

Supporting Information

Axial ligand effect on the rate constant of aromatic hydroxylation by iron(IV)-oxo complexes mimicking cytochrome P450 enzymes.

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Reference 31b for Gaussian-03:

Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Montgomery, Jr., J. A.; Vreven, T.; Kudin, K. N.; Burant, J. C.; Millam, J. M.; Iyengar, S. S.; Tomasi, J.; Barone, V.; Mennucci, B.; Cossi, M.; Scalmani, G.; Rega, N.; Petersson, G. A.; Nakatsuji, H.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, N.; Klene, M.; Li, X.; Knox, J. E.; Hratchian, H. P.; Cross, J. B.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Ayala, P. Y.; Morokuma, K.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Zakrzewski, V. G.; Dapprich, S.; Daniels, A. D.; Strain, M. C.; Farkas, O.; Malick, D. K.; Rabuck, A. D.; Raghavachari, K.; Foresman, J. B.; Ortiz, J. V.; Cui, Q.; Baboul, A. G.; Clifford, S.; Cioslowski, J.; Stefanov, B. B.; Liu, G.; Liashenko, A.; Piskorz, P.; Komaromi, I.; Martin, R. L.; Fox, D. J.; Keith, T.; Al-Laham, M. A.; Peng, C. Y.; Nanayakkara, A.; Challacombe, M.; Gill, P. M. W.; Johnson, B.; Chen, W.; Wong, M. W.; Gonzalez, C.; Pople, J. A. In Gaussian 03; revision C.02 ed.; Gaussian, Inc.: Wallingford, CT, 2004

Reference 31c for Gaussian-09:

Gaussian 09, Revision B.01,

Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Mennucci, B.; Petersson, G. A.; Nakatsuji, H.; Caricato, M.; Li, X.; Hratchian, H. P.; Izmaylov, A. F.; Bloino, J.; Zheng, G.; Sonnenberg, J. L.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Montgomery, Jr., J. A.; Peralta, J. E.; Ogliaro, F.; Bearpark, M.; Heyd, J. J.; Brothers, E.; Kudin, K. N.; Staroverov, V. N.; Keith, T.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Rega, N.; Millam, J. M.; Klene, M.; Knox, J. E.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Zakrzewski, V. G.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Dapprich, S.; Daniels, A. D.; Farkas, O.; Foresman, J. B.; Ortiz, J. V.; Cioslowski, J.; Fox, D. J. Gaussian, Inc., Wallingford CT, 2010.

Table S1: Absolute energies, free energies and zero-point energies (in au) of optimized UB3LYP/B1 geometries of substrate ethylbenzene (EB) and subsequent UB3LYP/B2//UB3LYP/B1 single points.

B1 -> LACVP				B2 -> LACV3P+*	
Multip	E	E+ZPE	G	E	E+ZPE
M1	-310.810795	-310.652110	-310.684225	-310.946968	-310.788282

Table S2: Absolute energies, free energies and zero-point energies (in au) and relative (free) energies (in kcal mol⁻¹) of optimized UB3LYP/B1 geometries of Cpd I(F) and subsequent UB3LYP/B2//UB3LYP/B1 single points.

B1 -> LACVP						
Multip	E	E+ZPE	G	ΔE^a	$\Delta E+ZPE^a$	ΔG^a
M2	-1286.573456	-1286.291754	-1286.338617	0.00	0.00	0.00
M4	-1286.574191	-1286.292474	-1286.339991	-0.46	-0.45	-0.86

^a with respect to ²Cpd I(F).

B2 -> LACV3P+*				
Multip	E	E+ZPE	ΔE^a	$\Delta E+ZPE^a$
M2	-1287.160866	-1286.879164	0.00	0.00
M4	-1287.161085	-1286.879367	-0.14	-0.13

^a with respect to ²Cpd I(F).

Table S3: Group spin densities and charges of optimized UB3LYP/B1 geometries of Cpd I(F).

	Spin densities				Charges			
	Fe	O	Por	F	Fe	O	Por	F
M2	1.06	0.98	-1.06	0.02	0.60	-0.35	0.14	-0.39
M4	0.99	1.02	0.89	0.10	0.60	-0.34	0.14	-0.39

Table S4: Group spin densities and group charges of UB3LYP/B2//UB3LYP/B1 single point calculations Cpd I(F).

	Spin densities				Charges			
	Fe	O	Por	F	Fe	O	Por	F
M2	1.20	0.91	-1.12	0.01	0.41	-0.28	0.11	-0.25
M4	1.10	0.94	0.88	0.07	0.41	-0.27	0.10	-0.25

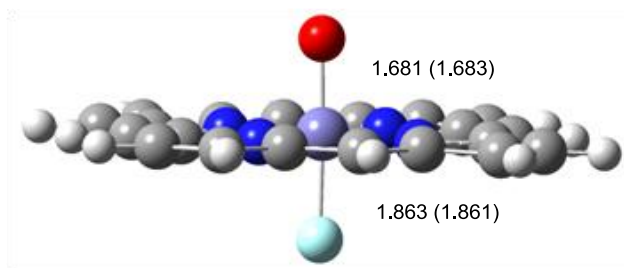


Figure S1. Optimized UB3LYP/B1 geometry of 4,2 Cpd I(F) with bond lengths in angstroms. High spin data in parenthesis.

Table S5: Absolute energies, free energies and zero-point energies (in au) and relative (free) energies (in kcal mol⁻¹) of optimized UB3LYP/B1 geometries of TS1_F and subsequent UB3LYP/B2//UB3LYP/B1 single points.

B1 -> LACVP						
Multip	E	E+ZPE	G	ΔE^a	$\Delta E+ZPE^a$	ΔG^a
M2	-1597.371309	-1596.929177	-1596.988976	8.12	9.22	21.25
M4	-1597.366248	-1596.924576	-1596.983669	11.30	12.10	24.58

^a with respect to ²Cpd I(F) + EB.

B2 -> LACV3P+*				
Multip	E	E+ZPE	ΔE^a	$\Delta E+ZPE^a$
M2	-1598.093667	-1597.651535	8.89	9.98
M4	-1598.087410	-1597.645739	12.82	13.62

^a with respect to ²Cpd I(F) + EB.

Table S6: Group spin densities and charges of optimized UB3LYP/B1 geometries of TS1_F.

	Spin densities					Charges				
	Fe	O	Por	F	EB	Fe	O	Por	F	EB
M2	1.54	-0.10	-0.17	0.11	-0.38	0.73	-0.36	-0.37	-0.33	0.33
M4	1.53	0.88	-0.01	0.15	0.46	0.72	-0.35	-0.36	-0.32	0.31

Table S7: Group spin densities and group charges of UB3LYP/B2//UB3LYP/B1 single point calculations for TS1_F.

	Spin densities					Charges				
	Fe	O	Por	F	EB	Fe	O	Por	F	EB
M2	1.65	-0.11	-0.20	0.08	-0.42	0.33	-0.02	-0.37	-0.07	0.13
M4	1.66	0.79	-0.05	0.11	0.49	0.32	0.01	-0.38	-0.05	0.10

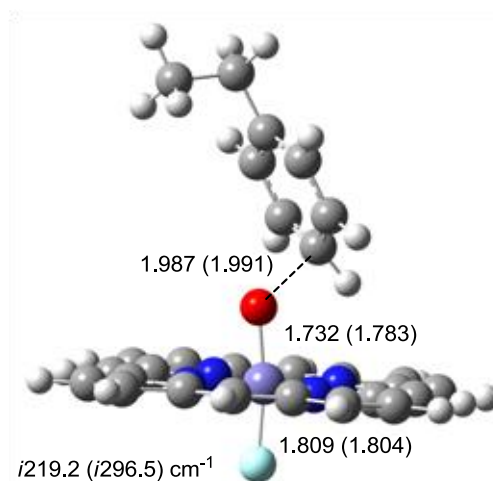


Figure S2. Optimized UB3LYP/B1 geometry of $^{4,2}\text{TS1}_\text{F}$ with bond lengths in angstroms and the imaginary frequency in the transition state in wavenumbers. High spin data in parenthesis.

Table S8: Absolute energies, free energies and zero-point energies (in au) and relative (free) energies (in kcal mol⁻¹) of optimized UB3LYP/B1 geometries of A_F and subsequent UB3LYP/B2//UB3LYP/B1 single points.

B1 -> LACVP						
Multip	E	E+ZPE	G	ΔE^a	$\Delta E+ZPE^a$	ΔG^a
M2	-1597.378691	-1596.936434	-1596.995027	3.49	4.66	17.45
M4	-1597.378492	-1596.936007	-1596.994510	3.61	4.93	17.78

^a with respect to ²Cpd I(F) + EB.

B2 -> LACV3P+*				
Multip	E	E+ZPE	ΔE^a	$\Delta E+ZPE^a$
M2	-1598.106875	-1597.664618	0.60	1.78
M4	-1598.107405	-1597.664921	0.27	1.58

^a with respect to ²Cpd I(F) + EB.

Table S9: Group spin densities and charges of optimized UB3LYP/B1 geometries of A_F.

	Spin densities					Charges				
	Fe	O	Por	F	EB	Fe	O	Por	F	EB
M2	1.53	0.19	-0.10	0.11	-0.73	0.75	-0.48	-0.39	-0.32	0.43
M4	1.84	0.29	-0.14	0.14	0.87	0.78	-0.49	-0.37	-0.31	0.38

Table S10: Group spin densities and group charges of UB3LYP/B2//UB3LYP/B1 single point calculations for A_F.

	Spin densities					Charges				
	Fe	O	Por	F	EB	Fe	O	Por	F	EB
M2	1.63	0.19	-0.13	0.09	-0.77	0.38	-0.06	-0.43	-0.04	0.15
M4	1.92	0.23	-0.18	0.11	0.91	0.40	-0.07	-0.41	-0.03	0.11

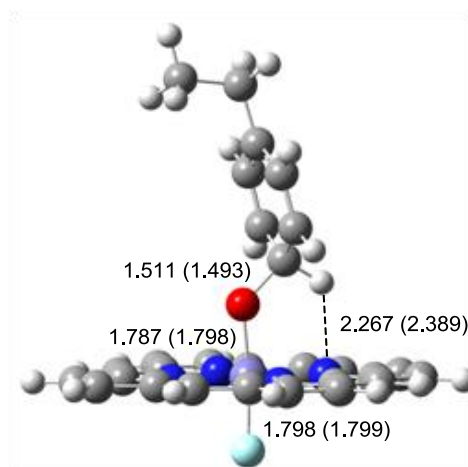


Figure S3. Optimized UB3LYP/B1 geometry of $^{4,2}A_F$ with bond lengths in angstroms. High spin data in parenthesis.

