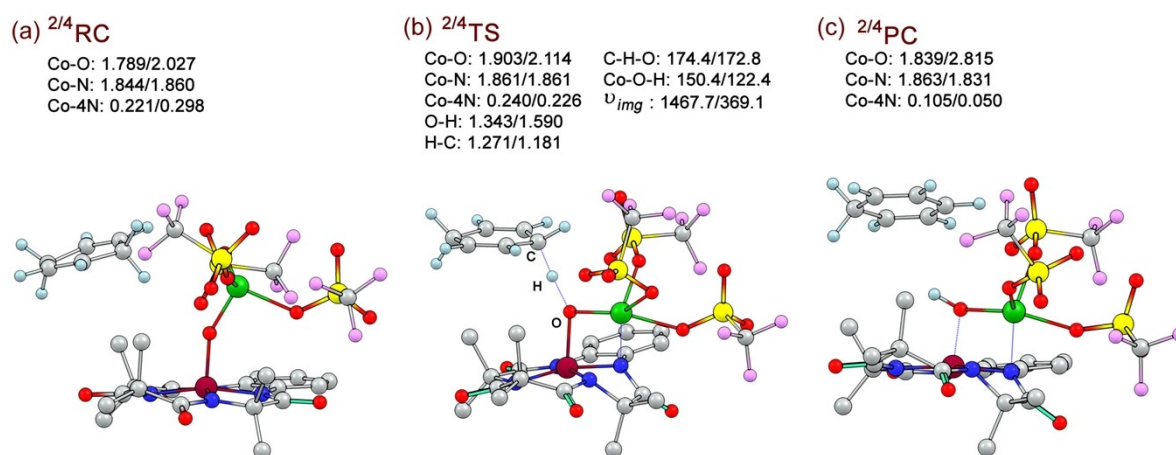


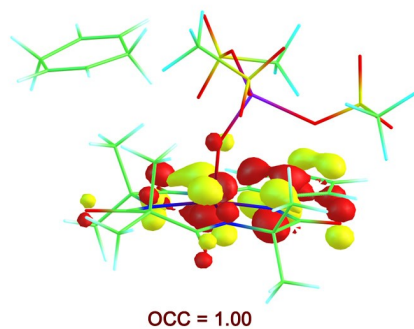
Figure S7. Molecular geometries of key intermediates in C-H bond activation of CHD by 1-Sc(OTf)₃. Values on the left side of slash are for the doublet spin state and the quartet spin state ones are presented on the right side of slash. Lengths are in Å unit and angles are in ° degree unit. Co-N denotes the average of four Co-N distance and Co-4N denotes the deviation of Co atom from the 4N plane (N1-N2-N3-N4). Hydrogen atoms in the TAML ligand are omitted for clarity. Calculations were done at the UMN12L/B1 level in solvent.

Table S8. Mulliken atomic spin densities and charges of key intermediates in C-H bond activation of CHD by **1-Sc(OTf)₃**. Calculations were done at the UMN12L/B1 level in solvent.

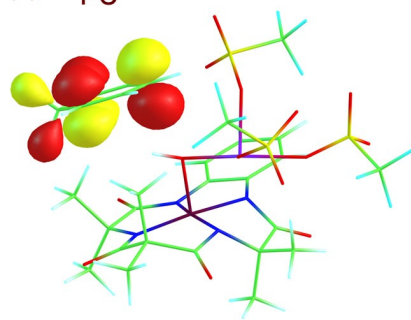
	charge						spin					
	Co	O	TAML	H	sub	ScX ^a	Co	O	TAML	H	Sub	ScX
2-RC	1.09	-0.82	-1.57	0.21	-0.19	-0.72	0.24	0.02	0.74	0.00	0.00	0.00
4-RC	1.02	-0.79	-1.43	0.22	-0.23	-0.79	1.84	0.12	1.03	0.00	0.00	0.02
2-TS	0.81	-0.83	-1.72	0.37	-0.06	-0.57	1.62	-0.16	-0.05	0.01	-0.44	0.01
4-TS	0.94	-0.78	-1.70	0.35	-0.02	-0.78	1.86	0.34	0.41	0.00	0.42	-0.03
2-PC	0.84	-0.91	-1.84	0.50	0.05	-0.64	0.00	0.00	0.01	0.00	0.97	0.02
4-PC	0.89	-0.89	-1.94	0.49	0.04	-0.58	1.81	0.00	0.21	0.00	0.98	0.01

a. ScX denotes Sc(OTf)₃.

(a) ²RC



(c) ²PC



(b) ²TS

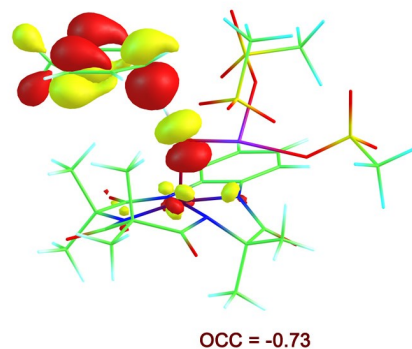
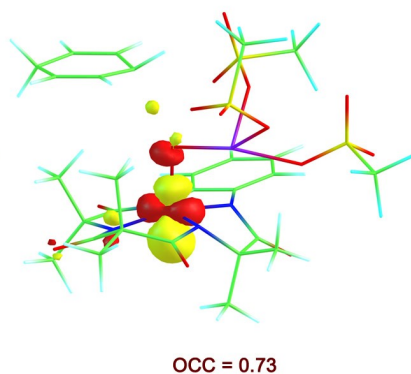
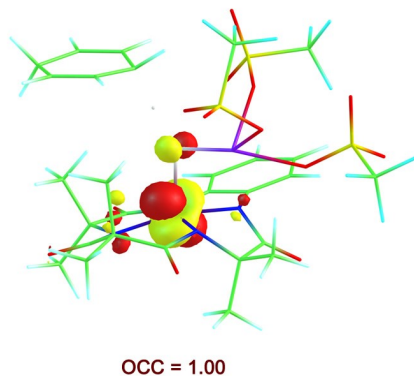


Figure S8. Singly occupied natural orbitals of key intermediates in C-H bond activation of CHD by **1-Sc(OTf)₃**. Calculations were done at the UMN12L/B1 level in solvent.

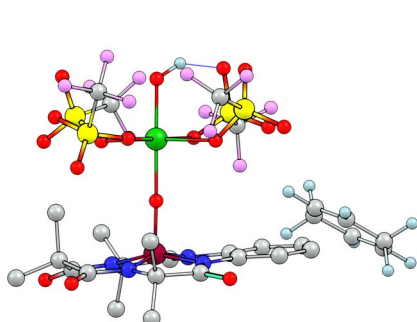
2.4 HAT by 1-Sc

Table S9. Various SCRF energies of C-H bond activation of CHD by **1-Sc**. Calculations were done at the UMN12L/B2//B1 computational level

	OPT/B1+ZPE/B1		SOLV/B2+ZPE/B1		Free Energy, G/B1	
	E^a	ΔE	E	ΔE	G	ΔG
^2RC	-5673.912288	0.0	-5675.180956	0.0	-5674.005814	0.0
^4RC	-5673.888719	14.8	-5675.154253	16.8	-5673.985786	12.6
^2TS	-5673.897262	9.4	-5675.169521	7.2	-5673.984217	13.6
^4TS	-5673.894421	11.2	-5675.164036	10.6	-5673.986074	12.4
^2PC	-5673.952939	-25.5	-5675.226753	-28.7	-5674.041192	-22.2
^4PC	-5673.951607	-24.7	-5675.227432	-29.2	-5674.040520	-21.8

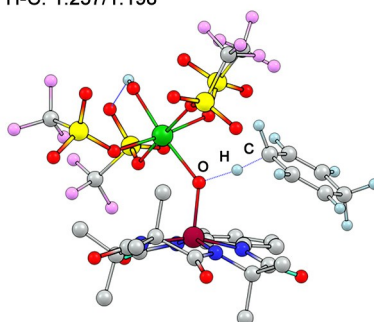
(a) $^2/4\text{RC}$

Co-O: 1.715/2.055
Co-N: 1.853/1.859
Co-4N: 0.349/0.251



(b) $^2/4\text{TS}$

Co-O: 1.914/2.067
Co-N: 1.869/1.872
Co-4N: 0.328/0.304
O-H: 1.385/1.487
H-C: 1.257/1.198
C-H-O: 171.7/166.6
Co-O-H: 113.5/101.1
 ν_{img} : 1384.7/529.6



(c) $^2/4\text{PC}$

Co-O: 1.855/2.095
Co-N: 1.864/1.864
Co-4N: 0.247/0.274

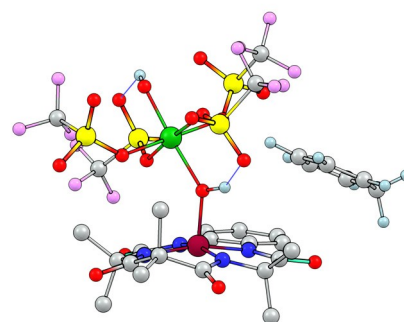
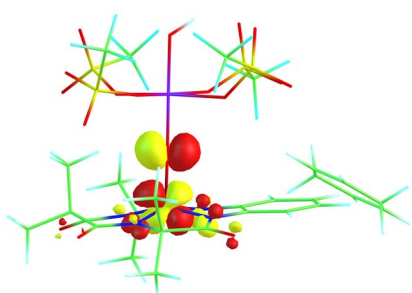


Figure S9. Molecular geometries of key intermediates in C-H bond activation of CHD by **1-Sc**. Values on the left side of slash are for the doublet spin state and the quartet spin state ones are presented on the right side of slash. Lengths are in Å unit and angles are in ° degree unit. Co-N denotes the average of four Co-N distance and Co-4N denotes the deviation of Co atom from the 4N plane (N1-N2-N3-N4). Hydrogen atoms in the TAML ligand are omitted for clarity. Calculations were done at the UMN12L/B1 level in solvent.

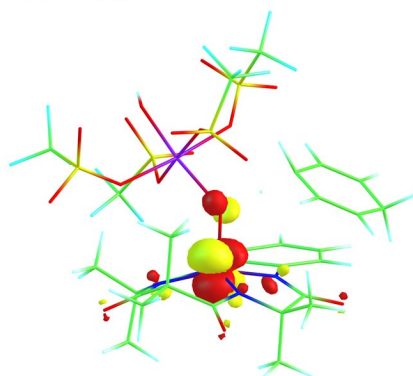
Table S10. Mulliken atomic spin densities and charges of key intermediates in C-H bond activation of CHD by **1-Sc**. Calculations were done at the UMN12L/B1 level in solvent.

	charge							spin					
	Co	O	TAML	H	sub	ScX		Co	O	TAML	H	Sub	ScX
2-RC	1.27	-0.83	-2.01	0.23	-0.25	-2.40		0.74	0.17	0.08	0.00	0.00	0.01
4-RC	1.02	-0.55	-2.25	0.19	-0.23	-2.19		1.83	1.05	0.10	0.00	0.00	0.01
2-TS	1.01	-0.80	-2.07	0.37	-0.20	-2.31		1.69	-0.27	-0.08	0.03	-0.38	0.01
4-TS	0.94	-0.69	-2.21	0.32	-0.06	-2.28		1.88	0.71	0.05	-0.06	0.41	0.01
2-PC	0.95	-0.92	-2.30	0.50	-0.03	-2.19		0.00	0.01	0.01	0.00	0.98	0.01
4-PC	0.98	-0.93	-2.26	0.47	-0.02	-2.22		1.89	0.07	0.05	0.00	0.98	0.01

(a) ^2RC



(b) ^2TS



(c) ^2PC

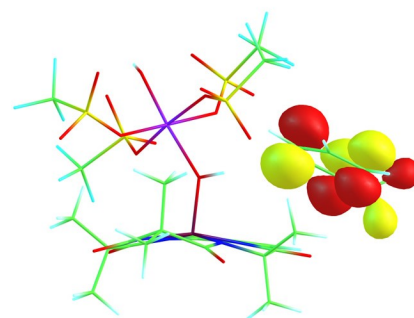


Figure S10. Singly occupied natural orbitals key intermediates in C-H bond activation of CHD by **1-Sc**. Calculations were done at the UMN12L/B1 level in solvent.

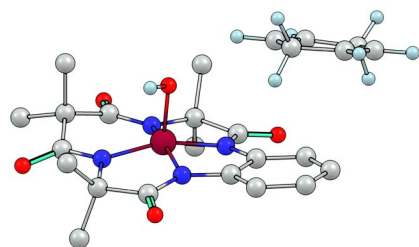
2.5 HAT by protonated 1, 1-H, [Co(OH)(TAML)]¹⁻

Table S11. Various SCRF energies of C-H bond activation of CHD by **1-H**. Calculations were done at the UMN12L/B2//B1 computational level

	OPT/B1+ZPE/B1		SOLV/B2+ZPE/B1		Free Energy, G/B1	
	E^a	ΔE	E	ΔE	G	ΔG
² RC	-1708.051911	0.0	-1708.447627	0.0	-1708.109491	0.0
⁴ RC	-1708.021618	19.0	-1708.419322	17.8	-1708.078718	19.3
² TS	-1708.024368	17.3	-1708.422228	15.9	-1708.087251	14.0
⁴ TS	-1708.012009	25.0	-1708.407573	25.1	-1708.077624	20.0
² PC	-1708.072636	-13.0	-1708.473493	-16.2	-1708.131115	-13.6
⁴ PC	-1708.069718	-11.2	-1708.470104	-14.1	-1708.127522	-11.3

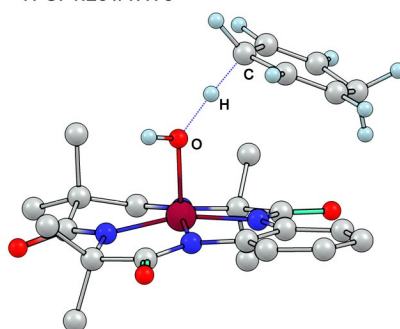
(a) ^{2/4}RC

Co-O: 1.766/1.989
Co-N: 1.841/1.861
Co-4N: 0.268/0.305



(b) ^{2/4}TS

Co-O: 1.961/2.169
Co-N: 1.853/1.852
Co-4N: 0.246/0.223
O-H: 1.345/1.597
H-C: 1.261/1.170
C-H-O: 175.4/179.9
Co-O-H: 141.8/115.8
 ν_{img} : 1383.1/372.9



(c) ^{2/4}PC

Co-O: 2.751/2.776
Co-N: 1.831/1.832
Co-4N: 0.026/0.118

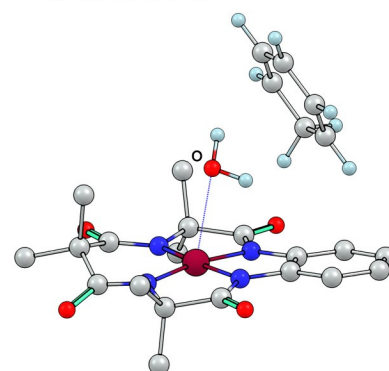


Figure S11. Molecular geometries of key intermediates in C-H bond activation of CHD by **1-H**. Values on the left side of slash are for the doublet spin state and the quartet spin state ones are presented on the right side of slash. Lengths are in Å unit and angles are in ° degree unit. Co-N denotes the average of four Co-N distance and Co-4N denotes the deviation of Co atom from the 4N plane (N1-N2-N3-N4). Hydrogen atoms in the TAML ligand are omitted for clarity. Calculations were done at the UMN12L/B1 level in solvent.

Table S12. Mulliken atomic spin densities and charges of key intermediates in C-H bond activation of CHD by **1-H**. Calculations were done at the UMN12L/B1 level in solvent.

	charge						spin				
	Co	OH	TAML	H	sub		Co	OH	TAML	H	Sub
2-RC	1.07	-0.31	-1.75	0.19	-0.20		0.72	0.05	0.23	0.00	0.00
4-RC	0.96	-0.44	-1.50	0.18	-0.19		1.78	0.24	0.96	0.00	0.02
2-TS	1.02	-0.34	-2.00	0.42	-0.10		1.65	-0.15	-0.06	0.01	-0.45
4-TS	0.96	-0.31	-1.86	0.33	-0.12		1.84	0.39	0.46	-0.01	0.32
2-PC	0.88	-0.40	-1.95	0.48	0.00		1.80	-0.01	0.20	0.00	-0.99
4-PC	0.87	-0.41	-1.96	0.49	0.02		1.80	0.00	0.21	-0.01	0.99

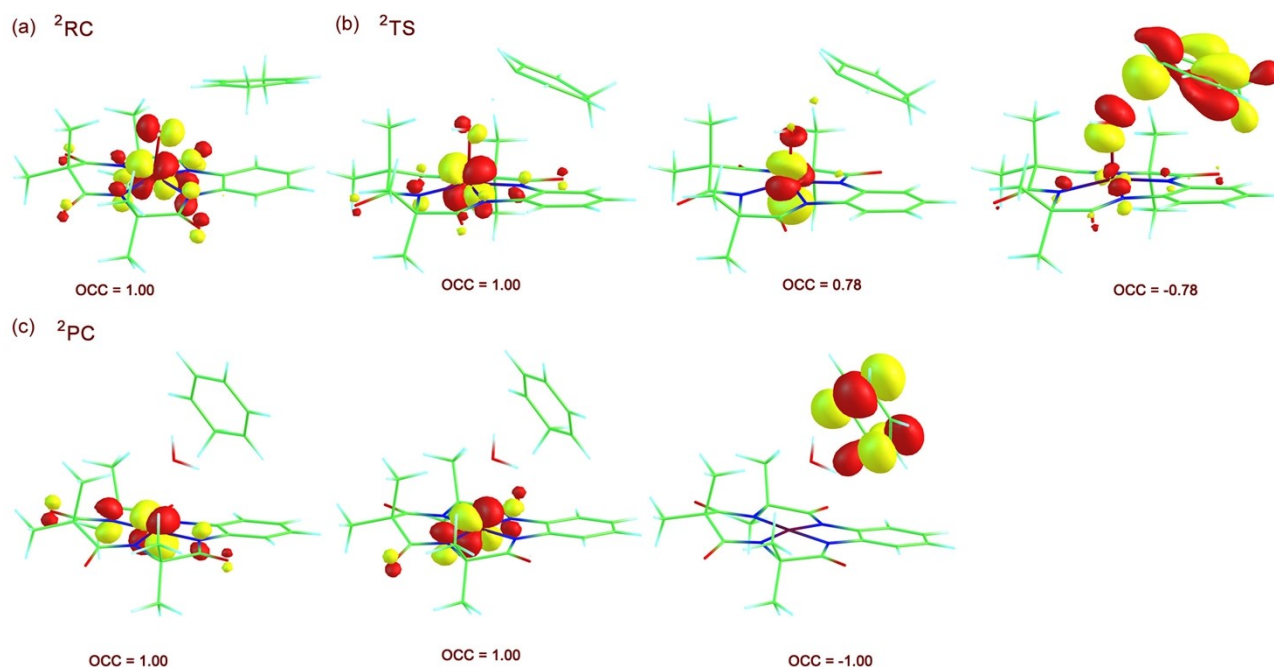


Figure S12. Singly occupied natural orbitals of key intermediates in C-H bond activation of CHD by **1-H**. Calculations were done at the UMN12L/B1 level in solvent.

Part III: C-H bond activation of substrates with normal C-H bond mediated by **1**

3.1 HAT of toluene by **1**

Table S13. Various SCRF energies of C-H bond activation of toluene by **1**. Calculations were done at the UMN12L/B2//B1 level

	OPT/B1+ZPE/B1		SOLV/B2+ZPE/B1		Free Energy, G/B1	
	E^a	ΔE	E	ΔE	G	ΔG
² RC	-1745.674749	0.0	-1746.074600	0.0	-1745.732783	0.0
⁴ RC	-1745.652914	13.7	-1746.058399	10.2	-1745.710296	14.1
² TS	-1745.657660	10.7	-1746.060057	9.1	-1745.714818	11.3
⁴ TS	-1745.633025	26.2	-1746.043151	19.7	-1745.688363	27.9
² PC	-1745.686399	-7.3	-1746.093574	-11.9	-1745.745768	-8.1
⁴ PC	-1745.668661	3.8	-1746.082159	-4.7	-1745.724958	4.9

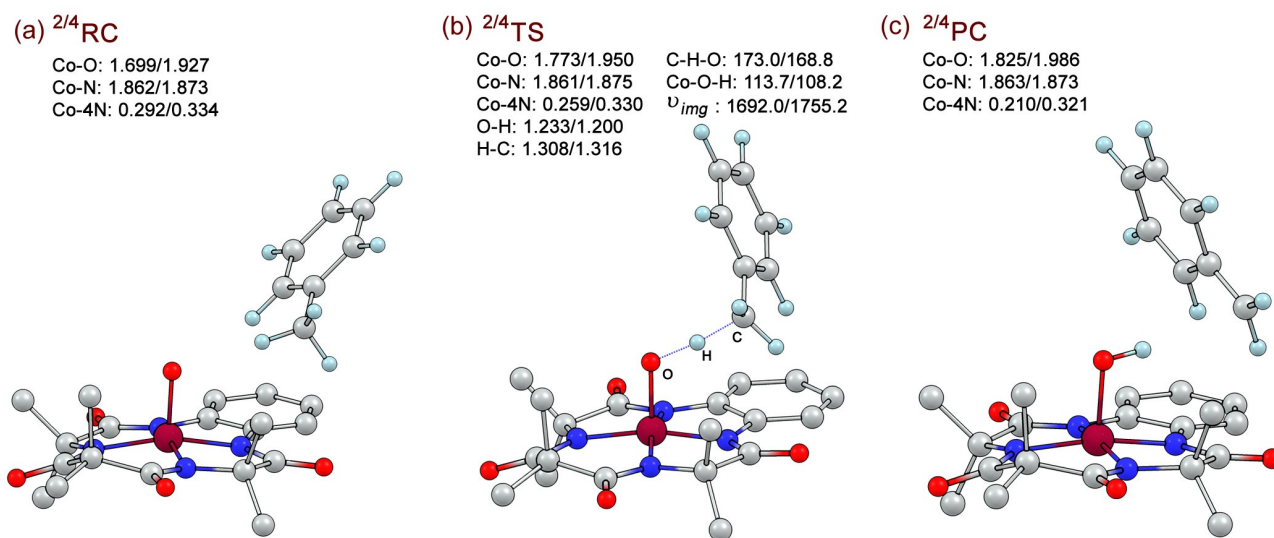
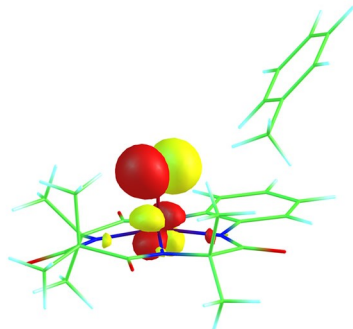


Figure S13. Molecular geometries of key intermediates in C-H bond activation of toluene by **1**. Values on the left side of slash are for the doublet spin state and the quartet spin state ones are presented on the right side of slash. Lengths are in Å unit and angles are in ° degree unit. Co-N denotes the average of four Co-N distance and Co-4N denotes the deviation of Co atom from the 4N plane (N1-N2-N3-N4). Hydrogen atoms in the TAMC ligand are omitted for clarity. Calculations were done at the UMN12L/B1 level in solvent.

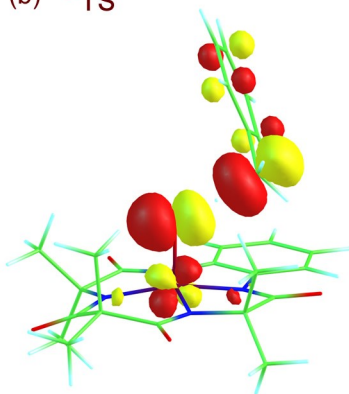
Table S14. Mulliken atomic spin and charges of key intermediates in C-H bond activation of toluene by **1**. Calculations were done at the UMN12L/B1 level in solvent.

	charge						spin				
	Co	O	TAML	H	sub		Co	O	TAML	H	Sub
2-RC	0.93	-0.61	-2.26	0.25	-0.30		0.24	0.70	0.06	0.00	0.01
4-RC	0.92	-0.54	-2.33	0.22	-0.27		1.73	1.16	0.09	-0.01	0.03
2-TS	0.87	-0.71	-2.31	0.41	-0.25		0.07	0.51	0.04	-0.08	0.46
4-TS	0.88	-0.74	-2.34	0.40	-0.20		1.77	0.73	0.07	-0.10	0.53
2-PC	0.83	-0.86	-2.38	0.44	-0.03		0.00	0.01	0.01	-0.01	0.98
4-PC	0.87	-0.90	-2.34	0.40	-0.04		1.80	0.18	0.04	-0.01	0.99

(a) ^2RC



(b) ^2TS



(c) ^2PC

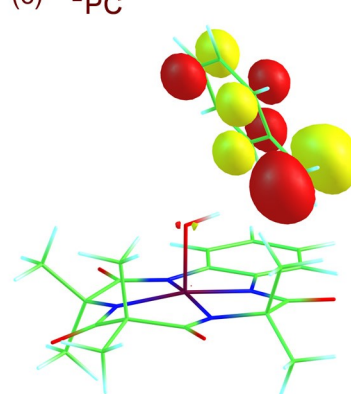


Figure S14. Singly occupied natural orbitals of key intermediates in C-H bond activation of toluene by **1**. Calculations were done at the UMN12L/B1 level in solvent.

Part IV: C-H bond activation of substrates with acidic C-H bond mediated by complex 1

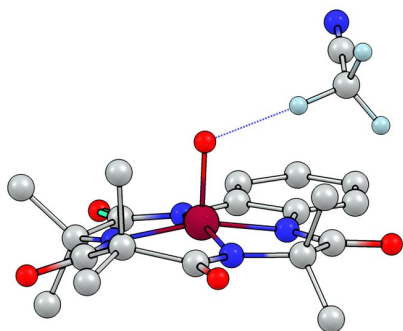
4.1 C-H bond activation of acetonitrile by 1

Table S15. Various SCRF energies of C-H bond activation of acetonitrile by **1**. Calculations were done at the UMN12L/B2//B1 level

	OPT/B1+ZPE/B1		SOLV/B2+ZPE/B1		Free Energy, G/B1	
	E^a	ΔE	E	ΔE	G	ΔG
^2RC	-1607.097631	0.0	-1607.470370	0.0	-1607.150942	0.0
^4RC	-1607.073912	14.9	-1607.450434	12.5	-1607.129406	13.5
^2TS	-1607.083578	8.8	-1607.462210	5.1	-1607.136280	9.2
^4TS	-1607.059166	24.1	-1607.438758	19.8	-1607.112400	24.2
^2PC	-1607.097531	0.1	-1607.474754	-2.8	-1607.151722	-0.5
^4PC	-1607.081490	10.1	-1607.465429	3.1	-1607.136544	9.0

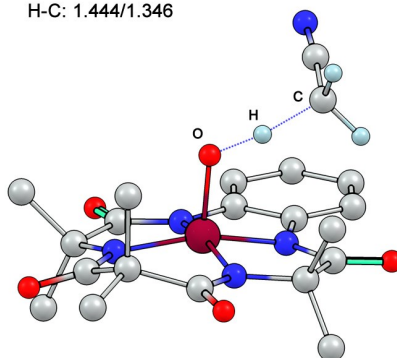
(a) $^2/4\text{RC}$

Co-O: 1.694/1.932
Co-N: 1.861/1.869
Co-4N: 0.297/0.307



(b) $^2/4\text{TS}$

Co-O: 1.721/1.980
Co-N: 1.851/1.868
Co-4N: 0.289/0.286
O-H: 1.167/1.174
H-C: 1.444/1.346
C-H-O: 170.8/168.4
Co-O-H: 114.6/114.6
 ν_{img} : 1113.8/1579.3



(c) $^2/4\text{PC}$

Co-O: 1.825/1.965
Co-N: 1.863/1.871
Co-4N: 0.204/0.323

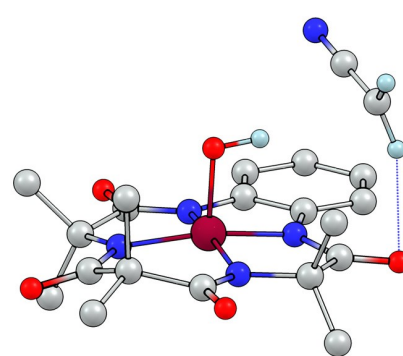


Figure S15. Molecular geometries of key intermediates in C-H bond activation of acetonitrile by **1**. Values on the left side of slash are for the doublet spin state and the quartet spin state ones are presented on the right side of slash. Lengths are in Å unit and angles are in ° degree unit. Co-N denotes the average of four Co-N distance and Co-4N denotes the deviation of Co atom from the 4N plane (N1-N2-N3-N4). Hydrogen atoms in the TAMC ligand are omitted for clarity. Calculations were done at the UMN12L/B1 level in solvent.

Table S16. Mulliken atomic spin densities and charges of key intermediates in C-H bond activation of acetonitrile by **1**. Calculations were done at the UMN12L/B1 level in solvent.

	charge						spin				
	Co	O	TAML	H	sub		Co	O	TAML	H	Sub
2-RC	0.95	-0.63	-2.24	0.32	-0.39		0.31	0.63	0.06	0.00	0.01
4-RC	0.93	-0.54	-2.32	0.30	-0.37		1.73	1.17	0.09	-0.01	0.01
2-TS	1.00	-0.78	-2.03	0.49	-0.67		0.66	0.20	0.08	-0.01	0.06
4-TS	0.93	-0.71	-2.28	0.45	-0.39		1.80	0.77	0.09	-0.08	0.41
2-PC	0.85	-0.85	-2.35	0.43	-0.08		0.01	0.02	0.05	-0.01	0.94
4-PC	0.90	-0.88	-2.36	0.40	-0.06		1.79	0.21	0.04	-0.01	0.97

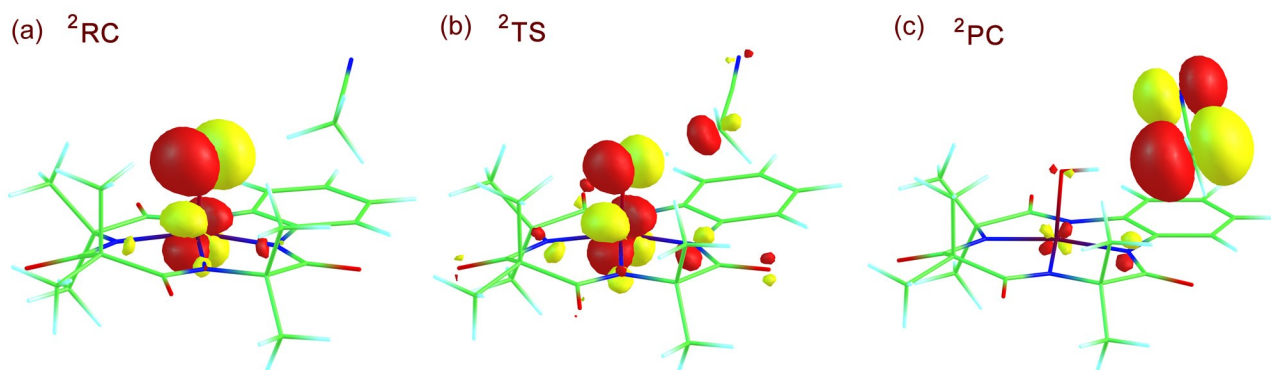


Figure S16. Singly occupied natural orbitals of key intermediates on the ground spin state in C-H bond activation of acetonitrile by **1**. Calculations were done at the UMN12L/B1 level in solvent.

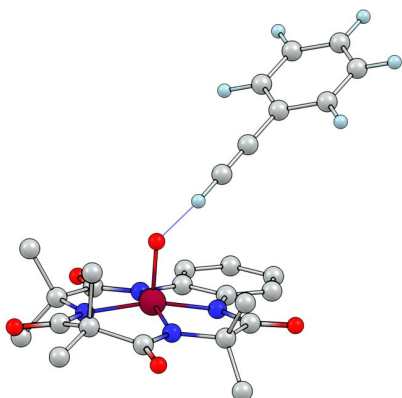
4.2 C-H bond activation of phenylacetylene by **1**

Table S17. Various SCRF energies of C-H bond activation of phenylacetylene by **1**. Calculations were done at the UMN12L/B2//B1 computational level

	OPT/B1+ZPE/B1		SOLV/B2+ZPE/B1		Free Energy, G/B1	
	E^a	ΔE	E	ΔE	G	ΔG
^2RC	-1782.515744	0.0	-1782.921574	0.0	-1782.575158	0.0
^4RC	-1782.478205	23.6	-1782.887074	21.6	-1782.538997	22.7
^2TS	-1782.510440	3.3	-1782.920299	0.8	-1782.568217	4.4
^4TS	-1782.479805	22.6	-1782.892131	18.5	-1782.540090	22.0
^2PC	-1782.510050	3.6	-1782.924360	-1.7	-1782.572392	1.7
^4PC	-1782.488097	17.3	-1782.905926	9.8	-1782.548489	16.7

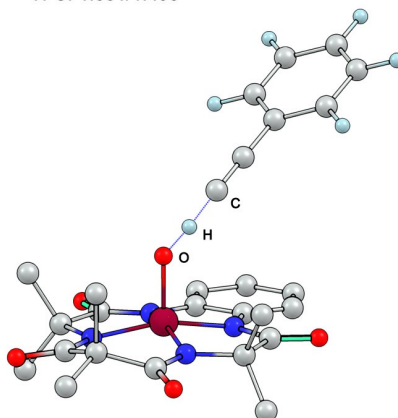
(a) $^2/^4\text{RC}$

Co-O: 1.692/1.722
Co-N: 1.862/1.883
Co-4N: 0.291/0.462



(b) $^2/^4\text{TS}$

Co-O: 1.703/2.152
Co-N: 1.854/1.854
Co-4N: 0.311/0.180
O-H: 1.230/1.123
H-C: 1.351/1.498
C-H-O: 172.7/176.0
Co-O-H: 114.8/117.1
 ν_{img} : 1187.3/635.7



(c) $^2/^4\text{PC}$

Co-O: 1.732/1.928
Co-N: 1.848/1.877
Co-4N: 0.301/0.357

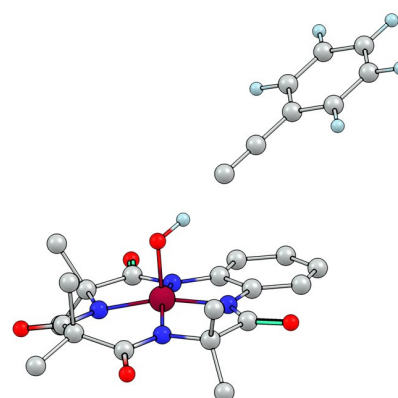


Figure S17. Molecular geometries of key intermediates in C-H bond activation of phenylacetylene by **1**. Values on the left side of slash are for the doublet spin state and the quartet spin state ones are presented on the right side of slash. Lengths are in Å unit and angles are in ° degree unit. Co-N denotes the average of four Co-N distance and Co-4N denotes the deviation of Co atom from the 4N plane (N1-N2-N3-N4). Hydrogen atoms in the TAML ligand are omitted for clarity. Calculations were done at the UMN12L/B1 level in solvent.