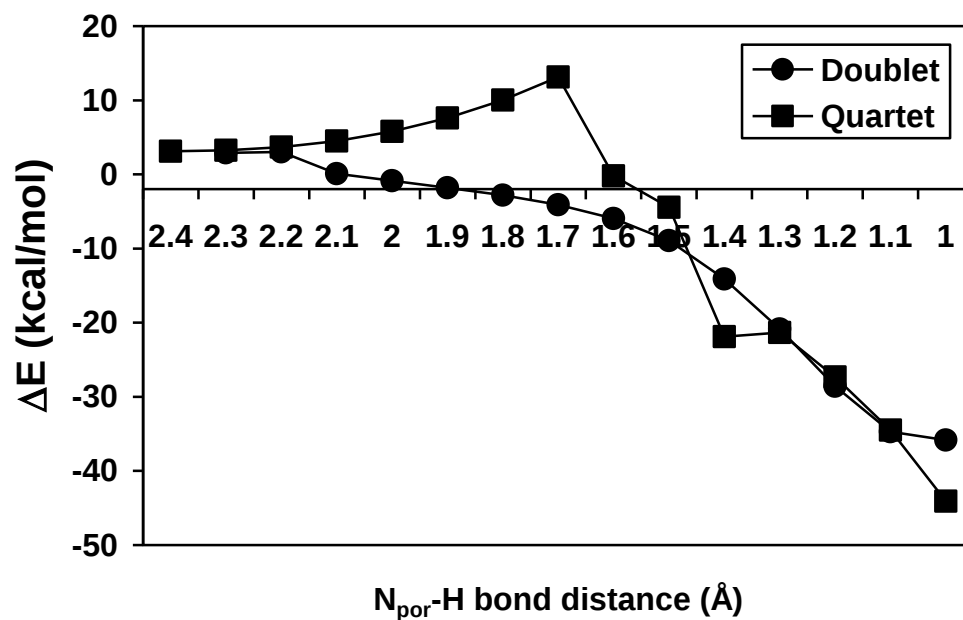


Figure S4. UB3LYP/B1 geometry scan for the proton transfer from $^{4,2}A_F$ in the direction of $^{4,2}B_F$. Each point in the figure represents a full geometry optimization with fixed N-H bond distance.

Table S11: Absolute energies, free energies and zero-point energies (in au) and relative (free) energies (in kcal mol⁻¹) of optimized UB3LYP/B1 geometries of ⁴TS2_F and subsequent UB3LYP/B2//UB3LYP/B1 single points.

B1 -> LACVP						
Multip	E	E+ZPE	G	ΔE^a	$\Delta E+ZPE^a$	ΔG^a
M4	-1597.360379	-1596.919647	-1596.976056	14.98	15.20	29.36

^a with respect to ²Cpd I(F) + EB.

B2 -> LACV3P+*				
Multip	E	E+ZPE	ΔE^a	$\Delta E+ZPE^a$
M4	-1598.087267	-1597.646535	12.91	13.12

^a with respect to ²Cpd I(F) + EB.

Table S12: Group spin densities and charges of optimized UB3LYP/B1 geometries of ⁴TS2_F.

	Spin densities					Charges				
	Fe	O	Por	F	EB	Fe	O	Por	F	EB
M4	1.99	0.24	-0.09	0.16	0.70	0.75	-0.48	-0.38	-0.33	0.44

Table S13: Group spin densities and group charges of UB3LYP/B2//UB3LYP/B1 single point calculations for ⁴TS2_F.

	Spin densities					Charges				
	Fe	O	Por	F	EB	Fe	O	Por	F	EB
M4	2.05	0.20	-0.12	0.12	0.75	0.46	-0.11	-0.50	-0.09	0.24

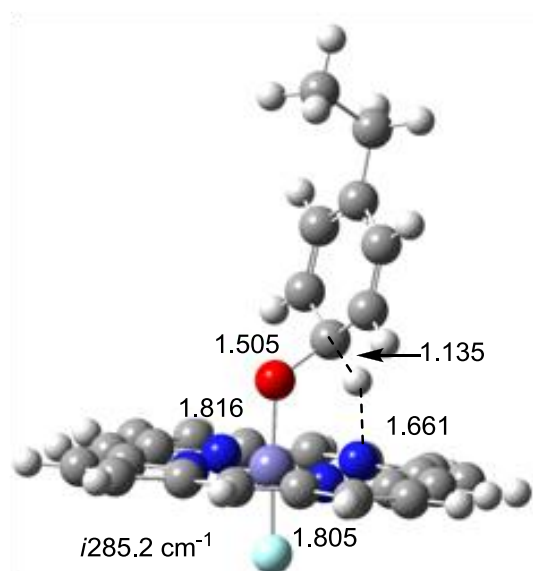


Figure S5. Optimized UB3LYP/B1 geometry of ${}^4\text{TS2}_\text{F}$ with bond lengths in angstroms and the imaginary frequency in the transition state in wavenumbers. High spin data in parenthesis.

Table S14: Absolute energies, free energies and zero-point energies (in au) and relative (free) energies (in kcal mol⁻¹) of optimized UB3LYP/B1 geometries of ^{4,2}B_F and subsequent UB3LYP/B2//UB3LYP/B1 single points.

B1 -> LACVP						
Multip	E	E+ZPE	G	ΔE ^a	ΔE+ZPE ^a	ΔG ^a
M2	-1597.442801	-1596.998307	-1597.057531	-36.74	-34.16	-21.77
M4	-1597.458274	-1597.014789	-1597.074802	-46.45	-44.51	-32.61

^a with respect to ²Cpd I(F) + EB.

B2 -> LACV3P+*				
Multip	E	E+ZPE	ΔE ^a	ΔE+ZPE ^a
M2	-1598.16827	-1597.723777	-37.92	-35.35
M4	-1598.178693	-1597.735208	-44.46	-42.52

^a with respect to ²Cpd I(F) + EB.

Table S15: Group spin densities and charges of optimized UB3LYP/B1 geometries of ^{4,2}B_F.

	Spin densities					Charges				
	Fe	O	Por	F	EB	Fe	O	Por	F	EB
M2	0.93	0.08	-0.06	0.05	0.00	0.65	-0.60	-0.29	-0.37	0.62
M4	2.71	0.05	0.06	0.16	0.02	0.79	-0.72	-0.44	-0.38	0.75

Table S16: Group spin densities and group charges of UB3LYP/B2//UB3LYP/B1 single point calculations for ^{4,2}B_F.

	Spin densities					Charges				
	Fe	O	Por	F	EB	Fe	O	Por	F	EB
M2	0.96	0.07	-0.07	0.04	0.00	0.46	-0.28	-0.38	-0.19	0.39
M4	2.80	0.04	0.01	0.13	0.01	0.49	-0.46	-0.43	-0.18	0.58

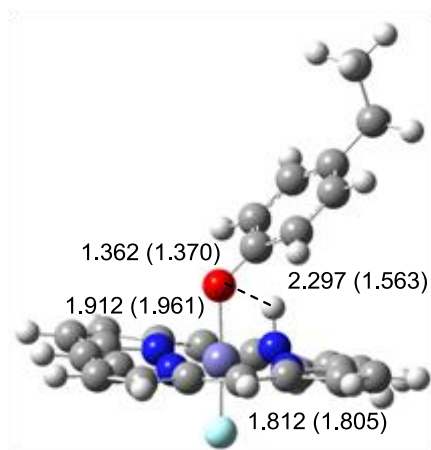


Figure S6. Optimized UB3LYP/B1 geometry of $^{4,2}\text{B}_\text{F}$ with bond lengths in angstroms. High spin data in parenthesis.

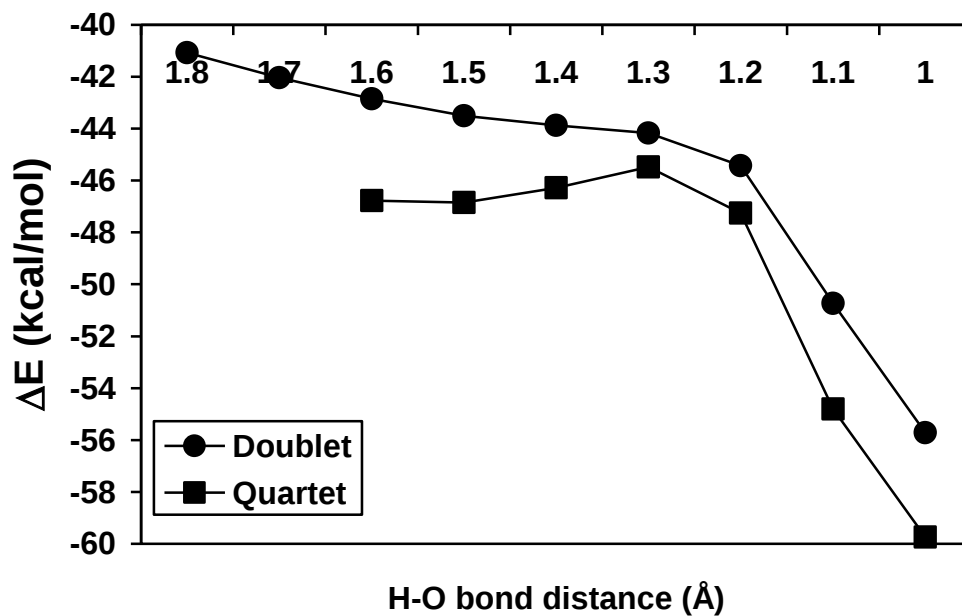


Figure S7. UB3LYP/B1 geometry scan for the proton transfer from $^{4,2}\text{B}_\text{F}$ in the direction of $^{4,2}\text{C}_\text{F}$. Each point in the figure represents a full geometry optimization with fixed O-H bond distance

Table S17: Absolute energies, free energies and zero-point energies (in au) and relative (free) energies (in kcal mol⁻¹) of optimized UB3LYP/B1 geometries of ^{4,2}C_F and subsequent UB3LYP/B2//UB3LYP/B1 single points.