Table S18. Mulliken atomic spin and charges of key intermediates in C-H bond activation of phenylacetylene by **1**. Calculations were done at the UMN12L/B1 level in solvent.

	charge						spin				
	Co	O	TAML	H	sub		Co	O	TAML	H	Sub
2-RC	0.92	-0.62	-2.25	0.26	-0.32		0.26	0.68	0.06	0.00	0.01
4-RC	0.94	-0.65	-2.23	0.25	-0.30		1.68	1.08	0.24	0.00	0.01
2-TS	0.98	-0.77	-2.06	0.47	-0.63		0.71	0.20	0.07	-0.01	0.03
4-TS	0.88	-0.73	-2.31	0.41	-0.26		1.80	0.74	0.06	-0.10	0.50
2-PC	0.87	-0.84	-2.35	0.42	-0.10		0.00	0.00	0.04	0.00	0.96
4-PC	0.91	-0.87	-2.37	0.39	-0.06		1.79	0.18	0.05	0.00	0.98

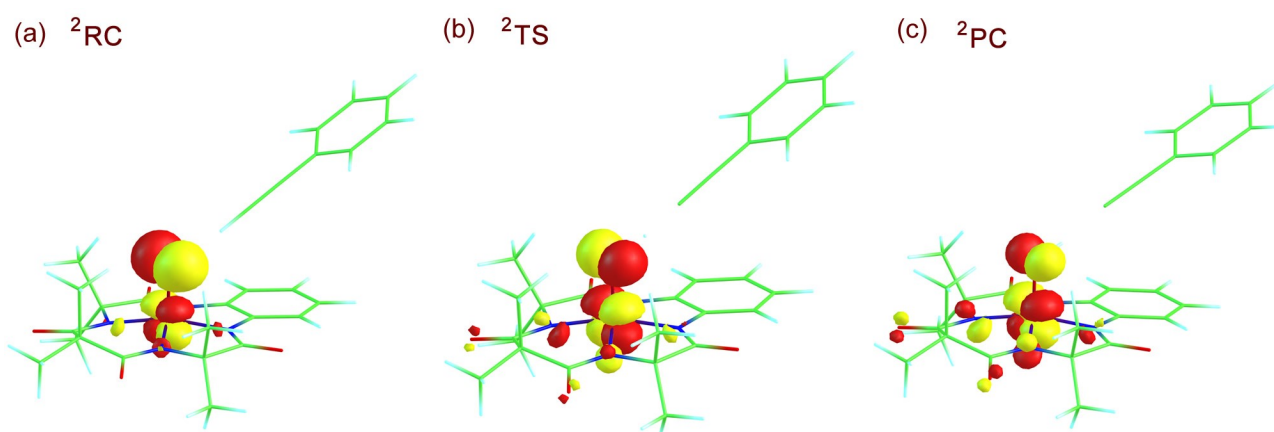


Figure S18. Singly occupied natural orbitals of key intermediates on the ground spin state in C-H bond activation of phenylacetylene by **1**. Calculations were done at the UMN12L/B1 level in solvent.

Part V: Cartesian coordinates

I) Complexes [Co(O)(TAML)]²⁻ binding redox-inactive scandium ion with multiple coordination states

I-1) [Co(O)(TAML)]²⁻, 1

a. ²¹

Co	-0.013799000	-0.166429000	-0.012942000
O	0.065623000	0.098225000	4.016424000
O	3.763369000	-0.017309000	1.409048000
O	1.917382000	0.502231000	-3.396085000
O	-3.815407000	0.683610000	0.652422000
N	1.848778000	-0.077052000	0.161043000
C	-2.299043000	0.564986000	-4.490355000
H	-2.394714000	0.622596000	-5.572107000
N	-1.766951000	0.330056000	-0.351865000
C	-2.601808000	0.459685000	0.691992000
C	-1.870008000	0.359020000	2.044326000
N	-0.466071000	0.002834000	1.796073000
C	0.367434000	-0.131150000	2.834006000
C	1.771190000	-0.716471000	2.542768000
C	1.564805000	-2.230087000	2.315410000
H	1.088986000	-2.676194000	3.198634000
H	2.538143000	-2.717690000	2.172034000
H	0.936509000	-2.410036000	1.435857000
C	2.540438000	-0.201418000	1.300581000
C	2.566664000	0.212709000	-1.088162000
C	1.541315000	0.323001000	-2.233770000
N	0.274606000	0.255231000	-1.793923000
C	-0.901384000	0.364720000	-2.532291000
C	-2.065422000	0.406471000	-1.709920000
C	-3.326532000	0.528656000	-2.298401000
H	-4.204099000	0.564894000	-1.663860000
C	-3.435440000	0.605755000	-3.687270000
H	-4.419802000	0.695173000	-4.140927000
C	-1.030426000	0.446074000	-3.920931000
H	-0.139405000	0.417192000	-4.537425000
C	3.292105000	1.566756000	-1.048661000
H	2.591187000	2.360333000	-0.761839000
H	3.682720000	1.794204000	-2.046578000
H	4.109380000	1.538073000	-0.325564000
C	3.555685000	-0.899170000	-1.455424000
H	4.378292000	-0.926642000	-0.737787000
H	3.949265000	-0.714606000	-2.460697000
H	3.051959000	-1.872799000	-1.453109000
C	2.648753000	-0.532223000	3.779238000
H	2.150432000	-0.962079000	4.651117000

H	2.837308000	0.526719000	3.984907000
H	3.612734000	-1.022832000	3.625224000
C	-2.594769000	-0.695909000	2.887554000
H	-2.484542000	-1.688902000	2.435891000
H	-3.661806000	-0.451832000	2.927552000
H	-2.182646000	-0.719154000	3.898793000
C	-2.013913000	1.741553000	2.699546000
H	-1.594063000	1.727195000	3.707402000
H	-3.074765000	2.012734000	2.738665000
H	-1.484660000	2.495589000	2.103728000
O	-0.261712000	-1.827905000	-0.264327000

(a) ⁴¹

Co	-0.017878000	-0.258146000	-0.014917000
O	0.069334000	0.100720000	4.006106000
O	3.757103000	-0.034073000	1.405865000
O	1.909171000	0.563629000	-3.386153000
O	-3.809640000	0.709478000	0.646555000
N	1.850490000	-0.134044000	0.150660000
C	-2.300147000	0.592164000	-4.491293000
H	-2.392826000	0.675852000	-5.571573000
N	-1.780902000	0.250709000	-0.355390000
C	-2.604576000	0.446276000	0.687348000
C	-1.869634000	0.359062000	2.040401000
N	-0.482488000	-0.065620000	1.795984000
C	0.363557000	-0.161567000	2.829129000
C	1.771534000	-0.745332000	2.545010000
C	1.582965000	-2.265533000	2.346028000
H	1.112518000	-2.698667000	3.238807000
H	2.563798000	-2.742674000	2.217613000
H	0.959723000	-2.472889000	1.469792000
C	2.537326000	-0.235703000	1.296144000
C	2.562650000	0.221188000	-1.086884000
C	1.536154000	0.330350000	-2.233071000
N	0.272188000	0.183472000	-1.804091000
C	-0.907316000	0.323884000	-2.537138000
C	-2.071349000	0.360507000	-1.715740000
C	-3.328909000	0.514915000	-2.301809000
H	-4.206816000	0.546398000	-1.667615000
C	-3.436318000	0.627331000	-3.689109000
H	-4.419376000	0.738740000	-4.140609000
C	-1.033724000	0.443399000	-3.922491000
H	-0.142507000	0.418798000	-4.538736000

C	3.244572000	1.595738000	-1.004639000
H	2.519791000	2.360438000	-0.698979000
H	3.631192000	1.863069000	-1.993980000
H	4.060684000	1.572608000	-0.280189000
C	3.588027000	-0.846789000	-1.483315000
H	4.403662000	-0.875298000	-0.757968000
H	3.985355000	-0.615245000	-2.477245000
H	3.113100000	-1.834379000	-1.520486000
C	2.647766000	-0.531404000	3.777899000
H	2.154142000	-0.953076000	4.656429000
H	2.825953000	0.532203000	3.967308000
H	3.616131000	-1.015291000	3.630447000
C	-2.628752000	-0.637240000	2.922768000
H	-2.557932000	-1.648723000	2.505648000
H	-3.685682000	-0.352437000	2.959690000
H	-2.211188000	-0.640986000	3.931932000
C	-1.955470000	1.767122000	2.650431000
H	-1.535451000	1.769838000	3.658131000
H	-3.004526000	2.081054000	2.682129000
H	-1.398920000	2.481002000	2.030411000
O	-0.314682000	-2.116441000	-0.349231000

I-2) {Sc-[Co(O)(TAML)]}¹⁺, 1-Sc³⁺

a. ²¹Sc³⁺

Co	-0.217697000	0.178220000	-0.014560000
O	0.072946000	0.138351000	3.983959000
O	3.584543000	-0.527836000	1.075739000
O	1.523017000	0.575690000	-3.509697000
O	-3.948333000	1.034680000	0.882773000
N	1.619689000	-0.031254000	0.033112000
C	-2.617393000	1.464943000	-4.279164000
H	-2.768829000	1.646198000	-5.339287000
N	-1.953671000	0.768462000	-0.243881000
C	-2.747628000	0.808867000	0.871466000
C	-1.953991000	0.579958000	2.164929000
N	-0.578016000	0.199646000	1.800147000
C	0.306279000	-0.054930000	2.786985000
C	1.622083000	-0.758845000	2.407021000
C	1.237208000	-2.246533000	2.217815000
H	0.749101000	-2.621137000	3.125936000
H	2.143510000	-2.838195000	2.040377000
H	0.558710000	-2.365693000	1.367530000
C	2.358315000	-0.383262000	1.103729000
C	2.277248000	0.021523000	-1.285077000
C	1.233298000	0.435923000	-2.331427000
N	-0.014762000	0.609363000	-1.794762000
C	-1.175486000	0.907472000	-2.442352000

C	-2.304126000	1.003344000	-1.541070000
C	-3.574639000	1.342075000	-2.044310000
H	-4.414449000	1.422576000	-1.366870000
C	-3.716534000	1.566592000	-3.398675000
H	-4.693327000	1.825048000	-3.797093000
C	-1.357636000	1.141940000	-3.819684000
H	-0.510976000	1.067720000	-4.489739000
C	3.414136000	1.049504000	-1.372079000
H	3.083879000	2.020417000	-0.986357000
H	3.700427000	1.170418000	-2.421795000
H	4.274695000	0.713737000	-0.794662000
C	2.774920000	-1.370235000	-1.702039000
H	3.583322000	-1.685922000	-1.039322000
H	3.140195000	-1.340665000	-2.733758000
H	1.952759000	-2.093140000	-1.635171000
C	2.598113000	-0.660535000	3.578685000
H	2.123930000	-1.039515000	4.486014000
H	2.900676000	0.375772000	3.762064000
H	3.493733000	-1.244826000	3.360479000
C	-2.659471000	-0.524437000	2.958813000
H	-2.586173000	-1.483193000	2.430488000
H	-3.717475000	-0.270294000	3.076107000
H	-2.197865000	-0.628579000	3.942497000
C	-2.031217000	1.914296000	2.926897000
H	-1.587048000	1.808003000	3.916294000
H	-3.081075000	2.209663000	3.025105000
H	-1.497453000	2.698087000	2.377303000
O	-0.681554000	-1.524363000	-0.461825000
Sc	-1.880578000	-2.806111000	-0.673827000

b. ⁴¹Sc³⁺

Co	-0.157004000	0.016953000	-0.003429000
O	0.095038000	0.151938000	3.994119000
O	3.626610000	-0.173402000	1.270298000
O	1.654728000	0.349578000	-3.476600000
O	-3.879510000	0.988053000	0.801312000
N	1.679946000	-0.154961000	0.078279000
C	-2.442646000	1.370694000	-4.332804000
H	-2.574474000	1.543675000	-5.396738000
N	-1.869141000	0.698707000	-0.286617000
C	-2.680133000	0.763884000	0.819549000
C	-1.904452000	0.572966000	2.128824000
N	-0.536473000	0.128499000	1.800915000
C	0.337116000	-0.090626000	2.812226000
C	1.644364000	-0.820887000	2.450756000
C	1.244559000	-2.285484000	2.153892000
H	0.735854000	-2.710189000	3.028196000
H	2.144254000	-2.882676000	1.961954000

H	0.580081000	-2.350667000	1.286321000	C	-2.582354000	0.493423000	0.075813000
C	2.405506000	-0.312137000	1.211307000	C	-2.023205000	0.181540000	1.469508000
C	2.390838000	0.115270000	-1.186670000	N	-0.583853000	-0.099339000	1.330573000
C	1.349144000	0.289774000	-2.298024000	C	0.125264000	-0.395939000	2.439662000
N	0.077672000	0.443920000	-1.800008000	C	1.547447000	-0.953215000	2.244685000
C	-1.053602000	0.781248000	-2.471165000	C	1.358085000	-2.408928000	1.756471000
C	-2.192982000	0.935597000	-1.585608000	H	0.693267000	-2.954578000	2.439575000
C	-3.442916000	1.316801000	-2.109951000	H	2.329449000	-2.919114000	1.741671000
H	-4.289529000	1.437957000	-1.447524000	H	0.921888000	-2.433369000	0.754134000
C	-3.553051000	1.525528000	-3.468433000	C	2.466192000	-0.290882000	1.199074000
H	-4.512022000	1.814975000	-3.887881000	C	2.806293000	0.440434000	-1.090245000
C	-1.202799000	1.006712000	-3.853693000	C	1.937554000	0.801335000	-2.302225000
H	-0.350620000	0.888857000	-4.510199000	N	0.600417000	0.789691000	-2.013728000
C	3.152396000	1.453397000	-1.153476000	C	-0.446548000	1.038876000	-2.853683000
H	2.476802000	2.265569000	-0.859751000	C	-1.723181000	0.945351000	-2.185181000
H	3.547262000	1.669846000	-2.151784000	C	-2.908124000	1.200512000	-2.899626000
H	3.974216000	1.396353000	-0.438212000	H	-3.862592000	1.131595000	-2.393851000
C	3.327369000	-1.028317000	-1.580255000	C	-2.822661000	1.531844000	-4.238129000
H	4.170176000	-1.078306000	-0.889439000	H	-3.732806000	1.723380000	-4.799478000
H	3.698949000	-0.854739000	-2.594597000	C	-0.395123000	1.384355000	-4.217123000
H	2.793540000	-1.984468000	-1.561455000	H	0.563487000	1.455227000	-4.714639000
C	2.580154000	-0.801479000	3.654746000	C	3.645332000	1.694578000	-0.794175000
H	2.073061000	-1.229894000	4.522033000	H	2.999070000	2.514816000	-0.460691000
H	2.888058000	0.217372000	3.907110000	H	4.157888000	2.005152000	-1.710813000
H	3.478139000	-1.382638000	3.432851000	H	4.379565000	1.482450000	-0.016775000
C	-2.649093000	-0.460589000	2.978083000	C	3.713724000	-0.722704000	-1.507641000
H	-2.581781000	-1.453957000	2.518042000	H	4.426414000	-0.941707000	-0.710184000
H	-3.703726000	-0.178565000	3.052784000	H	4.257244000	-0.454138000	-2.419133000
H	-2.212066000	-0.506425000	3.977146000	H	3.114232000	-1.618756000	-1.706152000
C	-1.934852000	1.951680000	2.811813000	C	2.259710000	-0.980676000	3.594744000
H	-1.484860000	1.887732000	3.802451000	H	1.662906000	-1.545618000	4.314144000
H	-2.974428000	2.283908000	2.901512000	H	2.405010000	0.028497000	3.993468000
H	-1.383294000	2.685771000	2.213619000	H	3.239846000	-1.448667000	3.483280000
O	-0.889512000	-1.880175000	-0.557554000	C	-2.792095000	-1.015889000	2.035379000
Sc	-2.324445000	-2.887125000	-0.566740000	H	-2.544140000	-1.928105000	1.479645000

I-3) {(OTf)Sc-[Co(O)(TAML)]}⁰, 1-Sc(OTf)²⁺

a. ²¹Sc(OTf)²⁺

Co	0.105712000	0.117275000	-0.375320000
O	-0.334596000	-0.342178000	3.583987000
O	3.672994000	-0.208572000	1.446926000
O	2.428999000	1.086516000	-3.384092000
O	-3.779401000	0.640337000	-0.123872000
N	1.914889000	0.063600000	0.019649000
C	-1.576859000	1.622858000	-4.890973000
H	-1.546691000	1.883179000	-5.945227000
N	-1.594946000	0.630625000	-0.861290000

H	-2.531097000	-1.164616000	3.084833000
C	-2.308217000	1.441833000	2.305922000
H	-2.019649000	1.274627000	3.344209000
H	-3.377445000	1.673716000	2.253308000
H	-1.745666000	2.295970000	1.910820000
O	-0.144800000	-1.517789000	-1.104748000
Sc	-1.238575000	-2.876190000	-1.520963000
O	-1.691286000	-5.088077000	2.352755000
S	-1.540017000	-5.193629000	0.920865000
O	-1.216877000	-3.863226000	0.298023000
O	-2.516510000	-5.946987000	0.163829000

C	0.052675000	-6.055588000	0.644776000
F	1.030986000	-5.426455000	1.273038000
F	0.324241000	-6.081471000	-0.655074000
F	-0.024865000	-7.297610000	1.090856000

b. ⁴¹Sc(OTf)²⁺

Co	0.145687000	-0.003356000	-0.408595000
O	-0.252387000	-0.292129000	3.558142000
O	3.693916000	-0.109672000	1.462672000
O	2.437557000	1.137361000	-3.390111000
O	-3.763919000	0.325961000	-0.191134000
N	1.948186000	0.043342000	0.000571000
C	-1.570202000	1.756425000	-4.852186000
H	-1.548588000	2.088881000	-5.885901000
N	-1.579481000	0.496573000	-0.906837000
C	-2.564023000	0.284586000	0.027454000
C	-1.984832000	0.074723000	1.432343000
N	-0.545297000	-0.213716000	1.295509000
C	0.185425000	-0.423412000	2.414884000
C	1.598862000	-0.998542000	2.210072000
C	1.404762000	-2.438010000	1.675981000
H	0.745110000	-3.002295000	2.348529000
H	2.374773000	-2.949429000	1.641462000
H	0.959486000	-2.439353000	0.676068000
C	2.503208000	-0.273055000	1.193175000
C	2.821521000	0.520377000	-1.087658000
C	1.951481000	0.833345000	-2.312725000
N	0.608670000	0.777791000	-2.037307000
C	-0.433124000	1.065436000	-2.858377000
C	-1.714994000	0.895301000	-2.199254000
C	-2.905557000	1.168917000	-2.899206000
H	-3.859282000	1.041715000	-2.403872000
C	-2.819786000	1.590207000	-4.209499000
H	-3.730134000	1.798413000	-4.764091000
C	-0.384598000	1.503742000	-4.196124000
H	0.573054000	1.629584000	-4.684152000
C	3.526334000	1.845267000	-0.748428000
H	2.794296000	2.597147000	-0.431794000
H	4.040981000	2.214116000	-1.641907000
H	4.249476000	1.692752000	0.053179000
C	3.846430000	-0.539716000	-1.503779000
H	4.562145000	-0.703613000	-0.696163000
H	4.377746000	-0.198731000	-2.397593000
H	3.345221000	-1.486571000	-1.733736000
C	2.311128000	-1.064436000	3.557162000
H	1.712386000	-1.646275000	4.262044000
H	2.461051000	-0.067466000	3.982440000
H	3.289453000	-1.534270000	3.433695000

C	-2.741921000	-1.064119000	2.116302000
H	-2.460054000	-2.029193000	1.679203000
H	-3.817515000	-0.912639000	1.982863000
H	-2.512131000	-1.081443000	3.182568000
C	-2.244860000	1.411209000	2.153404000
H	-1.909504000	1.344047000	3.189567000
H	-3.316351000	1.637680000	2.127792000
H	-1.703294000	2.222868000	1.652608000
O	-0.079532000	-1.783999000	-1.410709000
Sc	-1.272751000	-3.074800000	-1.634659000
O	-1.897453000	-4.905828000	2.412981000
S	-1.695381000	-5.133296000	1.000567000
O	-1.238080000	-3.893250000	0.291476000
O	-2.699962000	-5.870685000	0.261393000
C	-0.170595000	-6.137493000	0.860795000
F	0.821209000	-5.570122000	1.526885000
F	0.174121000	-6.235474000	-0.418432000
F	-0.378941000	-7.351891000	1.341226000

I-4) {(OTf)₂Sc-[Co(O)(TAML)]}¹⁺, 1-Sc(OTf)₂⁺

a. ²¹Sc(OTf)₂⁺

Co	0.105522000	0.102104000	-0.386900000
O	-0.354787000	-0.427702000	3.565770000
O	3.658154000	-0.203683000	1.469546000
O	2.448025000	1.164679000	-3.350876000
O	-3.749288000	0.803613000	-0.109828000
N	1.912808000	0.066362000	0.025696000
C	-1.567053000	1.570115000	-4.907265000
H	-1.535751000	1.819418000	-5.964458000
N	-1.580519000	0.634329000	-0.868448000
C	-2.566634000	0.560230000	0.074235000
C	-2.021089000	0.202194000	1.460844000
N	-0.592105000	-0.125922000	1.317466000
C	0.109542000	-0.454301000	2.421609000
C	1.535478000	-1.002611000	2.223365000
C	1.366490000	-2.446482000	1.696209000
H	0.707039000	-3.020128000	2.361376000
H	2.345132000	-2.942538000	1.671268000
H	0.934569000	-2.450189000	0.691446000
C	2.456026000	-0.302529000	1.204554000
C	2.810328000	0.481573000	-1.065065000
C	1.947913000	0.848737000	-2.280124000
N	0.612428000	0.805666000	-2.005369000
C	-0.434654000	1.036599000	-2.858394000
C	-1.708707000	0.924827000	-2.199046000
C	-2.896600000	1.118771000	-2.924365000
H	-3.851271000	0.978226000	-2.431141000

C	-2.813202000	1.434654000	-4.266615000	O	-3.757062000	1.059224000	0.304353000
H	-3.725775000	1.565512000	-4.841515000	N	1.859516000	-0.023405000	0.204848000
C	-0.381572000	1.372962000	-4.222183000	C	-1.873133000	0.949370000	-4.687929000
H	0.577994000	1.463610000	-4.714949000	H	-1.923224000	0.967462000	-5.772476000
C	3.619112000	1.746559000	-0.733586000	N	-1.644306000	0.745693000	-0.562481000
H	2.951046000	2.546796000	-0.394271000	C	-2.561576000	0.853914000	0.449712000
H	4.137083000	2.085090000	-1.637320000	C	-1.926452000	0.718425000	1.840544000
H	4.347237000	1.535404000	0.050022000	N	-0.508553000	0.350834000	1.677758000
C	3.748314000	-0.652652000	-1.493384000	C	0.251192000	0.190689000	2.782901000
H	4.459077000	-0.870330000	-0.693775000	C	1.593009000	-0.544823000	2.601336000
H	4.293083000	-0.353872000	-2.394787000	C	1.203293000	-2.029945000	2.395865000
H	3.172982000	-1.558987000	-1.715443000	H	0.620109000	-2.371615000	3.259710000
C	2.237399000	-1.059143000	3.578269000	H	2.106762000	-2.649289000	2.330399000
H	1.640216000	-1.648835000	4.277311000	H	0.607925000	-2.167133000	1.485028000
H	2.369847000	-0.059947000	4.005612000	C	2.475967000	-0.160286000	1.399608000
H	3.222760000	-1.515148000	3.462091000	C	2.680842000	0.057315000	-1.016829000
C	-2.846593000	-0.972504000	1.990953000	C	1.747638000	0.219525000	-2.225341000
H	-2.710148000	-1.858434000	1.359479000	N	0.440423000	0.411779000	-1.862634000
H	-3.906704000	-0.701080000	1.973338000	C	-0.632910000	0.644062000	-2.662966000
H	-2.544365000	-1.213961000	3.011625000	C	-1.848922000	0.859559000	-1.901241000
C	-2.256224000	1.450102000	2.329463000	C	-3.055703000	1.143501000	-2.567754000
H	-1.991259000	1.242388000	3.366746000	H	-3.961522000	1.293560000	-1.995009000
H	-3.312156000	1.734353000	2.268799000	C	-3.055845000	1.172089000	-3.944244000
H	-1.647770000	2.286509000	1.965335000	H	-3.985795000	1.353428000	-4.475314000
O	-0.149254000	-1.513861000	-1.129637000	C	-0.668494000	0.698186000	-4.068782000
Sc	-1.293403000	-2.872272000	-1.506901000	H	0.237659000	0.530713000	-4.635510000
O	-3.068904000	-1.822279000	-1.915140000	C	3.596743000	1.292249000	-1.038697000
S	-4.372285000	-2.253511000	-2.532394000	H	3.012771000	2.201035000	-0.852224000
O	-4.533324000	-3.695212000	-2.512169000	H	4.065174000	1.373257000	-2.025223000
O	-4.667853000	-1.547859000	-3.759065000	H	4.367466000	1.200857000	-0.273045000
C	-5.582519000	-1.617378000	-1.302366000	C	3.497775000	-1.221357000	-1.229996000
F	-5.127022000	-1.780078000	-0.073216000	H	4.258944000	-1.309180000	-0.452446000
F	-6.711838000	-2.302657000	-1.433230000	H	3.981083000	-1.186033000	-2.211230000
F	-5.840740000	-0.341291000	-1.520202000	H	2.844701000	-2.100892000	-1.190923000
O	-1.441687000	-4.979347000	2.488113000	C	2.410681000	-0.427495000	3.884018000
S	-1.510505000	-5.152417000	1.054977000	H	1.819924000	-0.784642000	4.730340000
O	-1.290263000	-3.861121000	0.326425000	H	2.701036000	0.608878000	4.083623000
O	-2.587627000	-5.943388000	0.500436000	H	3.321242000	-1.024045000	3.796087000
C	0.020249000	-6.045139000	0.591661000	C	-2.690241000	-0.378363000	2.590677000
F	1.086965000	-5.377876000	0.999460000	H	-2.526770000	-1.350113000	2.105845000
F	0.079594000	-6.177514000	-0.729140000	H	-3.761710000	-0.154878000	2.581945000
F	0.023699000	-7.247980000	1.142067000	H	-2.336950000	-0.435247000	3.623055000
b. ⁴¹ Sc(OTf) ₂ ⁺				C	-2.129909000	2.083933000	2.517717000
Co	0.037251000	0.099012000	-0.069648000	H	-1.828394000	2.037462000	3.564475000
O	-0.122205000	0.472877000	3.923157000	H	-3.187535000	2.360224000	2.450090000
O	3.698097000	-0.109320000	1.553190000	H	-1.535785000	2.852126000	2.009582000
O	2.171849000	0.214100000	-3.370521000	O	-0.567186000	-1.786371000	-0.549314000

Sc	-1.951477000	-2.832151000	-0.976512000
O	-2.636438000	-2.028427000	-2.837341000
S	-3.453085000	-2.588678000	-3.961822000
O	-3.453594000	-4.039124000	-3.983113000
O	-3.253514000	-1.885815000	-5.208863000
C	-5.147200000	-2.147454000	-3.422388000
F	-5.370485000	-2.616799000	-2.199586000
F	-6.028778000	-2.687572000	-4.249774000
F	-5.316138000	-0.835625000	-3.409950000
O	-2.620533000	-6.202284000	1.954153000
S	-1.821946000	-5.641808000	0.887029000
O	-2.098027000	-4.186244000	0.666665000
O	-1.699774000	-6.387177000	-0.350092000
C	-0.120226000	-5.552666000	1.552382000
F	-0.104681000	-4.853006000	2.675862000
F	0.680918000	-4.968972000	0.670885000
F	0.331796000	-6.772565000	1.798875000

I-5) {(OTf)₃Sc-[Co(O)(TAML)]}²⁻, 1-Sc(OTf)₃

a. ²¹Sc(OTf)₃

Co	-0.100595000	0.007047000	-0.022262000
O	-0.278417000	0.406779000	3.962845000
O	3.500339000	-0.633708000	1.621699000
O	2.063458000	-0.179906000	-3.293825000
O	-3.661456000	1.614748000	0.288108000
N	1.692204000	-0.344315000	0.265817000
C	-1.965097000	0.582252000	-4.664192000
H	-2.025680000	0.463338000	-5.742793000
N	-1.630007000	0.897006000	-0.523304000
C	-2.523772000	1.190811000	0.455439000
C	-1.963197000	0.926615000	1.857709000
N	-0.580822000	0.446283000	1.707218000
C	0.109760000	0.130854000	2.824928000
C	1.367360000	-0.740067000	2.683251000
C	0.829885000	-2.185312000	2.549056000
H	0.203819000	-2.420143000	3.418903000
H	1.671990000	-2.888226000	2.529655000
H	0.238559000	-2.315100000	1.636160000
C	2.281339000	-0.528551000	1.469492000
C	2.530718000	-0.413602000	-0.940387000
C	1.632239000	-0.145677000	-2.149367000
N	0.357322000	0.160803000	-1.785980000
C	-0.714837000	0.427176000	-2.621316000
C	-1.866498000	0.841684000	-1.891731000
C	-3.059860000	1.120911000	-2.566869000
H	-3.933286000	1.434275000	-2.009321000
C	-3.096145000	0.983229000	-3.948605000

H	-4.025785000	1.177595000	-4.476237000
C	-0.767261000	0.315635000	-4.014551000
H	0.110160000	-0.007993000	-4.559540000
C	3.615280000	0.675450000	-0.986311000
H	3.172109000	1.662341000	-0.808693000
H	4.070562000	0.673322000	-1.982109000
H	4.378654000	0.486532000	-0.231690000
C	3.152627000	-1.803268000	-1.110763000
H	3.953175000	-1.948372000	-0.382509000
H	3.558355000	-1.897055000	-2.123572000
H	2.390523000	-2.575878000	-0.958056000
C	2.195981000	-0.643993000	3.961927000
H	1.571136000	-0.891249000	4.822317000
H	2.597078000	0.364336000	4.108164000
H	3.035760000	-1.339685000	3.908072000
C	-2.837376000	-0.166059000	2.489053000
H	-2.678820000	-1.122337000	1.971804000
H	-3.894133000	0.109403000	2.408737000
H	-2.576456000	-0.291592000	3.542197000
C	-2.088588000	2.244086000	2.634543000
H	-1.862366000	2.090655000	3.689246000
H	-3.112921000	2.614046000	2.523992000
H	-1.402726000	2.995849000	2.227621000
O	-0.931571000	-1.543409000	-0.190935000
Sc	-2.363995000	-2.453951000	-0.956766000
O	-2.390606000	-2.192777000	-3.025351000
S	-2.928301000	-2.986227000	-4.179136000
O	-3.287057000	-4.336444000	-3.792354000
O	-2.165590000	-2.793598000	-5.391098000
C	-4.550461000	-2.147698000	-4.493665000
F	-4.985079000	-1.523829000	-3.408283000
F	-5.448553000	-3.059178000	-4.840910000
F	-4.442273000	-1.273808000	-5.479555000
O	-4.479639000	-3.167554000	2.800609000
S	-4.131309000	-3.993610000	1.666260000
O	-3.667780000	-3.185465000	0.493818000
O	-5.036633000	-5.053151000	1.281771000
C	-2.570121000	-4.828740000	2.146830000
F	-1.582816000	-3.944714000	2.174832000
F	-2.264520000	-5.786015000	1.285429000
F	-2.702512000	-5.360214000	3.351811000
O	-1.454683000	-4.303788000	-1.149366000
S	-0.069844000	-4.880961000	-1.223587000
O	-0.100392000	-6.281186000	-1.583664000
O	0.796698000	-4.471608000	-0.141504000
C	0.540929000	-4.010942000	-2.716460000
F	-0.185478000	-4.376005000	-3.763470000

F	1.809547000	-4.310824000	-2.941273000
F	0.429606000	-2.697398000	-2.564311000
b. ⁴¹Sc(OTf)₃			
Co	-0.194512000	0.071137000	0.125478000
O	0.912932000	0.053629000	3.979985000
O	3.801384000	-0.228093000	0.367534000
O	0.715085000	0.723466000	-3.653343000
O	-3.574405000	1.283472000	1.761155000
N	1.623318000	0.076120000	-0.233240000
C	-3.588616000	0.784446000	-3.561029000
H	-4.006576000	0.754719000	-4.563524000
N	-1.964090000	0.654443000	0.242201000
C	-2.458848000	0.862786000	1.501137000
C	-1.441942000	0.505754000	2.597555000
N	-0.128142000	0.269675000	1.963038000
C	0.932763000	-0.009896000	2.747460000
C	2.188958000	-0.606541000	2.080537000
C	1.869182000	-2.117728000	1.949693000
H	1.646520000	-2.530169000	2.941878000
H	2.743363000	-2.643008000	1.544416000
H	1.009955000	-2.280848000	1.287300000
C	2.602144000	-0.180065000	0.657414000
C	1.964301000	0.133586000	-1.668894000
C	0.690455000	0.460307000	-2.462686000
N	-0.433557000	0.441720000	-1.683225000
C	-1.724277000	0.602217000	-2.072629000
C	-2.615566000	0.766968000	-0.943182000
C	-3.986789000	0.995674000	-1.163809000
H	-4.651267000	1.108459000	-0.316887000
C	-4.452750000	0.996879000	-2.461380000
H	-5.514950000	1.132320000	-2.644256000
C	-2.234659000	0.595066000	-3.384808000
H	-1.564160000	0.400059000	-4.215470000
C	2.995722000	1.212039000	-2.018723000
H	2.704296000	2.173906000	-1.581644000
H	3.031736000	1.322836000	-3.106939000
H	3.980302000	0.937844000	-1.642138000
C	2.421609000	-1.246478000	-2.164359000
H	3.378276000	-1.506824000	-1.703601000
H	2.530833000	-1.235834000	-3.255226000
H	1.671973000	-2.000067000	-1.890334000
C	3.382111000	-0.438342000	3.019616000
H	3.135893000	-0.845290000	4.002061000
H	3.649758000	0.616857000	3.144649000
H	4.248027000	-0.962554000	2.610863000
C	-1.954395000	-0.795972000	3.231478000
H	-1.969207000	-1.592257000	2.475595000

H	-2.970629000	-0.652993000	3.615260000
H	-1.292649000	-1.085075000	4.053074000
C	-1.449258000	1.655320000	3.610518000
H	-0.925895000	1.370908000	4.522010000
H	-2.488309000	1.907953000	3.843244000
H	-0.963869000	2.541586000	3.185928000
O	-0.736057000	-1.844170000	-0.193821000
Sc	-1.452970000	-2.930518000	-1.443738000
O	-0.834318000	-2.104697000	-3.307895000
S	-0.522181000	-2.557815000	-4.698421000
O	0.198304000	-3.815333000	-4.733218000
O	-0.069442000	-1.484024000	-5.553256000
C	-2.197342000	-2.946448000	-5.328490000
F	-2.715629000	-3.980657000	-4.676570000
F	-2.133040000	-3.248508000	-6.616564000
F	-2.997488000	-1.901540000	-5.170899000
O	-4.302047000	-1.484293000	0.686494000
S	-4.641713000	-2.179527000	-0.537182000
O	-3.484271000	-2.359397000	-1.472961000
O	-5.845065000	-1.789357000	-1.241092000
C	-4.957121000	-3.914364000	-0.005262000
F	-4.116392000	-4.256300000	0.961466000
F	-4.811612000	-4.756497000	-1.017460000
F	-6.194556000	-4.014380000	0.457938000
O	-1.727727000	-4.843949000	-0.558252000
S	-1.414705000	-5.556563000	0.721537000
O	-2.122332000	-6.814653000	0.825570000
O	-1.375552000	-4.694354000	1.883326000
C	0.333151000	-6.011578000	0.423269000
F	0.437159000	-6.750060000	-0.672124000
F	0.803399000	-6.699532000	1.452567000
F	1.069825000	-4.917727000	0.268925000

I-6) {(OTf)₄Sc-[Co(O)(TAML)]}³⁻, 1-Sc(OTf)₄⁻

a. ²¹Sc(OTf)₄⁻			
Co	-0.137626000	-0.008846000	0.005551000
O	-0.178438000	0.224037000	4.010467000
O	3.532396000	-0.629591000	1.499143000
O	1.903928000	-0.011824000	-3.350623000
O	-3.562984000	1.840960000	0.490300000
N	1.680375000	-0.291128000	0.217468000
C	-2.250795000	0.545119000	-4.509338000
H	-2.361396000	0.436653000	-5.584751000
N	-1.713812000	0.811893000	-0.400210000
C	-2.507220000	1.237206000	0.615790000
C	-1.912082000	0.904056000	1.989179000
N	-0.554081000	0.378556000	1.768961000

C	0.169392000	0.006808000	2.845861000
C	1.431589000	-0.839902000	2.615380000
C	0.910276000	-2.286695000	2.438300000
H	0.324642000	-2.571545000	3.321150000
H	1.758871000	-2.977276000	2.350995000
H	0.283462000	-2.400289000	1.545819000
C	2.305752000	-0.540099000	1.387138000
C	2.471852000	-0.287171000	-1.021325000
C	1.512405000	-0.027021000	-2.189293000
N	0.248157000	0.224078000	-1.768997000
C	-0.883483000	0.426869000	-2.542897000
C	-2.016997000	0.765976000	-1.750375000
C	-3.261089000	0.982175000	-2.349636000
H	-4.117835000	1.214976000	-1.726913000
C	-3.366336000	0.862187000	-3.729278000
H	-4.333985000	0.996180000	-4.206113000
C	-1.006478000	0.330428000	-3.931014000
H	-0.145008000	0.064208000	-4.530459000
C	3.499291000	0.854753000	-1.063742000
H	3.008733000	1.816014000	-0.869328000
H	3.949198000	0.889691000	-2.061818000
H	4.275389000	0.691267000	-0.314513000
C	3.158188000	-1.635713000	-1.263169000
H	4.018824000	-1.745883000	-0.600143000
H	3.489501000	-1.689721000	-2.305666000
H	2.457383000	-2.455604000	-1.071442000
C	2.301828000	-0.794526000	3.869959000
H	1.709432000	-1.092134000	4.737451000
H	2.696323000	0.210862000	4.052433000
H	3.148589000	-1.474440000	3.753635000
C	-2.809888000	-0.170227000	2.622071000
H	-2.646573000	-1.138073000	2.129449000
H	-3.864157000	0.103242000	2.496807000
H	-2.574015000	-0.272829000	3.684617000
C	-1.943984000	2.198631000	2.809309000
H	-1.685641000	2.002533000	3.849703000
H	-2.951649000	2.621991000	2.748713000
H	-1.238008000	2.929850000	2.397863000
O	-0.825593000	-1.595787000	-0.258334000
Sc	-2.324225000	-2.618113000	-0.687537000
O	-2.768722000	-2.237709000	-2.741094000
S	-2.975440000	-3.003514000	-4.005779000
O	-3.336574000	-4.390036000	-3.770581000
O	-1.979628000	-2.730773000	-5.020672000
C	-4.534502000	-2.244478000	-4.678241000
F	-5.240835000	-1.648779000	-3.735226000
F	-5.278821000	-3.206657000	-5.215086000

F	-4.266487000	-1.364234000	-5.633170000
O	-2.238824000	-3.609231000	3.604624000
S	-2.585056000	-4.393725000	2.436549000
O	-2.503650000	-3.621164000	1.168842000
O	-3.756259000	-5.242493000	2.520223000
C	-1.209353000	-5.587850000	2.232111000
F	-0.035028000	-5.010207000	2.393661000
F	-1.259533000	-6.143862000	1.026581000
F	-1.334503000	-6.550025000	3.140592000
O	-1.313574000	-4.359403000	-1.383778000
S	0.098940000	-4.843770000	-1.379684000
O	0.191084000	-6.251973000	-1.711745000
O	0.893145000	-4.359138000	-0.270883000
C	0.746916000	-3.982534000	-2.859778000
F	0.162665000	-4.461140000	-3.948235000
F	2.056702000	-4.179538000	-2.961100000
F	0.517190000	-2.678990000	-2.786736000
O	-5.850558000	-0.113962000	0.839810000
S	-5.431326000	-1.290748000	0.110699000
O	-3.956244000	-1.364057000	-0.105181000
O	-6.202204000	-1.666505000	-1.057534000
C	-5.690862000	-2.664117000	1.289511000
F	-4.919708000	-2.511378000	2.357941000
F	-5.414849000	-3.822935000	0.709691000
F	-6.958434000	-2.681737000	1.683661000

b. ⁴¹Sc(OTf)₄⁻

Co	-0.107484000	-0.030867000	0.095057000
O	-0.188691000	0.418897000	4.086026000
O	3.591151000	-0.415318000	1.609488000
O	1.923195000	-0.259055000	-3.281788000
O	-3.583091000	1.793004000	0.456209000
N	1.719034000	-0.258010000	0.312921000
C	-2.135949000	0.564620000	-4.503145000
H	-2.232093000	0.482730000	-5.581775000
N	-1.726857000	0.744857000	-0.400844000
C	-2.529092000	1.198571000	0.612112000
C	-1.944600000	0.900901000	2.000812000
N	-0.542266000	0.462006000	1.831389000
C	0.185853000	0.189143000	2.931933000
C	1.495835000	-0.604756000	2.744888000
C	1.033631000	-2.078622000	2.634555000
H	0.483826000	-2.367263000	3.538611000
H	1.906806000	-2.736450000	2.533154000
H	0.376659000	-2.219902000	1.768421000
C	2.362219000	-0.362908000	1.493168000
C	2.488694000	-0.377595000	-0.939229000
C	1.531536000	-0.186524000	-2.124906000

N	0.256699000	0.097193000	-1.731536000
C	-0.831581000	0.333046000	-2.511239000
C	-1.990529000	0.718579000	-1.729568000
C	-3.211697000	1.008438000	-2.366779000
H	-4.076031000	1.266888000	-1.767462000
C	-3.268291000	0.931194000	-3.740817000
H	-4.206142000	1.129577000	-4.252007000
C	-0.927447000	0.266777000	-3.910061000
H	-0.072568000	-0.047930000	-4.493326000
C	3.575371000	0.696741000	-1.095540000
H	3.153907000	1.694528000	-0.925894000
H	3.968043000	0.654073000	-2.116852000
H	4.382484000	0.528251000	-0.383114000
C	3.092590000	-1.779768000	-1.077648000
H	3.833789000	-1.941113000	-0.290650000
H	3.573185000	-1.877141000	-2.056942000
H	2.309759000	-2.544489000	-0.997349000
C	2.361024000	-0.452043000	3.992956000
H	1.778807000	-0.719051000	4.876948000
H	2.716024000	0.577167000	4.114325000
H	3.234183000	-1.103698000	3.918364000
C	-2.791363000	-0.245173000	2.575851000
H	-2.605016000	-1.167598000	2.011771000
H	-3.859130000	-0.005612000	2.495277000
H	-2.523444000	-0.408810000	3.623760000
C	-2.099300000	2.178016000	2.833641000
H	-1.885165000	1.980557000	3.882984000
H	-3.124798000	2.543660000	2.725356000
H	-1.415756000	2.955954000	2.473642000
O	-0.924135000	-1.813142000	-0.171413000
Sc	-2.350910000	-2.786565000	-0.733474000
O	-2.743546000	-2.219572000	-2.789309000

a. ²¹Sc

Co	-0.016983000	0.086220000	0.056396000
O	-0.165600000	0.300025000	4.074028000
O	3.660621000	-0.186470000	1.649005000
O	2.148359000	0.409236000	-3.223615000
O	-3.647591000	1.550073000	0.500902000
N	1.817107000	-0.020230000	0.323141000
C	-1.899157000	1.228141000	-4.520853000
H	-1.926389000	1.313579000	-5.604258000
N	-1.627859000	0.874612000	-0.373592000
C	-2.502129000	1.122403000	0.625738000
C	-1.912512000	0.819917000	2.007271000
N	-0.523022000	0.371708000	1.823637000
C	0.215673000	0.094171000	2.916222000
C	1.572768000	-0.606867000	2.717179000

S	-2.965923000	-2.882522000	-4.103167000
O	-3.313851000	-4.287401000	-3.983316000
O	-1.994986000	-2.515404000	-5.113367000
C	-4.540328000	-2.080303000	-4.685643000
F	-5.199571000	-1.508953000	-3.692799000
F	-5.325658000	-2.998473000	-5.237515000
F	-4.287448000	-1.159754000	-5.609851000
O	-2.107997000	-3.497030000	3.327727000
S	-2.566733000	-4.484017000	2.371049000
O	-2.775918000	-3.956807000	0.999255000
O	-3.635980000	-5.372023000	2.784664000
C	-1.113419000	-5.578966000	2.115251000
F	0.002398000	-4.871750000	2.094692000
F	-1.221843000	-6.247865000	0.973197000
F	-1.035173000	-6.457783000	3.109759000
O	-1.400675000	-4.542253000	-1.547449000
S	-0.003067000	-5.021549000	-1.732384000
O	0.047605000	-6.376114000	-2.250013000
O	0.897993000	-4.696869000	-0.645599000
C	0.543440000	-3.962627000	-3.129719000
F	0.031167000	-4.414113000	-4.264997000
F	1.868168000	-3.984497000	-3.225462000
F	0.151944000	-2.708737000	-2.951584000
O	-5.896659000	-0.217875000	0.719722000
S	-5.467637000	-1.467183000	0.124190000
O	-4.000063000	-1.524655000	-0.113219000
O	-6.257564000	-1.988951000	-0.975932000
C	-5.728319000	-2.698376000	1.460938000
F	-4.877920000	-2.513711000	2.461465000
F	-5.601263000	-3.933694000	1.002881000
F	-6.963982000	-2.556039000	1.932866000

I-6) {(OH)(OTf)₃Sc-[Co(O)(TAML)]⁺, 1-Sc

C	1.244577000	-2.107431000	2.533867000
H	0.811575000	-2.501058000	3.460154000
H	2.160512000	-2.669533000	2.306861000
H	0.536925000	-2.261599000	1.711461000
C	2.432976000	-0.215651000	1.505945000
C	2.644857000	0.091265000	-0.886587000
C	1.710388000	0.322662000	-2.078595000
N	0.423971000	0.476083000	-1.696220000
C	-0.670347000	0.772275000	-2.501531000
C	-1.848624000	1.003006000	-1.741308000
C	-3.041147000	1.341596000	-2.387318000
H	-3.934742000	1.515472000	-1.801597000
C	-3.055366000	1.452746000	-3.775770000
H	-3.983307000	1.713369000	-4.278334000
C	-0.703006000	0.885896000	-3.894246000

H	0.197567000	0.704863000	-4.465997000
C	3.570344000	1.319190000	-0.862479000
H	2.991289000	2.224920000	-0.644232000
H	4.030085000	1.431052000	-1.850332000
H	4.345565000	1.199808000	-0.105436000
C	3.451067000	-1.185021000	-1.140479000
H	4.263244000	-1.269476000	-0.415477000
H	3.868411000	-1.152348000	-2.152624000
H	2.809308000	-2.068929000	-1.051196000
C	2.408658000	-0.451007000	3.987041000
H	1.832093000	-0.794332000	4.848126000
H	2.693967000	0.592654000	4.158020000
H	3.323349000	-1.041312000	3.899067000
C	-2.771935000	-0.291781000	2.619254000
H	-2.664643000	-1.215481000	2.036378000
H	-3.822682000	0.019399000	2.614654000
H	-2.452781000	-0.493805000	3.643337000
C	-2.036195000	2.114460000	2.822842000
H	-1.806161000	1.933168000	3.872369000
H	-3.060541000	2.488514000	2.725173000
H	-1.350052000	2.877263000	2.435626000
O	-0.513001000	-1.530765000	-0.225027000
Sc	-1.038120000	-3.435570000	-0.593991000
S	2.058210000	-5.013306000	-0.439879000
S	-1.523732000	-4.197710000	2.792826000
S	-1.315633000	-3.578927000	-3.949596000
S	-4.296302000	-3.383963000	-1.604637000
O	-1.836474000	-3.670497000	1.442342000
O	-0.569215000	-3.160991000	-2.734660000
O	-3.036173000	-2.745130000	-1.141741000
O	1.027320000	-3.969837000	-0.210727000
O	-1.690851000	-3.219053000	3.851826000
O	-0.341595000	-5.040078000	2.841976000
O	-1.508882000	-5.284156000	-1.007186000
F	-0.628457000	-3.403863000	-6.440535000
O	3.377846000	-4.576397000	-0.018104000
F	2.346447000	-3.835590000	-2.750151000
O	-1.506617000	-5.011666000	-4.090400000
F	-2.908340000	-6.371289000	2.255372000
F	-4.996756000	-3.034390000	0.895461000
F	0.261361000	-1.896333000	-5.183549000
F	-4.070672000	-4.731740000	3.048219000
O	1.666285000	-6.360289000	-0.069511000
F	-2.761777000	-5.853878000	4.336584000
F	1.072368000	-5.576396000	-2.796438000
O	-4.123775000	-4.591758000	-2.389685000
F	3.204331000	-5.807312000	-2.628781000

F	-6.253373000	-4.384615000	-0.216048000
O	-2.446788000	-2.723289000	-4.265133000
O	-5.264562000	-2.411544000	-2.080695000
F	0.998014000	-3.918629000	-5.129662000
C	2.164835000	-5.056195000	-2.267904000
C	-0.092219000	-3.173854000	-5.245281000
C	-2.903221000	-5.357789000	3.109047000
F	-4.298532000	-5.019322000	0.418466000
C	-4.995920000	-3.988459000	-0.025895000
H	-1.932735000	-5.541485000	-1.830218000
b. ⁴¹Sc			
Co	-0.033596000	0.254669000	0.102835000
O	-0.056853000	0.370605000	4.125252000
O	3.695857000	-0.054234000	1.604676000
O	2.023120000	0.694842000	-3.230821000
O	-3.793396000	1.302381000	0.657342000
N	1.809840000	0.208021000	0.341285000
C	-2.108638000	1.399905000	-4.428555000
H	-2.157400000	1.536629000	-5.506214000
N	-1.749183000	0.837010000	-0.301184000
C	-2.602549000	0.989126000	0.726168000
C	-1.928051000	0.789604000	2.099099000
N	-0.540095000	0.337084000	1.891350000
C	0.260056000	0.133825000	2.952897000
C	1.621395000	-0.545837000	2.680072000
C	1.331846000	-2.029853000	2.350624000
H	0.912481000	-2.533976000	3.228897000
H	2.260363000	-2.543484000	2.063842000
H	0.625163000	-2.126637000	1.517859000
C	2.464825000	-0.050878000	1.485662000
C	2.567233000	0.245944000	-0.923021000
C	1.596260000	0.557744000	-2.081499000
N	0.319492000	0.659566000	-1.678701000
C	-0.811799000	0.940289000	-2.448014000
C	-1.992955000	1.040399000	-1.662856000
C	-3.214694000	1.318867000	-2.275797000
H	-4.109501000	1.390631000	-1.669473000
C	-3.263828000	1.496685000	-3.660962000
H	-4.218386000	1.708171000	-4.136688000
C	-0.876871000	1.124026000	-3.829640000
H	0.028525000	1.044450000	-4.418933000
C	3.653173000	1.327746000	-0.961213000
H	3.235041000	2.296820000	-0.662300000
H	4.022363000	1.413564000	-1.988473000
H	4.474784000	1.078431000	-0.289517000
C	3.162774000	-1.141190000	-1.196671000
H	3.938310000	-1.364744000	-0.457543000

H	3.598625000	-1.174271000	-2.201557000
H	2.371461000	-1.900011000	-1.122779000
C	2.470189000	-0.494313000	3.948322000
H	1.908248000	-0.914072000	4.785804000
H	2.745296000	0.533865000	4.206538000
H	3.389996000	-1.064437000	3.799312000
C	-2.747811000	-0.244106000	2.874543000
H	-2.674590000	-1.228704000	2.397400000
H	-3.797023000	0.070155000	2.888009000
H	-2.376383000	-0.328480000	3.898290000
C	-1.999659000	2.158898000	2.792543000
H	-1.649652000	2.084536000	3.823373000
H	-3.037178000	2.510072000	2.776903000
H	-1.378388000	2.887594000	2.256619000
O	-0.392050000	-1.702208000	-0.430905000
Sc	-1.059575000	-3.712364000	-0.648898000
S	2.026833000	-5.245183000	-0.289262000
S	-1.421070000	-4.195874000	2.709604000
S	-1.120553000	-3.755085000	-4.012148000
S	-4.236415000	-3.326557000	-1.758802000
O	-1.714622000	-3.521072000	1.414778000
O	-0.461355000	-3.424889000	-2.717224000
O	-2.937977000	-2.810214000	-1.245474000
O	0.934238000	-4.245936000	-0.161126000
O	-1.512685000	-3.298773000	3.846223000
O	-0.290346000	-5.103465000	2.656389000
O	-1.743771000	-5.494199000	-0.907377000
F	-0.183046000	-3.513787000	-6.417705000
O	3.277450000	-4.763275000	0.265007000
F	2.516435000	-4.030419000	-2.547774000
O	-1.364833000	-5.167079000	-4.231374000
F	-2.921211000	-6.227014000	1.998656000
F	-4.960052000	-2.875521000	0.717350000
F	0.646085000	-2.109556000	-5.010476000
F	-3.995957000	-4.580606000	2.892294000
O	1.635469000	-6.605679000	0.024697000
F	-2.789568000	-5.878309000	4.116480000
F	1.246519000	-5.765785000	-2.727417000
O	-4.137166000	-4.568202000	-2.505972000
F	3.358042000	-6.006225000	-2.383949000
F	-6.334241000	-4.087208000	-0.416348000
O	-2.173826000	-2.823509000	-4.376109000
O	-5.076935000	-2.278415000	-2.303132000
F	1.271712000	-4.171518000	-4.973466000
C	2.296286000	-5.256416000	-2.101566000
C	0.240008000	-3.362241000	-5.166448000
C	-2.874230000	-5.286577000	2.927333000

F	-4.472376000	-4.927226000	0.267234000
C	-5.048792000	-3.829369000	-0.197408000
H	-2.528884000	-5.791820000	-1.370485000

I-7) [Co(OH)(TAML)]¹⁻, 1-H

a. ²1-H

Co	0.00366500	0.05745000	-0.01359200
O	-0.03518500	-0.04507800	3.99203000
O	3.73028900	-0.05138600	1.45917100
O	1.99564100	0.95090200	-3.27986100
O	-3.78049400	0.93905100	0.61421000
N	1.83844300	0.10329100	0.20204000
C	-2.16827300	1.03652600	-4.46710000
H	-2.24524400	1.15529600	-5.54454200
N	-1.72188700	0.57662700	-0.35203200
C	-2.58826100	0.66902500	0.68838700
C	-1.90124700	0.43042500	2.03675300
N	-0.49897700	0.06533400	1.76747000
C	0.31657000	-0.17571800	2.81761000
C	1.71626100	-0.74726700	2.53109300
C	1.51310500	-2.24887700	2.21719600
H	1.01911800	-2.73405600	3.06775600
H	2.49065900	-2.72457500	2.07257400
H	0.90824000	-2.39548500	1.31787900
C	2.50812700	-0.16591400	1.34535300
C	2.61106900	0.44340800	-1.00418300
C	1.61808900	0.68339300	-2.14620100
N	0.32725400	0.59106200	-1.73472800
C	-0.82144400	0.73208400	-2.50045600
C	-2.00089800	0.72019400	-1.70520200
C	-3.25434100	0.86655400	-2.30620400
H	-4.14764100	0.85917900	-1.69457300
C	-3.32574000	1.02271000	-3.68591600
H	-4.29788900	1.13163300	-4.15919300
C	-0.91311900	0.89395900	-3.88667700
H	-0.01127000	0.90575400	-4.48562500
C	3.40331600	1.75034000	-0.85048000
H	2.74548100	2.55725000	-0.50780000
H	3.81512100	2.02840300	-1.82621200
H	4.21387000	1.62119600	-0.13292600
C	3.54078300	-0.69589500	-1.43753800
H	4.35119300	-0.81864700	-0.71713900
H	3.95905600	-0.45794900	-2.42073800
H	2.98430100	-1.63681000	-1.51362000
C	2.56435800	-0.63575000	3.79677900
H	2.04476300	-1.11623900	4.62832000
H	2.74797300	0.40883600	4.06706700

H	3.52900100	-1.12138000	3.63651300	N	0.30679700	0.59004000	-1.72200000
C	-2.66271500	-0.68919700	2.75441700	C	-0.80696900	0.87325700	-2.45145400
H	-2.55274800	-1.63818100	2.21567800	C	-2.00809700	0.84652800	-1.64334400
H	-3.72644400	-0.43277600	2.78808500	C	-3.25388400	1.14227400	-2.22885500
H	-2.28309500	-0.81415200	3.77046400	H	-4.14966900	1.11876500	-1.62221600
C	-2.03371500	1.74848000	2.81481900	C	-3.29904000	1.44895100	-3.57299200
H	-1.68119300	1.62164900	3.83858800	H	-4.25523200	1.67185200	-4.03754100
H	-3.08666100	2.04871000	2.82069600	C	-0.89003700	1.19605600	-3.81948100
H	-1.44831400	2.53755500	2.32903800	H	0.00996600	1.21521600	-4.42015500
O	-0.29971600	-1.62437500	-0.45737900	C	3.33491900	1.77569600	-0.86900900
H	-1.08366500	-1.89710400	0.03614800	H	2.63329700	2.56656800	-0.57914600

b. ⁴¹H

Co	0.00484500	0.00194200	0.02764800	H	3.76352900	2.03012000	-1.84413400
O	0.01423600	0.14793400	4.04275300	H	4.12724900	1.71206300	-0.12224500
O	3.73260600	0.11369200	1.53442200	C	3.58533600	-0.68535600	-1.35692200
O	1.99191900	0.77743700	-3.28290000	H	4.38693100	-0.74527400	-0.61854900
O	-3.82750000	0.68553900	0.63617600	H	4.01215000	-0.47036200	-2.34160600
N	1.84718600	0.09489800	0.24602900	H	3.06947200	-1.65105900	-1.40127700
C	-2.12759200	1.47607700	-4.36123400	C	2.57766900	-0.60141100	3.84678400
H	-2.20503400	1.72020600	-5.41677700	H	2.05285700	-1.08940500	4.67153000
N	-1.74462600	0.54755900	-0.34186400	H	2.77791900	0.43442200	4.13720200
C	-2.61753200	0.53870800	0.71523600	H	3.53547900	-1.09838800	3.67671500
C	-1.90144100	0.40636600	2.06573600	C	-2.62221800	-0.66417300	2.88851100
N	-0.49116400	0.06111600	1.81814100	H	-2.48615200	-1.65141900	2.43312500
C	0.33844100	-0.07201100	2.87243700	H	-3.69263500	-0.43743400	2.91792800
C	1.72780400	-0.67354200	2.58262200	H	-2.22504100	-0.68403300	3.90507400
C	1.49187200	-2.16091400	2.22611900	C	-2.05638800	1.78927700	2.72515300
H	0.98455600	-2.66259800	3.05992500	H	-1.62968200	1.77169800	3.72920400
H	2.45814400	-2.65751800	2.07130200	H	-3.11892400	2.04997900	2.77768600
H	0.88550600	-2.26914800	1.32125600	H	-1.53856700	2.55072600	2.12945700
C	2.51988000	-0.07364600	1.40275200	O	-0.33576800	-1.83423700	-0.56583100
C	2.60282800	0.42612600	-0.97417200	H	-0.87880300	-1.82186900	-1.36225000
C	1.61339900	0.60017400	-2.13491900				

II) C-H bond activation of CHD by complex [Co(O)(TAML)]²⁻ binding multiple coordinated redox-inactive scandium ion

II-1) C-H bond activation by 1

²RC

Co	0.230059000	-0.358067000	-0.109103000
O	-0.229719000	-0.294926000	3.897210000
O	3.744969000	0.510760000	1.668474000
O	2.406329000	0.427970000	-3.319999000
O	-3.710765000	-0.075111000	0.098224000
N	2.011900000	0.077385000	0.245775000
C	-1.649963000	0.213495000	-4.835298000
H	-1.635643000	0.324803000	-5.917378000

N	-1.535566000	-0.196985000	-0.673404000
C	-2.492247000	-0.172373000	0.270180000
C	-1.915080000	-0.272075000	1.697596000
N	-0.448137000	-0.189911000	1.625245000
C	0.260808000	-0.272703000	2.755587000
C	1.794897000	-0.460225000	2.649865000
C	1.999368000	-1.989558000	2.556137000
H	1.546064000	-2.472982000	3.431309000
H	3.072908000	-2.220125000	2.550134000
H	1.537996000	-2.385790000	1.643948000
C	2.583227000	0.125021000	1.453947000

C	2.821339000	0.369275000	-0.945292000	Co	0.259650000	-0.344700000	-0.065245000
C	1.928049000	0.246410000	-2.195218000	O	0.128952000	-0.223973000	3.979898000
N	0.646068000	-0.008543000	-1.888819000	O	3.918341000	0.363782000	1.493529000
C	-0.453391000	-0.003182000	-2.748205000	O	2.238890000	0.389135000	-3.409079000
C	-1.694644000	-0.080720000	-2.054302000	O	-3.627868000	0.070630000	0.435244000
C	-2.892033000	0.001983000	-2.768736000	N	2.101035000	-0.066253000	0.171219000
H	-3.830687000	-0.070153000	-2.232317000	C	-1.941483000	0.258373000	-4.644716000
C	-2.861706000	0.160785000	-4.154058000	H	-2.007426000	0.311677000	-5.729382000
H	-3.799855000	0.224922000	-4.702585000	N	-1.518159000	0.031134000	-0.495390000
C	-0.443173000	0.128288000	-4.140277000	C	-2.395603000	0.006342000	0.516878000
H	0.506620000	0.186517000	-4.658293000	C	-1.720133000	-0.148430000	1.896691000
C	3.349184000	1.812635000	-0.959173000	N	-0.255674000	-0.128313000	1.727117000
H	2.519743000	2.517163000	-0.819065000	C	0.527215000	-0.256964000	2.805569000
H	3.815043000	2.015047000	-1.929914000	C	2.013532000	-0.619338000	2.565540000
H	4.076550000	1.959012000	-0.158935000	C	2.010393000	-2.151447000	2.358042000
C	3.987317000	-0.613331000	-1.101327000	H	1.572345000	-2.639786000	3.238539000
H	4.714701000	-0.466686000	-0.299560000	H	3.038505000	-2.517818000	2.238836000
H	4.469673000	-0.449685000	-2.071251000	H	1.428559000	-2.428985000	1.471402000
H	3.623741000	-1.647403000	-1.064581000	C	2.747524000	-0.018984000	1.343494000
C	2.440164000	0.024563000	3.949632000	C	2.814815000	0.281681000	-1.067893000
H	1.957171000	-0.458371000	4.801369000	C	1.830542000	0.216159000	-2.255948000
H	2.338807000	1.109529000	4.069027000	N	0.558671000	0.037295000	-1.866801000
H	3.505881000	-0.213925000	3.943531000	C	-0.597880000	0.121866000	-2.647262000
C	-2.357963000	-1.635604000	2.246232000	C	-1.783049000	0.114195000	-1.862644000
H	-1.850284000	-2.427994000	1.681654000	C	-3.030847000	0.169408000	-2.484486000
H	-3.442331000	-1.748236000	2.125853000	H	-3.927936000	0.136928000	-1.877598000
H	-2.094809000	-1.724732000	3.303603000	C	-3.100811000	0.238493000	-3.876293000
C	-2.541359000	0.866261000	2.510502000	H	-4.075411000	0.265729000	-4.359929000
H	-2.284054000	0.770910000	3.566134000	C	-0.684792000	0.203107000	-4.036895000
H	-3.628342000	0.835632000	2.383630000	H	0.224157000	0.210491000	-4.626780000
H	-2.180162000	1.835516000	2.144955000	C	3.327695000	1.731534000	-1.061335000
O	0.355994000	-2.057918000	-0.152658000	H	2.503295000	2.418034000	-0.829791000
H	-0.988103000	-2.664759000	-1.756223000	H	3.716280000	1.979583000	-2.055272000
C	-1.740233000	-3.405740000	-2.079748000	H	4.112561000	1.856294000	-0.313718000
H	-1.311206000	-4.367751000	-1.746805000	C	3.968789000	-0.684332000	-1.344638000
C	-3.027058000	-3.141354000	-1.367385000	H	4.743579000	-0.573457000	-0.582352000
H	-2.981713000	-3.079066000	-0.278711000	H	4.391077000	-0.471722000	-2.332415000
C	-4.190453000	-2.948482000	-1.987680000	H	3.609086000	-1.720191000	-1.335676000
H	-5.085499000	-2.737897000	-1.402288000	C	2.814208000	-0.311745000	3.829224000
C	-4.345887000	-2.962305000	-3.477550000	H	2.349152000	-0.802291000	4.687054000
H	-5.099397000	-3.709309000	-3.782235000	H	2.851265000	0.764429000	4.029525000
H	-4.775834000	-2.000775000	-3.812851000	H	3.841172000	-0.666012000	3.712696000
C	-3.051632000	-3.202384000	-4.191853000	C	-2.162599000	-1.522527000	2.419615000
H	-3.083966000	-3.190496000	-5.281496000	H	-1.780299000	-2.293259000	1.736762000
C	-1.890458000	-3.392914000	-3.567061000	H	-3.256800000	-1.576179000	2.449440000
H	-0.984408000	-3.544975000	-4.154608000	H	-1.760078000	-1.689650000	3.423236000
⁴ RC				C	-2.253494000	0.977230000	2.788786000

H	-1.971698000	0.815042000	3.829439000	C	-0.643792000	0.301664000	-4.175090000
H	-3.344370000	1.008613000	2.697346000	H	0.293003000	0.355180000	-4.716870000
H	-1.851564000	1.944333000	2.462589000	C	3.571656000	1.427367000	-1.157105000
O	0.044607000	-2.251130000	-0.187443000	H	2.930850000	2.298832000	-0.974030000
H	-2.687774000	-2.246809000	-0.759688000	H	4.004349000	1.521474000	-2.159012000
C	-2.839948000	-3.098644000	-1.443900000	H	4.364067000	1.410039000	-0.407487000
H	-2.644883000	-3.978583000	-0.805324000	C	3.653943000	-1.085814000	-1.261748000
C	-4.251266000	-3.124134000	-1.940260000	H	4.418383000	-1.093543000	-0.480022000
H	-5.039593000	-3.120952000	-1.186751000	H	4.133412000	-1.057475000	-2.246552000
C	-4.580960000	-3.144674000	-3.232258000	H	3.051904000	-1.999680000	-1.184821000
H	-5.632613000	-3.158173000	-3.519891000	C	2.482853000	-0.124090000	3.816820000
C	-3.576393000	-3.152863000	-4.343670000	H	1.988698000	-0.568320000	4.683115000
H	-3.715311000	-4.050588000	-4.971877000	H	2.477024000	0.964569000	3.945980000
H	-3.773564000	-2.313711000	-5.033203000	H	3.523094000	-0.453142000	3.773392000
C	-2.165936000	-3.065702000	-3.845188000	C	-2.464353000	-1.443304000	2.364705000
H	-1.384667000	-2.984634000	-4.601225000	H	-2.003542000	-2.309871000	1.873901000
C	-1.838214000	-3.033110000	-2.554536000	H	-3.553762000	-1.512699000	2.262556000
H	-0.796387000	-2.921240000	-2.250707000	H	-2.188746000	-1.450929000	3.422776000
² TS				C	-2.490145000	1.073151000	2.441585000
Co	0.124262000	-0.276006000	-0.185656000	H	-2.188454000	1.045502000	3.489254000
O	-0.198272000	-0.133595000	3.850102000	H	-3.582493000	1.092860000	2.365645000
O	3.778355000	0.154965000	1.482638000	H	-2.096397000	1.988806000	1.982689000
O	2.260350000	0.269409000	-3.454285000	O	0.223914000	-2.021211000	-0.378258000
O	-3.803007000	-0.032244000	0.146582000	H	-0.759003000	-2.514481000	-1.131038000
N	1.940648000	0.018558000	0.133148000	C	-1.557211000	-3.298310000	-1.681081000
C	-1.868939000	0.398356000	-4.834863000	H	-1.068451000	-4.206010000	-1.291988000
H	-1.885455000	0.520483000	-5.915853000	C	-2.907305000	-3.089656000	-1.131158000
N	-1.646035000	-0.069319000	-0.684717000	H	-3.009203000	-3.067899000	-0.045137000
C	-2.576786000	-0.094792000	0.282891000	C	-3.990189000	-2.886245000	-1.892883000
C	-1.958761000	-0.159830000	1.697025000	H	-4.956208000	-2.703697000	-1.422878000
N	-0.493493000	-0.177701000	1.581728000	C	-3.953816000	-2.913079000	-3.387765000
C	0.247177000	-0.222315000	2.691725000	H	-4.565292000	-3.752328000	-3.770094000
C	1.754716000	-0.542066000	2.538703000	H	-4.455931000	-2.020359000	-3.796264000
C	1.812392000	-2.083919000	2.429739000	C	-2.560674000	-3.002444000	-3.927232000
H	1.338875000	-2.533162000	3.313000000	H	-2.440175000	-2.911302000	-5.006422000
H	2.859946000	-2.411625000	2.393368000	C	-1.487232000	-3.195807000	-3.149287000
H	1.290194000	-2.420039000	1.525812000	H	-0.501332000	-3.271332000	-3.609639000
C	2.562745000	-0.046701000	1.314079000	⁴ TS			
C	2.743723000	0.136851000	-1.093146000	Co	0.144981000	-0.425047000	-0.157966000
C	1.795959000	0.168627000	-2.311846000	O	-0.210046000	-0.137586000	3.866517000
N	0.504391000	0.099715000	-1.961368000	O	3.746611000	0.313641000	1.537422000
C	-0.616351000	0.145192000	-2.786348000	O	2.291465000	0.185870000	-3.418908000
C	-1.840374000	0.069451000	-2.057197000	O	-3.775824000	-0.017908000	0.133453000
C	-3.055405000	0.188605000	-2.733895000	N	1.964963000	-0.095033000	0.165722000
H	-3.978854000	0.135159000	-2.168088000	C	-1.809115000	0.420230000	-4.829613000
C	-3.061764000	0.353766000	-4.119934000	H	-1.813754000	0.562426000	-5.908089000
H	-4.013274000	0.437980000	-4.641654000	N	-1.622438000	-0.127131000	-0.690576000