B1 -> LACVP						
Multip	E	E+ZPE	G	ΔE ^a	ΔE+ZPE ^a	ΔG ^a
M2	-1597.472304	-1597.027731	-1597.087623	-55.25	-52.63	-40.65
M4	-1597.478977	-1597.035832	-1597.095355	-59.44	-57.71	-45.50

^a with respect to ²Cpd I(F) + EB.

B2 -> LACV3P+*				
Multip	E	E+ZPE	ΔE ^a	ΔE+ZPE ^a
M2	-1598.197782	-1597.754297	-56.44	-54.50
M4	-1598.210108	-1597.766623	-64.18	-62.23

^a with respect to ²Cpd I(F) + EB.

Table S18: Group spin densities and charges of optimized UB3LYP/B1 geometries of ^{4,2}C_F.

	Spin densities					Charges				
	Fe	O	Por	F	EB	Fe	O	Por	F	EB
M2	1.00	-0.01	-0.04	0.05	0.00	0.73	-0.66	-0.53	-0.35	0.82
M4	2.69	0.01	-0.02	0.32	0.00	0.80	-0.65	-0.45	-0.40	0.70

Table S19: Group spin densities and group charges of UB3LYP/B2//UB3LYP/B1 single point calculations for ^{4,2}C_F.

	Spin densities					Charges				
	Fe	O	Por	F	EB	Fe	O	Por	F	EB
M2	1.03	-0.01	-0.05	0.04	0.00	0.55	-0.46	-0.58	-0.15	0.64
M4	2.79	-0.01	-0.04	0.26	-0.01	0.38	-0.39	-0.44	-0.13	0.59

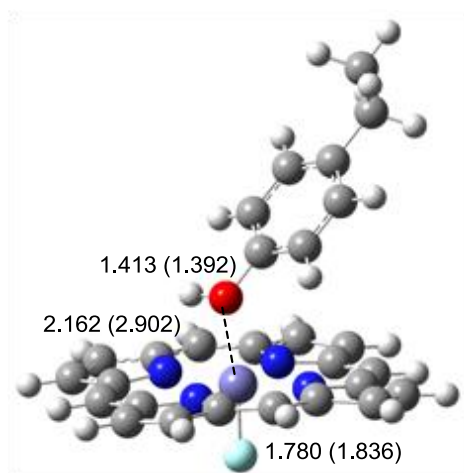


Figure S8. Optimized UB3LYP/B1 geometry of $^{4,2}\text{C}_\text{F}$ with bond lengths in angstroms. High spin data in parenthesis.

Table S20: Absolute energies, free energies and zero-point energies (in au) of optimized UB3LYP/B1 geometries of ²Cpd I(SH) and subsequent UB3LYP/B2//UB3LYP/B1 single points.

B1 -> LACVP				B2 -> LACV3P+*	
Multip	E	E+ZPE	G	E	E+ZPE
M2	-1585.520444	-1585.231208	-1585.280035	-1586.101842	-1585.812607

Table S21: Group spin densities and charges of optimized UB3LYP/B1 geometries of ²Cpd I(SH).

	Spin densities				Charges			
	Fe	O	Por	SH	Fe	O	Por	SH
M2	1.17	0.93	-0.50	-0.59	0.51	-0.32	-0.13	-0.06

Table S22: Group spin densities and group charges of UB3LYP/B2//UB3LYP/B1 single point calculations for ²Cpd I(SH).

	Spin densities				Charges			
	Fe	O	Por	SH	Fe	O	Por	SH
M2	1.24	0.88	-0.50	-0.61	0.24	-0.18	0.08	-0.14

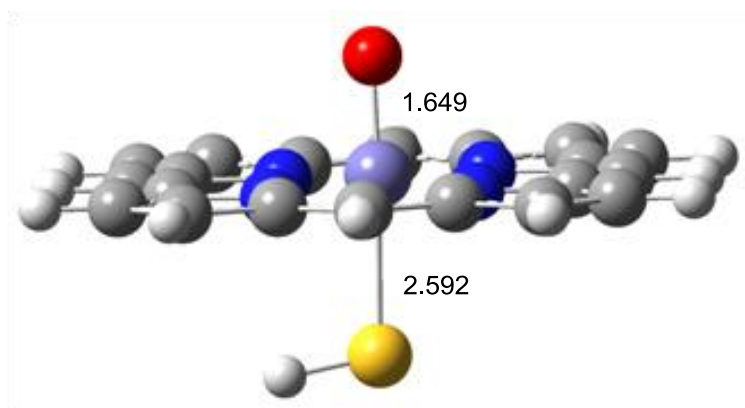


Figure S9. Optimized UB3LYP/B1 geometry of ²Cpd I(SH) with bond lengths in angstroms.

Table S23: Absolute energies, free energies and zero-point energies (in au) and relative (free) energies (in kcal mol⁻¹) of optimized UB3LYP/B1 geometries of ²TS1_{SH} and subsequent UB3LYP/B2//UB3LYP/B1 single points.

B1 -> LACVP						
Multip	E	E+ZPE	G	ΔE^a	$\Delta E+ZPE^a$	ΔG^a
M2	-1896.305175	-1895.857544	-1895.918414	16.36	16.17	28.77

^a with respect to ²Cpd I(SH) + EB.

B2 -> LACV3P+*				
Multip	E	E+ZPE	ΔE^a	$\Delta E+ZPE^a$
M2	-1897.024552	-1896.576921	15.22	15.04

^a with respect to ²Cpd I(SH) + EB.

Table S24: Group spin densities and charges of optimized UB3LYP/B1 geometries of ²TS1_{SH}.

	Spin densities					Charges				
	Fe	O	Por	SH	EB	Fe	O	Por	SH	EB
M2	1.64	0.12	-0.20	-0.17	-0.39	0.45	-0.41	-0.34	-0.04	0.33

Table S25: Group spin densities and group charges of UB3LYP/B2//UB3LYP/B1 single point calculations for ²TS1_{SH}.

	Spin densities					Charges				
	Fe	O	Por	SH	EB	Fe	O	Por	SH	EB
M2	1.70	0.09	-0.22	-0.15	-0.43	0.12	-0.05	0.04	-0.21	0.10

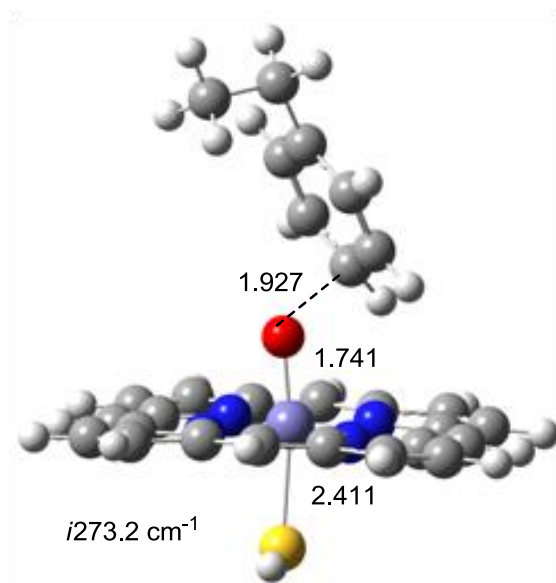


Figure S10. Optimized UB3LYP/B1 geometry of $^2\text{TS1}_{\text{SH}}$ with bond lengths in angstroms and the imaginary frequency in the transition state in wavenumbers.

Table S26: Absolute energies, free energies and zero-point energies (in au) of optimized UB3LYP/B1 geometries of $^2\text{Cpd I}(\text{OH})$ and subsequent UB3LYP/B2//UB3LYP/B1 single points.

B1 -> LACVP				B2 -> LACV3P+*	
Multip	E	E+ZPE	G	E	E+ZPE
M2	-1262.52602	-1262.23343	-1262.28109	-1263.105959	-1262.813366

Table S27: Group spin densities and charges of optimized UB3LYP/B1 geometries of $^2\text{Cpd I}(\text{OH})$.

	Spin densities				Charges			
	Fe	O	Por	OH	Fe	O	Por	OH
M2	1.06	0.97	-0.61	-0.42	0.60	-0.30	-0.13	-0.16

Table S28: Group spin densities and group charges of UB3LYP/B2//UB3LYP/B1 single point calculations for $^2\text{Cpd I}(\text{OH})$.

	Spin densities				Charges			
	Fe	O	Por	OH	Fe	O	Por	OH
M2	1.18	0.89	-0.71	-0.36	0.50	-0.22	-0.11	-0.17

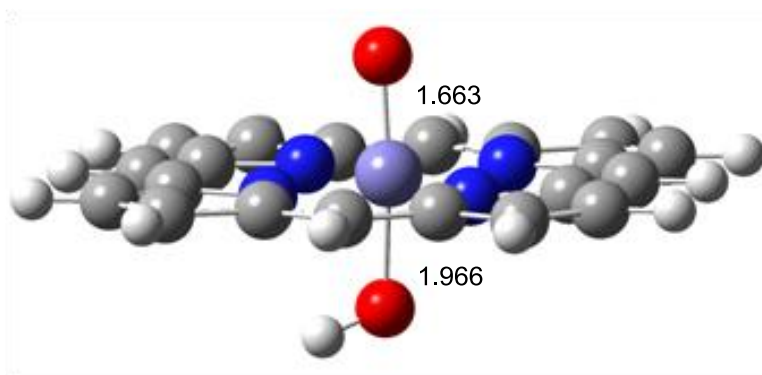


Figure S11. Optimized UB3LYP/B1 geometry of $^2\text{Cpd I}(\text{OH})$ with bond lengths in angstroms.

Table S29: Absolute energies, free energies and zero-point energies (in au) and relative (free) energies (in kcal mol⁻¹) of optimized UB3LYP/B1 geometries of ²TS1_{OH} and subsequent UB3LYP/B2//UB3LYP/B1 single points.

B1 -> LACVP						
Multip	E	E+ZPE	G	ΔE^a	$\Delta E+ZPE^a$	ΔG^a
M2	-1573.327038	-1572.874587	-1572.931036	6.14	6.87	21.51

^a with respect to ²Cpd I(OH) + EB.

B2 -> LACV3P+*				
Multip	E	E+ZPE	ΔE^a	$\Delta E+ZPE^a$
M2	-1574.044874	-1573.592423	5.05	5.79

^a with respect to ²Cpd I(OH) + EB.

Table S30: Group spin densities and charges of optimized UB3LYP/B1 geometries of ²TS1_{OH}.