C	-2.551660000	-0.107674000	0.274923000	C	-4.027212000	-2.883548000	-1.958816000
C	-1.941755000	-0.191975000	1.692798000	H	-4.982965000	-2.697859000	-1.469438000
N	-0.470888000	-0.132058000	1.595216000	C	-4.007283000	-2.837154000	-3.453956000
C	0.256140000	-0.196219000	2.717376000	H	-4.630566000	-3.651974000	-3.868033000
C	1.764932000	-0.516558000	2.586626000	H	-4.505018000	-1.921758000	-3.813351000
C	1.821613000	-2.060617000	2.511416000	C	-2.621387000	-2.913012000	-4.013820000
H	1.346700000	-2.486686000	3.405016000	H	-2.510320000	-2.749109000	-5.085348000
H	2.867542000	-2.393591000	2.484101000	C	-1.543375000	-3.169956000	-3.262590000
H	1.300442000	-2.426127000	1.617997000	H	-0.562563000	-3.225455000	-3.735926000
C	2.562786000	-0.017090000	1.360620000	² PC			
C	2.755475000	0.138061000	-1.053236000	Co	0.317252000	-0.296126000	-0.221080000
C	1.822514000	0.072949000	-2.280910000	O	-0.055940000	-0.458997000	3.811569000
N	0.528423000	-0.049898000	-1.947097000	O	3.865279000	0.299213000	1.610072000
C	-0.584090000	0.071642000	-2.782242000	O	2.477775000	0.661959000	-3.379693000
C	-1.810110000	0.040038000	-2.060879000	O	-3.610830000	0.045883000	0.077565000
C	-3.015796000	0.221137000	-2.738426000	N	2.126438000	-0.006618000	0.152316000
H	-3.944007000	0.190365000	-2.178777000	C	-1.599634000	0.257999000	-4.903190000
C	-3.005937000	0.411035000	-4.122221000	H	-1.594789000	0.354001000	-5.986695000
H	-3.950120000	0.541118000	-4.647769000	N	-1.454334000	-0.125898000	-0.740028000
C	-0.591651000	0.256801000	-4.165390000	C	-2.393006000	-0.112616000	0.218559000
H	0.348981000	0.276032000	-4.702221000	C	-1.796285000	-0.268422000	1.635775000
C	3.375805000	1.544502000	-1.100197000	N	-0.332162000	-0.374717000	1.538580000
H	2.601626000	2.301125000	-0.920954000	C	0.396740000	-0.485198000	2.653298000
H	3.800435000	1.712628000	-2.095919000	C	1.908545000	-0.787753000	2.477250000
H	4.152704000	1.648870000	-0.341717000	C	1.981949000	-2.294071000	2.140268000
C	3.844695000	-0.923664000	-1.224227000	H	1.522526000	-2.875168000	2.951722000
H	4.582402000	-0.836075000	-0.422906000	H	3.031983000	-2.606159000	2.055177000
H	4.336113000	-0.789760000	-2.193761000	H	1.461618000	-2.505710000	1.201361000
H	3.405033000	-1.927933000	-1.193153000	C	2.706186000	-0.072874000	1.354012000
C	2.481115000	-0.072824000	3.861880000	C	2.910337000	0.425661000	-1.013358000
H	1.981336000	-0.503578000	4.731743000	C	1.999215000	0.427014000	-2.263429000
H	2.472976000	1.017688000	3.969388000	N	0.710420000	0.214212000	-1.959385000
H	3.523071000	-0.399205000	3.833538000	C	-0.389820000	0.178525000	-2.813298000
C	-2.367028000	-1.548095000	2.270170000	C	-1.625221000	0.003072000	-2.117002000
H	-1.873528000	-2.337456000	1.688178000	C	-2.824049000	-0.034514000	-2.833086000
H	-3.454782000	-1.663829000	2.191111000	H	-3.753570000	-0.194654000	-2.297470000
H	-2.064133000	-1.624882000	3.318643000	C	-2.803159000	0.094709000	-4.222304000
C	-2.545228000	0.964689000	2.497273000	H	-3.740266000	0.060518000	-4.775029000
H	-2.275905000	0.884715000	3.550541000	C	-0.391654000	0.301138000	-4.206509000
H	-3.633708000	0.942335000	2.383452000	H	0.551144000	0.434851000	-4.723970000
H	-2.180096000	1.924959000	2.112126000	C	3.425117000	1.867917000	-0.877559000
O	0.068536000	-2.348735000	-0.207386000	H	2.592099000	2.545000000	-0.649887000
H	-0.804541000	-2.709714000	-1.170148000	H	3.877517000	2.181462000	-1.825188000
C	-1.607217000	-3.389241000	-1.804892000	H	4.162068000	1.930884000	-0.074544000
H	-1.174590000	-4.357860000	-1.506914000	C	4.089273000	-0.513615000	-1.291268000
C	-2.944409000	-3.161144000	-1.223167000	H	4.812816000	-0.456108000	-0.474489000
H	-3.025961000	-3.197625000	-0.136050000	H	4.571277000	-0.224853000	-2.231287000

H	3.743989000	-1.550344000	-1.383809000	C	2.551899000	0.049828000	1.581142000
C	2.617690000	-0.561251000	3.810992000	C	2.964088000	0.458828000	-0.780278000
H	2.121660000	-1.138855000	4.594501000	C	2.189581000	0.346228000	-2.112584000
H	2.598475000	0.493932000	4.105332000	N	0.892785000	0.061981000	-1.930553000
H	3.663328000	-0.868048000	3.730900000	C	-0.124961000	0.018383000	-2.884681000
C	-2.424093000	-1.527573000	2.246944000	C	-1.411938000	-0.142025000	-2.299546000
H	-2.145777000	-2.418170000	1.667707000	C	-2.543813000	-0.195853000	-3.110881000
H	-3.516523000	-1.435599000	2.228540000	H	-3.514394000	-0.344591000	-2.650898000
H	-2.080573000	-1.653316000	3.277413000	C	-2.403631000	-0.095972000	-4.495938000
C	-2.245544000	0.969225000	2.426040000	H	-3.287859000	-0.166230000	-5.125804000
H	-1.982057000	0.868265000	3.479678000	C	-0.001812000	0.123163000	-4.271360000
H	-3.329381000	1.087099000	2.322274000	H	0.981540000	0.250974000	-4.708474000
H	-1.759236000	1.867586000	2.025416000	C	3.325649000	1.947999000	-0.655377000
O	0.403962000	-2.070381000	-0.654493000	H	2.411635000	2.544885000	-0.542916000
H	-0.203611000	-2.131742000	-1.402792000	H	3.841104000	2.271619000	-1.566422000
C	-2.603652000	-3.178197000	-1.287944000	H	3.965796000	2.114034000	0.212673000
H	-1.879548000	-3.193507000	-0.478838000	C	4.235262000	-0.385986000	-0.891179000
C	-3.956703000	-2.853353000	-1.042589000	H	4.875468000	-0.220826000	-0.021332000
H	-4.265399000	-2.636483000	-0.020942000	H	4.774582000	-0.112829000	-1.804155000
C	-4.866810000	-2.782797000	-2.055757000	H	3.979193000	-1.451005000	-0.943985000
H	-5.904096000	-2.529635000	-1.847366000	C	2.268174000	-0.376523000	4.032314000
C	-4.484545000	-3.006855000	-3.482729000	H	1.712298000	-0.936570000	4.788087000
H	-5.135049000	-3.776005000	-3.944440000	H	2.211641000	0.686798000	4.286722000
H	-4.724598000	-2.103857000	-4.083037000	H	3.319948000	-0.672953000	4.055375000
C	-3.045613000	-3.361449000	-3.666223000	C	-2.597454000	-1.432714000	2.042188000
H	-2.698781000	-3.551844000	-4.679242000	H	-2.245744000	-2.344076000	1.539449000
C	-2.181230000	-3.432589000	-2.615221000	H	-3.682712000	-1.357593000	1.904398000
H	-1.138739000	-3.693988000	-2.797835000	H	-2.366835000	-1.502515000	3.108457000
⁴ PC				C	-2.434526000	1.076549000	2.108420000
Co	0.360267000	-0.454238000	-0.210859000	H	-2.275239000	1.031924000	3.186747000
O	-0.395873000	-0.231286000	3.765063000	H	-3.501886000	1.186109000	1.891372000
O	3.645992000	0.521987000	1.925197000	H	-1.908487000	1.952527000	1.709302000
O	2.761242000	0.575565000	-3.184214000	O	0.482953000	-2.386572000	-0.617867000
O	-3.574785000	0.035989000	-0.310347000	H	0.018084000	-2.456545000	-1.461615000
N	2.100873000	0.001432000	0.320041000	C	-2.138872000	-3.593533000	-2.817563000
C	-1.146953000	0.063636000	-5.070351000	H	-1.116426000	-3.897995000	-3.025730000
H	-1.046493000	0.137341000	-6.150931000	C	-2.537868000	-3.287637000	-1.494066000
N	-1.361485000	-0.236880000	-0.908053000	H	-1.789295000	-3.315910000	-0.702851000
C	-2.379342000	-0.130011000	-0.042396000	C	-3.815865000	-2.910963000	-1.210204000
C	-1.920256000	-0.200767000	1.431174000	H	-4.093750000	-2.643924000	-0.193195000
N	-0.452358000	-0.316005000	1.478529000	C	-4.865332000	-2.790327000	-2.264168000
C	0.168187000	-0.341328000	2.666132000	H	-5.751056000	-3.404949000	-2.005570000
C	1.684160000	-0.657894000	2.650684000	H	-5.285043000	-1.762306000	-2.249033000
C	1.795278000	-2.174472000	2.374286000	C	-4.375370000	-3.134153000	-3.632686000
H	1.259305000	-2.729027000	3.156519000	H	-5.085921000	-3.073092000	-4.454091000
H	2.849260000	-2.481738000	2.407980000	C	-3.085231000	-3.510031000	-3.865477000
H	1.375469000	-2.434768000	1.397559000	H	-2.772447000	-3.742942000	-4.881923000

II-2) C-H bond activation by 1-Sc³⁺

²RC

Co	-0.303878000	0.108027000	0.133846000
O	0.148497000	0.388547000	4.102538000
O	3.498581000	-0.745695000	1.088655000
O	1.345659000	0.495012000	-3.409037000
O	-3.990168000	1.080861000	1.102151000
N	1.537927000	-0.096778000	0.126701000
C	-2.866572000	1.017265000	-4.127976000
H	-3.061966000	1.102324000	-5.193656000
N	-2.048785000	0.678387000	-0.074346000
C	-2.794629000	0.829944000	1.062355000
C	-1.949181000	0.705061000	2.337866000
N	-0.598720000	0.254731000	1.953849000
C	0.328907000	0.087558000	2.918231000
C	1.630460000	-0.651062000	2.553385000
C	1.255346000	-2.152217000	2.584910000
H	0.805915000	-2.403974000	3.553117000
H	2.161190000	-2.754889000	2.449723000
H	0.546625000	-2.389003000	1.784671000
C	2.299618000	-0.460248000	1.176028000
C	2.131370000	-0.170309000	-1.221822000
C	1.077621000	0.297476000	-2.234540000
N	-0.166403000	0.426030000	-1.672864000
C	-1.353953000	0.648387000	-2.303906000
C	-2.451908000	0.798543000	-1.373335000
C	-3.745236000	1.068169000	-1.856753000
H	-4.564456000	1.186515000	-1.159306000
C	-3.934706000	1.178211000	-3.220543000
H	-4.929358000	1.386324000	-3.604509000
C	-1.585978000	0.748895000	-3.690156000
H	-0.764431000	0.602758000	-4.383240000
C	3.370001000	0.711292000	-1.410596000
H	3.176817000	1.725241000	-1.043384000
H	3.601253000	0.767976000	-2.478625000
H	4.221340000	0.297421000	-0.872261000
C	2.434212000	-1.630252000	-1.599715000
H	3.237344000	-2.014436000	-0.965902000
H	2.741700000	-1.688784000	-2.650767000
H	1.534157000	-2.241241000	-1.452999000
C	2.668760000	-0.394085000	3.647224000
H	2.254230000	-0.662060000	4.620868000
H	2.958255000	0.661840000	3.683053000
H	3.561323000	-0.990072000	3.450591000
C	-2.647876000	-0.288889000	3.270198000
H	-2.623917000	-1.299950000	2.845478000

H	-3.692685000	0.009427000	3.400857000
H	-2.150270000	-0.304089000	4.240783000
C	-1.955379000	2.111641000	2.962497000
H	-1.458274000	2.092529000	3.932102000
H	-2.991240000	2.444562000	3.086144000
H	-1.435956000	2.820495000	2.307360000
O	-0.778679000	-1.627917000	-0.153204000
Sc	-2.019857000	-2.893462000	-0.123135000
H	-0.357576000	-1.900440000	-2.883330000
C	-0.454230000	-2.555415000	-3.771372000
H	-0.051611000	-3.521663000	-3.423747000
C	-1.897148000	-2.694808000	-4.149758000
H	-2.557274000	-3.184717000	-3.434242000
C	-2.401754000	-2.259293000	-5.304122000
H	-3.464070000	-2.384351000	-5.510328000
C	-1.580054000	-1.595461000	-6.364659000
H	-1.763722000	-2.073434000	-7.340118000
H	-1.929465000	-0.557706000	-6.517344000
C	-0.116459000	-1.596909000	-6.049430000
H	0.552902000	-1.216091000	-6.819495000
C	0.385369000	-2.021593000	-4.889380000
H	1.459681000	-1.975352000	-4.715826000

⁴RC

Co	-0.281924000	-0.104111000	0.070544000
O	0.116862000	0.497673000	3.992374000
O	3.551013000	-0.579147000	1.160869000
O	1.462213000	0.489601000	-3.411415000
O	-4.034344000	0.718203000	0.926190000
N	1.565945000	-0.152259000	0.124632000
C	-2.680799000	1.258355000	-4.211994000
H	-2.818742000	1.533530000	-5.253851000
N	-2.047663000	0.422963000	-0.205585000
C	-2.824059000	0.558839000	0.917260000
C	-1.979580000	0.592401000	2.198610000
N	-0.629769000	0.088125000	1.876469000
C	0.306928000	0.069270000	2.853463000
C	1.620031000	-0.674521000	2.550298000
C	1.268104000	-2.180756000	2.505278000
H	0.752128000	-2.477126000	3.426531000
H	2.191934000	-2.765585000	2.422006000
H	0.629910000	-2.402273000	1.642907000
C	2.331577000	-0.415296000	1.207816000
C	2.208909000	-0.157385000	-1.207153000
C	1.163753000	0.254478000	-2.252414000
N	-0.109477000	0.292596000	-1.741567000
C	-1.261436000	0.600760000	-2.396368000
C	-2.403424000	0.634942000	-1.504251000

C	-3.679423000	0.933968000	-2.012109000	O	-3.690663000	1.899799000	0.772440000
H	-4.533949000	0.942033000	-1.348519000	N	1.511950000	-0.363933000	0.018592000
C	-3.801955000	1.239762000	-3.353321000	C	-2.162791000	2.190201000	-4.336509000
H	-4.780771000	1.484053000	-3.755804000	H	-2.203694000	2.511183000	-5.373377000
C	-1.421725000	0.925923000	-3.758908000	N	-1.870555000	1.031859000	-0.347662000
H	-0.562844000	0.910013000	-4.417895000	C	-2.620172000	1.304666000	0.756240000
C	3.383303000	0.818627000	-1.339479000	C	-1.921586000	0.857803000	2.054165000
H	3.110610000	1.801008000	-0.938779000	N	-0.761335000	0.014966000	1.692213000
H	3.624235000	0.930792000	-2.400740000	C	0.033298000	-0.450307000	2.680291000
H	4.255664000	0.449699000	-0.802970000	C	1.244307000	-1.320364000	2.267787000
C	2.628159000	-1.586605000	-1.583866000	C	0.721980000	-2.676170000	1.744550000
H	3.429735000	-1.920308000	-0.919706000	H	-0.009576000	-3.104635000	2.440688000
H	2.981777000	-1.614827000	-2.621228000	H	1.559469000	-3.379757000	1.660025000
H	1.766998000	-2.259832000	-1.476108000	H	0.272767000	-2.567632000	0.754757000
C	2.603004000	-0.435803000	3.694166000	C	2.141634000	-0.747250000	1.147333000
H	2.150942000	-0.741774000	4.640134000	C	2.323987000	-0.001473000	-1.154999000
H	2.871831000	0.622070000	3.776761000	C	1.367035000	0.381463000	-2.296709000
H	3.513553000	-1.011569000	3.519358000	N	0.113166000	0.661882000	-1.831149000
C	-2.673776000	-0.236928000	3.278498000	C	-0.952867000	1.206434000	-2.500703000
H	-2.621655000	-1.305691000	3.041848000	C	-2.101425000	1.404407000	-1.652869000
H	-3.726293000	0.056652000	3.335817000	C	-3.270951000	1.966329000	-2.183885000
H	-2.197495000	-0.070450000	4.245894000	H	-4.130701000	2.111648000	-1.541677000
C	-1.959987000	2.080727000	2.598328000	C	-3.292160000	2.348520000	-3.516329000
H	-1.409611000	2.204935000	3.532309000	H	-4.196137000	2.787280000	-3.929678000
H	-2.987950000	2.436723000	2.725526000	C	-0.999657000	1.626987000	-3.844739000
H	-1.477362000	2.677138000	1.814698000	H	-0.122561000	1.506704000	-4.469540000
O	-0.823462000	-2.101186000	-0.301581000	C	3.138328000	1.285520000	-0.911843000
Sc	-2.068920000	-3.202628000	0.259095000	H	2.470569000	2.107267000	-0.624981000
H	-0.217778000	-2.073562000	-2.704164000	H	3.666890000	1.567509000	-1.829314000
C	-0.489148000	-2.585710000	-3.644096000	H	3.861251000	1.113501000	-0.111953000
H	-0.153479000	-3.622603000	-3.464611000	C	3.254548000	-1.127490000	-1.608250000
C	-1.973486000	-2.551461000	-3.831448000	H	4.135790000	-1.172714000	-0.966312000
H	-2.589326000	-2.952937000	-3.027658000	H	3.565419000	-0.948700000	-2.642445000
C	-2.569569000	-2.089019000	-4.931677000	H	2.742454000	-2.094509000	-1.551484000
H	-3.656843000	-2.095000000	-5.000916000	C	2.095359000	-1.583996000	3.506912000
C	-1.821039000	-1.544276000	-6.105317000	H	1.491913000	-2.079612000	4.271515000
H	-2.089160000	-2.101804000	-7.018577000	H	2.484284000	-0.655013000	3.932712000
H	-2.167091000	-0.518199000	-6.325717000	H	2.942635000	-2.220419000	3.240931000
C	-0.338565000	-1.548922000	-5.907861000	C	-2.946910000	0.160535000	2.950926000
H	0.266476000	-1.142726000	-6.717124000	H	-3.234232000	-0.818554000	2.551626000
C	0.254997000	-2.005285000	-4.802085000	H	-3.845377000	0.783122000	3.007814000
H	1.340522000	-1.963489000	-4.715362000	H	-2.538308000	0.017739000	3.952059000
² TS				C	-1.469871000	2.171799000	2.720148000
Co	-0.282006000	0.122307000	-0.107977000	H	-0.999752000	1.958977000	3.682251000
O	-0.177240000	-0.262801000	3.881430000	H	-2.338537000	2.821241000	2.873022000
O	3.366280000	-0.746013000	1.297976000	H	-0.751309000	2.694361000	2.076651000
O	1.746005000	0.503917000	-3.454970000	O	-1.056236000	-1.441618000	-0.793573000

Sc	-2.609397000	-2.354453000	-0.361210000	H	2.985632000	1.935238000	-0.932765000
H	-0.379671000	-1.760365000	-1.769370000	H	3.535940000	1.097985000	-2.400568000
C	-0.008345000	-2.420639000	-2.925643000	H	4.196663000	0.641815000	-0.804386000
H	1.082060000	-2.448258000	-2.921089000	C	2.670363000	-1.466930000	-1.582508000
C	-0.718428000	-3.611463000	-2.503043000	H	3.462245000	-1.776169000	-0.895078000
H	-0.222872000	-4.291001000	-1.808205000	H	3.059963000	-1.474242000	-2.607016000
C	-2.028716000	-3.817512000	-2.814271000	H	1.834950000	-2.180033000	-1.509145000
H	-2.525056000	-4.718878000	-2.451043000	C	2.581987000	-0.663925000	3.674046000
C	-2.740034000	-3.013098000	-3.869137000	H	2.111383000	-1.052898000	4.580254000
H	-2.995608000	-3.680897000	-4.713616000	H	2.876992000	0.371544000	3.866892000
H	-3.731827000	-2.676676000	-3.524151000	H	3.479784000	-1.243762000	3.451096000
C	-1.928170000	-1.856466000	-4.358153000	C	-2.679478000	-0.022551000	3.363721000
H	-2.380554000	-1.206682000	-5.105195000	H	-2.749581000	-1.097926000	3.165898000
C	-0.652731000	-1.640327000	-3.965937000	H	-3.694647000	0.381002000	3.427006000
H	-0.088456000	-0.816895000	-4.398169000	H	-2.169156000	0.123613000	4.316975000
⁴ TS				C	-1.765365000	2.188295000	2.595174000
Co	-0.299425000	-0.016294000	0.087958000	H	-1.202090000	2.293600000	3.523998000
O	0.181862000	0.440693000	4.006845000	H	-2.753128000	2.647589000	2.710484000
O	3.553106000	-0.417600000	1.164297000	H	-1.230600000	2.706390000	1.789232000
O	1.399920000	0.516100000	-3.424528000	O	-0.983278000	-2.178456000	-0.523026000
O	-3.998836000	0.973655000	1.013314000	Sc	-2.116750000	-3.098680000	0.522627000
N	1.544220000	-0.106060000	0.120999000	H	-0.783916000	-2.392701000	-1.832882000
C	-2.792790000	1.321520000	-4.153988000	C	-0.789217000	-2.913252000	-3.026265000
H	-2.933856000	1.609585000	-5.192739000	H	-0.348495000	-3.849933000	-2.654604000
N	-2.064698000	0.481891000	-0.143292000	C	-2.207984000	-2.987029000	-3.373647000
C	-2.802753000	0.706248000	0.973800000	H	-2.875147000	-3.540994000	-2.714517000
C	-1.934802000	0.698297000	2.242355000	C	-2.723644000	-2.390669000	-4.467559000
N	-0.638537000	0.072932000	1.906511000	H	-3.789446000	-2.459054000	-4.674610000
C	0.320072000	0.007824000	2.862906000	C	-1.873914000	-1.695813000	-5.469528000
C	1.606877000	-0.757805000	2.504465000	H	-1.946657000	-2.218768000	-6.443162000
C	1.241255000	-2.243268000	2.282174000	H	-2.292758000	-0.702776000	-5.709343000
H	0.636440000	-2.627499000	3.111988000	C	-0.448433000	-1.583927000	-5.068642000
H	2.160297000	-2.838420000	2.220283000	H	0.221557000	-1.032577000	-5.725184000
H	0.698749000	-2.362079000	1.338587000	C	0.046951000	-2.188152000	-3.962257000
C	2.324860000	-0.357432000	1.198383000	H	1.112823000	-2.114632000	-3.758919000
C	2.177912000	-0.061590000	-1.212498000	² PC			
C	1.104479000	0.312297000	-2.250158000	Co	-0.232773000	0.464961000	0.032686000
N	-0.139728000	0.348487000	-1.720070000	O	0.124139000	0.225165000	3.966921000
C	-1.330459000	0.659273000	-2.360837000	O	3.520120000	-0.437251000	1.086981000
C	-2.444920000	0.680226000	-1.464955000	O	1.480382000	0.905578000	-3.464816000
C	-3.727129000	0.951561000	-1.947722000	O	-3.987680000	1.124938000	0.933642000
H	-4.566900000	0.950155000	-1.264326000	N	1.564374000	0.113332000	0.043033000
C	-3.891132000	1.263616000	-3.295314000	C	-2.717239000	1.697939000	-4.237312000
H	-4.884958000	1.489656000	-3.671854000	H	-2.854929000	1.936646000	-5.288316000
C	-1.512320000	1.016732000	-3.700379000	N	-1.995109000	0.876656000	-0.203735000
H	-0.655475000	1.055178000	-4.361955000	C	-2.778217000	0.927327000	0.904267000
C	3.305273000	0.968808000	-1.338707000	C	-1.950796000	0.783918000	2.194756000

N	-0.622742000	0.273224000	1.808564000	H	-3.707586000	-3.299797000	-3.966390000
C	0.283357000	-0.021934000	2.773091000	C	-2.062085000	-1.820939000	-4.115149000
C	1.513414000	-0.833073000	2.324702000	H	-2.438029000	-1.370130000	-5.054499000
C	1.006824000	-2.232852000	1.897022000	H	-2.477258000	-1.124484000	-3.354535000
H	0.411322000	-2.685557000	2.699209000	C	-0.567283000	-1.782658000	-4.093661000
H	1.866287000	-2.884998000	1.699080000	H	-0.077233000	-0.828504000	-4.279615000
H	0.400495000	-2.172443000	0.985940000	C	0.181227000	-2.909972000	-3.887350000
C	2.296804000	-0.317703000	1.099484000	H	1.267415000	-2.836490000	-3.900934000
C	2.229981000	0.251017000	-1.267219000	⁴ PC			
C	1.176147000	0.688590000	-2.296507000	Co	-0.230810000	0.467303000	0.033568000
N	-0.066637000	0.770261000	-1.759810000	O	0.123114000	0.227390000	3.968042000
C	-1.258175000	1.121310000	-2.412824000	O	3.520546000	-0.438086000	1.090061000
C	-2.369862000	1.121889000	-1.532732000	O	1.483239000	0.895597000	-3.465476000
C	-3.651296000	1.364107000	-2.026839000	O	-3.986141000	1.128667000	0.931701000
H	-4.498164000	1.349733000	-1.352277000	N	1.565784000	0.113215000	0.044687000
C	-3.815560000	1.640007000	-3.386205000	C	-2.712694000	1.696780000	-4.239157000
H	-4.813637000	1.829366000	-3.771954000	H	-2.849859000	1.934285000	-5.290505000
C	-1.430483000	1.445156000	-3.758372000	N	-1.992809000	0.879566000	-0.204184000
H	-0.571789000	1.480548000	-4.418202000	C	-2.776669000	0.930768000	0.903181000
C	3.347579000	1.297896000	-1.289035000	C	-1.950264000	0.787116000	2.194310000
H	2.992052000	2.246322000	-0.871000000	N	-0.621997000	0.276137000	1.809123000
H	3.647269000	1.468319000	-2.327942000	C	0.283149000	-0.019805000	2.774368000
H	4.206741000	0.956503000	-0.712250000	C	1.512948000	-0.831768000	2.326921000
C	2.742719000	-1.115024000	-1.740938000	C	1.005494000	-2.231378000	1.899527000
H	3.569482000	-1.453864000	-1.112510000	H	0.409754000	-2.683551000	2.701829000
H	3.078428000	-1.044211000	-2.781105000	H	1.864543000	-2.884071000	1.701630000
H	1.928696000	-1.853153000	-1.682015000	H	0.399097000	-2.170763000	0.988487000
C	2.464495000	-0.996736000	3.505587000	C	2.297332000	-0.317590000	1.101870000
H	1.935010000	-1.449593000	4.347211000	C	2.231901000	0.248002000	-1.265634000
H	2.860687000	-0.032002000	3.835973000	C	1.178813000	0.684789000	-2.295995000
H	3.304546000	-1.631954000	3.217351000	N	-0.063188000	0.772305000	-1.759222000
C	-2.687846000	-0.149547000	3.153566000	C	-1.254583000	1.122047000	-2.413279000
H	-2.637687000	-1.185771000	2.799067000	C	-2.366704000	1.123607000	-1.533791000
H	-3.738723000	0.151337000	3.200880000	C	-3.647822000	1.365416000	-2.028766000
H	-2.250097000	-0.104038000	4.151485000	H	-4.495046000	1.351826000	-1.354646000
C	-1.868753000	2.199611000	2.787499000	C	-3.811445000	1.639715000	-3.388571000
H	-1.337093000	2.175735000	3.740647000	H	-4.809334000	1.828668000	-3.775012000
H	-2.880135000	2.589796000	2.945957000	C	-1.426169000	1.444620000	-3.759238000
H	-1.340135000	2.868248000	2.097330000	H	-0.567132000	1.479409000	-4.418663000
O	-1.208765000	-2.180357000	-1.080734000	C	3.350406000	1.293928000	-1.288876000
Sc	-2.593155000	-2.848371000	-0.156896000	H	2.995481000	2.243440000	-0.872804000
H	-0.628334000	-1.898135000	-1.800834000	H	3.650729000	1.462095000	-2.327983000
C	-0.421543000	-4.171126000	-3.665872000	H	4.209062000	0.952906000	-0.711089000
H	0.192162000	-5.050238000	-3.501722000	C	2.743797000	-1.119188000	-1.736871000
C	-1.832330000	-4.278820000	-3.697278000	H	3.570516000	-1.457327000	-1.108027000
H	-2.291299000	-5.255985000	-3.559942000	H	3.079311000	-1.050291000	-2.777205000
C	-2.626607000	-3.188669000	-3.920507000	H	1.929589000	-1.857011000	-1.676501000

C	2.463366000	-0.995676000	3.508311000	H	1.962123000	-2.627346000	2.644246000
H	1.933131000	-1.447595000	4.349950000	H	0.460493000	-2.314713000	1.720251000
H	2.860292000	-0.031102000	3.838299000	C	2.181794000	-0.290371000	1.449318000
H	3.302990000	-1.631761000	3.220754000	C	2.339492000	-0.162932000	-0.964813000
C	-2.688196000	-0.146389000	3.152367000	C	1.411259000	0.172230000	-2.141710000
H	-2.637850000	-1.182548000	2.797668000	N	0.102314000	0.241426000	-1.761180000
H	-3.739078000	0.154616000	3.198790000	C	-1.000325000	0.343934000	-2.562753000
H	-2.251304000	-0.101161000	4.150678000	C	-2.215493000	0.474029000	-1.803888000
C	-1.868223000	2.202696000	2.787285000	C	-3.443328000	0.647829000	-2.465784000
H	-1.337404000	2.178529000	3.740891000	H	-4.356112000	0.721364000	-1.887067000
H	-2.879598000	2.593237000	2.944893000	C	-3.452754000	0.697738000	-3.847278000
H	-1.338773000	2.871193000	2.097623000	H	-4.398129000	0.827262000	-4.371092000
O	-1.212746000	-2.176862000	-1.083353000	C	-1.047005000	0.369546000	-3.968377000
Sc	-2.596882000	-2.844778000	-0.159036000	H	-0.129926000	0.241208000	-4.531460000
H	-0.632092000	-1.896148000	-1.803824000	C	3.557214000	0.760919000	-1.043902000
C	-0.426218000	-4.171884000	-3.662540000	H	3.297233000	1.773417000	-0.707021000
H	0.187246000	-5.050632000	-3.495501000	H	3.885204000	0.816329000	-2.088754000
C	-1.836813000	-4.279600000	-3.695654000	H	4.372227000	0.385109000	-0.424124000
H	-2.296094000	-5.256295000	-3.556006000	C	2.722152000	-1.634618000	-1.181140000
C	-2.630813000	-3.189907000	-3.922828000	H	3.336634000	-1.988791000	-0.342905000
H	-3.711762000	-3.301071000	-3.969346000	H	3.279247000	-1.757816000	-2.120351000
C	-2.065967000	-1.822739000	-4.121100000	H	1.801341000	-2.229229000	-1.239487000
H	-2.441213000	-1.374664000	-5.061995000	C	2.156982000	-0.283716000	3.952287000
H	-2.481335000	-1.124256000	-3.362569000	H	1.603341000	-0.601701000	4.840183000
C	-0.571161000	-1.784821000	-4.098748000	H	2.387555000	0.783964000	4.060785000
H	-0.080403000	-0.831171000	-4.285419000	H	3.098967000	-0.834941000	3.889744000
C	0.176912000	-2.911077000	-3.886979000	C	-3.009717000	-0.499628000	2.735508000
H	1.263143000	-2.837845000	-3.898327000	H	-2.968204000	-1.472097000	2.224563000

II-3) C-H bond activation by 1-Sc(OTf)₃

²RC

Co	-0.275032000	-0.014687000	0.014540000
O	-0.418865000	0.439967000	3.997837000
O	3.405921000	-0.422496000	1.563067000
O	1.832534000	0.325198000	-3.279675000
O	-4.091493000	0.849430000	0.403690000
N	1.556872000	-0.051351000	0.280053000
C	-2.265808000	0.556476000	-4.591909000
H	-2.312537000	0.571315000	-5.679228000
N	-1.986251000	0.461905000	-0.455373000
C	-2.896928000	0.630687000	0.546176000
C	-2.252884000	0.564740000	1.935715000
N	-0.834825000	0.209241000	1.767066000
C	-0.053351000	0.121002000	2.860150000
C	1.321495000	-0.552355000	2.701122000
C	1.014814000	-2.067550000	2.634765000
H	0.414204000	-2.374516000	3.503804000