	Spin densities					Charges				
	Fe	O	Por	OH	EB	Fe	O	Por	OH	EB
M2	1.48	-0.16	-0.15	0.19	-0.35	0.65	-0.34	-0.40	-0.19	0.28

Table S31: Group spin densities and group charges of UB3LYP/B2//UB3LYP/B1 single point calculations for ²TS1_{OH}.

	Spin densities					Charges				
	Fe	O	Por	OH	EB	Fe	O	Por	OH	EB
M2	1.58	-0.18	-0.18	0.16	-0.39	0.53	-0.02	-0.48	-0.14	0.10

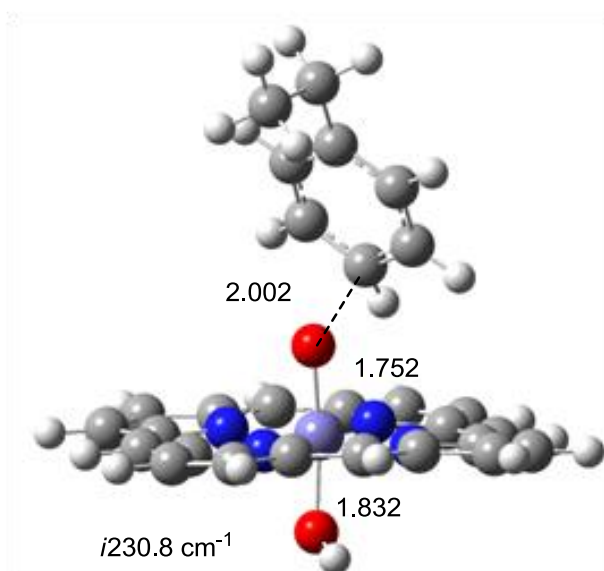


Figure S12. Optimized UB3LYP/B1 geometry of $^2\text{TS1}_{\text{OH}}$ with bond lengths in angstroms and the imaginary frequency in the transition state in wavenumbers.

Table S32: Absolute energies, free energies and zero-point energies (in au) of optimized UB3LYP/B1 geometries of ²Cpd I(CF₃COO) and subsequent UB3LYP/B2//UB3LYP/B1 single points.

B1 -> LACVP				B2 -> LACV3P+*	
Multip	E	E+ZPE	G	E	E+ZPE
M2	-1712.80198	-1712.49524	-1712.55264	-1713.651610	-1713.344867

Table S33: Group spin densities and charges of optimized UB3LYP/B1 geometries of ²Cpd I(CF₃COO).

	Spin densities				Charges			
	Fe	O	Por	CF ₃ COO	Fe	O	Por	CF ₃ COO
M2	1.07	1.00	-1.05	-0.02	0.63	-0.30	0.24	-0.58

Table S34: Group spin densities and group charges of UB3LYP/B2//UB3LYP/B1 single point calculations for ²Cpd I(CF₃COO).

	Spin densities				Charges			
	Fe	O	Por	CF ₃ COO	Fe	O	Por	CF ₃ COO
M2	1.18	0.93	-1.09	-0.02	0.43	-0.13	0.14	-0.44

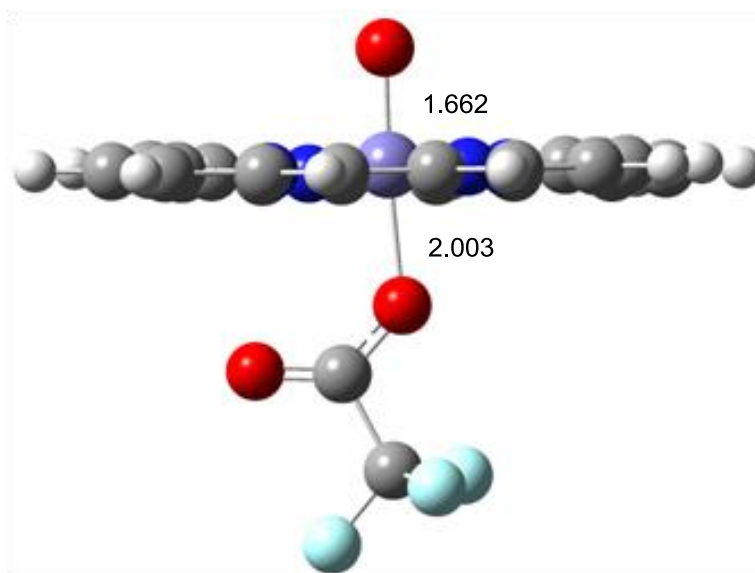


Figure S13. Optimized UB3LYP/B1 geometry of ²Cpd I(CF₃COO) with bond lengths in angstroms.

Table S35: Absolute energies, free energies and zero-point energies (in au) and relative (free) energies (in kcal mol⁻¹) of optimized UB3LYP/B1 geometries of ²TS1_{CF₃COO} and subsequent UB3LYP/B2//UB3LYP/B1 single points.

B1 -> LACVP						
Multip	E	E+ZPE	G	ΔE ^a	ΔE+ZPE ^a	ΔG ^a
M2	-2023.588816	-2023.122950	-2023.186868	15.03	15.31	31.37

^a with respect to ²Cpd I(CF₃COO) + EB.

B2 -> LACV3P+*				
Multip	E	E+ZPE	ΔE ^a	ΔE+ZPE ^a
M2	-2024.571377	-2024.105510	17.07	17.34

^a with respect to ²Cpd I(CF₃COO) + EB.

Table S36: Group spin densities and charges of optimized UB3LYP/B1 geometries of ²TS1_{CF₃COO}.

	Spin densities					Charges				
	Fe	O	Por	CF ₃ COO	EB	Fe	O	Por	CF ₃ COO	EB
M2	1.07	0.58	-0.56	-0.01	-0.07	0.65	-0.33	-0.10	-0.53	0.30

Table S37: Group spin densities and group charges of UB3LYP/B2//UB3LYP/B1 single point calculations for ²TS1_{CF₃COO}.

	Spin densities					Charges				
	Fe	O	Por	CF ₃ COO	EB	Fe	O	Por	CF ₃ COO	EB
M2	1.14	0.53	-0.57	-0.01	-0.09	0.47	0.00	-0.10	-0.46	0.08

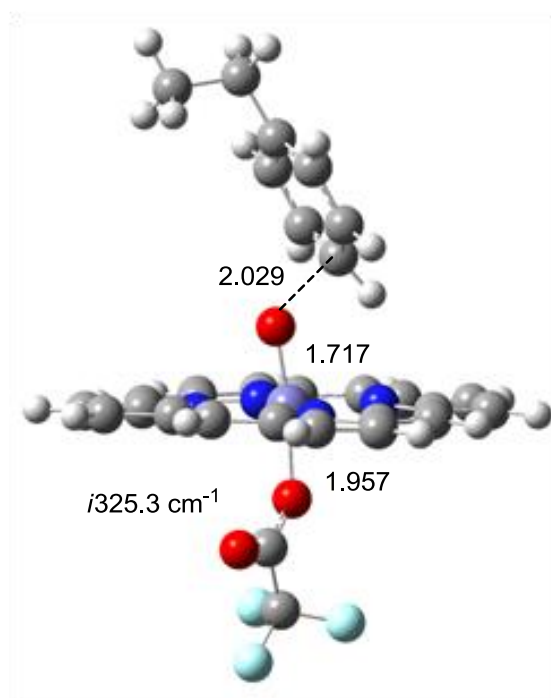


Figure S14. Optimized UB3LYP/B1 geometry of $^2\text{TS1}_{\text{CF}_3\text{COO}}$ with bond lengths in angstroms and the imaginary frequency in the transition state in wavenumbers.

Table S38: Absolute energies, free energies and zero-point energies (in au) of optimized UB3LYP/B1 geometries of ²Cpd I(CH₃COO) and subsequent UB3LYP/B2//UB3LYP/B1 single points.

B1 -> LACVP				B2 -> LACV3P+*	
Multip	E	E+ZPE	G	E	E+ZPE
M2	-1415.155999	-1414.825383	-1414.879470	-1415.829866	-1415.499250

Table S39: Group spin densities and charges of optimized UB3LYP/B1 geometries of ²Cpd I(CH₃COO).

	Spin densities				Charges			
	Fe	O	Por	CH ₃ COO	Fe	O	Por	CH ₃ COO
M2	1.08	1.00	-0.92	-0.16	0.62	-0.31	0.10	-0.41

Table S40: Group spin densities and group charges of UB3LYP/B2//UB3LYP/B1 single point calculations for ²Cpd I(CH₃COO).

	Spin densities				Charges			
	Fe	O	Por	CH ₃ COO	Fe	O	Por	CH ₃ COO
M2	1.18	0.93	-0.97	-0.14	0.50	-0.16	0.09	-0.42

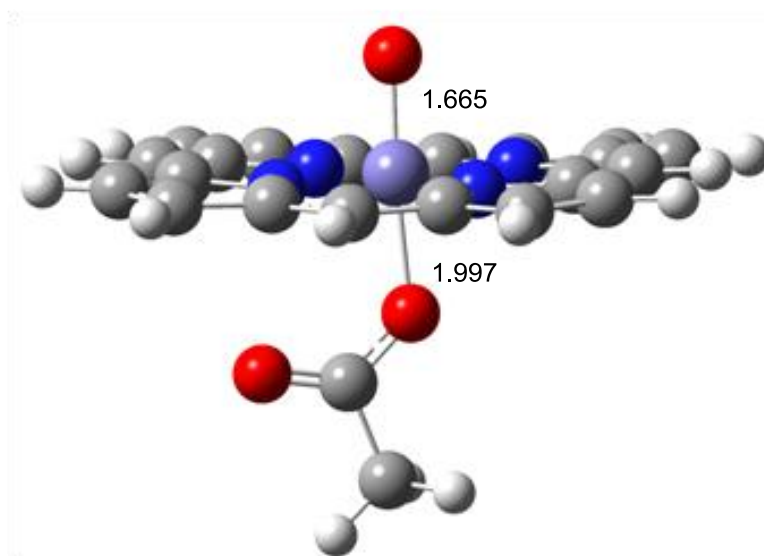


Figure S15. Optimized UB3LYP/B1 geometry of ²Cpd I(CH₃COO) with bond lengths in angstroms.

Table S41: Absolute energies, free energies and zero-point energies (in au) and relative (free) energies (in kcal mol⁻¹) of optimized UB3LYP/B1 geometries of ²TS1_{CH₃COO} and subsequent UB3LYP/B2//UB3LYP/B1 single points.

B1 -> LACVP						
Multip	E	E+ZPE	G	ΔE ^a	ΔE+ZPE ^a	ΔG ^a
M2	-1725.946020	-1725.455046	-1725.520066	13.04	14.09	27.38

^a with respect to ²CpdI + EB.

B2 -> LACV3P+*				
Multip	E	E+ZPE	ΔE ^a	ΔE+ZPE ^a
M2	-1726.756365	-1726.265391	12.84	13.89

^a with respect to ²CpdI + EB.

Table S42: Group spin densities and charges of optimized UB3LYP/B1 geometries of ²TS1_{CH₃COO}.

	Spin densities					Charges				
	Fe	O	Por	CH ₃ COO	EB	Fe	O	Por	CH ₃ COO	EB
M2	1.51	-0.02	-0.16	0.06	-0.38	0.71	-0.34	-0.34	-0.38	0.35

Table S43: Group spin densities and group charges of UB3LYP/B2//UB3LYP/B1 single point calculations for ²TS1_{CH₃COO}.

	Spin densities					Charges				
	Fe	O	Por	CH ₃ COO	EB	Fe	O	Por	CH ₃ COO	EB
M2	1.59	-0.03	-0.19	0.04	-0.42	0.49	-0.03	-0.25	-0.37	0.15

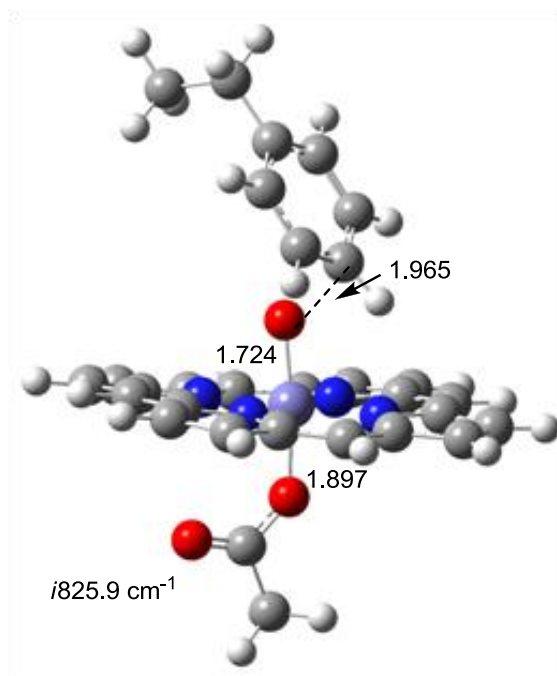


Figure S16. Optimized UB3LYP/B1 geometry of ${}^2\text{TS1}_{\text{CH}_3\text{COO}}$ with bond lengths in angstroms and the imaginary frequency in the transition state in wavenumbers.

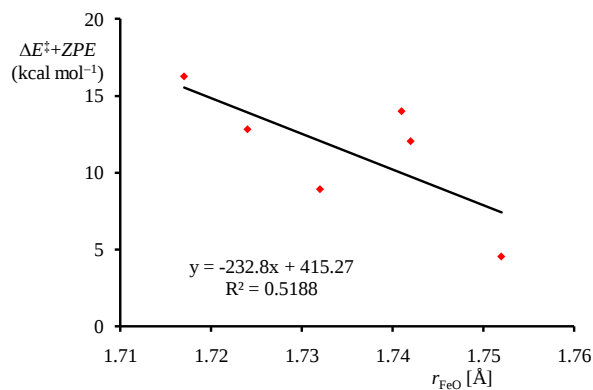


Figure S17. Correlation between Fe–O bond length with barrier height for the various **TS1_x** transition states.

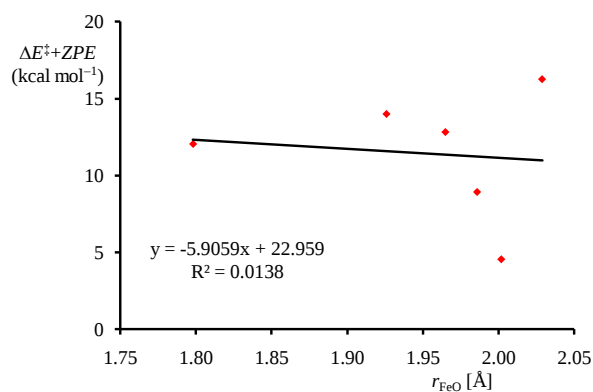


Figure S18. Correlation between C–O bond length with barrier height for the various **TS1_x** transition states.

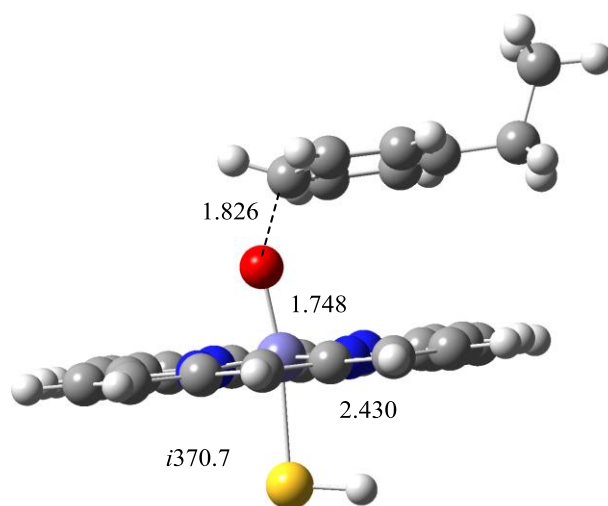


Figure S19. Face-on optimized geometry of **²TS1_{SH}** as calculated with UB3LYP/B1. Bond lengths are given in angstroms and the value of the imaginary frequency in wavenumbers.

Table S44: Absolute and relative energies of OPBE/B2 calculated reactants and rate determining transition states.

OPBE

B2 -> LACV3P+*			
Ethylbenzene	-310.8046626		
Axial Ligand	² Cpdl (Hartree)	² TS1 (Hartree)	$\Delta E^\ddagger$ (kcal/mol)
SH-	-1585.867046	-1896.649862	13.71
OH-	-1262.882032	-1573.668355	11.51
F-	-1286.913286	-1597.701713	10.19
Cl-	-1647.296507	-1958.084366	10.54
CF ₃ COO-	-1713.184661	-2023.970554	11.78
CH ₃ COO-	-1415.52262	-1726.305698	13.54

Table S45: Group spin densities and charges of OPBE/B2 calculated reactants and rate determining transition states.

Axial Ligand : - SH-										
	Spin densities					Charges				
	Fe	O	Por	SH	EB	Fe	O	Por	SH	EB
² Cpdl	1.32	0.83	-0.53	-0.62	-	-0.18	0.32	0.06	-0.20	-
² TS1	1.29	0.25	-0.17	-0.09	-0.27	-3.86	1.28	3.24	-0.32	-0.34
Axial Ligand : - OH-										
	Spin densities					Charges				
	Fe	O	Por	OH	EB	Fe	O	Por	OH	EB
² Cpdl	0.97	0.73	-0.35	-0.35	-	-0.27	0.33	-0.59	0.53	-
² TS1	1.19	0.07	-0.11	0.13	-0.29	2.17	1.37	-4.38	1.17	-0.34
Axial Ligand : - F-										
	Spin densities					Charges				
	Fe	O	Por	F	EB	Fe	O	Por	F	EB
² Cpdl	1.09	0.56	-0.67	0.02	-	-0.57	0.32	0.14	0.10	-
² TS1	1.22	0.07	-0.07	0.10	-0.31	2.34	1.28	-3.58	0.28	-0.31
Axial Ligand : - Cl-										
	Spin densities					Charges				
	Fe	O	Por	Cl	EB	Fe	O	Por	Cl	EB
² Cpdl	1.23	0.77	-0.83	-0.17	-	-0.75	0.44	0.75	-0.43	-
² TS1	1.44	0.19	-0.22	0.00	-0.40	-4.51	1.32	3.80	-0.42	-0.20
Axial Ligand : - CF ₃ COO-										
	Spin densities					Charges				
	Fe	O	Por	CF ₃ COO	EB	Fe	O	Por	CF ₃ COO	EB
² Cpdl	1.19	0.78	-0.87	-0.11	-	1.60	1.11	-3.04	0.33	-
² TS1	1.35	0.20	-0.30	0.00	-0.25	-4.61	1.56	2.60	0.61	-0.17
Axial Ligand : - CH ₃ COO-										
	Spin densities					Charges				
	Fe	O	Por	CF ₃ COO	EB	Fe	O	Por	CF ₃ COO	EB
² Cpdl	1.13	0.81	-0.64	-0.30	-	1.72	0.96	-3.18	0.50	-
² TS1	1.34	0.15	-0.23	0.03	-0.29	-4.27	1.55	2.18	0.82	-0.27

**Table S46: Absolute and relative energies of UB3LYP(15% HF exchange)/B2
calculated reactants and rate determining transition states.**

B2 -> LACV3P+*			
Ethyl Benzene	-310.5135442		
Axial Ligand	² Cpdl (Hartree)	² TS1 (Hartree)	$\Delta E^\ddagger$ (kcal/mol)
SH-	-1584.578134	-1895.072161	12.25
OH-	-1261.676159	-1572.184563	3.23
F-	-1285.722679	-1596.226665	6.00
Cl-	-1645.999017	-1956.497788	9.27
CF ₃ COO-	-1711.833910	-2022.328867	11.66
CH ₃ COO-	-1415.522620	-1726.305698	13.54

Table S47: Group spin densities and charges of UB3LYP(15% HF exchange)/B2 calculated reactants and rate determining transition states.