H	-2.565494000	-0.599784000	3.731325000
C	-2.464113000	1.953380000	2.561037000
H	-2.193424000	1.944848000	3.618714000
H	-3.519911000	2.232468000	2.455086000
H	-1.850481000	2.702733000	2.042599000
O	-0.587893000	-1.757755000	-0.241856000
Sc	-1.728639000	-3.169903000	-0.327319000
O	-3.533860000	-2.082324000	-0.483860000
S	-4.939460000	-2.510315000	-0.780415000
O	-5.012766000	-3.890309000	-1.229070000
O	-5.699546000	-1.520651000	-1.508410000
C	-5.657525000	-2.542276000	0.908658000
F	-4.852506000	-3.207098000	1.727590000
F	-6.829781000	-3.163334000	0.870800000
F	-5.836538000	-1.321569000	1.377346000
O	-1.931478000	-3.730289000	4.124626000
S	-2.129484000	-4.518243000	2.927166000
O	-1.916723000	-3.725008000	1.681806000

O	-3.281453000	-5.391309000	2.866183000	C	2.458229000	-0.118154000	-0.941023000
C	-0.691457000	-5.645945000	2.837179000	C	1.467865000	-0.053582000	-2.112499000
F	0.439803000	-4.957896000	2.785016000	N	0.164626000	0.005659000	-1.701374000
F	-0.780102000	-6.400321000	1.747034000	C	-0.942941000	0.164780000	-2.472726000
F	-0.665935000	-6.434178000	3.900019000	C	-2.138592000	0.359670000	-1.678112000
O	-1.021742000	-4.105326000	-2.098622000	C	-3.383290000	0.555231000	-2.310580000
S	-0.486751000	-3.607008000	-3.412460000	H	-4.280448000	0.644758000	-1.709218000
O	0.002858000	-4.696905000	-4.231656000	C	-3.419687000	0.608623000	-3.686936000
O	0.313974000	-2.408438000	-3.313278000	H	-4.371243000	0.760003000	-4.192345000
C	-2.058591000	-3.081343000	-4.195708000	C	-1.022580000	0.203225000	-3.877737000
F	-2.830747000	-4.134908000	-4.423877000	H	-0.129587000	0.029082000	-4.465741000
F	-1.821418000	-2.466015000	-5.341541000	C	3.379339000	1.100625000	-1.102761000
F	-2.707094000	-2.253816000	-3.383401000	H	2.825174000	2.026663000	-0.898245000
H	1.232293000	-3.886256000	0.133421000	H	3.741910000	1.132546000	-2.137026000
C	1.846516000	-4.808516000	0.028223000	H	4.226084000	1.036586000	-0.417335000
H	1.179128000	-5.622614000	0.352302000	C	3.243251000	-1.425361000	-1.089722000
C	2.242844000	-5.000191000	-1.404008000	H	3.981863000	-1.505422000	-0.284569000
H	1.446697000	-5.247469000	-2.108088000	H	3.754003000	-1.452893000	-2.060598000
C	3.499573000	-4.891395000	-1.835936000	H	2.559765000	-2.283773000	-1.031112000
H	3.722833000	-5.039728000	-2.893646000	C	2.429335000	-0.092187000	3.987946000
C	4.657760000	-4.569996000	-0.940141000	H	1.910266000	-0.412555000	4.895478000
H	5.488620000	-5.271401000	-1.127774000	H	2.620016000	0.985708000	4.063627000
H	5.077689000	-3.581914000	-1.207592000	H	3.393634000	-0.603396000	3.915836000
C	4.284761000	-4.594267000	0.511568000	C	-2.723355000	-0.721654000	2.723209000
H	5.101085000	-4.521516000	1.231818000	H	-2.556859000	-1.627109000	2.121000000
C	3.028458000	-4.708432000	0.944073000	H	-3.803892000	-0.558661000	2.812981000
H	2.823460000	-4.737122000	2.015010000	H	-2.290949000	-0.872925000	3.718814000
⁴ RC				C	-2.392376000	1.778709000	2.838148000
Co	-0.148255000	-0.170617000	0.128947000	H	-2.178615000	1.651809000	3.900093000
O	-0.216624000	0.393846000	4.106650000	H	-3.455417000	2.008972000	2.702132000
O	3.593553000	0.031224000	1.577653000	H	-1.800880000	2.621119000	2.455614000
O	1.850209000	-0.017618000	-3.271951000	O	-0.710574000	-2.114128000	0.003877000
O	-3.902294000	0.964109000	0.559920000	Sc	-2.022761000	-3.273153000	-0.429985000
N	1.695008000	-0.120569000	0.320666000	O	-3.736077000	-1.992022000	-0.341913000
C	-2.247642000	0.441932000	-4.463380000	S	-5.168986000	-2.378867000	-0.528554000
H	-2.324698000	0.465890000	-5.548596000	O	-5.322249000	-3.791430000	-0.837356000
N	-1.874853000	0.355844000	-0.347311000	O	-5.921941000	-1.427422000	-1.316868000
C	-2.733463000	0.635124000	0.683667000	C	-5.817779000	-2.201881000	1.175726000
C	-2.068014000	0.496859000	2.059870000	F	-5.028785000	-2.813824000	2.044781000
N	-0.624272000	0.260297000	1.866801000	F	-7.027145000	-2.746521000	1.239779000
C	0.164701000	0.161545000	2.955930000	F	-5.911101000	-0.925650000	1.504813000
C	1.576785000	-0.426614000	2.766367000	O	-2.862697000	-3.899416000	3.704725000
C	1.364118000	-1.959161000	2.718090000	S	-2.781382000	-4.882319000	2.647310000
H	0.883259000	-2.293858000	3.647844000	O	-2.691638000	-4.287884000	1.283416000
H	2.337599000	-2.464692000	2.627665000	O	-3.684909000	-6.012409000	2.695344000
H	0.734688000	-2.244310000	1.863866000	C	-1.103266000	-5.599481000	2.797136000
C	2.369263000	-0.099822000	1.488981000	F	-0.204839000	-4.624533000	2.872660000

F	-0.820482000	-6.350850000	1.741141000	C	-0.505708000	0.169110000	-2.533875000
F	-1.016715000	-6.344661000	3.887981000	C	-1.748682000	-0.152374000	-1.943773000
O	-1.400866000	-4.203692000	-2.250211000	C	-2.871856000	-0.414083000	-2.711662000
S	-0.622733000	-3.789923000	-3.461853000	H	-3.804837000	-0.675616000	-2.215800000
O	-0.088263000	-4.933216000	-4.174665000	C	-2.764088000	-0.352774000	-4.100441000
O	0.245458000	-2.651847000	-3.247137000	H	-3.633858000	-0.565197000	-4.719313000
C	-1.990282000	-3.165281000	-4.517789000	C	-0.413345000	0.242251000	-3.925466000
F	-2.675025000	-4.179389000	-5.026838000	H	0.533013000	0.496438000	-4.391198000
F	-1.506069000	-2.434550000	-5.509772000	C	3.524623000	1.831256000	-0.399777000
F	-2.819562000	-2.419502000	-3.798378000	H	2.924910000	2.694240000	-0.082243000
H	0.997873000	-3.933813000	-1.038328000	H	3.953152000	2.050328000	-1.385114000
C	1.650006000	-4.815609000	-0.890204000	H	4.327283000	1.677538000	0.323595000
H	0.948627000	-5.669192000	-0.911031000	C	3.482758000	-0.688617000	-0.723466000
C	2.629675000	-4.914126000	-2.018805000	H	4.128767000	-0.851614000	0.149000000
H	2.212418000	-5.053879000	-3.017095000	H	4.102521000	-0.605185000	-1.626227000
C	3.949857000	-4.821305000	-1.855619000	H	2.804929000	-1.553229000	-0.827255000
H	4.608300000	-4.891938000	-2.723144000	C	1.973398000	-0.330327000	4.288945000
C	4.610264000	-4.614684000	-0.525812000	H	1.448111000	-0.947128000	5.024906000
H	5.382141000	-5.386810000	-0.358807000	H	1.861749000	0.719014000	4.584019000
H	5.183475000	-3.668840000	-0.534838000	H	3.037038000	-0.583539000	4.296670000
C	3.632918000	-4.607639000	0.610794000	C	-3.213404000	-0.160258000	2.634829000
H	4.048153000	-4.512453000	1.616075000	H	-3.267249000	-1.254992000	2.554851000
C	2.312798000	-4.708039000	0.447898000	H	-4.177291000	0.250667000	2.310867000
H	1.655267000	-4.682101000	1.318122000	H	-3.034588000	0.096339000	3.682409000
² TS				C	-1.846906000	1.889927000	2.127402000
Co	0.055326000	-0.184743000	0.088227000	H	-1.581328000	1.978384000	3.183982000
O	-0.630459000	-0.004774000	3.998759000	H	-2.756833000	2.469366000	1.934151000
O	3.407421000	0.466712000	2.149599000	H	-1.032649000	2.308871000	1.516179000
O	2.305733000	1.020986000	-2.880548000	O	0.116975000	-2.035495000	-0.348865000
O	-3.570001000	1.077412000	-0.065002000	Sc	-1.672675000	-2.406649000	0.393407000
N	1.732579000	0.343686000	0.607963000	O	-3.771759000	-1.917171000	0.118629000
C	-1.546872000	-0.023574000	-4.693097000	S	-5.077613000	-2.575795000	-0.172645000
H	-1.470704000	0.022556000	-5.778422000	O	-5.011216000	-4.017632000	-0.290574000
N	-1.711973000	-0.220278000	-0.527430000	O	-5.850729000	-1.849147000	-1.162495000
C	-2.578030000	0.470306000	0.286622000	C	-6.001880000	-2.276909000	1.380680000
C	-2.105969000	0.421691000	1.753335000	F	-5.338147000	-2.710766000	2.439823000
N	-0.839228000	-0.388875000	1.759097000	F	-7.162294000	-2.920537000	1.314816000
C	-0.109565000	-0.305591000	2.932743000	F	-6.248463000	-0.981781000	1.534117000
C	1.402348000	-0.590268000	2.895884000	O	-1.389164000	-4.807154000	3.735209000
C	1.657953000	-2.066399000	2.531520000	S	-1.592514000	-4.573470000	2.328854000
H	1.147721000	-2.737560000	3.235221000	O	-0.459514000	-4.030454000	1.544174000
H	2.740473000	-2.257113000	2.582344000	O	-2.761690000	-3.750018000	1.931340000
H	1.315113000	-2.296049000	1.518580000	C	-1.914295000	-6.236902000	1.602208000
C	2.251720000	0.173933000	1.845081000	F	-1.100184000	-7.118206000	2.158829000
C	2.646487000	0.587236000	-0.524227000	F	-1.711830000	-6.224079000	0.299604000
C	1.800642000	0.712396000	-1.806317000	F	-3.165678000	-6.582994000	1.853223000
N	0.508871000	0.373827000	-1.594829000	O	-2.050262000	-3.817396000	-1.079654000

S	-1.661518000	-4.151891000	-2.487553000	H	-3.723947000	-0.242384000	-2.209525000
O	-1.159499000	-5.506738000	-2.609224000	C	-2.580085000	-0.208762000	-4.051556000
O	-0.945320000	-3.097197000	-3.167956000	H	-3.458433000	-0.230405000	-4.693054000
C	-3.318498000	-4.204937000	-3.268552000	C	-0.161456000	-0.153215000	-3.822905000
F	-3.993915000	-5.259786000	-2.844621000	H	0.829763000	-0.124851000	-4.261823000
F	-3.169956000	-4.294093000	-4.585341000	C	3.510297000	1.494878000	-0.414381000
F	-4.010785000	-3.110224000	-2.995466000	H	2.763935000	2.299695000	-0.376708000
H	0.816949000	-3.146026000	-0.630265000	H	4.060543000	1.576218000	-1.359550000
C	1.396296000	-4.259411000	-0.827985000	H	4.200014000	1.610628000	0.423905000
H	0.515737000	-4.912733000	-0.726819000	C	3.854366000	-1.003804000	-0.340594000
C	1.977418000	-4.194408000	-2.173837000	H	4.523499000	-0.890352000	0.518213000
H	1.294065000	-4.247343000	-3.020838000	H	4.436675000	-0.975427000	-1.270824000
C	3.298101000	-4.038719000	-2.383401000	H	3.344684000	-1.978395000	-0.275207000
H	3.684479000	-3.975743000	-3.401065000	C	1.991132000	0.016394000	4.506117000
C	4.296353000	-3.981223000	-1.274185000	H	1.360659000	-0.372726000	5.310922000
H	5.116367000	-4.698109000	-1.464419000	H	2.070072000	1.103266000	4.628339000
H	4.818041000	-3.002763000	-1.282518000	H	2.995093000	-0.410666000	4.589831000
C	3.696237000	-4.230712000	0.069959000	C	-3.026007000	-0.416110000	2.500034000
H	4.381245000	-4.308085000	0.914927000	H	-2.834541000	-1.450597000	2.178593000
C	2.373446000	-4.388374000	0.258842000	H	-4.069651000	-0.173497000	2.262918000
H	1.985730000	-4.580605000	1.258788000	H	-2.869375000	-0.373092000	3.582717000
4TS				C	-2.328058000	1.994819000	2.324131000
Co	0.128111000	-0.314342000	0.284544000	H	-2.204597000	2.024142000	3.407821000
O	-0.626764000	0.477465000	4.154004000	H	-3.344720000	2.304326000	2.058356000
O	3.488989000	0.424463000	2.317746000	H	-1.621332000	2.697225000	1.863857000
O	2.602191000	0.038409000	-2.763103000	O	-0.133221000	-2.396287000	0.030811000
O	-3.447265000	1.157277000	-0.121294000	Sc	-1.981760000	-2.591240000	-0.289013000
N	1.877737000	-0.011590000	0.762076000	O	-4.009353000	-1.813655000	-0.246613000
C	-1.303120000	-0.162357000	-4.615205000	S	-5.281753000	-2.592580000	-0.374048000
H	-1.195036000	-0.147740000	-5.698170000	O	-5.062349000	-4.006194000	-0.603381000
N	-1.605252000	-0.198188000	-0.441862000	O	-6.270143000	-1.912190000	-1.184808000
C	-2.477978000	0.568944000	0.313798000	C	-5.929110000	-2.468986000	1.337658000
C	-2.087025000	0.575465000	1.800572000	F	-5.025124000	-2.860598000	2.224089000
N	-0.673961000	0.161691000	1.894932000	F	-7.004534000	-3.233747000	1.461388000
C	-0.067533000	0.162946000	3.101353000	F	-6.268065000	-1.213454000	1.601818000
C	1.384479000	-0.355725000	3.155610000	O	-1.639306000	-3.403470000	3.454935000
C	1.326255000	-1.899012000	3.056077000	S	-2.174322000	-4.424182000	2.579846000
H	0.715451000	-2.301886000	3.873969000	O	-2.532312000	-3.914139000	1.218112000
H	2.344571000	-2.304128000	3.150349000	O	-3.188061000	-5.315064000	3.100828000
H	0.896895000	-2.236443000	2.104127000	C	-0.756788000	-5.516083000	2.180996000
C	2.334683000	0.101318000	2.030799000	F	0.284512000	-4.805842000	1.779123000
C	2.819890000	0.124253000	-0.361968000	F	-1.093940000	-6.362539000	1.217700000
C	2.031287000	-0.003701000	-1.675700000	F	-0.413512000	-6.209254000	3.257503000
N	0.701335000	-0.135753000	-1.476027000	O	-2.104424000	-4.171081000	-1.654868000
C	-0.298489000	-0.180460000	-2.428873000	S	-1.911269000	-4.291732000	-3.140956000
C	-1.605882000	-0.194860000	-1.858300000	O	-1.560450000	-5.641240000	-3.527418000
C	-2.740296000	-0.221374000	-2.668692000	O	-1.152913000	-3.192766000	-3.699911000

C	-3.630615000	-4.042540000	-3.722277000
F	-4.401781000	-5.038608000	-3.327104000
F	-3.642738000	-3.984795000	-5.046165000
F	-4.107945000	-2.900488000	-3.244240000
H	0.822751000	-3.269044000	-0.892248000
C	1.409094000	-3.970325000	-1.640770000
H	0.558069000	-4.594987000	-1.965981000
C	1.949394000	-3.128425000	-2.718144000
H	1.233979000	-2.531436000	-3.288160000
C	3.267651000	-3.039606000	-2.978257000
H	3.621545000	-2.366729000	-3.758833000
C	4.290858000	-3.840338000	-2.247578000
H	4.852127000	-4.476444000	-2.959087000
H	5.079425000	-3.175754000	-1.846511000
C	3.728774000	-4.681589000	-1.151216000
H	4.433796000	-5.273016000	-0.567065000
C	2.411853000	-4.747879000	-0.889634000
H	2.047314000	-5.385942000	-0.085044000
² PC			
Co	0.036355000	-0.256990000	-0.294302000
O	-0.198111000	-0.838706000	3.600852000
O	3.607392000	-0.211592000	1.501386000
O	2.082865000	1.297758000	-3.243082000
O	-3.625169000	0.826571000	0.145292000
N	1.809334000	-0.014264000	0.108702000
C	-1.998548000	0.778259000	-4.797252000
H	-2.023585000	1.048409000	-5.851879000
N	-1.783398000	-0.261341000	-0.753529000
C	-2.576713000	0.224453000	0.264250000
C	-1.922768000	-0.049179000	1.643884000
N	-0.687696000	-0.864638000	1.368226000
C	0.163876000	-1.020872000	2.446273000
C	1.633515000	-1.401992000	2.164912000
C	1.737924000	-2.801251000	1.497731000
H	2.010964000	-3.554658000	2.247237000
H	2.515824000	-2.816568000	0.715985000
H	0.805585000	-3.147604000	1.045131000
C	2.427407000	-0.435435000	1.225535000
C	2.599056000	0.536214000	-1.008078000
C	1.644301000	0.847230000	-2.186339000
N	0.358256000	0.562259000	-1.897549000
C	-0.748848000	0.538424000	-2.748601000
C	-1.940563000	0.090637000	-2.122042000
C	-3.132633000	-0.023964000	-2.822774000
H	-4.019507000	-0.388847000	-2.304545000
C	-3.159137000	0.324532000	-4.173855000
H	-4.085318000	0.238570000	-4.738209000

C	-0.794569000	0.889122000	-4.101792000
H	0.106619000	1.241489000	-4.593221000
C	3.334300000	1.833506000	-0.659106000
H	2.644864000	2.553792000	-0.199497000
H	3.733960000	2.271600000	-1.581933000
H	4.153712000	1.636689000	0.036330000
C	3.585075000	-0.523009000	-1.514747000
H	4.326224000	-0.746887000	-0.739828000
H	4.092539000	-0.165610000	-2.418602000
H	3.044113000	-1.449661000	-1.764596000
C	2.368875000	-1.467134000	3.504642000
H	1.854003000	-2.164658000	4.173372000
H	2.407715000	-0.487742000	3.993114000
H	3.393116000	-1.813155000	3.339025000
C	-2.917753000	-0.734686000	2.585443000
H	-2.908025000	-1.825145000	2.465932000
H	-3.927485000	-0.366053000	2.369412000
H	-2.662243000	-0.513907000	3.625608000
C	-1.588034000	1.349973000	2.195891000
H	-1.150838000	1.263444000	3.194411000
H	-2.514776000	1.932649000	2.259351000
H	-0.885374000	1.899282000	1.550202000
O	0.126551000	-1.937640000	-1.035590000
Sc	-1.631322000	-2.491428000	-0.157759000
O	-3.696469000	-2.311252000	0.048093000
S	-5.113232000	-2.663175000	-0.297989000
O	-5.283829000	-4.032251000	-0.721855000
O	-5.762988000	-1.624018000	-1.068778000
C	-5.887822000	-2.572284000	1.368278000
F	-5.110862000	-3.117261000	2.290136000
F	-7.040930000	-3.225610000	1.338955000
F	-6.126249000	-1.311562000	1.701348000
O	-2.670874000	-4.277371000	3.534090000
S	-2.359300000	-4.758844000	2.206359000
O	-1.476440000	-3.804766000	1.448875000
O	-3.415351000	-5.320869000	1.396232000
C	-1.163722000	-6.121625000	2.470275000
F	-0.009051000	-5.648891000	2.914123000
F	-0.953050000	-6.776726000	1.336227000
F	-1.656384000	-6.965374000	3.363280000
O	-1.913957000	-4.070088000	-1.497355000
S	-1.733455000	-4.355367000	-2.962365000
O	-1.351368000	-5.731967000	-3.190718000
O	-1.016787000	-3.319022000	-3.676111000
C	-3.458350000	-4.198067000	-3.560109000
F	-4.200600000	-5.197348000	-3.124984000
F	-3.458965000	-4.209070000	-4.885892000

F	-3.968332000	-3.044332000	-3.147322000	H	2.488212000	2.441646000	-0.298332000
H	1.021496000	-2.304509000	-0.973722000	H	3.735423000	2.235319000	-1.556922000
C	1.079108000	-5.415967000	-0.675349000	H	4.045013000	1.668597000	0.110139000
H	0.021102000	-5.668513000	-0.691822000	C	3.797308000	-0.522865000	-1.545029000
C	1.629117000	-4.598497000	-1.694276000	H	4.602025000	-0.617176000	-0.812037000
H	0.978586000	-4.216216000	-2.481782000	H	4.195872000	-0.120402000	-2.483566000
C	2.956947000	-4.279215000	-1.720426000	H	3.377894000	-1.516175000	-1.745597000
H	3.359128000	-3.673395000	-2.531039000	C	2.574304000	-1.495736000	3.528846000
C	3.913559000	-4.773409000	-0.684967000	H	2.007750000	-2.085620000	4.256598000
H	4.761923000	-5.298606000	-1.168694000	H	2.861312000	-0.551546000	4.004698000
H	4.420330000	-3.916370000	-0.190553000	H	3.487121000	-2.033652000	3.254742000
C	3.272507000	-5.655087000	0.335874000	C	-2.564067000	-0.876391000	2.668469000
H	3.912534000	-6.072682000	1.111580000	H	-2.473931000	-1.816707000	2.107068000
C	1.939378000	-5.941872000	0.320154000	H	-3.621635000	-0.596410000	2.713697000
H	1.526977000	-6.593637000	1.087777000	H	-2.185540000	-1.044018000	3.681305000
⁴ PC				C	-1.844009000	1.531223000	2.802738000
Co	0.114005000	0.061683000	-0.061032000	H	-1.465269000	1.359532000	3.813437000
O	0.139117000	-0.443408000	3.888448000	H	-2.886476000	1.868598000	2.853807000
O	3.791088000	-0.421331000	1.394208000	H	-1.246061000	2.319846000	2.325432000
O	2.113674000	0.970542000	-3.312724000	O	-0.449222000	-2.332423000	-1.430251000
O	-3.654327000	0.891611000	0.607963000	Sc	-2.029457000	-3.189036000	-0.902129000
N	1.931542000	-0.166044000	0.087909000	O	-3.672839000	-1.935348000	-0.553420000
C	-2.093430000	1.172257000	-4.494634000	S	-5.161024000	-2.115269000	-0.689111000
H	-2.169162000	1.362965000	-5.563910000	O	-5.510678000	-3.420123000	-1.219139000
N	-1.636417000	0.424449000	-0.411929000	O	-5.821891000	-0.956931000	-1.243038000
C	-2.480891000	0.541356000	0.643092000	C	-5.681250000	-2.181935000	1.069117000
C	-1.780022000	0.238686000	1.979358000	F	-4.855047000	-2.945400000	1.769327000
N	-0.396848000	-0.175599000	1.681840000	F	-6.898289000	-2.705534000	1.129916000
C	0.420923000	-0.544399000	2.694635000	F	-5.713575000	-0.974634000	1.598289000
C	1.723588000	-1.260284000	2.284496000	O	-2.584475000	-4.280671000	3.191327000
C	1.300211000	-2.637813000	1.722741000	S	-2.391303000	-4.927844000	1.914621000
H	0.599577000	-3.129477000	2.413037000	O	-1.634068000	-4.065792000	0.936788000
H	2.182583000	-3.282737000	1.628145000	O	-3.504642000	-5.617365000	1.297105000
H	0.810197000	-2.563956000	0.741662000	C	-1.129791000	-6.209726000	2.251401000
C	2.578585000	-0.546574000	1.214842000	F	-0.008452000	-5.643164000	2.667457000
C	2.698753000	0.406486000	-1.035517000	F	-0.878099000	-6.928577000	1.166924000
C	1.714066000	0.660437000	-2.193750000	F	-1.583963000	-7.014733000	3.199300000
N	0.426966000	0.556449000	-1.794715000	O	-2.028485000	-5.022967000	-1.901044000
C	-0.734950000	0.771414000	-2.548736000	S	-1.671333000	-5.494933000	-3.285583000
C	-1.911326000	0.686163000	-1.760909000	O	-0.935199000	-6.738003000	-3.258232000
C	-3.165541000	0.831961000	-2.347754000	O	-1.196940000	-4.425129000	-4.139005000
H	-4.056036000	0.734724000	-1.735451000	C	-3.335711000	-5.904031000	-3.927926000
C	-3.246457000	1.074054000	-3.721466000	F	-3.914856000	-6.818894000	-3.168289000
H	-4.224776000	1.182150000	-4.187263000	F	-3.226765000	-6.369549000	-5.161770000
C	-0.830275000	1.021971000	-3.916543000	F	-4.084678000	-4.812797000	-3.941532000
H	0.072407000	1.090649000	-4.514416000	H	0.506002000	-2.443021000	-1.502308000
C	3.282999000	1.778356000	-0.667563000	C	1.131615000	-5.586387000	-0.793995000

H	0.170174000	-6.086512000	-0.870231000
C	1.557952000	-4.722950000	-1.832004000
H	0.916886000	-4.583220000	-2.704024000
C	2.758362000	-4.078162000	-1.777520000
H	3.085463000	-3.461400000	-2.612990000
C	3.678737000	-4.217646000	-0.607095000
H	4.713063000	-4.412831000	-0.947786000
H	3.780715000	-3.234704000	-0.084415000
C	3.236168000	-5.262442000	0.366099000
H	3.907663000	-5.498619000	1.190298000
C	2.017811000	-5.869974000	0.272709000
H	1.722581000	-6.600993000	1.023578000

II-4) C-H bond activation by 1-Sc(OH)(OTf)₄

²RC

Co	0.003524000	0.034891000	0.087082000
O	-0.054740000	0.240838000	4.108671000
O	3.716685000	-0.208178000	1.595468000
O	2.087235000	0.391146000	-3.240818000
O	-3.584639000	1.583745000	0.621948000
N	1.843062000	-0.054142000	0.311546000
C	-2.003158000	1.139793000	-4.444614000
H	-2.060397000	1.213089000	-5.529426000
N	-1.624185000	0.811149000	-0.303995000
C	-2.454165000	1.108245000	0.717604000
C	-1.838119000	0.794411000	2.084113000
N	-0.460178000	0.325896000	1.866559000
C	0.302345000	0.043354000	2.941935000
C	1.657277000	-0.649691000	2.709945000
C	1.332590000	-2.151652000	2.537145000
H	0.915585000	-2.543759000	3.473877000
H	2.248210000	-2.712015000	2.296110000
H	0.610102000	-2.312385000	1.726974000
C	2.486534000	-0.249527000	1.479826000
C	2.642088000	0.078023000	-0.915245000
C	1.678022000	0.294230000	-2.086184000
N	0.398499000	0.429695000	-1.674462000
C	-0.719080000	0.707819000	-2.454153000
C	-1.878030000	0.940643000	-1.665463000
C	-3.086305000	1.278774000	-2.281698000
H	-3.964537000	1.470063000	-1.673146000
C	-3.138061000	1.376614000	-3.670396000
H	-4.078592000	1.638795000	-4.153681000
C	-0.789519000	0.806553000	-3.846903000
H	0.097044000	0.622347000	-4.442380000
C	3.540969000	1.325435000	-0.902446000
H	2.944462000	2.220471000	-0.676843000

H	3.990050000	1.447709000	-1.896015000
H	4.326950000	1.220383000	-0.151529000
C	3.470034000	-1.179068000	-1.192108000
H	4.308232000	-1.243759000	-0.492536000
H	3.854245000	-1.140549000	-2.219148000
H	2.849242000	-2.077011000	-1.078314000
C	2.521687000	-0.490237000	3.960363000
H	1.966020000	-0.838364000	4.835421000
H	2.805256000	0.556955000	4.125599000
H	3.438798000	-1.076493000	3.850510000
C	-2.702906000	-0.305740000	2.710257000
H	-2.622056000	-1.229346000	2.120332000
H	-3.750732000	0.021150000	2.728876000
H	-2.366427000	-0.518690000	3.728307000
C	-1.922942000	2.087017000	2.907195000
H	-1.680943000	1.895658000	3.953829000
H	-2.942163000	2.483730000	2.827946000
H	-1.225603000	2.838496000	2.512276000
O	-0.475021000	-1.587877000	-0.195525000
Sc	-0.910794000	-3.511396000	-0.584613000
S	2.218917000	-5.020290000	-0.383043000
S	-1.436996000	-4.262958000	2.790532000
S	-1.107175000	-3.688899000	-3.939724000
S	-4.139568000	-3.574103000	-1.678918000
O	-1.751890000	-3.745592000	1.436153000
O	-0.388867000	-3.240695000	-2.717827000
O	-2.908131000	-2.886919000	-1.208400000
O	1.168462000	-3.989652000	-0.187269000
O	-1.612823000	-3.280166000	3.844280000
O	-0.248411000	-5.095633000	2.845772000
O	-1.328825000	-5.375439000	-0.990263000
F	-0.398244000	-3.502993000	-6.423163000
O	3.525091000	-4.550971000	0.046155000
F	2.537756000	-3.898172000	-2.719183000
O	-1.262703000	-5.127541000	-4.066062000
F	-2.794762000	-6.451157000	2.254660000
F	-4.878925000	-3.163566000	0.800214000
F	0.459785000	-1.986200000	-5.155175000
F	-3.980917000	-4.816721000	3.022418000
O	1.846978000	-6.366870000	0.009502000
F	-2.677822000	-5.919072000	4.334399000
F	1.271266000	-5.644069000	-2.741336000
O	-3.921466000	-4.799234000	-2.424080000
F	3.401172000	-5.861874000	-2.532188000
F	-6.123774000	-4.534425000	-0.299106000
O	-2.253922000	-2.865486000	-4.282975000
O	-5.120720000	-2.641964000	-2.207869000

F	1.222131000	-3.999227000	-5.097956000	H	-4.484019000	1.398966000	-1.101999000
C	2.352551000	-5.105993000	-2.207984000	C	-3.841564000	1.520982000	-3.166523000
C	0.123965000	-3.268082000	-5.222676000	H	-4.846685000	1.727764000	-3.533936000
C	-2.808986000	-5.432512000	3.102191000	C	-1.479503000	1.175375000	-3.579477000
F	-4.186218000	-5.164115000	0.388334000	H	-0.636191000	1.113406000	-4.258953000
C	-4.867567000	-4.140929000	-0.096418000	C	3.364337000	1.310282000	-1.178305000
H	-1.702663000	-5.644577000	-1.837524000	H	3.026529000	2.284555000	-0.798405000
H	-5.670807000	0.729259000	-0.392375000	H	3.618198000	1.421488000	-2.239373000
C	-6.574313000	0.421812000	-0.950078000	H	4.246523000	1.000502000	-0.613799000
H	-6.284825000	-0.542039000	-1.403649000	C	2.753647000	-1.129063000	-1.425683000
C	-7.716455000	0.226286000	-0.000999000	H	3.584324000	-1.411010000	-0.768260000
H	-7.568889000	-0.504598000	0.795897000	H	3.099987000	-1.138585000	-2.467575000
C	-8.870896000	0.888352000	-0.081859000	H	1.942053000	-1.863641000	-1.312563000
H	-9.658463000	0.693367000	0.648013000	C	2.644597000	-0.499849000	3.805852000
C	-9.169346000	1.909820000	-1.137592000	H	2.173074000	-0.923431000	4.697344000
H	-10.092286000	1.636398000	-1.679918000	H	2.935891000	0.533503000	4.033173000
H	-9.420820000	2.878583000	-0.669188000	H	3.549934000	-1.064388000	3.565143000
C	-8.038514000	2.085600000	-2.106157000	C	-2.642309000	-0.398379000	3.213032000
H	-8.193880000	2.799007000	-2.917145000	H	-2.586492000	-1.352921000	2.672527000
C	-6.885245000	1.422301000	-2.020075000	H	-3.696290000	-0.128096000	3.353573000
H	-6.108131000	1.598459000	-2.767935000	H	-2.160427000	-0.525111000	4.187401000
⁴ RC				C	-2.003330000	2.039995000	3.166548000
Co	-0.232516000	0.261247000	0.234765000	H	-1.561523000	1.942767000	4.160500000
O	0.127404000	0.303958000	4.242285000	H	-3.052421000	2.348509000	3.255523000
O	3.627508000	-0.133212000	1.332656000	H	-1.458994000	2.814686000	2.608104000
O	1.475916000	0.826041000	-3.272187000	O	-0.534987000	-1.693097000	-0.325471000
O	-3.947346000	1.193473000	1.169293000	Sc	-0.937943000	-3.752313000	-0.647705000
N	1.627329000	0.226982000	0.289234000	S	2.195554000	-5.157582000	-0.228874000
C	-2.769312000	1.442287000	-4.048309000	S	-1.309243000	-4.345922000	2.685506000
H	-2.927547000	1.588089000	-5.115994000	S	-0.874646000	-3.755000000	-3.983509000
N	-1.989981000	0.815740000	0.011385000	S	-4.100559000	-3.498986000	-1.850838000
C	-2.746174000	0.918770000	1.118187000	O	-1.611458000	-3.630333000	1.414587000
C	-1.941157000	0.702228000	2.414418000	O	-0.228752000	-3.424993000	-2.681012000
N	-0.564180000	0.309621000	2.063975000	O	-2.811901000	-2.937607000	-1.366077000
C	0.337220000	0.099291000	3.039728000	O	1.070081000	-4.189352000	-0.152489000
C	1.671227000	-0.562911000	2.630386000	O	-1.431820000	-3.497900000	3.856556000
C	1.347085000	-2.049488000	2.352621000	O	-0.152329000	-5.218224000	2.607538000
H	0.980031000	-2.531645000	3.269124000	O	-1.586979000	-5.546128000	-0.937375000
H	2.247620000	-2.581425000	2.010703000	F	0.036185000	-3.432169000	-6.384997000
H	0.579543000	-2.149379000	1.573776000	O	3.420347000	-4.618193000	0.330226000
C	2.391412000	-0.082320000	1.350180000	F	2.714677000	-4.023203000	-2.529756000
C	2.245539000	0.270527000	-1.050638000	O	-1.083240000	-5.170502000	-4.218586000
C	1.166865000	0.635353000	-2.093020000	F	-2.741574000	-6.379274000	1.868591000
N	-0.066902000	0.696735000	-1.566433000	F	-4.733186000	-3.022370000	0.657414000
C	-1.273070000	0.976024000	-2.213998000	F	0.852438000	-2.049184000	-4.949509000
C	-2.371416000	1.047897000	-1.313951000	F	-3.876184000	-4.795205000	2.798083000
C	-3.650679000	1.329716000	-1.794809000	O	1.841942000	-6.518287000	0.125016000

F	-2.671288000	-6.113646000	4.001794000	C	2.065744000	-0.602287000	1.183384000
F	1.482701000	-5.789481000	-2.664205000	C	1.948123000	-0.078603000	-1.181913000
O	-3.984739000	-4.765973000	-2.553337000	C	0.853746000	0.207619000	-2.216863000
F	3.588931000	-5.971697000	-2.257805000	N	-0.374724000	0.232966000	-1.665083000
F	-6.201807000	-4.148832000	-0.444101000	C	-1.575636000	0.552206000	-2.287414000
O	-1.952069000	-2.849901000	-4.344347000	C	-2.591891000	0.919692000	-1.361666000
O	-4.963060000	-2.492532000	-2.436789000	C	-3.826904000	1.368721000	-1.833817000
F	1.523830000	-4.095029000	-4.977986000	H	-4.590279000	1.667289000	-1.122338000
C	2.505612000	-5.231239000	-2.034857000	C	-4.062191000	1.405987000	-3.207809000
C	0.471599000	-3.305358000	-5.135065000	H	-5.031245000	1.742580000	-3.574308000
C	-2.739330000	-5.477122000	2.834783000	C	-1.831846000	0.570871000	-3.659041000
F	-4.367849000	-5.091953000	0.183757000	H	-1.054363000	0.256059000	-4.347170000
C	-4.896907000	-3.962382000	-0.261659000	C	2.760599000	1.223447000	-1.071790000
H	-2.347888000	-5.832832000	-1.453122000	H	2.137967000	2.022230000	-0.641185000
H	-5.329026000	-0.588733000	-0.407768000	H	3.079670000	1.532326000	-2.075200000
C	-6.428084000	-0.537149000	-0.508446000	H	3.636695000	1.073348000	-0.435199000
H	-6.742536000	-1.595389000	-0.455350000	C	2.815273000	-1.206007000	-1.741718000
C	-7.001651000	0.247482000	0.628359000	H	3.569151000	-1.508875000	-1.009325000
H	-6.714683000	-0.066595000	1.632771000	H	3.307140000	-0.852122000	-2.656556000
C	-7.810869000	1.295840000	0.472042000	H	2.186288000	-2.059186000	-2.010440000
H	-8.187752000	1.824702000	1.349322000	C	2.390149000	-0.914325000	3.639818000
C	-8.243892000	1.817544000	-0.865163000	H	1.903673000	-1.148413000	4.593152000
H	-9.344686000	1.766904000	-0.956442000	H	2.899878000	0.049411000	3.742921000
H	-8.027253000	2.898210000	-0.936999000	H	3.144001000	-1.677685000	3.419474000
C	-7.596440000	1.086721000	-2.002922000	C	-2.513402000	1.154254000	3.538638000
H	-7.813661000	1.453397000	-3.008121000	H	-2.767718000	0.096854000	3.673301000
C	-6.790106000	0.036256000	-1.842617000	H	-3.444207000	1.732755000	3.478335000
H	-6.340386000	-0.446465000	-2.710687000	H	-1.929683000	1.484443000	4.402255000
² TS				C	-1.081036000	2.771020000	2.273788000
Co	-0.553611000	-0.104041000	0.139612000	H	-0.370179000	2.835565000	3.103046000
O	0.322925000	0.733284000	3.971289000	H	-1.859413000	3.535205000	2.396743000
O	3.303756000	-0.574154000	1.173662000	H	-0.551561000	2.959682000	1.327655000
O	1.134017000	0.463484000	-3.386011000	O	-1.326316000	-1.816548000	-0.226419000
O	-3.690660000	2.146573000	1.068932000	Sc	-0.693317000	-3.625795000	-1.061187000
N	1.295942000	-0.415530000	0.096776000	S	2.368831000	-4.758351000	-0.193699000
C	-3.080967000	0.997236000	-4.110379000	S	-1.631348000	-4.831374000	2.174329000
H	-3.287576000	1.011239000	-5.179764000	S	-0.334777000	-3.079921000	-4.349776000
N	-2.167911000	0.814761000	-0.040808000	S	-3.507348000	-4.586388000	-2.827053000
C	-2.678650000	1.446687000	1.036345000	O	-1.511715000	-4.621495000	0.713139000
C	-1.726787000	1.369084000	2.244831000	O	-0.081927000	-2.636526000	-2.951012000
N	-0.709822000	0.340466000	1.969403000	O	-2.693392000	-3.689611000	-1.969490000
C	0.267160000	0.157439000	2.876683000	O	1.311682000	-3.713577000	-0.277138000
C	1.347397000	-0.887518000	2.524205000	O	-2.292396000	-3.756780000	2.891234000
C	0.687090000	-2.276836000	2.466502000	O	-0.451494000	-5.403999000	2.796138000
H	0.200820000	-2.497297000	3.427645000	O	-0.310434000	-5.367425000	-1.858007000
H	1.453007000	-3.042934000	2.283974000	F	1.256668000	-2.872425000	-6.389723000
H	-0.062558000	-2.347547000	1.670008000	O	3.608312000	-4.213928000	0.336175000

F	2.284725000	-4.290051000	-2.815697000	N	-0.854237000	0.376864000	1.816784000
O	-0.007326000	-4.470918000	-4.617205000	C	0.124242000	0.255479000	2.733807000
F	-2.450103000	-7.220258000	1.494960000	C	1.229288000	-0.775695000	2.426979000
F	-5.092728000	-4.866368000	-0.775244000	C	0.592869000	-2.174473000	2.320055000
F	0.543766000	-0.980617000	-5.687479000	H	0.090468000	-2.430221000	3.265073000
F	-4.028486000	-5.765448000	1.737809000	H	1.368342000	-2.928598000	2.129450000
O	1.939410000	-6.022718000	0.374189000	H	-0.136291000	-2.234124000	1.502866000
F	-3.040807000	-6.586590000	3.464848000	C	2.012447000	-0.512982000	1.115515000
F	2.363014000	-6.379946000	-2.293124000	C	1.985360000	0.136991000	-1.229982000
O	-2.762283000	-5.534462000	-3.631802000	C	0.941859000	0.629846000	-2.248165000
F	4.110394000	-5.158853000	-2.105159000	N	-0.319232000	0.468597000	-1.804700000
F	-5.127395000	-6.508289000	-2.168220000	C	-1.496991000	0.820526000	-2.465614000
O	-1.587174000	-2.589550000	-4.902931000	C	-2.598664000	0.996061000	-1.584222000
O	-4.600643000	-3.886217000	-3.481401000	C	-3.839971000	1.375354000	-2.099075000
F	2.067867000	-2.041154000	-4.581379000	H	-4.675226000	1.507590000	-1.419145000
C	2.783640000	-5.169329000	-1.967109000	C	-3.989131000	1.558141000	-3.475470000
C	0.962844000	-2.172308000	-5.292584000	H	-4.962330000	1.842617000	-3.873413000
C	-2.860724000	-6.181503000	2.210844000	C	-1.662124000	1.001561000	-3.839699000
F	-3.457684000	-6.269963000	-0.830506000	H	-0.812237000	0.851400000	-4.498805000
C	-4.340097000	-5.617592000	-1.569183000	C	3.035509000	1.243981000	-1.086654000
H	-0.452096000	-5.553850000	-2.793058000	H	2.602365000	2.120610000	-0.584727000
H	-2.660524000	-1.908348000	0.135390000	H	3.368939000	1.546559000	-2.086159000
C	-3.837107000	-2.167389000	0.493093000	H	3.890305000	0.891553000	-0.505121000
H	-3.690616000	-3.254279000	0.605448000	C	2.620265000	-1.116827000	-1.840130000
C	-4.095809000	-1.472441000	1.764572000	H	3.405074000	-1.495621000	-1.178442000
H	-3.457247000	-1.740022000	2.605838000	H	3.050735000	-0.867989000	-2.819807000
C	-5.044560000	-0.534235000	1.914373000	H	1.869596000	-1.905842000	-1.991853000
H	-5.165633000	-0.031414000	2.875995000	C	2.220914000	-0.801475000	3.588544000
C	-5.961469000	-0.115458000	0.811946000	H	1.689433000	-1.020861000	4.521377000
H	-7.018626000	-0.213461000	1.127591000	H	2.734367000	0.159319000	3.707609000
H	-5.839666000	0.969092000	0.632690000	H	2.975412000	-1.574072000	3.409124000
C	-5.725659000	-0.876313000	-0.451564000	C	-2.652609000	1.223204000	3.366505000
H	-6.373209000	-0.640238000	-1.298695000	H	-2.653834000	0.174578000	3.679851000
C	-4.769573000	-1.810758000	-0.584545000	H	-3.692206000	1.552114000	3.229493000
H	-4.660939000	-2.328143000	-1.536211000	H	-2.186011000	1.817315000	4.158338000
⁴ TS				C	-1.295559000	2.805862000	1.975226000
Co	-0.575292000	0.030517000	-0.012817000	H	-0.564293000	2.929849000	2.780816000
O	0.150626000	0.871454000	3.808270000	H	-2.087568000	3.558748000	2.082243000
O	3.239739000	-0.681080000	1.120132000	H	-0.796800000	2.957427000	1.005642000
O	1.285220000	1.105086000	-3.331269000	O	-1.198760000	-1.884659000	-0.478148000
O	-3.920066000	1.974488000	0.838488000	Sc	-0.971480000	-3.896295000	-1.036687000
N	1.294425000	-0.152580000	0.039990000	S	2.134242000	-5.040124000	-0.093670000
C	-2.913096000	1.367572000	-4.338888000	S	-1.313923000	-5.006828000	2.256157000
H	-3.043344000	1.501134000	-5.411973000	S	-0.248503000	-3.546129000	-4.318031000
N	-2.257745000	0.797765000	-0.243629000	S	-3.848354000	-4.272568000	-2.907867000
C	-2.851439000	1.361735000	0.828593000	O	-1.713327000	-4.440267000	0.942110000
C	-1.899635000	1.385621000	2.044807000	O	-0.042106000	-3.235238000	-2.880748000

O	-2.886723000	-3.482081000	-2.101351000
O	1.029760000	-4.066778000	-0.300361000
O	-1.948788000	-4.339100000	3.379520000
O	0.094510000	-5.322538000	2.379401000
O	-1.130657000	-5.713136000	-1.703517000
F	1.251535000	-2.826180000	-6.317384000
O	3.154640000	-4.527495000	0.803700000
F	3.558304000	-3.927057000	-2.007499000
O	-0.067267000	-4.941125000	-4.673759000
F	-1.701848000	-7.382380000	1.218098000
F	-5.657726000	-4.239980000	-1.021579000
F	1.141627000	-1.390062000	-4.712338000
F	-3.461649000	-6.471124000	2.064126000
O	1.726422000	-6.420623000	0.076131000
F	-1.933784000	-7.276208000	3.353958000
F	2.047079000	-5.301984000	-2.690822000
O	-3.266743000	-5.366449000	-3.667699000
F	3.842996000	-6.043867000	-1.762930000
F	-5.536814000	-6.098323000	-2.103339000
O	-1.379224000	-2.852986000	-4.913579000
O	-4.816939000	-3.438502000	-3.597814000
F	2.333051000	-3.167140000	-4.483608000
C	2.937142000	-5.066149000	-1.741803000
C	1.210462000	-2.682467000	-4.995298000
C	-2.152885000	-6.631933000	2.212016000
F	-4.026823000	-5.591222000	-0.650802000
C	-4.823282000	-5.101978000	-1.590948000
H	-1.418046000	-5.933763000	-2.596988000
H	-2.599591000	-1.858435000	0.019330000
C	-3.698761000	-2.115041000	0.419844000
H	-3.669580000	-3.199551000	0.236250000
C	-3.773379000	-1.803939000	1.857524000
H	-3.018792000	-2.265221000	2.499911000
C	-4.735444000	-1.028859000	2.379680000
H	-4.766907000	-0.852001000	3.455593000
C	-5.793861000	-0.368767000	1.561603000
H	-6.796978000	-0.678474000	1.911209000
H	-5.765801000	0.721092000	1.744945000
C	-5.649793000	-0.633498000	0.099240000
H	-6.372771000	-0.153769000	-0.563191000
C	-4.703902000	-1.433854000	-0.413621000
H	-4.658531000	-1.612123000	-1.490204000
² PC			
Co	-0.344949000	-0.056067000	0.050097000
O	0.283099000	0.535379000	3.986450000
O	3.550779000	-0.437151000	1.079139000
O	1.307508000	0.366052000	-3.504817000

O	-3.861769000	1.467092000	1.032138000
N	1.518936000	-0.306661000	0.033844000
C	-2.897848000	0.952788000	-4.229899000
H	-3.087356000	0.993496000	-5.302148000
N	-2.040805000	0.669034000	-0.145967000
C	-2.722405000	0.999080000	0.966246000
C	-1.833749000	0.916421000	2.229758000
N	-0.588423000	0.201906000	1.895837000
C	0.365788000	0.087414000	2.829903000
C	1.617115000	-0.748190000	2.461516000
C	1.170942000	-2.221219000	2.420353000
H	0.720471000	-2.508984000	3.381125000
H	2.041789000	-2.867443000	2.232172000
H	0.442954000	-2.385280000	1.620947000
C	2.308285000	-0.456591000	1.104926000
C	2.138862000	-0.080939000	-1.285213000
C	1.025093000	0.152497000	-2.322718000
N	-0.198034000	0.175701000	-1.769009000
C	-1.402508000	0.482594000	-2.395050000
C	-2.441867000	0.799745000	-1.472673000
C	-3.676113000	1.247075000	-1.954111000
H	-4.450189000	1.514714000	-1.243511000
C	-3.896684000	1.319774000	-3.330145000
H	-4.864360000	1.660108000	-3.698485000
C	-1.646907000	0.540175000	-3.769226000
H	-0.854975000	0.261908000	-4.455533000
C	2.989816000	1.200791000	-1.294757000
H	2.401522000	2.048006000	-0.911606000
H	3.292314000	1.424507000	-2.325471000
H	3.875956000	1.072647000	-0.666352000
C	2.979965000	-1.261692000	-1.777192000
H	3.771374000	-1.484302000	-1.054867000
H	3.422767000	-1.001605000	-2.747063000
H	2.354775000	-2.149456000	-1.921291000
C	2.650965000	-0.603798000	3.577922000
H	2.198560000	-0.877443000	4.536382000
H	3.022204000	0.425235000	3.659030000
H	3.504879000	-1.257663000	3.375202000
C	-2.616865000	0.260257000	3.365627000
H	-2.654468000	-0.824838000	3.217220000
H	-3.643895000	0.647116000	3.360670000
H	-2.141968000	0.473622000	4.328425000
C	-1.559331000	2.394329000	2.570413000
H	-0.959721000	2.466169000	3.481782000
H	-2.512339000	2.920886000	2.711585000
H	-1.015958000	2.874930000	1.742771000
O	-0.998823000	-1.787795000	-0.071747000

Sc	-0.660769000	-3.595904000	-1.135557000	C	-4.909388000	-1.433791000	-0.476560000
S	2.374980000	-4.765034000	-0.228319000	H	-4.492784000	-1.634878000	-1.464207000
S	-1.593907000	-4.345171000	2.170875000	⁴ PC			
S	-0.362791000	-3.103543000	-4.404175000	Co	-0.295295000	0.027101000	0.051655000
S	-3.602028000	-4.321362000	-2.719762000	O	0.297549000	0.583396000	3.997014000
O	-1.475666000	-4.467239000	0.697031000	O	3.572844000	-0.402253000	1.082792000
O	-0.110366000	-2.642508000	-3.006494000	O	1.358628000	0.435659000	-3.510140000
O	-2.711092000	-3.473788000	-1.881926000	O	-3.780862000	1.668215000	1.004173000
O	1.313328000	-3.728630000	-0.330278000	N	1.558769000	-0.223364000	0.023239000
O	-1.983842000	-3.018427000	2.618261000	C	-2.851547000	1.016322000	-4.234337000
O	-0.543441000	-5.019435000	2.909558000	H	-3.043945000	1.040528000	-5.306297000
O	-0.392895000	-5.372828000	-1.858140000	N	-1.979890000	0.799840000	-0.150966000
F	1.269260000	-3.041452000	-6.415552000	C	-2.649314000	1.182740000	0.951834000
O	3.621761000	-4.202236000	0.260978000	C	-1.790968000	1.055648000	2.226726000
F	2.225217000	-4.343877000	-2.846191000	N	-0.531407000	0.377132000	1.877615000
O	-0.104688000	-4.516676000	-4.623016000	C	0.400165000	0.188307000	2.826043000
F	-2.883320000	-6.610513000	2.036761000	C	1.627514000	-0.678516000	2.454079000
F	-5.246048000	-4.567438000	-0.704581000	C	1.125144000	-2.137365000	2.407400000
F	0.648826000	-1.094415000	-5.783210000	H	0.686345000	-2.406972000	3.379313000
F	-4.125232000	-4.861466000	1.825692000	H	1.968833000	-2.812775000	2.203258000
O	1.943612000	-6.009599000	0.382186000	H	0.370701000	-2.279724000	1.624469000
F	-3.350582000	-5.403490000	3.759931000	C	2.332887000	-0.395806000	1.105072000
F	2.305552000	-6.426516000	-2.294951000	C	2.190778000	-0.010287000	-1.291178000
O	-2.916199000	-5.299929000	-3.541662000	C	1.081534000	0.236540000	-2.327516000
F	4.067262000	-5.214180000	-2.176425000	N	-0.145322000	0.258173000	-1.772763000
F	-5.210070000	-6.244151000	-2.053480000	C	-1.351182000	0.573736000	-2.399365000
O	-1.582698000	-2.563872000	-4.978460000	C	-2.385127000	0.905530000	-1.480918000
O	-4.668763000	-3.559080000	-3.344065000	C	-3.624977000	1.333989000	-1.960975000
F	2.096515000	-2.201805000	-4.618896000	H	-4.398018000	1.605094000	-1.250776000
C	2.746833000	-5.215369000	-2.000265000	C	-3.851317000	1.384359000	-3.337205000
C	0.999001000	-2.291505000	-5.345440000	H	-4.824409000	1.706955000	-3.706435000
C	-3.079064000	-5.368857000	2.459036000	C	-1.596832000	0.615943000	-3.772180000
F	-3.591537000	-5.946542000	-0.664696000	H	-0.806957000	0.329996000	-4.456649000
C	-4.458275000	-5.325728000	-1.450643000	C	3.076280000	1.245055000	-1.304326000
H	-0.562640000	-5.559186000	-2.789555000	H	2.512075000	2.110791000	-0.927391000
H	-1.577815000	-1.854981000	0.707612000	H	3.387615000	1.454440000	-2.335327000
C	-4.328344000	-2.065275000	0.646204000	H	3.957159000	1.095422000	-0.673574000
H	-3.533871000	-2.794892000	0.506278000	C	2.988617000	-1.225126000	-1.771792000
C	-4.882131000	-1.839007000	1.928742000	H	3.783196000	-1.461141000	-1.057726000
H	-4.446507000	-2.359319000	2.781795000	H	3.424390000	-0.995241000	-2.752182000
C	-5.936955000	-0.995579000	2.112628000	H	2.330848000	-2.094787000	-1.888691000
H	-6.341890000	-0.830300000	3.111238000	C	2.661815000	-0.574653000	3.574074000
C	-6.564035000	-0.249207000	0.980703000	H	2.197493000	-0.840255000	4.528587000
H	-7.663153000	-0.404240000	0.972673000	H	3.065881000	0.441424000	3.661448000
H	-6.467029000	0.843084000	1.153975000	H	3.494661000	-1.254172000	3.368966000
C	-5.973254000	-0.592030000	-0.346839000	C	-2.595716000	0.271350000	3.262311000
H	-6.397467000	-0.107896000	-1.226933000	H	-2.695283000	-0.773544000	2.940932000

H	-3.602127000	0.703091000	3.335157000
H	-2.101464000	0.307546000	4.237772000
C	-1.566299000	2.500327000	2.702585000
H	-1.043477000	2.511417000	3.661925000
H	-2.537895000	2.999955000	2.806744000
H	-0.968643000	3.053965000	1.963814000
O	-1.118382000	-1.891274000	-0.126022000
Sc	-0.733751000	-3.674252000	-1.111204000
S	2.344844000	-4.750337000	-0.225034000
S	-1.636402000	-4.472077000	2.174295000
S	-0.429800000	-3.142878000	-4.378574000
S	-3.661478000	-4.487667000	-2.720759000
O	-1.527422000	-4.613817000	0.702401000
O	-0.174726000	-2.682783000	-2.982545000
O	-2.783872000	-3.631386000	-1.881853000
O	1.258158000	-3.739382000	-0.317779000
O	-2.058778000	-3.157591000	2.624308000
O	-0.561746000	-5.113276000	2.909904000
O	-0.404902000	-5.448105000	-1.850701000
F	1.209684000	-3.054301000	-6.388620000
O	3.577136000	-4.160827000	0.270984000
F	2.190041000	-4.310603000	-2.838564000
O	-0.159409000	-4.551628000	-4.609153000
F	-2.893647000	-6.760430000	2.043133000
F	-5.312272000	-4.742196000	-0.712277000
F	0.560739000	-1.117633000	-5.750867000
F	-4.162934000	-5.026504000	1.867694000
O	1.947354000	-6.011014000	0.375076000
F	-3.350142000	-5.575680000	3.784409000
F	2.325144000	-6.395730000	-2.306533000
O	-2.963627000	-5.460383000	-3.539831000
F	4.052887000	-5.137912000	-2.171784000
F	-5.257271000	-6.422756000	-2.056190000
O	-1.658057000	-2.611776000	-4.945312000
O	-4.734566000	-3.737871000	-3.350234000
F	2.015470000	-2.209448000	-4.583514000
C	2.731734000	-5.175644000	-1.999617000
C	0.923413000	-2.313817000	-5.317130000
C	-3.097896000	-5.524860000	2.479830000
F	-3.647473000	-6.108131000	-0.660791000
C	-4.514655000	-5.496640000	-1.453060000
H	-0.587861000	-5.637793000	-2.778390000
H	-1.815683000	-1.899529000	0.549784000
C	-4.375495000	-2.209058000	0.635191000
H	-3.637460000	-2.995704000	0.493889000
C	-4.914986000	-1.949267000	1.917977000
H	-4.524691000	-2.509208000	2.767917000

C	-5.890723000	-1.016250000	2.105437000
H	-6.282688000	-0.823948000	3.104255000
C	-6.448995000	-0.210632000	0.978234000
H	-7.556447000	-0.287878000	0.956612000
H	-6.276585000	0.868857000	1.167365000
C	-5.871733000	-0.578122000	-0.348428000
H	-6.246313000	-0.048594000	-1.224291000
C	-4.888784000	-1.513600000	-0.484101000
H	-4.482374000	-1.738396000	-1.471317000

II-5) C-H bond activation by 1-H

² RC			
Co	0.032237000	-0.033077000	0.190889000
O	0.115506000	0.374203000	4.174205000
O	3.815187000	-0.144856000	1.512950000
O	1.913566000	0.637751000	-3.194757000
O	-3.754364000	0.841957000	0.825297000
N	1.872252000	0.064939000	0.345653000
C	-2.269806000	0.413831000	-4.278309000
H	-2.372637000	0.398862000	-5.361635000
N	-1.714183000	0.410932000	-0.152206000
C	-2.553392000	0.608511000	0.894589000
C	-1.821602000	0.553171000	2.240067000
N	-0.423260000	0.174383000	1.973994000
C	0.430974000	0.089729000	3.015933000
C	1.826339000	-0.507889000	2.767207000
C	1.626813000	-2.041290000	2.707300000
H	1.145072000	-2.384904000	3.633022000
H	2.607996000	-2.529006000	2.626322000
H	1.010370000	-2.332991000	1.848984000
C	2.582132000	-0.145236000	1.475549000
C	2.601878000	0.171259000	-0.929348000
C	1.574090000	0.404948000	-2.041723000
N	0.298361000	0.315212000	-1.583589000
C	-0.871462000	0.367465000	-2.327079000
C	-2.031341000	0.395598000	-1.504708000
C	-3.303555000	0.415429000	-2.084652000
H	-4.183973000	0.428149000	-1.452038000
C	-3.410207000	0.419867000	-3.471685000
H	-4.397634000	0.426474000	-3.929581000
C	-0.997707000	0.387929000	-3.718640000
H	-0.107996000	0.350979000	-4.338962000
C	3.590745000	1.341031000	-0.970461000
H	3.101846000	2.263950000	-0.631779000
H	3.919624000	1.482230000	-2.006688000
H	4.453103000	1.141763000	-0.331751000
C	3.298982000	-1.152137000	-1.270275000

H	4.077407000	-1.369327000	-0.532552000	H	1.150345000	-2.280828000	3.616986000
H	3.750028000	-1.081364000	-2.268431000	H	2.674982000	-2.410096000	2.703013000
H	2.562742000	-1.970022000	-1.272256000	H	1.133782000	-2.233626000	1.827965000
C	2.720734000	-0.191568000	3.966141000	C	2.617002000	-0.037103000	1.484200000
H	2.240583000	-0.539356000	4.884846000	C	2.625620000	0.137875000	-0.937960000
H	2.897726000	0.886929000	4.060709000	C	1.600974000	0.311171000	-2.068139000
H	3.686511000	-0.689014000	3.843314000	N	0.311497000	0.232334000	-1.625595000
C	-2.543561000	-0.473841000	3.118580000	C	-0.827169000	0.377489000	-2.359608000
H	-2.435942000	-1.484863000	2.701954000	C	-2.008608000	0.467953000	-1.529326000
H	-3.611402000	-0.227062000	3.153624000	C	-3.280328000	0.569039000	-2.126754000
H	-2.132135000	-0.463712000	4.131040000	H	-4.164132000	0.621161000	-1.501774000
C	-1.952044000	1.959393000	2.846256000	C	-3.365523000	0.592876000	-3.504302000
H	-1.550521000	1.974329000	3.862512000	H	-4.342245000	0.658303000	-3.979019000
H	-3.012100000	2.240937000	2.861635000	C	-0.947202000	0.436254000	-3.758165000
H	-1.405593000	2.688843000	2.233617000	H	-0.059798000	0.357550000	-4.376624000
O	-0.240207000	-1.765215000	-0.018318000	C	3.577663000	1.338808000	-1.020607000
H	-0.991091000	-1.978860000	0.556297000	H	3.063194000	2.253909000	-0.698622000
H	-1.817772000	-2.191034000	-2.890571000	H	3.895555000	1.464981000	-2.061893000
C	-1.196661000	-2.918248000	-3.452264000	H	4.450211000	1.182692000	-0.383961000
H	-1.526008000	-3.902993000	-3.075474000	C	3.373822000	-1.168523000	-1.234468000
C	-1.486932000	-2.803062000	-4.916999000	H	4.138766000	-1.339091000	-0.470008000
H	-2.510853000	-3.012507000	-5.232687000	H	3.851944000	-1.107070000	-2.220843000
C	-0.577849000	-2.447865000	-5.825499000	H	2.671052000	-2.015324000	-1.237647000
H	-0.863280000	-2.375834000	-6.876529000	C	2.745970000	-0.058256000	3.982418000
C	0.846596000	-2.128805000	-5.488141000	H	2.268545000	-0.411966000	4.900536000
H	1.530313000	-2.720761000	-6.122418000	H	2.901863000	1.023657000	4.074648000
H	1.078175000	-1.081469000	-5.762928000	H	3.722373000	-0.536540000	3.866037000
C	1.158777000	-2.344367000	-4.039768000	C	-2.444324000	-0.672575000	3.046937000
H	2.192296000	-2.171863000	-3.734104000	H	-2.232418000	-1.644286000	2.579357000
C	0.249938000	-2.695005000	-3.129762000	H	-3.530959000	-0.539846000	3.103932000
H	0.533796000	-2.795749000	-2.080974000	H	-2.022443000	-0.663584000	4.055688000
⁴ RC				C	-2.109468000	1.823375000	2.850431000
Co	0.049031000	-0.057437000	0.193702000	H	-1.757508000	1.846581000	3.883161000
O	0.125120000	0.463172000	4.177839000	H	-3.190479000	2.009168000	2.826965000
O	3.848799000	0.027793000	1.531941000	H	-1.606023000	2.617649000	2.283209000
O	1.948108000	0.510696000	-3.223762000	O	-0.542604000	-1.940323000	-0.055574000
O	-3.777170000	0.556112000	0.796512000	H	-0.587340000	-2.288931000	0.845254000
N	1.900415000	0.047971000	0.345074000	H	-1.889896000	-2.105778000	-2.851454000
C	-2.208256000	0.533794000	-4.312036000	C	-1.293350000	-2.854729000	-3.411723000
H	-2.314750000	0.539616000	-5.394730000	H	-1.658065000	-3.822466000	-3.023814000
N	-1.704629000	0.453651000	-0.204865000	C	-1.583073000	-2.740968000	-4.876251000
C	-2.558754000	0.480738000	0.862335000	H	-2.617008000	-2.901455000	-5.187975000
C	-1.825647000	0.453059000	2.213373000	C	-0.658193000	-2.444087000	-5.791029000
N	-0.392922000	0.204649000	1.971715000	H	-0.941852000	-2.370686000	-6.842439000
C	0.451511000	0.179626000	3.021624000	C	0.782179000	-2.199007000	-5.460696000
C	1.863347000	-0.393107000	2.781662000	H	1.429396000	-2.845524000	-6.079826000
C	1.687178000	-1.929584000	2.725015000	H	1.073290000	-1.174145000	-5.763643000

C	1.082277000	-2.389372000	-4.005623000
H	2.120331000	-2.241108000	-3.700548000
C	0.159345000	-2.677851000	-3.087837000
H	0.422272000	-2.742604000	-2.029445000
² TS			
Co	-0.023968000	-0.043774000	-0.136997000
O	0.007788000	-0.007031000	3.876419000
O	3.732282000	-0.111555000	1.284539000
O	1.936146000	0.681688000	-3.481525000
O	-3.818032000	0.815258000	0.527552000
N	1.823698000	-0.042645000	0.039760000
C	-2.259910000	1.106991000	-4.563153000
H	-2.344110000	1.307755000	-5.629759000
N	-1.767984000	0.467459000	-0.470107000
C	-2.615838000	0.569451000	0.578163000
C	-1.897890000	0.398526000	1.926006000
N	-0.507255000	-0.008887000	1.658408000
C	0.329537000	-0.192107000	2.698057000
C	1.729059000	-0.774234000	2.405983000
C	1.527835000	-2.286106000	2.151578000
H	1.025838000	-2.742360000	3.016335000
H	2.507964000	-2.768840000	2.031558000
H	0.929881000	-2.464193000	1.251443000
C	2.507947000	-0.241895000	1.183236000
C	2.568630000	0.275335000	-1.190486000
C	1.557970000	0.465452000	-2.332475000
N	0.275056000	0.410107000	-1.903837000
C	-0.887581000	0.637689000	-2.637709000
C	-2.055655000	0.627376000	-1.823855000
C	-3.314122000	0.807730000	-2.403946000
H	-4.199342000	0.784992000	-1.778092000
C	-3.407415000	1.039480000	-3.774042000
H	-4.387749000	1.181020000	-4.225759000
C	-0.999361000	0.910450000	-4.004923000
H	-0.104124000	0.966247000	-4.615359000
C	3.334307000	1.603709000	-1.087184000
H	2.654962000	2.412581000	-0.785464000
H	3.755535000	1.851559000	-2.069175000
H	4.137364000	1.519006000	-0.350886000
C	3.520047000	-0.857276000	-1.589953000
H	4.355052000	-0.917794000	-0.886733000
H	3.902558000	-0.667067000	-2.600390000
H	2.984573000	-1.816115000	-1.595383000
C	2.596747000	-0.616043000	3.653450000
H	2.091689000	-1.068987000	4.511435000
H	2.781610000	0.439868000	3.884751000
H	3.562234000	-1.104748000	3.494563000

C	-2.662687000	-0.651184000	2.737728000
H	-2.582149000	-1.639929000	2.264505000
H	-3.722673000	-0.372914000	2.775390000
H	-2.260271000	-0.712433000	3.752775000
C	-1.984647000	1.768681000	2.617084000
H	-1.582583000	1.706159000	3.631111000
H	-3.034244000	2.085541000	2.653076000
H	-1.413284000	2.515994000	2.049713000
O	-0.466257000	-1.920999000	-0.490429000
H	-1.190981000	-2.155944000	0.111731000
H	-0.493388000	-2.833121000	-1.478053000
C	-0.448477000	-3.633262000	-2.451244000
H	-0.786812000	-4.561250000	-1.972413000
C	-1.372439000	-3.065439000	-3.435285000
H	-2.441623000	-3.186242000	-3.259239000
C	-0.943789000	-2.357352000	-4.496934000
H	-1.662635000	-1.906593000	-5.181463000
C	0.503684000	-2.162388000	-4.805858000
H	0.708234000	-2.447575000	-5.855126000
H	0.755439000	-1.086484000	-4.781636000
C	1.416446000	-2.902659000	-3.885535000
H	2.483618000	-2.864930000	-4.106674000
C	0.968735000	-3.607173000	-2.831364000
H	1.675515000	-4.133858000	-2.189152000
⁴ TS			
Co	0.024399000	-0.090076000	-0.126504000
O	0.026539000	0.113810000	3.884707000
O	3.777702000	-0.144598000	1.284917000
O	1.977707000	0.487443000	-3.496165000
O	-3.806735000	0.620109000	0.485102000
N	1.862108000	-0.124071000	0.048319000
C	-2.167971000	1.209386000	-4.556498000
H	-2.232633000	1.471120000	-5.611119000
N	-1.734764000	0.394765000	-0.502980000
C	-2.590439000	0.457634000	0.544154000
C	-1.869641000	0.349406000	1.899141000
N	-0.440601000	0.095242000	1.655755000
C	0.377972000	-0.070525000	2.716407000
C	1.772053000	-0.677038000	2.462115000
C	1.527558000	-2.198309000	2.317954000
H	1.066231000	-2.582004000	3.238999000
H	2.487443000	-2.713603000	2.174298000
H	0.862705000	-2.415145000	1.472633000
C	2.551667000	-0.253955000	1.202080000
C	2.607085000	0.147802000	-1.196104000
C	1.595622000	0.305963000	-2.343117000
N	0.310266000	0.272628000	-1.917031000