Axial Ligand : - SH-										
	Spin densities					Charges				
	Fe	O	Por	SH	EB	Fe	O	Por	SH	EB
² Cpdl	1.31	0.88	-0.56	-0.64	-	0.13	0.14	-0.15	-0.12	-
² TS1	1.51	0.14	-0.13	-0.10	-0.41	-2.09	1.00	1.44	-0.20	-0.16
Axial Ligand : - OH-										
	Spin densities					Charges				
	Fe	O	Por	OH	EB	Fe	O	Por	OH	EB
² Cpdl	1.18	0.84	-0.69	-0.33	-	0.01	0.11	-0.46	0.34	-
² TS1	1.47	-0.09	-0.14	0.15	-0.38	2.59	1.10	-4.46	0.91	-0.14
Axial Ligand : - F-										
	Spin densities					Charges				
	Fe	O	Por	F	EB	Fe	O	Por	F	EB
² Cpdl	1.23	0.89	-1.14	0.02	-	-0.23	0.09	0.19	-0.06	-
² TS1	1.46	-0.04	-0.10	0.09	-0.41	2.77	1.03	-3.85	0.16	-0.11
Axial Ligand : - Cl-										
	Spin densities					Charges				
	Fe	O	Por	Cl	EB	Fe	O	Por	Cl	EB
² Cpdl	1.29	0.90	-1.05	-0.14	-	-0.55	0.22	0.75	-0.42	-
² TS1	1.53	0.16	-0.17	0.00	-0.52	-3.14	1.04	2.41	-0.32	0.01
Axial Ligand : - CF ₃ COO-										
	Spin densities					Charges				
	Fe	O	Por	CF ₃ COO	EB	Fe	O	Por	CF ₃ COO	EB
² Cpdl	1.26	0.92	-1.16	-0.02	-	1.61	0.79	-2.54	0.14	-
² TS1	1.52	0.09	-0.25	0.02	-0.37	-3.16	1.25	1.43	0.47	0.02
Axial Ligand : - CH ₃ COO-										
	Spin densities					Charges				
	Fe	O	Por	CF ₃ COO	EB	Fe	O	Por	CF ₃ COO	EB
² Cpdl	1.13	0.81	-0.64	-0.30	-	1.72	0.96	-3.18	0.50	-
² TS1	1.34	0.15	-0.23	0.03	-0.29	-4.27	1.55	2.18	0.82	-0.27

Cartesian coordinates of optimized geometries:**²CpdI(F):**

26	-0.000875000	0.020916000	-0.008422000
7	0.000040000	-0.019578000	2.010292000
7	2.025312000	0.005427000	-0.012691000
7	-2.027494000	-0.041516000	-0.012047000
7	-0.001482000	-0.030951000	-2.043109000
6	-1.101530000	-0.057576000	2.839515000
6	2.852442000	0.015578000	-1.115768000
6	1.102096000	-0.041479000	2.839481000
6	2.856815000	0.002529000	1.087237000
6	-2.858244000	-0.053659000	1.088324000
6	1.099558000	-0.017549000	-2.871789000
6	-2.855057000	-0.058787000	-1.114671000
6	-1.102640000	-0.051802000	-2.871465000
6	-0.682271000	-0.097015000	4.225969000
6	4.240945000	0.027025000	-0.699179000
6	0.683617000	-0.087475000	4.225941000
6	4.243542000	0.018351000	0.666358000
6	-4.245385000	-0.072037000	0.668231000
6	0.680875000	-0.028008000	-4.260095000
6	-4.243353000	-0.075405000	-0.697330000
6	-0.684309000	-0.049565000	-4.260021000
1	-1.352885000	-0.131326000	5.071852000
1	5.086210000	0.036014000	-1.371441000
1	1.354650000	-0.112079000	5.071827000
1	5.091010000	0.018904000	1.335609000
1	-5.092637000	-0.084928000	1.337879000
1	1.351694000	-0.020756000	-5.106328000
1	-5.088719000	-0.091014000	-1.369348000
1	-1.355068000	-0.063357000	-5.106413000
6	-2.425086000	-0.061729000	2.410214000
6	2.421337000	0.005039000	-2.438662000
6	-2.424346000	-0.065312000	-2.437720000
6	2.425174000	-0.021186000	2.409494000
1	-3.191021000	-0.084116000	3.179510000
1	3.190212000	0.013088000	-3.205379000
1	-3.193333000	-0.081133000	-3.204194000
1	3.192050000	-0.032923000	3.178080000
8	-0.022652000	1.700823000	-0.056388000
9	0.018578000	-1.842283000	-0.027331000

⁴CpdI(F):

26	-0.001370000	0.018552000	-0.011746000
7	-0.000264000	-0.020172000	2.009560000
7	2.024180000	0.006075000	-0.014507000
7	-2.026273000	-0.040704000	-0.013566000
7	-0.001618000	-0.030378000	-2.042458000
6	-1.101689000	-0.057534000	2.839081000
6	2.852400000	0.017035000	-1.116879000
6	1.101958000	-0.041812000	2.838758000
6	2.855816000	0.002628000	1.086569000
6	-2.857383000	-0.053143000	1.087941000
6	1.100030000	-0.017293000	-2.872082000
6	-2.854982000	-0.057570000	-1.115733000
6	-1.103088000	-0.051817000	-2.871798000

6	-0.682325000	-0.096281000	4.225583000
6	4.240607000	0.028553000	-0.699661000
6	0.683615000	-0.086962000	4.225376000
6	4.242543000	0.019016000	0.665781000
6	-4.244424000	-0.071107000	0.667674000
6	0.680843000	-0.028879000	-4.259944000
6	-4.242938000	-0.074070000	-0.697761000
6	-0.684199000	-0.050625000	-4.259922000
1	-1.352825000	-0.129882000	5.071589000
1	5.086165000	0.038110000	-1.371532000
1	1.354719000	-0.111048000	5.071227000
1	5.089774000	0.019365000	1.335337000
1	-5.091519000	-0.084017000	1.337521000
1	1.351612000	-0.022142000	-5.106208000
1	-5.088537000	-0.089357000	-1.369475000
1	-1.354817000	-0.065112000	-5.106400000
6	-2.425135000	-0.061617000	2.409606000
6	2.421613000	0.006665000	-2.439814000
6	-2.424704000	-0.064125000	-2.438763000
6	2.424877000	-0.021668000	2.408578000
1	-3.191362000	-0.083897000	3.178597000
1	3.190355000	0.015496000	-3.206620000
1	-3.193610000	-0.079375000	-3.205294000
1	3.191977000	-0.033475000	3.176932000
8	-0.022022000	1.700657000	-0.042653000
9	0.020248000	-1.842657000	-0.019026000

²TS1_F:

26	0.005360000	-0.005166000	-0.001518000
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7	2.027531000	-0.033820000	-0.002682000
7	-2.016994000	-0.039673000	-0.010703000
7	0.009896000	-0.064745000	-2.035478000
6	-1.115124000	-0.057997000	2.823644000
6	2.852381000	-0.055953000	-1.114029000
6	1.111712000	-0.023693000	2.827596000
6	2.858646000	-0.019452000	1.101583000
6	-2.853113000	-0.055468000	1.089950000
6	1.119755000	-0.082701000	-2.858221000
6	-2.836824000	-0.041830000	-1.126426000
6	-1.096317000	-0.062708000	-2.863320000
6	-0.687263000	-0.096294000	4.202111000
6	4.238051000	-0.050544000	-0.690913000
6	0.679577000	-0.073686000	4.204490000
6	4.242662000	-0.026794000	0.673956000
6	-4.234808000	-0.060439000	0.656075000
6	0.697072000	-0.097145000	-4.244216000
6	-4.224191000	-0.051052000	-0.709281000
6	-0.667709000	-0.083712000	-4.247560000
1	-1.357703000	-0.142542000	5.048111000
1	5.082637000	-0.067665000	-1.364353000
1	1.347825000	-0.099090000	5.052779000
1	5.091259000	-0.022129000	1.342839000
1	-5.086061000	-0.075087000	1.321327000
1	1.370170000	-0.116825000	-5.088670000
1	-5.065723000	-0.056981000	-1.386739000

1	-1.337040000	-0.090977000	-5.095499000
6	-2.437782000	-0.068094000	2.412512000
6	2.439495000	-0.081745000	-2.436383000
6	-2.417947000	-0.050205000	-2.447251000
6	2.436906000	-0.013787000	2.422332000
1	-3.202053000	-0.097919000	3.181467000
1	3.209333000	-0.099959000	-3.200177000
1	-3.184393000	-0.054698000	-3.214665000
1	3.197740000	-0.022723000	3.195308000
8	0.002792000	1.704858000	-0.274975000
9	0.009869000	-1.814131000	-0.027276000
6	-0.084599000	3.080845000	1.155109000
6	1.241473000	3.604329000	1.065466000
6	1.477194000	4.816473000	0.430113000
6	0.411126000	5.578158000	-0.101335000
6	-0.911617000	5.087811000	0.036643000
6	-1.163374000	3.879764000	0.667901000
1	-0.288699000	2.289991000	1.865646000
1	2.062329000	3.022727000	1.470353000
1	2.492304000	5.195364000	0.341695000
1	-1.735879000	5.679184000	-0.353832000
1	-2.178092000	3.509508000	0.770451000
6	0.676325000	6.878464000	-0.830754000
6	0.850034000	6.680856000	-2.356640000
1	1.581354000	7.350495000	-0.426448000
1	-0.153577000	7.576320000	-0.653006000
1	1.037676000	7.642021000	-2.850964000
1	-0.049248000	6.236604000	-2.797939000
1	1.692619000	6.013072000	-2.571165000

⁴TS1_F:

26	0.004081000	-0.033894000	-0.039786000
7	0.003352000	0.009970000	1.980584000
7	2.028949000	-0.045784000	-0.031834000
7	-2.020208000	-0.079271000	-0.031263000
7	0.004882000	-0.060955000	-2.032142000
6	-1.106115000	-0.053160000	2.812000000
6	2.857555000	-0.053556000	-1.135853000
6	1.113765000	-0.004745000	2.811012000
6	2.857305000	-0.021128000	1.078053000
6	-2.848536000	-0.094821000	1.078662000
6	1.116535000	-0.062968000	-2.864783000
6	-2.848646000	-0.079194000	-1.135782000
6	-1.106989000	-0.060851000	-2.864764000
6	-0.678595000	-0.076040000	4.191494000
6	4.243189000	-0.039914000	-0.711084000
6	0.688773000	-0.044715000	4.190739000
6	4.243153000	-0.018509000	0.653122000
6	-4.234039000	-0.109676000	0.653628000
6	0.687683000	-0.066560000	-4.245093000
6	-4.233930000	-0.099287000	-0.711077000
6	-0.678126000	-0.064416000	-4.245146000
1	-1.347254000	-0.121509000	5.038776000
1	5.088869000	-0.047125000	-1.383046000
1	1.359679000	-0.060913000	5.037051000
1	5.089233000	-0.006317000	1.324587000