C	-0.833633000	0.585405000	-2.650917000	O	3.792996000	0.067838000	1.369302000
C	-2.011752000	0.587773000	-1.846592000	O	2.019873000	1.093592000	-3.362805000
C	-3.261381000	0.830672000	-2.430485000	O	-3.832784000	0.352036000	0.433905000
H	-4.152383000	0.807253000	-1.812791000	N	1.880728000	0.380922000	0.164398000
C	-3.330164000	1.130037000	-3.786907000	C	-2.142134000	1.169057000	-4.574850000
H	-4.298995000	1.322357000	-4.243907000	H	-2.208481000	1.380398000	-5.640565000
C	-0.919382000	0.943786000	-3.998213000	N	-1.716750000	0.442429000	-0.478838000
H	-0.016995000	1.004940000	-4.596611000	C	-2.611264000	0.361460000	0.536694000
C	3.365106000	1.483698000	-1.135832000	C	-1.923413000	0.356799000	1.913282000
H	2.680068000	2.296922000	-0.859078000	N	-0.476942000	0.181610000	1.692518000
H	3.783124000	1.702388000	-2.125772000	C	0.350808000	0.091260000	2.759174000
H	4.170435000	1.429642000	-0.399049000	C	1.758377000	-0.471279000	2.488028000
C	3.564299000	-0.990408000	-1.561309000	C	1.551260000	-1.970502000	2.154748000
H	4.404903000	-1.023822000	-0.863233000	H	1.020024000	-2.467574000	2.978674000
H	3.938811000	-0.826887000	-2.579512000	H	2.530411000	-2.454716000	2.033918000
H	3.036648000	-1.952607000	-1.536880000	H	0.971534000	-2.094523000	1.230929000
C	2.649589000	-0.439929000	3.689854000	C	2.563978000	0.069271000	1.289231000
H	2.140175000	-0.814070000	4.582095000	C	2.632915000	0.527202000	-1.098515000
H	2.857205000	0.627304000	3.834893000	C	1.635533000	0.855709000	-2.221233000
H	3.604546000	-0.958593000	3.566760000	N	0.350201000	0.763123000	-1.809601000
C	-2.519659000	-0.798098000	2.679313000	C	-0.805632000	0.863166000	-2.596327000
H	-2.253933000	-1.754890000	2.206943000	C	-1.986784000	0.640477000	-1.842000000
H	-3.609284000	-0.678232000	2.656934000	C	-3.231411000	0.655956000	-2.471005000
H	-2.171278000	-0.803797000	3.715864000	H	-4.129860000	0.477914000	-1.889752000
C	-2.108473000	1.694917000	2.603973000	C	-3.298296000	0.918497000	-3.841012000
H	-1.717254000	1.663272000	3.623919000	H	-4.269304000	0.933991000	-4.332483000
H	-3.186250000	1.898177000	2.623630000	C	-0.887692000	1.139543000	-3.961698000
H	-1.611141000	2.505153000	2.054078000	H	0.019292000	1.318490000	-4.529249000
O	-0.796878000	-2.097171000	-0.109070000	C	3.700805000	1.622493000	-1.078474000
H	-1.759992000	-1.994705000	-0.157881000	H	3.290774000	2.547992000	-0.653323000
H	-0.632748000	-2.926364000	-1.464521000	H	4.012948000	1.823501000	-2.110286000
C	-0.511492000	-3.534460000	-2.456328000	H	4.565641000	1.317445000	-0.487364000
H	-0.805228000	-4.545516000	-2.131358000	C	3.228513000	-0.833561000	-1.494045000
C	-1.439414000	-2.960048000	-3.451111000	H	3.976755000	-1.148112000	-0.758488000
H	-2.508276000	-3.068774000	-3.262782000	H	3.693887000	-0.768120000	-2.485793000
C	-1.018013000	-2.294920000	-4.538537000	H	2.421358000	-1.584314000	-1.528819000
H	-1.742908000	-1.861544000	-5.228777000	C	2.598103000	-0.362470000	3.757237000
C	0.424729000	-2.113854000	-4.872174000	H	2.075638000	-0.846326000	4.588098000
H	0.624907000	-2.483864000	-5.895517000	H	2.774380000	0.684491000	4.032443000
H	0.663217000	-1.038223000	-4.935754000	H	3.566923000	-0.845306000	3.601909000
C	1.350277000	-2.766016000	-3.900427000	C	-2.517916000	-0.782006000	2.742947000
H	2.418745000	-2.691306000	-4.107769000	H	-2.226758000	-1.753994000	2.322967000
C	0.917907000	-3.437911000	-2.823811000	H	-3.611278000	-0.706101000	2.720549000
H	1.636832000	-3.906786000	-2.150061000	H	-2.171051000	-0.725148000	3.778071000
² PC				C	-2.263090000	1.716245000	2.542487000
Co	0.058748000	0.371784000	-0.045778000	H	-1.885972000	1.765870000	3.566873000
O	0.005388000	0.308060000	3.921150000	H	-3.352173000	1.850278000	2.546794000

H	-1.813195000	2.528715000	1.955239000	H	-3.889561000	1.945406000	-1.859623000
O	-0.263521000	-2.218821000	-0.912038000	C	-3.105583000	1.964446000	-3.879089000
H	-0.907475000	-1.836530000	-1.526545000	H	-4.041009000	2.307606000	-4.317458000
H	0.229084000	-2.854079000	-1.451394000	C	-0.796562000	1.282557000	-4.146281000
C	-0.749533000	-4.631878000	-3.327758000	H	0.069468000	1.093783000	-4.772404000
H	-1.180254000	-5.589874000	-3.051059000	C	3.281677000	1.688651000	-1.046443000
C	-1.586404000	-3.533151000	-3.635823000	H	2.496403000	2.421416000	-0.812272000
H	-2.667302000	-3.663133000	-3.588984000	H	3.819560000	2.024793000	-1.942356000
C	-1.072173000	-2.315004000	-3.980250000	H	3.979995000	1.629014000	-0.204900000
H	-1.735202000	-1.479647000	-4.207997000	C	3.756332000	-0.693311000	-1.678395000
C	0.402869000	-2.073247000	-4.062558000	H	4.641321000	-0.554708000	-1.052314000
H	0.673994000	-1.682670000	-5.065243000	H	4.025208000	-0.539356000	-2.730735000
H	0.691514000	-1.228121000	-3.401951000	H	3.407654000	-1.726126000	-1.547647000
C	1.224389000	-3.275876000	-3.726164000	C	2.409793000	-1.452973000	3.309215000
H	2.308135000	-3.170434000	-3.761336000	H	1.795729000	-1.981205000	4.044947000
C	0.657379000	-4.470104000	-3.381160000	H	2.794416000	-0.539474000	3.776233000
H	1.297592000	-5.318274000	-3.140249000	H	3.264500000	-2.077878000	3.030526000
⁴ PC				C	-2.660971000	-0.438353000	2.354676000
Co	0.084873000	0.322568000	-0.270030000	H	-2.617634000	-1.318880000	1.699465000
O	0.016164000	-0.286558000	3.681993000	H	-3.697955000	-0.085894000	2.405292000
O	3.688426000	-0.387229000	1.199554000	H	-2.321414000	-0.717296000	3.355933000
O	2.081271000	0.643802000	-3.626275000	C	-1.775639000	1.898008000	2.705388000
O	-3.588869000	1.506521000	0.422151000	H	-1.433711000	1.618759000	3.705668000
N	1.856615000	-0.128450000	-0.141010000	H	-2.792924000	2.304665000	2.764223000
C	-2.002213000	1.725847000	-4.692882000	H	-1.112491000	2.677548000	2.306465000
H	-2.074345000	1.880503000	-5.767871000	O	-1.550623000	-1.810414000	-0.963813000
N	-1.571952000	1.038040000	-0.590085000	H	-1.801251000	-1.257851000	-1.717048000
C	-2.424800000	1.118810000	0.456892000	H	-1.256028000	-2.646574000	-1.350799000
C	-1.777779000	0.674367000	1.780347000	C	0.244809000	-4.585965000	-1.802917000
N	-0.420948000	0.177883000	1.486889000	H	0.368362000	-5.338312000	-1.028831000
C	0.326099000	-0.332395000	2.491100000	C	-0.883421000	-4.620942000	-2.661605000
C	1.575340000	-1.137099000	2.072901000	H	-1.617210000	-5.416816000	-2.537950000
C	1.050097000	-2.466278000	1.477248000	C	-1.074918000	-3.673951000	-3.628738000
H	0.449206000	-2.993825000	2.231631000	H	-1.951617000	-3.716914000	-4.272581000
H	1.897470000	-3.112802000	1.205808000	C	-0.108426000	-2.554411000	-3.841970000
H	0.432147000	-2.305978000	0.583042000	H	0.199277000	-2.509198000	-4.905313000
C	2.476036000	-0.479816000	1.009382000	H	-0.610641000	-1.567078000	-3.709518000
C	2.660083000	0.302301000	-1.295207000	C	1.090608000	-2.627291000	-2.956906000
C	1.686477000	0.516388000	-2.471865000	H	1.873636000	-1.892743000	-3.131378000
N	0.407344000	0.643133000	-2.039266000	C	1.226248000	-3.581946000	-1.990967000
C	-0.708549000	1.078631000	-2.769213000	H	2.113887000	-3.587066000	-1.356527000
C	-1.836034000	1.317017000	-1.938280000				
C	-3.032753000	1.763611000	-2.499452000				

III)C-H bond activation of substrates with normal C-H bond mediated by 1

III-1) C-H bond activation of toluene by 1

² RC	Co	0.204223000	0.063770000	0.008043000
-----------------	----	-------------	-------------	-------------

O	0.259857000	-0.545305000	3.991185000	H	-3.408954000	0.413127000	3.090959000
O	3.820210000	1.009386000	1.504052000	H	-2.085996000	1.595339000	2.952384000
O	1.911529000	1.413550000	-3.293769000	O	0.357366000	-1.587903000	-0.360505000
O	-3.684404000	-0.074629000	0.689625000	H	-1.748686000	-2.509464000	-0.815520000
N	1.989400000	0.571350000	0.209333000	C	-2.732078000	-2.967516000	-1.002310000
C	-2.237122000	0.686557000	-4.411890000	H	-2.876814000	-3.796635000	-0.296017000
H	-2.353975000	0.815170000	-5.487277000	H	-3.479129000	-2.196831000	-0.754231000
N	-1.619236000	0.175651000	-0.308560000	C	-3.857290000	-4.905167000	-4.087956000
C	-2.448881000	-0.051783000	0.721477000	C	-3.706435000	-4.501224000	-2.763339000
C	-1.691438000	-0.333167000	2.032337000	C	-2.873747000	-3.428588000	-2.424485000
N	-0.259159000	-0.073099000	1.815537000	C	-2.186286000	-2.777291000	-3.454938000
C	0.595016000	-0.288758000	2.823402000	C	-2.337697000	-3.173234000	-4.780859000
C	2.109405000	-0.333035000	2.501560000	C	-3.174375000	-4.239924000	-5.104593000
C	2.378191000	-1.802831000	2.103271000	H	-4.509285000	-5.744396000	-4.327335000
H	2.084007000	-2.464172000	2.931291000	H	-4.243624000	-5.026923000	-1.972163000
H	3.451704000	-1.946111000	1.910685000	H	-1.533829000	-1.937853000	-3.206978000
H	1.808541000	-2.073583000	1.204044000	H	-1.797273000	-2.643040000	-5.564850000
C	2.690813000	0.516791000	1.347958000	H	-3.291292000	-4.553306000	-6.140832000
C	2.613164000	1.124312000	-1.000882000	⁴ RC			
C	1.589587000	1.071930000	-2.151469000	Co	-0.298413000	-0.464834000	0.167020000
N	0.373159000	0.689069000	-1.731865000	O	0.674640000	0.465449000	3.986624000
C	-0.806639000	0.609612000	-2.466902000	O	3.714365000	-0.297894000	0.710878000
C	-1.944613000	0.336527000	-1.652608000	O	0.864052000	-0.084446000	-3.597031000
C	-3.212954000	0.262909000	-2.236368000	O	-3.831525000	0.766300000	1.455626000
H	-4.074566000	0.064405000	-1.606842000	N	1.565430000	-0.380777000	-0.066522000
C	-3.350470000	0.437316000	-3.613723000	C	-3.466061000	-0.134968000	-3.829888000
H	-4.339733000	0.367326000	-4.064258000	H	-3.786965000	-0.238940000	-4.865764000
C	-0.964394000	0.778284000	-3.845928000	N	-2.083606000	0.091477000	0.109732000
H	-0.091630000	0.984148000	-4.457254000	C	-2.651390000	0.450860000	1.271322000
C	2.985327000	2.607828000	-0.850864000	C	-1.645279000	0.504212000	2.441398000
H	2.111742000	3.182646000	-0.512248000	N	-0.329067000	0.036380000	1.976792000
H	3.302929000	3.000454000	-1.825470000	C	0.708524000	0.035397000	2.823189000
H	3.791244000	2.726360000	-0.122068000	C	2.001404000	-0.668395000	2.343253000
C	3.842954000	0.315332000	-1.423846000	C	1.722236000	-2.185572000	2.415656000
H	4.638440000	0.422156000	-0.680018000	H	1.423658000	-2.462314000	3.437334000
H	4.198570000	0.674292000	-2.397577000	H	2.636586000	-2.742956000	2.164526000
H	3.584711000	-0.748315000	-1.517293000	H	0.926313000	-2.479996000	1.720021000
C	2.896806000	-0.038004000	3.778635000	C	2.491978000	-0.392421000	0.900378000
H	2.556346000	-0.699393000	4.580044000	C	1.988615000	-0.299281000	-1.474382000
H	2.759043000	1.000613000	4.107083000	C	0.738127000	-0.238447000	-2.378494000
H	3.964574000	-0.194470000	3.598840000	N	-0.410275000	-0.319768000	-1.688292000
C	-1.915442000	-1.826506000	2.318917000	C	-1.706877000	-0.178200000	-2.184253000
H	-1.412026000	-2.411252000	1.535645000	C	-2.663043000	0.067033000	-1.161733000
H	-2.989964000	-2.055524000	2.307101000	C	-4.007603000	0.239073000	-1.495844000
H	-1.495232000	-2.088695000	3.296077000	H	-4.730866000	0.439196000	-0.712088000
C	-2.319540000	0.535513000	3.125360000	C	-4.400412000	0.136507000	-2.833731000
H	-1.943124000	0.249312000	4.109785000	H	-5.451548000	0.261312000	-3.091189000

C	-2.114687000	-0.287431000	-3.512606000	N	-1.859984000	0.427414000	-0.217550000
H	-1.378655000	-0.540068000	-4.271927000	C	-2.653799000	0.165304000	0.835409000
C	2.794643000	0.973924000	-1.769665000	C	-1.857900000	-0.140169000	2.120561000
H	2.242528000	1.859225000	-1.423946000	N	-0.420783000	-0.073049000	1.818622000
H	2.940544000	1.058441000	-2.853134000	C	0.458145000	-0.339396000	2.788062000
H	3.761777000	0.940160000	-1.261359000	C	1.929133000	-0.610300000	2.381051000
C	2.793157000	-1.533239000	-1.897491000	C	1.957234000	-2.116125000	2.031425000
H	3.738363000	-1.574775000	-1.345800000	H	1.606103000	-2.699038000	2.895824000
H	2.998369000	-1.481214000	-2.975097000	H	2.987313000	-2.426157000	1.800201000
H	2.222917000	-2.452162000	-1.695937000	H	1.309312000	-2.318329000	1.169001000
C	3.131422000	-0.350424000	3.321096000	C	2.554764000	0.090562000	1.151822000
H	2.830041000	-0.624778000	4.336597000	C	2.411611000	0.600445000	-1.218449000
H	3.377668000	0.718548000	3.317903000	C	1.315175000	0.696062000	-2.301369000
H	4.030928000	-0.906633000	3.040248000	N	0.082630000	0.576323000	-1.787335000
C	-2.196360000	-0.378203000	3.566148000	C	-1.138406000	0.752030000	-2.428855000
H	-2.205981000	-1.431546000	3.253639000	C	-2.245649000	0.680007000	-1.532870000
H	-3.225399000	-0.074693000	3.794968000	C	-3.543249000	0.884783000	-2.013160000
H	-1.576198000	-0.279522000	4.462144000	H	-4.377921000	0.830227000	-1.321582000
C	-1.613228000	1.973401000	2.889812000	C	-3.744362000	1.158927000	-3.368436000
H	-0.998773000	2.081752000	3.787158000	H	-4.757020000	1.318200000	-3.736469000
H	-2.637135000	2.311033000	3.092514000	C	-1.361689000	1.020507000	-3.782757000
H	-1.191686000	2.600062000	2.091175000	H	-0.512988000	1.077278000	-4.456690000
O	-0.623483000	-2.361346000	0.276971000	C	3.037747000	2.004141000	-1.168067000
H	-2.311959000	-2.961347000	-1.113622000	H	2.298875000	2.732583000	-0.804696000
C	-2.856287000	-3.307749000	-2.003464000	H	3.343239000	2.297673000	-2.180546000
H	-3.335741000	-4.268637000	-1.765204000	H	3.903454000	2.016296000	-0.501687000
H	-3.657261000	-2.583581000	-2.213344000	C	3.452665000	-0.421876000	-1.680788000
C	0.295469000	-3.268621000	-4.126379000	H	4.306524000	-0.426695000	-0.996641000
C	-0.553129000	-3.260427000	-3.021248000	H	3.791441000	-0.165701000	-2.692127000
C	-1.931929000	-3.416610000	-3.181410000	H	3.013231000	-1.428307000	-1.705784000
C	-2.439125000	-3.607969000	-4.471108000	C	2.831009000	-0.384364000	3.594446000
C	-1.593774000	-3.628389000	-5.575399000	H	2.456942000	-0.964941000	4.442174000
C	-0.219949000	-3.451647000	-5.407357000	H	2.855247000	0.673450000	3.887986000
H	1.364546000	-3.109689000	-3.985048000	H	3.853982000	-0.691524000	3.357899000
H	-0.165214000	-3.081473000	-2.014610000	C	-2.243792000	-1.561900000	2.549917000
H	-3.516626000	-3.716445000	-4.608326000	H	-1.862289000	-2.273080000	1.803964000
H	-2.006959000	-3.771138000	-6.573463000	H	-3.335802000	-1.653229000	2.610944000
H	0.442106000	-3.453158000	-6.272066000	H	-1.797035000	-1.789707000	3.523777000
² TS				C	-2.314198000	0.879383000	3.172016000
Co	-0.066382000	0.039651000	-0.014570000	H	-1.878201000	0.639990000	4.144938000
O	0.168902000	-0.488656000	3.988617000	H	-3.409568000	0.861495000	3.237555000
O	3.757297000	0.398281000	1.212516000	H	-2.001406000	1.892551000	2.883306000
O	1.620131000	0.925887000	-3.477180000	O	-0.193062000	-1.692755000	-0.368381000
O	-3.889430000	0.149350000	0.845234000	H	-1.332283000	-2.055477000	-0.669510000
N	1.793200000	0.206356000	0.057189000	C	-2.478339000	-2.585932000	-1.008290000
C	-2.663664000	1.223469000	-4.244488000	H	-2.631830000	-3.325688000	-0.213440000
H	-2.829191000	1.434494000	-5.300224000	H	-3.191431000	-1.755714000	-0.943852000

C	-1.638782000	-5.005499000	-3.785766000	H	3.634222000	-1.456759000	-1.557389000
C	-1.847936000	-4.479231000	-2.517132000	H	2.817216000	-1.404479000	-3.152179000
C	-2.309045000	-3.160227000	-2.342465000	H	2.144047000	-2.400328000	-1.838597000
C	-2.542677000	-2.388284000	-3.496680000	C	3.061902000	-0.447079000	3.157958000
C	-2.329998000	-2.915132000	-4.764173000	H	2.781752000	-0.761805000	4.167881000
C	-1.877168000	-4.226668000	-4.918977000	H	3.306781000	0.621651000	3.190530000
H	-1.289634000	-6.031400000	-3.894878000	H	3.956375000	-0.990168000	2.837626000
H	-1.661691000	-5.093846000	-1.635234000	C	-2.256259000	-0.510684000	3.516111000
H	-2.901240000	-1.365395000	-3.380064000	H	-2.264705000	-1.552874000	3.168069000
H	-2.521386000	-2.297807000	-5.641477000	H	-3.282712000	-0.222639000	3.774816000
H	-1.712575000	-4.638410000	-5.913072000	H	-1.620135000	-0.438417000	4.403225000
⁴ TS				C	-1.702636000	1.868013000	2.911281000
Co	-0.433504000	-0.455241000	0.067798000	H	-1.078917000	1.951828000	3.804300000
O	0.616612000	0.337774000	3.901571000	H	-2.725624000	2.193132000	3.137839000
O	3.585029000	-0.262255000	0.543914000	H	-1.294688000	2.523233000	2.128527000
O	0.670941000	-0.112799000	-3.719907000	O	-0.782776000	-2.373080000	0.092122000
O	-3.943482000	0.696469000	1.487340000	H	-1.567056000	-2.621521000	-0.780861000
N	1.425616000	-0.384464000	-0.198833000	C	-2.346163000	-3.135560000	-1.708585000
C	-3.660697000	0.286504000	-3.842496000	H	-2.628897000	-4.043817000	-1.161983000
H	-3.993603000	0.319700000	-4.879297000	H	-3.208713000	-2.481335000	-1.883883000
N	-2.214444000	0.117109000	0.074049000	C	0.568869000	-4.180960000	-3.869079000
C	-2.763836000	0.404692000	1.263600000	C	-0.229520000	-3.939760000	-2.757714000
C	-1.734291000	0.414330000	2.412562000	C	-1.509140000	-3.374297000	-2.894443000
N	-0.427617000	-0.028335000	1.899527000	C	-1.954867000	-3.056350000	-4.187131000
C	0.628652000	-0.051847000	2.723834000	C	-1.163047000	-3.313426000	-5.301952000
C	1.912948000	-0.731728000	2.192923000	C	0.103750000	-3.875069000	-5.149106000
C	1.635390000	-2.251133000	2.211674000	H	1.563088000	-4.607204000	-3.738455000
H	1.371103000	-2.567534000	3.231689000	H	0.134637000	-4.153457000	-1.752232000
H	2.543065000	-2.796183000	1.912501000	H	-2.939125000	-2.601736000	-4.305684000
H	0.817784000	-2.515228000	1.529214000	H	-1.534613000	-3.070001000	-6.296460000
C	2.369590000	-0.397144000	0.752479000	H	0.727555000	-4.067502000	-6.020281000
C	1.824421000	-0.265056000	-1.610363000	² PC			
C	0.559517000	-0.206072000	-2.492742000	Co	-0.032715000	0.097289000	-0.088747000
N	-0.576392000	-0.189887000	-1.777565000	O	0.200711000	-0.758346000	3.853088000
C	-1.873716000	0.028168000	-2.241032000	O	3.786659000	0.426063000	1.154179000
C	-2.812417000	0.190800000	-1.184371000	O	1.637714000	1.119048000	-3.519433000
C	-4.162747000	0.388760000	-1.475800000	O	-3.864081000	0.299861000	0.827067000
H	-4.870831000	0.505043000	-0.662177000	N	1.829687000	0.242088000	-0.020848000
C	-4.580795000	0.427764000	-2.809115000	C	-2.653839000	1.271135000	-4.304223000
H	-5.636605000	0.574134000	-3.033343000	H	-2.821446000	1.475448000	-5.360922000
C	-2.304576000	0.092090000	-3.565495000	N	-1.846139000	0.413595000	-0.289517000
H	-1.582871000	-0.043999000	-4.363917000	C	-2.631162000	0.208076000	0.780416000
C	2.579799000	1.044257000	-1.891126000	C	-1.828616000	-0.226648000	2.026892000
H	1.992664000	1.902123000	-1.533683000	N	-0.388488000	-0.106761000	1.739276000
H	2.724253000	1.149288000	-2.973354000	C	0.490146000	-0.472354000	2.677102000
H	3.547235000	1.040342000	-1.381761000	C	1.970082000	-0.678670000	2.256428000
C	2.665137000	-1.460374000	-2.066655000	C	2.029653000	-2.161694000	1.821513000

H	1.706697000	-2.800593000	2.656817000	H	-2.599552000	-5.133188000	-1.246014000
H	3.064009000	-2.431010000	1.559154000	H	-2.784870000	-1.330547000	-3.292216000
H	1.375048000	-2.328832000	0.957384000	H	-1.550619000	-2.303426000	-5.195724000
C	2.589295000	0.098222000	1.068492000	H	-0.840510000	-4.692048000	-5.147865000
C	2.435893000	0.716893000	-1.273973000	4PC			
C	1.335770000	0.844084000	-2.351837000	Co	-0.275174000	-0.439464000	0.150626000
N	0.104824000	0.696656000	-1.841318000	O	0.671027000	0.568518000	3.947129000
C	-1.120069000	0.845986000	-2.482523000	O	3.725436000	-0.334217000	0.762423000
C	-2.230942000	0.722297000	-1.593004000	O	0.949105000	-0.037496000	-3.598564000
C	-3.530194000	0.915276000	-2.075104000	O	-3.840307000	0.761835000	1.385710000
H	-4.365959000	0.838955000	-1.386300000	N	1.589434000	-0.378243000	-0.058666000
C	-3.734710000	1.186071000	-3.430445000	C	-3.396914000	-0.241894000	-3.881168000
H	-4.749674000	1.325407000	-3.800076000	H	-3.699660000	-0.361697000	-4.920921000
C	-1.347622000	1.108806000	-3.836666000	N	-2.062174000	0.111221000	0.066865000
H	-0.498336000	1.193614000	-4.507113000	C	-2.650749000	0.472729000	1.215526000
C	3.036186000	2.127779000	-1.152736000	C	-1.652314000	0.570002000	2.390813000
H	2.282555000	2.824654000	-0.758422000	N	-0.338855000	0.069324000	1.954411000
H	3.342036000	2.476902000	-2.147579000	C	0.696787000	0.085915000	2.804950000
H	3.897180000	2.120967000	-0.479522000	C	1.966361000	-0.677275000	2.354954000
C	3.497057000	-0.259295000	-1.786950000	C	1.605066000	-2.178859000	2.399932000
H	4.343468000	-0.288835000	-1.093729000	H	1.274325000	-2.450236000	3.413627000
H	3.841839000	0.058855000	-2.778514000	H	2.495805000	-2.780176000	2.163963000
H	3.074126000	-1.269611000	-1.872603000	H	0.809024000	-2.418827000	1.686198000
C	2.864195000	-0.504342000	3.484504000	C	2.498487000	-0.407534000	0.926094000
H	2.492050000	-1.130484000	4.299941000	C	2.036094000	-0.292352000	-1.459372000
H	2.877679000	0.538158000	3.829858000	C	0.801137000	-0.194628000	-2.382035000
H	3.891667000	-0.788683000	3.238308000	N	-0.355740000	-0.272191000	-1.709525000
C	-2.200104000	-1.702231000	2.246806000	C	-1.651437000	-0.185118000	-2.221396000
H	-1.823550000	-2.286471000	1.394794000	C	-2.629188000	0.012029000	-1.206414000
H	-3.291785000	-1.811916000	2.305639000	C	-3.981242000	0.071952000	-1.549904000
H	-1.741640000	-2.070791000	3.170789000	H	-4.722417000	0.221246000	-0.771333000
C	-2.302659000	0.630428000	3.203739000	C	-4.357141000	-0.062577000	-2.889676000
H	-1.897626000	0.246811000	4.142614000	H	-5.413692000	-0.026626000	-3.152721000
H	-3.398975000	0.616590000	3.236056000	C	-2.040710000	-0.297747000	-3.554967000
H	-1.973549000	1.671259000	3.077373000	H	-1.283679000	-0.469649000	-4.314772000
O	-0.178114000	-1.662412000	-0.551789000	C	2.886084000	0.955406000	-1.734245000
H	-1.110219000	-1.757243000	-0.795698000	H	2.365386000	1.854002000	-1.374661000
C	-3.461923000	-2.596026000	-1.019203000	H	3.033801000	1.051095000	-2.816679000
H	-3.693526000	-3.196440000	-0.142479000	H	3.852367000	0.883172000	-1.229459000
H	-3.778973000	-1.554890000	-1.015811000	C	2.799419000	-1.552864000	-1.881519000
C	-1.685295000	-5.054844000	-3.190131000	H	3.722183000	-1.649439000	-1.299762000
C	-2.369587000	-4.517168000	-2.115663000	H	3.044123000	-1.492866000	-2.950409000
C	-2.786049000	-3.155896000	-2.116295000	H	2.178431000	-2.446419000	-1.715834000
C	-2.469741000	-2.373573000	-3.264579000	C	3.085231000	-0.421616000	3.361172000
C	-1.781870000	-2.924117000	-4.330603000	H	2.744379000	-0.686453000	4.366956000
C	-1.382346000	-4.265556000	-4.306369000	H	3.385917000	0.633066000	3.371706000
H	-1.377643000	-6.099228000	-3.166954000	H	3.962282000	-1.022231000	3.100691000

C	-2.212528000	-0.260968000	3.548611000	C	-0.636221000	-3.357841000	-3.051104000
H	-2.217265000	-1.326729000	3.281608000	C	-2.024933000	-3.659621000	-3.169147000
H	-3.243411000	0.050906000	3.755832000	C	-2.603440000	-3.598578000	-4.468977000
H	-1.598470000	-0.123285000	4.443601000	C	-1.839627000	-3.279850000	-5.575207000
C	-1.609752000	2.056002000	2.777890000	C	-0.474478000	-3.001162000	-5.436682000
H	-0.994257000	2.196718000	3.670669000	H	1.167584000	-2.783965000	-4.051275000
H	-2.631123000	2.409792000	2.966835000	H	-0.193644000	-3.343101000	-2.052714000
H	-1.183587000	2.646300000	1.954271000	H	-3.667353000	-3.811813000	-4.576086000
O	-0.764385000	-2.364442000	0.142654000	H	-2.302381000	-3.245731000	-6.560608000
H	-1.421684000	-2.355312000	-0.568673000	H	0.123894000	-2.750290000	-6.310441000
C	-2.797431000	-4.004583000	-2.051881000				
H	-2.350279000	-4.098341000	-1.065590000				
H	-3.857489000	-4.223949000	-2.151551000				
C	0.113902000	-3.035365000	-4.165876000				

IV) C-H bond activation of substrates with acidic C-H bond by 1

IV-1) C-H bond activation of acetonitrile by 1

²RC

Co	0.120768000	0.031551000	-0.005719000
O	-0.026657000	-0.190646000	4.015549000
O	3.840504000	0.172184000	1.529589000
O	2.149695000	0.733187000	-3.324953000
O	-3.712543000	0.793374000	0.543538000
N	1.970725000	0.117277000	0.220218000
C	-2.030475000	0.908591000	-4.531909000
H	-2.095502000	0.988835000	-5.616174000
N	-1.616706000	0.554637000	-0.388528000
C	-2.496722000	0.582247000	0.623852000
C	-1.843080000	0.268848000	1.980753000
N	-0.388817000	0.163512000	1.788760000
C	0.376788000	-0.146390000	2.842808000
C	1.834594000	-0.596052000	2.581365000
C	1.728230000	-2.116186000	2.318435000
H	1.255277000	-2.602834000	3.183811000
H	2.733835000	-2.542242000	2.188927000
H	1.130153000	-2.313748000	1.418888000
C	2.624156000	-0.025347000	1.380966000
C	2.729297000	0.415645000	-1.002429000
C	1.740277000	0.541280000	-2.176552000
N	0.460102000	0.471791000	-1.774766000
C	-0.692219000	0.621600000	-2.543301000
C	-1.875117000	0.683325000	-1.751568000
C	-3.115584000	0.873244000	-2.367934000
H	-4.010517000	0.933484000	-1.756286000
C	-3.184701000	0.981303000	-3.756860000
H	-4.153943000	1.120177000	-4.233747000
C	-0.782493000	0.730826000	-3.933488000

H	0.123508000	0.682158000	-4.528789000
C	3.461691000	1.764553000	-0.928971000
H	2.757335000	2.562701000	-0.655989000
H	3.886000000	1.997819000	-1.913704000
H	4.256970000	1.722328000	-0.180183000
C	3.722803000	-0.700384000	-1.343984000
H	4.521876000	-0.737679000	-0.597587000
H	4.153654000	-0.512445000	-2.335251000
H	3.211982000	-1.672509000	-1.364709000
C	2.651490000	-0.389423000	3.857289000
H	2.144481000	-0.871914000	4.697659000
H	2.767129000	0.676575000	4.092946000
H	3.650619000	-0.817059000	3.732516000
C	-2.418817000	-1.089431000	2.409928000
H	-2.041198000	-1.863909000	1.726250000
H	-3.515643000	-1.064571000	2.361640000
H	-2.101742000	-1.327092000	3.430424000
C	-2.260263000	1.373966000	2.955959000
H	-1.961151000	1.119974000	3.975428000
H	-3.348799000	1.498576000	2.904197000
H	-1.789834000	2.326458000	2.675532000
O	-0.137468000	-1.625362000	-0.244633000
H	-2.142604000	-2.048500000	-0.589353000
C	-3.176673000	-2.245386000	-0.932562000
H	-3.579430000	-3.113493000	-0.398159000
H	-3.786979000	-1.362943000	-0.696395000
C	-3.177922000	-2.494240000	-2.356945000
N	-3.163853000	-2.705472000	-3.496333000