1	-5.080190000	-0.128598000	1.325078000
1	1.357694000	-0.073679000	-5.092218000
1	-5.079571000	-0.108177000	-1.383066000
1	-1.347928000	-0.070204000	-5.092517000
6	-2.430374000	-0.085877000	2.398701000
6	2.438673000	-0.064644000	-2.457037000
6	-2.429111000	-0.068957000	-2.456968000
6	2.439052000	-0.000821000	2.397643000
1	-3.193828000	-0.115589000	3.168474000
1	3.201776000	-0.071787000	-3.227539000
1	-3.192037000	-0.073590000	-3.227687000
1	3.202878000	0.000197000	3.167721000
8	-0.008312000	1.740357000	-0.214603000
9	0.017313000	-1.833140000	0.083332000
6	-0.125284000	3.118732000	1.217333000
6	1.187048000	3.678839000	1.124604000
6	1.389351000	4.889137000	0.480196000
6	0.304258000	5.621309000	-0.057052000
6	-1.004175000	5.099107000	0.088908000
6	-1.225227000	3.891626000	0.730322000
1	-0.309231000	2.327947000	1.929853000
1	2.022934000	3.122554000	1.533266000
1	2.393568000	5.294321000	0.390687000
1	-1.844233000	5.667744000	-0.300674000
1	-2.230086000	3.499206000	0.839822000
6	0.537614000	6.919999000	-0.797446000
6	0.714542000	6.714305000	-2.321746000
1	1.431158000	7.416855000	-0.397850000
1	-0.307736000	7.599360000	-0.625277000
1	0.878494000	7.674668000	-2.824335000
1	-0.173761000	6.244917000	-2.758698000
1	1.572068000	6.065428000	-2.531173000

²A_F:

26	0.008183000	-0.058652000	-0.021424000
7	-0.000401000	0.026464000	1.968617000
7	2.028442000	-0.089974000	-0.013272000
7	-2.013941000	-0.071032000	-0.030943000
7	0.015127000	-0.176157000	-2.046115000
6	-1.118611000	0.022942000	2.802355000
6	2.856203000	-0.134581000	-1.123717000
6	1.109117000	0.003589000	2.812358000
6	2.857842000	-0.061468000	1.092540000
6	-2.852232000	-0.026179000	1.067428000
6	1.124868000	-0.216687000	-2.866262000
6	-2.832682000	-0.120533000	-1.147353000
6	-1.088048000	-0.218044000	-2.875295000
6	-0.694519000	0.024701000	4.181661000
6	4.239889000	-0.127871000	-0.697082000
6	0.672278000	0.012200000	4.187809000
6	4.241404000	-0.083576000	0.667708000
6	-4.232574000	-0.041787000	0.631340000
6	0.706287000	-0.288890000	-4.251795000
6	-4.219827000	-0.100344000	-0.732670000
6	-0.658502000	-0.289980000	-4.257530000
1	-1.367662000	0.026224000	5.026661000

1	5.086300000	-0.160442000	-1.367754000
1	1.337183000	0.001531000	5.038858000
1	5.087776000	-0.072515000	1.338563000
1	-5.084714000	-0.017926000	1.295073000
1	1.381684000	-0.334808000	-5.093478000
1	-5.060051000	-0.133667000	-1.410517000
1	-1.326848000	-0.337080000	-5.104999000
6	-2.440114000	0.016917000	2.390720000
6	2.445477000	-0.193406000	-2.444825000
6	-2.411751000	-0.190567000	-2.464651000
6	2.434279000	-0.020733000	2.412464000
1	-3.205633000	0.031288000	3.158960000
1	3.216023000	-0.229924000	-3.207277000
1	-3.176236000	-0.229559000	-3.233019000
1	3.192756000	-0.020068000	3.187413000
8	0.010577000	1.713549000	-0.253692000
9	-0.003864000	-1.855746000	0.019194000
6	0.016920000	2.812869000	0.782887000
6	1.310728000	3.540311000	0.693903000
6	1.378682000	4.858771000	0.314789000
6	0.205519000	5.621519000	0.044976000
6	-1.064523000	4.989322000	0.187582000
6	-1.175863000	3.672367000	0.557128000
1	-0.063573000	2.281757000	1.744964000
1	2.209447000	2.967576000	0.898587000
1	2.345956000	5.347502000	0.227702000
1	-1.960698000	5.577836000	0.006852000
1	-2.146326000	3.198087000	0.659798000
6	0.306200000	7.053787000	-0.420364000
6	0.371976000	7.175123000	-1.962611000
1	1.200050000	7.522043000	0.012256000
1	-0.559295000	7.621901000	-0.056081000
1	0.443896000	8.225877000	-2.262879000
1	-0.522106000	6.745022000	-2.427167000
1	1.242964000	6.643986000	-2.358095000

⁴A_F:

26	0.002697000	-0.012684000	-0.007529000
7	0.013739000	-0.035077000	2.005231000
7	2.025478000	-0.007390000	-0.015358000
7	-2.019518000	-0.065239000	0.006501000
7	-0.007582000	-0.009441000	-2.019582000
6	-1.093368000	-0.101163000	2.841729000
6	2.844971000	0.027231000	-1.129515000
6	1.131061000	-0.073883000	2.829392000
6	2.861511000	-0.017633000	1.088199000
6	-2.843146000	-0.092372000	1.119075000
6	1.096890000	0.022937000	-2.852795000
6	-2.851071000	-0.062685000	-1.099351000
6	-1.121351000	-0.015975000	-2.841030000
6	-0.656288000	-0.160442000	4.217087000
6	4.231701000	0.038906000	-0.712666000
6	0.710838000	-0.143903000	4.209452000
6	4.242052000	0.011447000	0.652248000
6	-4.228522000	-0.106207000	0.697565000
6	0.662730000	0.034180000	-4.233128000

6	-4.233141000	-0.088767000	-0.667664000
6	-0.702493000	0.009796000	-4.225928000
1	-1.320603000	-0.215734000	5.067137000
1	5.073134000	0.061313000	-1.389794000
1	1.385729000	-0.182927000	5.052093000
1	5.093211000	0.006281000	1.317191000
1	-5.072477000	-0.131616000	1.371458000
1	1.329042000	0.056171000	-5.082817000
1	-5.081876000	-0.095840000	-1.335985000
1	-1.378033000	0.007832000	-5.068560000
6	-2.419178000	-0.110850000	2.437904000
6	2.421595000	0.041094000	-2.448078000
6	-2.441659000	-0.040996000	-2.422323000
6	2.452380000	-0.050915000	2.411476000
1	-3.178495000	-0.149243000	3.211016000
1	3.182563000	0.064360000	-3.220190000
1	-3.210768000	-0.044894000	-3.186676000
1	3.220670000	-0.071910000	3.176410000
8	-0.028488000	1.784004000	-0.064710000
9	0.027803000	-1.811735000	0.007442000
6	-0.087670000	2.856823000	0.972499000
6	1.202831000	3.614292000	0.917019000
6	1.258993000	4.937192000	0.563806000
6	0.085898000	5.690028000	0.259499000
6	-1.173267000	5.022926000	0.307877000
6	-1.282739000	3.701622000	0.656751000
1	-0.205001000	2.342981000	1.934758000
1	2.104204000	3.054657000	1.143312000
1	2.222603000	5.440004000	0.520198000
1	-2.069766000	5.590395000	0.068233000
1	-2.247454000	3.206232000	0.686205000
6	0.180576000	7.139454000	-0.153948000
6	0.346857000	7.325292000	-1.682778000
1	1.030969000	7.613023000	0.355138000
1	-0.721165000	7.675267000	0.172291000
1	0.411576000	8.389656000	-1.938505000
1	-0.502611000	6.893290000	-2.223529000
1	1.257154000	6.830488000	-2.039769000

²A_F:

26	0.000000000	0.000000000	0.000000000
7	0.000000000	0.000000000	2.152288810
7	2.018656291	0.000000000	0.012790432
7	-2.010798106	0.064494310	0.089289065
7	-0.024261185	0.195828072	-1.972059767
6	-1.115763165	-0.441456458	2.913872186
6	2.837647872	0.165587458	-1.086057200
6	1.135122358	-0.447592163	2.876971014
6	2.843668412	-0.100172814	1.112511640
6	-2.834849825	-0.049197124	1.195275507
6	1.072106748	0.271149148	-2.806856705
6	-2.849760660	0.254735910	-0.998565176
6	-1.138852245	0.308271342	-2.774018261
6	-0.660716624	-1.032994523	4.133737047
6	4.226409783	0.180286211	-0.663253117
6	0.713509736	-1.036012334	4.111284300

6	4.231133675	0.014294624	0.691644895
6	-4.221786184	0.089496406	0.794056180
6	0.631306786	0.412988751	-4.182025804
6	-4.230566457	0.279733296	-0.557882858
6	-0.733228056	0.440358316	-4.161426933
1	-1.310145908	-1.456894416	4.886360173
1	5.070750685	0.298807990	-1.326813059
1	1.384325337	-1.465203660	4.841982282
1	5.080467246	-0.032315219	1.358037748
1	-5.063203507	0.038605876	1.469980543
1	1.290773956	0.487204590	-5.034288717
1	-5.081306376	0.414634519	-1.210189578
1	-1.414494473	0.537038226	-4.994147271
6	-2.428940326	-0.331638590	2.498313071
6	2.401156753	0.272433743	-2.398633708
6	-2.451268212	0.353058639	-2.323126113
6	2.442157894	-0.356643795	2.425654690
1	-3.204851893	-0.552221210	3.224644896
1	3.158034264	0.369228666	-3.170154018
1	-3.231554098	0.473429876	-3.067608705
1	3.228289841	-0.581887262	3.140236683
8	0.120645186	1.835278850	0.205702492
9	-0.003178619	-1.809137006	-0.059352464
6	-0.240811501	2.487161506	1.375698663
6	0.750988637	2.840650553	2.356933422
6	0.389406627	3.530629579	3.514992801
6	-0.938374276	3.922123410	3.746726667
6	-1.910525709	3.610274536	2.767094351
6	-1.584760369	2.913671461	1.613098377
1	-0.094001534	1.366427775	1.938581469
1	1.782416778	2.579736309	2.150537054
1	1.156349877	3.778203602	4.243256195
1	-2.940807876	3.913448492	2.932847652
1	-2.330135202	2.699238370	0.857692447
6	-1.323417704	4.694240530	4.992402704
6	-1.299257511	6.225509138	4.781052763
1	-0.641886899	4.430670765	5.811152428
1	-2.328866409	4.391403221	5.313243308
1	-1.586450508	6.749914494	5.699456979
1	-1.993671120	6.522124913	3.986645617
1	-0.297949104	6.564097456	4.491801142