⁴RC

Co	0.129686000	-0.020040000	0.003191000
O	0.009320000	-0.073061000	4.046975000

O	3.849565000	0.263433000	1.550377000	H	-1.794866000	2.282941000	2.671331000
O	2.145298000	0.654626000	-3.326059000	O	-0.164650000	-1.912034000	-0.253754000
O	-3.715635000	0.677908000	0.543330000	H	-2.227523000	-2.167819000	-0.612799000
N	1.981842000	0.103401000	0.241855000	C	-3.250814000	-2.275716000	-1.015170000
C	-2.029639000	1.003568000	-4.527435000	H	-3.736698000	-3.133487000	-0.536398000
H	-2.091053000	1.124651000	-5.608073000	H	-3.811082000	-1.362187000	-0.774753000
N	-1.622344000	0.483996000	-0.400947000	C	-3.195623000	-2.474088000	-2.446753000
C	-2.492827000	0.499693000	0.616616000	N	-3.143078000	-2.646916000	-3.591303000
C	-1.829227000	0.222196000	1.982247000	² TS			
N	-0.367946000	0.143273000	1.803091000	Co	0.053082000	0.047025000	-0.027409000
C	0.405848000	-0.084391000	2.872473000	O	-0.066559000	-0.157430000	3.986866000
C	1.861809000	-0.542035000	2.615000000	O	3.776590000	0.043745000	1.478500000
C	1.745195000	-2.062820000	2.362160000	O	2.076923000	0.760547000	-3.335437000
H	1.266786000	-2.543886000	3.227620000	O	-3.756919000	0.831157000	0.543120000
H	2.745252000	-2.501085000	2.231602000	N	1.897129000	0.079222000	0.188903000
H	1.146545000	-2.267062000	1.464475000	C	-2.098180000	0.998938000	-4.520938000
C	2.640727000	0.026316000	1.405503000	H	-2.168558000	1.097475000	-5.603096000
C	2.723575000	0.393638000	-0.996325000	N	-1.661942000	0.606439000	-0.389661000
C	1.730276000	0.478315000	-2.176701000	C	-2.547240000	0.621829000	0.628765000
N	0.448297000	0.401522000	-1.784590000	C	-1.889387000	0.319923000	1.981161000
C	-0.700167000	0.610650000	-2.551615000	N	-0.443781000	0.161661000	1.762113000
C	-1.880653000	0.672225000	-1.759226000	C	0.330442000	-0.155176000	2.814573000
C	-3.115470000	0.913508000	-2.365423000	C	1.762779000	-0.661603000	2.547493000
H	-4.008745000	0.971135000	-1.750843000	C	1.597480000	-2.177222000	2.282808000
C	-3.181609000	1.073328000	-3.751317000	H	1.129500000	-2.646825000	3.159886000
H	-4.147345000	1.251775000	-4.222035000	H	2.585568000	-2.635101000	2.132227000
C	-0.785054000	0.774153000	-3.935214000	H	0.971957000	-2.355190000	1.399091000
H	0.119788000	0.725762000	-4.532123000	C	2.555559000	-0.109343000	1.346429000
C	3.425157000	1.760681000	-0.957159000	C	2.666365000	0.389185000	-1.025562000
H	2.704700000	2.547233000	-0.692177000	C	1.678365000	0.566507000	-2.187677000
H	3.832740000	1.983628000	-1.951027000	N	0.394997000	0.532126000	-1.775913000
H	4.229404000	1.754525000	-0.217135000	C	-0.755286000	0.692244000	-2.543796000
C	3.738666000	-0.709358000	-1.311407000	C	-1.933175000	0.737239000	-1.749266000
H	4.533824000	-0.716203000	-0.559359000	C	-3.180185000	0.912333000	-2.355224000
H	4.172549000	-0.534908000	-2.303705000	H	-4.073476000	0.946600000	-1.740891000
H	3.245355000	-1.690940000	-1.313876000	C	-3.252080000	1.045630000	-3.740801000
C	2.684043000	-0.331001000	3.885049000	H	-4.223524000	1.179836000	-4.214014000
H	2.179605000	-0.806388000	4.731177000	C	-0.847010000	0.821813000	-3.932357000
H	2.803408000	0.735789000	4.113075000	H	0.056030000	0.787657000	-4.532419000
H	3.681803000	-0.762004000	3.758984000	C	3.424988000	1.721570000	-0.918799000
C	-2.366307000	-1.142161000	2.437956000	H	2.737611000	2.526536000	-0.624464000
H	-2.016068000	-1.915420000	1.737221000	H	3.851045000	1.969545000	-1.899014000
H	-3.464111000	-1.132575000	2.448965000	H	4.222836000	1.645261000	-0.176061000
H	-1.991784000	-1.370863000	3.442350000	C	3.633201000	-0.739067000	-1.400176000
C	-2.280670000	1.333676000	2.935774000	H	4.438923000	-0.809530000	-0.664212000
H	-2.028075000	1.086551000	3.968956000	H	4.057729000	-0.533972000	-2.390437000
H	-3.365509000	1.461117000	2.836818000	H	3.103055000	-1.699819000	-1.440308000

C	2.597167000	-0.485850000	3.816111000
H	2.076407000	-0.944173000	4.661317000
H	2.760867000	0.574453000	4.047032000
H	3.575031000	-0.958141000	3.684699000
C	-2.509666000	-0.996082000	2.471892000
H	-2.204970000	-1.812948000	1.801641000
H	-3.604038000	-0.915074000	2.459688000
H	-2.169782000	-1.218118000	3.488003000
C	-2.243927000	1.477604000	2.921120000
H	-1.927805000	1.252385000	3.941922000
H	-3.328850000	1.636253000	2.891918000
H	-1.749129000	2.401082000	2.591273000
O	-0.259588000	-1.617267000	-0.336142000
H	-1.386805000	-1.880901000	-0.487488000
C	-2.707823000	-2.337391000	-0.850615000
H	-2.939469000	-3.217061000	-0.235710000
H	-3.405282000	-1.519319000	-0.623155000
C	-2.699093000	-2.654559000	-2.230162000
N	-2.601612000	-2.909884000	-3.367879000
⁴ TS			
Co	0.058171000	-0.015524000	-0.010192000
O	-0.004520000	0.027691000	4.031990000
O	3.797164000	0.108257000	1.484325000
O	2.053906000	0.603516000	-3.357704000
O	-3.777455000	0.657688000	0.559952000
N	1.914705000	-0.012521000	0.194965000
C	-2.112794000	1.126599000	-4.503850000
H	-2.178926000	1.275612000	-5.580597000
N	-1.679894000	0.559693000	-0.386997000
C	-2.548577000	0.534569000	0.631920000
C	-1.869039000	0.294645000	1.994796000
N	-0.412389000	0.190912000	1.791205000
C	0.372783000	-0.041554000	2.854546000
C	1.794101000	-0.591262000	2.589178000
C	1.581291000	-2.108565000	2.378034000
H	1.106372000	-2.538307000	3.272268000
H	2.550690000	-2.606044000	2.230442000
H	0.939027000	-2.299719000	1.507730000
C	2.580849000	-0.090981000	1.357645000
C	2.653241000	0.305347000	-1.039001000
C	1.651058000	0.443502000	-2.202731000
N	0.372002000	0.433297000	-1.788925000
C	-0.777168000	0.678950000	-2.544961000
C	-1.949551000	0.743965000	-1.742768000
C	-3.189310000	0.984520000	-2.339051000
H	-4.079064000	1.028752000	-1.719143000
C	-3.261909000	1.174221000	-3.721349000

H	-4.230189000	1.360219000	-4.183840000
C	-0.865997000	0.879111000	-3.923336000
H	0.034359000	0.836468000	-4.527069000
C	3.364004000	1.667360000	-0.963916000
H	2.649382000	2.449238000	-0.670296000
H	3.764164000	1.916931000	-1.954574000
H	4.175237000	1.635665000	-0.232325000
C	3.658006000	-0.792708000	-1.397562000
H	4.460897000	-0.826534000	-0.655101000
H	4.081800000	-0.587896000	-2.388151000
H	3.161687000	-1.771875000	-1.427289000
C	2.649539000	-0.397196000	3.839571000
H	2.128589000	-0.813221000	4.706535000
H	2.844352000	0.665175000	4.032748000
H	3.614024000	-0.898137000	3.712255000
C	-2.417356000	-1.039834000	2.519065000
H	-2.115733000	-1.846844000	1.834058000
H	-3.512840000	-1.000703000	2.571057000
H	-2.008609000	-1.243158000	3.515872000
C	-2.288015000	1.451737000	2.909746000
H	-2.010878000	1.247313000	3.946187000
H	-3.374615000	1.582730000	2.833374000
H	-1.802635000	2.384570000	2.591747000
O	-0.411067000	-1.929281000	-0.201521000
H	-1.537124000	-2.132486000	-0.464787000
C	-2.742248000	-2.345435000	-1.024589000
H	-3.086754000	-3.229659000	-0.477719000
H	-3.333442000	-1.453053000	-0.790906000
C	-2.605738000	-2.587215000	-2.414210000
N	-2.451076000	-2.811770000	-3.547285000
² PC			
Co	0.098558000	0.072816000	-0.025999000
O	-0.065422000	-0.278748000	4.000304000
O	3.822760000	0.176797000	1.510587000
O	2.128561000	0.619320000	-3.367969000
O	-3.735857000	0.831839000	0.533658000
N	1.951730000	0.079338000	0.198118000
C	-2.054079000	1.015478000	-4.551932000
H	-2.114116000	1.139520000	-5.632486000
N	-1.662688000	0.488181000	-0.421448000
C	-2.526532000	0.570463000	0.602710000
C	-1.873264000	0.225412000	1.957791000
N	-0.415175000	0.133365000	1.777289000
C	0.344136000	-0.185276000	2.830090000
C	1.818299000	-0.590560000	2.569660000
C	1.744440000	-2.114403000	2.315824000
H	1.295898000	-2.609130000	3.190197000

H	2.758050000	-2.517969000	2.172828000	N	1.951132000	0.011031000	0.171428000
H	1.135394000	-2.318141000	1.425691000	C	-2.045850000	0.935967000	-4.569817000
C	2.605314000	-0.027876000	1.359123000	H	-2.106317000	1.036585000	-5.652612000
C	2.702168000	0.362289000	-1.034483000	N	-1.648765000	0.491929000	-0.429655000
C	1.709476000	0.478928000	-2.213436000	C	-2.517226000	0.570617000	0.585883000
N	0.430510000	0.474009000	-1.807265000	C	-1.863376000	0.288627000	1.951611000
C	-0.718998000	0.648168000	-2.569770000	N	-0.431735000	0.023610000	1.742263000
C	-1.908992000	0.684197000	-1.780878000	C	0.346548000	-0.235874000	2.800019000
C	-3.146058000	0.902455000	-2.395295000	C	1.792040000	-0.726331000	2.526861000
H	-4.043006000	0.953969000	-1.784876000	C	1.655776000	-2.237231000	2.228160000
C	-3.211943000	1.064164000	-3.780119000	H	1.186535000	-2.736137000	3.089351000
H	-4.178515000	1.229038000	-4.254003000	H	2.653279000	-2.677909000	2.082532000
C	-0.808617000	0.812570000	-3.955953000	H	1.045575000	-2.404614000	1.329914000
H	0.099336000	0.786572000	-4.549976000	C	2.587858000	-0.119407000	1.343628000
C	3.433760000	1.714036000	-0.984214000	C	2.700368000	0.453348000	-1.014743000
H	2.727866000	2.514962000	-0.721733000	C	1.718834000	0.576137000	-2.198671000
H	3.857084000	1.934713000	-1.972552000	N	0.440088000	0.400710000	-1.822742000
H	4.229387000	1.685198000	-0.234921000	C	-0.714134000	0.591898000	-2.583897000
C	3.699569000	-0.754104000	-1.360582000	C	-1.898336000	0.651865000	-1.793057000
H	4.492625000	-0.780750000	-0.606854000	C	-3.133652000	0.871683000	-2.408719000
H	4.138009000	-0.577347000	-2.350540000	H	-4.029071000	0.937778000	-1.797884000
H	3.193020000	-1.728627000	-1.374243000	C	-3.200326000	1.009106000	-3.796750000
C	2.629643000	-0.352846000	3.843809000	H	-4.167143000	1.169826000	-4.271592000
H	2.125007000	-0.824428000	4.691777000	C	-0.801046000	0.732642000	-3.970243000
H	2.735921000	0.718715000	4.060312000	H	0.105247000	0.682263000	-4.565145000
H	3.633799000	-0.771907000	3.729794000	C	3.308350000	1.853900000	-0.836343000
C	-2.443851000	-1.150825000	2.340392000	H	2.529688000	2.570683000	-0.538637000
H	-2.057680000	-1.903052000	1.635625000	H	3.739975000	2.185877000	-1.789155000
H	-3.541533000	-1.137884000	2.288965000	H	4.083799000	1.832201000	-0.065577000
H	-2.126508000	-1.420005000	3.352881000	C	3.797580000	-0.540908000	-1.407492000
C	-2.311222000	1.292113000	2.965361000	H	4.579917000	-0.558233000	-0.643055000
H	-2.015040000	1.006634000	3.977251000	H	4.228911000	-0.241935000	-2.370864000
H	-3.400351000	1.408178000	2.911206000	H	3.380383000	-1.551447000	-1.512213000
H	-1.848426000	2.258210000	2.720904000	C	2.613604000	-0.566383000	3.805755000
O	-0.153568000	-1.710060000	-0.322839000	H	2.100824000	-1.064168000	4.633932000
H	-1.113193000	-1.779881000	-0.427809000	H	2.746772000	0.489883000	4.071769000
C	-3.573676000	-2.163441000	-0.859222000	H	3.605575000	-1.006879000	3.666764000
H	-3.772463000	-2.948892000	-0.136923000	C	-2.572551000	-0.951992000	2.511193000
H	-3.890248000	-1.144635000	-0.642946000	H	-2.372713000	-1.817922000	1.860463000
C	-2.981490000	-2.479847000	-2.057604000	H	-3.656062000	-0.782892000	2.539537000
N	-2.471318000	-2.774248000	-3.073805000	H	-2.205184000	-1.178310000	3.516547000
⁴ PC				C	-2.136928000	1.507067000	2.841416000
Co	0.094156000	-0.081897000	-0.058906000	H	-1.822503000	1.309557000	3.868835000
O	-0.035877000	-0.203919000	3.980647000	H	-3.210019000	1.733927000	2.816370000
O	3.792715000	0.122705000	1.516893000	H	-1.588085000	2.381354000	2.465381000
O	2.129658000	0.857261000	-3.327420000	O	-0.258750000	-1.981003000	-0.419164000
O	-3.731941000	0.802079000	0.510776000	H	-1.002016000	-2.198135000	0.161645000

C	-3.440155000	-2.244872000	-0.891508000	H	2.208621000	-0.605753000	4.743323000
H	-3.475663000	-3.002259000	-0.115376000	H	2.911190000	0.818770000	3.953160000
H	-3.790182000	-1.237753000	-0.676188000	H	3.658649000	-0.771302000	3.706341000
C	-3.013590000	-2.588821000	-2.153959000	C	-2.463994000	-0.758278000	2.735109000
N	-2.669507000	-2.908115000	-3.228718000	H	-2.255729000	-1.642742000	2.116099000

IV-2) C-H bond activation of PhCCH by 1

²RC

Co	0.017862000	0.068134000	0.038024000
O	0.063552000	0.200603000	4.080243000
O	3.818704000	-0.227251000	1.385463000
O	1.947967000	0.527377000	-3.361486000
O	-3.764991000	0.934120000	0.711676000
N	1.876621000	0.080036000	0.223125000
C	-2.225347000	1.172170000	-4.416855000
H	-2.314388000	1.299030000	-5.495046000
N	-1.714635000	0.641753000	-0.305635000
C	-2.551985000	0.705806000	0.742168000
C	-1.837530000	0.483899000	2.089842000
N	-0.402985000	0.264250000	1.846284000
C	0.405398000	0.063684000	2.894878000
C	1.807844000	-0.519369000	2.625217000
C	1.568138000	-2.044738000	2.519708000
H	1.088351000	-2.405296000	3.441363000
H	2.532280000	-2.560966000	2.404197000
H	0.924408000	-2.267796000	1.658395000
C	2.580143000	-0.162950000	1.336897000
C	2.578907000	0.098964000	-1.071197000
C	1.564547000	0.397498000	-2.194833000
N	0.303404000	0.489672000	-1.745708000
C	-0.854330000	0.741244000	-2.478740000
C	-2.008603000	0.837380000	-1.652888000
C	-3.252797000	1.111042000	-2.224666000
H	-4.126560000	1.189440000	-1.586534000
C	-3.352984000	1.278059000	-3.606718000
H	-4.325415000	1.489058000	-4.049706000
C	-0.972513000	0.907472000	-3.860752000
H	-0.087308000	0.830660000	-4.483602000
C	3.662343000	1.180305000	-1.162458000
H	3.254676000	2.151248000	-0.848548000
H	3.989379000	1.263459000	-2.205912000
H	4.512181000	0.933244000	-0.523455000
C	3.165539000	-1.286218000	-1.374257000
H	3.953268000	-1.523958000	-0.651452000
H	3.580051000	-1.304538000	-2.390191000
H	2.371105000	-2.042868000	-1.301061000
C	2.704073000	-0.253190000	3.834520000

H	2.208621000	-0.605753000	4.743323000
H	2.911190000	0.818770000	3.953160000
H	3.658649000	-0.771302000	3.706341000
C	-2.463994000	-0.758278000	2.735109000
H	-2.255729000	-1.642742000	2.116099000
H	-3.551263000	-0.631233000	2.812128000
H	-2.038432000	-0.912553000	3.732933000
C	-2.124333000	1.732095000	2.936736000
H	-1.781382000	1.586372000	3.963418000
H	-3.203247000	1.928746000	2.923084000
H	-1.607332000	2.604267000	2.512713000
O	-0.272932000	-1.579090000	-0.217927000
H	-1.524599000	-2.026124000	-1.618446000
C	-2.243520000	-2.426188000	-2.342036000
C	-3.040023000	-2.873402000	-3.140121000
C	-3.982794000	-3.386191000	-4.074301000
C	-3.607037000	-3.640108000	-5.405420000
C	-5.309653000	-3.642861000	-3.685356000
C	-4.532674000	-4.133373000	-6.315610000
H	-2.581943000	-3.442468000	-5.712700000
C	-6.228518000	-4.135776000	-4.602573000
H	-5.606700000	-3.447957000	-2.656667000
C	-5.845849000	-4.383055000	-5.920095000
H	-4.226904000	-4.323776000	-7.342635000
H	-7.252113000	-4.328042000	-4.286571000
H	-6.568832000	-4.768584000	-6.636103000

⁴RC

Co	-0.019494000	-0.273595000	0.038973000
O	0.110555000	0.199412000	4.063381000
O	3.791369000	-0.130139000	1.423266000
O	1.933796000	0.518307000	-3.327237000
O	-3.687681000	1.087228000	0.723327000
N	1.853893000	-0.101281000	0.218229000
C	-2.222365000	1.026019000	-4.398386000
H	-2.311200000	1.155913000	-5.476099000
N	-1.710725000	0.473442000	-0.291324000
C	-2.509284000	0.723895000	0.759917000
C	-1.786300000	0.558348000	2.103360000
N	-0.405419000	0.126079000	1.843011000
C	0.419381000	-0.043015000	2.886449000
C	1.801021000	-0.674060000	2.623326000
C	1.571756000	-2.197217000	2.502705000
H	1.095136000	-2.569761000	3.421205000
H	2.541095000	-2.704973000	2.392222000
H	0.935986000	-2.433924000	1.641162000
C	2.557876000	-0.243155000	1.350743000
C	2.580738000	0.143156000	-1.035979000

C	1.559266000	0.314602000	-2.169481000	O	0.022652000	0.207156000	4.005062000
N	0.290039000	0.262955000	-1.732810000	O	3.741221000	-0.300213000	1.291080000
C	-0.861694000	0.545669000	-2.466491000	O	1.838876000	0.431001000	-3.429682000
C	-2.007729000	0.675327000	-1.638329000	O	-3.817288000	0.907480000	0.665471000
C	-3.245490000	0.988385000	-2.203582000	N	1.789949000	0.012572000	0.152957000
H	-4.115437000	1.089574000	-1.564391000	C	-2.302397000	1.228154000	-4.453165000
C	-3.344029000	1.161208000	-3.584943000	H	-2.395294000	1.372683000	-5.528523000
H	-4.312034000	1.396855000	-4.024837000	N	-1.775313000	0.613649000	-0.361646000
C	-0.976234000	0.722164000	-3.847274000	C	-2.608937000	0.672784000	0.694795000
H	-0.096252000	0.622227000	-4.473251000	C	-1.887323000	0.452387000	2.034391000
C	3.384645000	1.452931000	-1.004299000	N	-0.453071000	0.238823000	1.775939000
H	2.735640000	2.287505000	-0.704990000	C	0.363562000	0.045176000	2.826711000
H	3.770789000	1.657175000	-2.010508000	C	1.751620000	-0.559291000	2.563936000
H	4.212468000	1.375023000	-0.295491000	C	1.493774000	-2.084216000	2.488920000
C	3.498225000	-1.026421000	-1.410600000	H	1.022513000	-2.420453000	3.423543000
H	4.324687000	-1.103936000	-0.698655000	H	2.451022000	-2.611655000	2.371672000
H	3.896250000	-0.861800000	-2.419633000	H	0.836946000	-2.322359000	1.642318000
H	2.936691000	-1.970545000	-1.407841000	C	2.506218000	-0.226940000	1.265589000
C	2.695937000	-0.427518000	3.837837000	C	2.486788000	0.008809000	-1.145937000
H	2.200310000	-0.798499000	4.739553000	C	1.469917000	0.309720000	-2.261013000
H	2.903421000	0.640814000	3.977155000	N	0.210131000	0.431230000	-1.802135000
H	3.650512000	-0.944334000	3.701452000	C	-0.937526000	0.739253000	-2.532493000
C	-2.566145000	-0.473303000	2.927382000	C	-2.080662000	0.849858000	-1.701491000
H	-2.514729000	-1.462495000	2.451998000	C	-3.321604000	1.163267000	-2.255741000
H	-3.619112000	-0.169414000	2.981360000	H	-4.190914000	1.251149000	-1.613787000
H	-2.149635000	-0.541613000	3.937034000	C	-3.422984000	1.346754000	-3.635546000
C	-1.855914000	1.934922000	2.783424000	H	-4.391970000	1.585877000	-4.071062000
H	-1.472972000	1.876096000	3.804422000	C	-1.051628000	0.929878000	-3.909973000
H	-2.899544000	2.271973000	2.793821000	H	-0.173042000	0.838395000	-4.539265000
H	-1.259919000	2.665718000	2.219616000	C	3.572392000	1.087714000	-1.251809000
O	-0.312605000	-1.960937000	-0.137945000	H	3.169306000	2.061880000	-0.943239000
H	-1.584891000	-2.270195000	-1.608043000	H	3.891216000	1.160159000	-2.298359000
C	-2.302975000	-2.598333000	-2.358107000	H	4.426629000	0.842504000	-0.618394000
C	-3.101434000	-2.987414000	-3.182794000	C	3.065294000	-1.380906000	-1.441420000
C	-4.051431000	-3.434178000	-4.143283000	H	3.864756000	-1.613298000	-0.730392000
C	-3.674902000	-3.650275000	-5.480555000	H	3.464409000	-1.405043000	-2.463176000
C	-5.386377000	-3.668790000	-3.768491000	H	2.272010000	-2.135807000	-1.351650000
C	-4.608496000	-4.088319000	-6.410858000	C	2.661119000	-0.278774000	3.759556000
H	-2.643491000	-3.469211000	-5.776527000	H	2.172714000	-0.614198000	4.678497000
C	-6.312854000	-4.106358000	-4.705846000	H	2.875889000	0.793285000	3.858171000
H	-5.682902000	-3.502835000	-2.734691000	H	3.610298000	-0.806209000	3.630405000
C	-5.929396000	-4.318391000	-6.029175000	C	-2.500967000	-0.792042000	2.686131000
H	-4.302799000	-4.250835000	-7.442598000	H	-2.284461000	-1.676473000	2.070944000
H	-7.342543000	-4.283186000	-4.401057000	H	-3.588910000	-0.671763000	2.762291000
H	-6.658020000	-4.660810000	-6.761144000	H	-2.076225000	-0.937395000	3.685417000
² TS				C	-2.170666000	1.704725000	2.877330000
Co	-0.060535000	0.001740000	-0.023329000	H	-1.835622000	1.560617000	3.906377000

H	-3.248720000	1.904044000	2.855967000
H	-1.648158000	2.573133000	2.453233000
O	-0.351276000	-1.663383000	-0.234049000
H	-1.124557000	-1.939297000	-1.150007000
C	-1.974449000	-2.401405000	-2.092814000
C	-2.785603000	-2.818647000	-2.919409000
C	-3.733461000	-3.287819000	-3.870756000
C	-3.367682000	-3.525098000	-5.210967000
C	-5.072158000	-3.529836000	-3.501409000
C	-4.298863000	-3.981917000	-6.134902000
H	-2.337883000	-3.342265000	-5.513879000
C	-5.998174000	-3.986146000	-4.430496000
H	-5.371680000	-3.351405000	-2.469827000
C	-5.619319000	-4.215808000	-5.752693000
H	-3.991296000	-4.156824000	-7.164796000
H	-7.026604000	-4.164309000	-4.119791000
H	-6.346968000	-4.572795000	-6.478897000

⁴TS

Co	0.011317000	0.055966000	0.052567000
O	0.178298000	-0.047173000	4.074552000
O	3.783917000	0.240209000	1.379071000
O	1.805374000	0.794505000	-3.374818000
O	-3.826229000	0.473749000	0.829406000
N	1.860712000	0.071652000	0.154246000
C	-2.421599000	1.153758000	-4.309057000
H	-2.541774000	1.343179000	-5.374618000
N	-1.787981000	0.420193000	-0.246534000
C	-2.599591000	0.368449000	0.829640000
C	-1.829299000	0.197513000	2.154405000
N	-0.388700000	0.082725000	1.863409000
C	0.470917000	-0.128933000	2.877192000
C	1.869630000	-0.668494000	2.499207000
C	1.644991000	-2.158780000	2.149266000
H	1.204527000	-2.677745000	3.012805000
H	2.606660000	-2.637721000	1.916543000
H	0.972613000	-2.272654000	1.289963000
C	2.583511000	-0.035751000	1.286690000
C	2.528690000	0.480036000	-1.095201000
C	1.469361000	0.583029000	-2.209251000
N	0.211866000	0.485016000	-1.735137000
C	-0.984528000	0.706142000	-2.427582000
C	-2.123618000	0.662058000	-1.580717000
C	-3.397578000	0.857761000	-2.112675000
H	-4.261836000	0.816246000	-1.458904000
C	-3.538737000	1.101569000	-3.480906000
H	-4.534098000	1.253682000	-3.896143000
C	-1.139599000	0.959471000	-3.789205000

H	-0.264258000	0.993352000	-4.428893000
C	3.137005000	1.888849000	-0.997671000
H	2.374086000	2.607444000	-0.666458000
H	3.493428000	2.193795000	-1.989542000
H	3.967544000	1.899510000	-0.287359000
C	3.594345000	-0.528168000	-1.527798000
H	4.431158000	-0.520589000	-0.823839000
H	3.953914000	-0.262477000	-2.528934000
H	3.172760000	-1.541047000	-1.567068000
C	2.787422000	-0.592125000	3.715476000
H	2.328045000	-1.115996000	4.558888000
H	2.971170000	0.446356000	4.015284000
H	3.752665000	-1.051684000	3.481076000
C	-2.355067000	-1.079477000	2.819466000
H	-2.085768000	-1.946986000	2.202595000
H	-3.447744000	-1.024242000	2.899895000
H	-1.921271000	-1.194088000	3.817688000
C	-2.162947000	1.426486000	3.011391000
H	-1.733707000	1.316502000	4.010808000
H	-3.252968000	1.528121000	3.081536000
H	-1.757717000	2.336933000	2.549017000
O	-0.818530000	-1.915062000	-0.190018000
H	-1.123563000	-2.218126000	-1.227193000
C	-1.623204000	-2.652234000	-2.570922000
C	-2.204153000	-2.948228000	-3.621642000
C	-2.885825000	-3.249529000	-4.833386000
C	-2.609108000	-4.421656000	-5.565924000
C	-3.871147000	-2.376159000	-5.340306000
C	-3.287115000	-4.704740000	-6.745279000
H	-1.850476000	-5.107382000	-5.191198000
C	-4.548744000	-2.667693000	-6.516895000
H	-4.087149000	-1.460675000	-4.788976000
C	-4.262004000	-3.832690000	-7.228408000
H	-3.053653000	-5.616610000	-7.293251000
H	-5.306736000	-1.977585000	-6.885248000
H	-4.792966000	-4.058346000	-8.151227000

²PC

Co	-0.055738000	0.001427000	0.023830000
O	0.082308000	0.294799000	4.039375000
O	3.762275000	-0.211863000	1.288475000
O	1.775162000	0.280122000	-3.422446000
O	-3.805312000	0.886968000	0.736453000
N	1.790215000	0.024070000	0.171759000
C	-2.346433000	1.198758000	-4.390998000
H	-2.447448000	1.354750000	-5.463876000
N	-1.777102000	0.579930000	-0.308608000
C	-2.598072000	0.658266000	0.760012000

C	-1.858042000	0.475274000	2.093012000
N	-0.424739000	0.267799000	1.818053000
C	0.411277000	0.106911000	2.864280000
C	1.800548000	-0.486565000	2.596839000
C	1.563066000	-2.016507000	2.549050000
H	1.109961000	-2.344171000	3.495277000
H	2.526121000	-2.531549000	2.426260000
H	0.899124000	-2.284223000	1.717707000
C	2.528331000	-0.166655000	1.284146000
C	2.467905000	-0.037790000	-1.136526000
C	1.433794000	0.218302000	-2.243560000
N	0.182807000	0.384269000	-1.763960000
C	-0.970298000	0.689793000	-2.487433000
C	-2.102381000	0.804745000	-1.646474000
C	-3.348896000	1.121532000	-2.185440000
H	-4.211805000	1.209718000	-1.535125000
C	-3.459757000	1.315532000	-3.562911000
H	-4.430742000	1.563179000	-3.988863000
C	-1.093053000	0.886946000	-3.862584000
H	-0.221369000	0.795750000	-4.500940000
C	3.551768000	1.034625000	-1.311287000
H	3.156912000	2.022324000	-1.037933000
H	3.848146000	1.058725000	-2.366545000
H	4.419218000	0.815316000	-0.686849000
C	3.038680000	-1.441422000	-1.374146000
H	3.854458000	-1.638690000	-0.670966000
H	3.415978000	-1.516002000	-2.401689000
H	2.247607000	-2.189857000	-1.229409000
C	2.721507000	-0.173557000	3.775263000
H	2.250511000	-0.500653000	4.706222000
H	2.922382000	0.902689000	3.852924000
H	3.675760000	-0.690713000	3.643086000
C	-2.456633000	-0.756709000	2.780983000
H	-2.232260000	-1.657032000	2.192253000
H	-3.545438000	-0.642703000	2.852813000
H	-2.034163000	-0.869253000	3.784751000
C	-2.139036000	1.748540000	2.904678000
H	-1.798820000	1.634210000	3.935379000
H	-3.218212000	1.941309000	2.885293000
H	-1.624117000	2.607155000	2.452812000
O	-0.323634000	-1.702383000	-0.131039000
H	-0.939008000	-1.899668000	-0.911157000
C	-2.017564000	-2.546970000	-2.193447000
C	-2.838501000	-2.909370000	-3.054208000
C	-3.782804000	-3.333030000	-4.029131000
C	-3.403580000	-3.577378000	-5.367084000
C	-5.141244000	-3.529879000	-3.696546000

C	-4.330381000	-3.994485000	-6.314217000
H	-2.361262000	-3.431913000	-5.648390000
C	-6.063541000	-3.946699000	-4.647859000
H	-5.458057000	-3.347187000	-2.670377000
C	-5.667361000	-4.183172000	-5.964210000
H	-4.005978000	-4.174812000	-7.338575000
H	-7.104460000	-4.089132000	-4.359274000
H	-6.391554000	-4.509874000	-6.708118000
⁴ PC			
Co	-0.006694000	-0.546215000	0.053675000
O	-0.020550000	0.732813000	3.888027000
O	3.688406000	0.428261000	1.372540000
O	1.921785000	-0.533576000	-3.391713000
O	-3.884536000	0.047939000	0.524852000
N	1.826682000	-0.181430000	0.192228000
C	-2.213792000	-0.080597000	-4.548005000
H	-2.296913000	-0.025447000	-5.632082000
N	-1.797742000	-0.231301000	-0.417873000
C	-2.660999000	-0.007071000	0.606796000
C	-1.944677000	0.261193000	1.941440000
N	-0.504016000	0.010436000	1.772362000
C	0.325378000	0.247803000	2.802701000
C	1.777875000	-0.251343000	2.648898000
C	1.710090000	-1.793453000	2.739569000
H	1.265314000	-2.085765000	3.702421000
H	2.727352000	-2.210365000	2.697775000
H	1.113080000	-2.215932000	1.922463000
C	2.504610000	0.068538000	1.324585000
C	2.539755000	-0.137209000	-1.093690000
C	1.541680000	-0.414144000	-2.231433000
N	0.250030000	-0.430352000	-1.804907000
C	-0.883191000	-0.359840000	-2.563609000
C	-2.075933000	-0.234830000	-1.758588000
C	-3.319064000	-0.038811000	-2.381807000
H	-4.214492000	0.041574000	-1.775791000
C	-3.376062000	0.039622000	-3.761504000
H	-4.341862000	0.158911000	-4.253262000
C	-0.978106000	-0.289462000	-3.967713000
H	-0.079361000	-0.384446000	-4.566487000
C	3.100538000	1.262534000	-1.403756000
H	2.300480000	2.012682000	-1.333409000
H	3.503690000	1.276532000	-2.424207000
H	3.888465000	1.516750000	-0.690799000
C	3.655118000	-1.183546000	-1.167030000
H	4.450113000	-0.933294000	-0.458451000
H	4.065038000	-1.210059000	-2.183922000
H	3.260933000	-2.178923000	-0.922697000

C	2.612794000	0.267878000	3.815334000
H	2.145144000	-0.020397000	4.761886000
H	2.697076000	1.361055000	3.796055000
H	3.622320000	-0.151486000	3.761530000
C	-2.558975000	-0.650956000	3.006747000
H	-2.333987000	-1.702663000	2.784813000
H	-3.648052000	-0.521501000	3.016510000
H	-2.151822000	-0.401207000	3.991030000
C	-2.256052000	1.734954000	2.257923000
H	-1.879737000	1.996711000	3.249090000
H	-3.341323000	1.890873000	2.219345000
H	-1.782282000	2.388716000	1.512345000
O	-0.111454000	-2.470736000	0.088028000
H	-0.570405000	-2.781640000	-0.712647000
C	-1.623537000	-3.465585000	-2.469983000
C	-2.641796000	-3.272399000	-3.178980000
C	-3.762988000	-3.012902000	-3.993616000
C	-3.623967000	-2.848229000	-5.392554000
C	-5.052715000	-2.839411000	-3.438333000
C	-4.712220000	-2.511989000	-6.185866000
H	-2.635003000	-2.970629000	-5.832465000
C	-6.135316000	-2.505916000	-4.236850000
H	-5.174070000	-2.951749000	-2.361728000
C	-5.972982000	-2.335737000	-5.614749000
H	-4.578048000	-2.382272000	-7.258792000
H	-7.117079000	-2.369958000	-3.785575000
H	-6.824918000	-2.069134000	-6.237316000