²B_F:

26	0.059146000	0.103848000	-0.024878000
7	0.173610000	0.402804000	2.136593000
7	2.077150000	-0.005624000	-0.074619000
7	-1.932244000	0.281665000	0.137755000
7	-0.027583000	-0.083720000	-1.991101000
6	-0.954861000	0.129713000	3.000723000
6	2.854752000	-0.091887000	-1.214449000
6	1.344606000	-0.010166000	2.880409000
6	2.950047000	0.022619000	0.990574000
6	-2.704423000	0.395180000	1.275467000
6	1.026516000	-0.223559000	-2.864015000
6	-2.810505000	0.295403000	-0.933339000
6	-1.174477000	-0.070558000	-2.751369000

6	-0.455144000	-0.326117000	4.247790000
6	4.260857000	-0.089672000	-0.854199000
6	0.924159000	-0.409005000	4.175906000
6	4.320723000	-0.022189000	0.506528000
6	-4.104113000	0.516895000	0.910466000
6	0.526234000	-0.331778000	-4.222708000
6	-4.168947000	0.458663000	-0.451365000
6	-0.833595000	-0.237965000	-4.153230000
1	-1.077659000	-0.618809000	5.080406000
1	5.076799000	-0.144684000	-1.559646000
1	1.589964000	-0.780371000	4.941010000
1	5.195904000	-0.011899000	1.139763000
1	-4.914801000	0.620573000	1.616750000
1	1.146127000	-0.455810000	-5.098285000
1	-5.044080000	0.503016000	-1.082789000
1	-1.550350000	-0.270479000	-4.960447000
6	-2.262901000	0.273932000	2.598603000
6	2.370369000	-0.211101000	-2.507191000
6	-2.463362000	0.120142000	-2.264264000
6	2.615348000	-0.032820000	2.349974000
1	-3.028137000	0.203122000	3.364631000
1	3.098182000	-0.299553000	-3.306855000
1	-3.269373000	0.129010000	-2.990587000
1	3.433711000	-0.198158000	3.043632000
8	0.243846000	1.984036000	-0.316704000
9	-0.044744000	-1.687146000	0.226928000
6	-0.093925000	3.026572000	0.491568000
6	0.838370000	3.541856000	1.424864000
6	0.502122000	4.619167000	2.253638000
6	-0.760589000	5.227377000	2.184371000
6	-1.678572000	4.723239000	1.240278000
6	-1.362459000	3.647996000	0.411137000
1	0.222143000	1.410771000	1.907502000
1	1.832789000	3.105318000	1.459155000
1	1.236418000	4.993820000	2.963401000
1	-2.662643000	5.180838000	1.164210000
1	-2.080276000	3.267156000	-0.306699000
6	-1.116369000	6.409772000	3.067062000
6	-0.837449000	7.775454000	2.400386000
1	-0.550963000	6.348734000	4.006880000
1	-2.179304000	6.357715000	3.341017000
1	-1.110457000	8.602948000	3.066868000
1	-1.411273000	7.880468000	1.472257000
1	0.224430000	7.875194000	2.147295000

⁴B_F:

26	0.079453000	-0.068100000	0.118405000
7	0.426728000	-0.617917000	2.488570000
7	2.047218000	-0.170080000	-0.072638000
7	-1.838909000	0.083497000	0.497896000
7	-0.158385000	0.645257000	-1.788775000
6	-0.666022000	-1.139225000	3.170735000
6	2.739064000	0.177986000	-1.221369000
6	1.579955000	-1.313115000	2.830444000
6	2.980079000	-0.617938000	0.858787000
6	-2.497174000	-0.251454000	1.679633000

6	0.847604000	0.857541000	-2.700404000
6	-2.799990000	0.481755000	-0.420066000
6	-1.352744000	0.952742000	-2.393558000
6	-0.152154000	-2.134664000	4.070807000
6	4.155651000	-0.045770000	-1.005511000
6	1.212308000	-2.241027000	3.863596000
6	4.301880000	-0.537364000	0.259588000
6	-3.920373000	-0.036660000	1.483831000
6	0.262186000	1.323552000	-3.948616000
6	-4.104131000	0.412887000	0.207596000
6	-1.093870000	1.380554000	-3.760098000
1	-0.757525000	-2.745813000	4.723492000
1	4.924718000	0.143802000	-1.739720000
1	1.883640000	-2.952139000	4.321902000
1	5.214457000	-0.827649000	0.759772000
1	-4.670602000	-0.217089000	2.239703000
1	0.816700000	1.568409000	-4.842844000
1	-5.032645000	0.672203000	-0.279611000
1	-1.848654000	1.682672000	-4.471555000
6	-1.988416000	-0.825277000	2.856653000
6	2.197336000	0.643077000	-2.423282000
6	-2.584983000	0.871602000	-1.744683000
6	2.778268000	-1.174174000	2.133321000
1	-2.740824000	-1.158824000	3.564929000
1	2.905858000	0.850398000	-3.219000000
1	-3.467552000	1.143443000	-2.314757000
1	3.656553000	-1.625557000	2.584686000
8	0.362326000	1.566087000	1.163905000
9	-0.075743000	-1.845210000	-0.153322000
6	-0.349002000	2.721622000	1.354719000
6	-0.703806000	3.109937000	2.661834000
6	-1.401242000	4.299126000	2.880940000
6	-1.768560000	5.138520000	1.814661000
6	-1.401929000	4.743393000	0.515288000
6	-0.702199000	3.557925000	0.279824000
1	0.461903000	0.395247000	2.194121000
1	-0.424263000	2.472550000	3.495160000
1	-1.671060000	4.578178000	3.896884000
1	-1.673377000	5.374795000	-0.327672000
1	-0.424831000	3.265562000	-0.725783000
6	-2.499737000	6.444870000	2.063351000
6	-1.546967000	7.635373000	2.314500000
1	-3.167024000	6.333698000	2.929060000
1	-3.142987000	6.676193000	1.203469000
1	-2.108623000	8.561032000	2.491096000
1	-0.886961000	7.793837000	1.453688000
1	-0.912748000	7.447765000	3.188848000

²C_F:

26	-0.003430000	0.002084000	0.006275000
7	0.004569000	-0.021933000	2.038511000
7	2.010374000	0.008108000	-0.001004000
7	-2.005613000	0.161649000	0.044799000
7	0.000530000	0.231772000	-1.983444000
6	-1.101162000	-0.037049000	2.885083000
6	2.845545000	0.128169000	-1.099692000

6	1.110723000	-0.267888000	2.847481000
6	2.837673000	-0.191789000	1.092223000
6	-2.836682000	0.166126000	1.155896000
6	1.103429000	0.309017000	-2.821235000
6	-2.842094000	0.161786000	-1.061590000
6	-1.111712000	0.216439000	-2.809815000
6	-0.671233000	-0.251746000	4.246792000
6	4.227393000	0.013652000	-0.683749000
6	0.688368000	-0.401987000	4.222546000
6	4.222403000	-0.192558000	0.666088000
6	-4.220678000	0.193635000	0.733641000
6	0.668655000	0.366374000	-4.200519000
6	-4.224096000	0.180994000	-0.631734000
6	-0.695766000	0.299002000	-4.193731000
1	-1.333729000	-0.297023000	5.098946000
1	5.075760000	0.074082000	-1.349992000
1	1.354162000	-0.590197000	5.052156000
1	5.066192000	-0.330267000	1.326530000
1	-5.065999000	0.205588000	1.405904000
1	1.332430000	0.432601000	-5.050330000
1	-5.073111000	0.186009000	-1.299761000
1	-1.370892000	0.304803000	-5.036907000
6	-2.420646000	0.094018000	2.477613000
6	2.428139000	0.288680000	-2.411811000
6	-2.431593000	0.171133000	-2.385670000
6	2.424330000	-0.340974000	2.409051000
1	-3.187284000	0.083947000	3.245132000
1	3.192545000	0.359868000	-3.177932000
1	-3.202510000	0.168089000	-3.148641000
1	3.191352000	-0.513035000	3.156472000
8	0.132325000	2.127783000	0.377728000
9	-0.067729000	-1.772626000	-0.112083000
6	-0.629273000	3.208598000	-0.121716000
6	-1.565352000	3.859687000	0.681356000
6	-2.287550000	4.934072000	0.149709000
6	-2.094466000	5.357745000	-1.174626000
6	-1.143144000	4.674857000	-1.956441000
6	-0.405860000	3.606870000	-1.439846000
1	0.116588000	2.048389000	1.357653000
1	-1.745115000	3.525852000	1.698455000
1	-3.019393000	5.441179000	0.772253000
1	-0.973268000	4.982944000	-2.984507000
1	0.328222000	3.081707000	-2.037959000
6	-2.871894000	6.533624000	-1.740069000
6	-2.022769000	7.815891000	-1.882668000
1	-3.732501000	6.741925000	-1.090552000
1	-3.285860000	6.267322000	-2.723180000
1	-2.635935000	8.653195000	-2.237699000
1	-1.201642000	7.669579000	-2.594964000
1	-1.581966000	8.099873000	-0.919404000

⁴C_F:

26	0.000667000	-0.008103000	-0.002530000
7	-0.000861000	-0.006516000	2.041185000
7	2.019692000	-0.005089000	0.039273000
7	-1.965976000	0.456553000	0.041850000

7	0.059016000	0.508218000	-1.949389000
6	-1.129171000	-0.082398000	2.862189000
6	2.866590000	0.049188000	-1.058667000
6	1.089069000	-0.289630000	2.868103000
6	2.835378000	-0.225424000	1.141754000
6	-2.816724000	0.376330000	1.137886000
6	1.171252000	0.478400000	-2.779431000
6	-2.775288000	0.742036000	-1.049082000
6	-1.027786000	0.773070000	-2.771818000
6	-0.729931000	-0.374979000	4.215604000
6	4.235460000	-0.138173000	-0.634277000
6	0.633966000	-0.500626000	4.218999000
6	4.216349000	-0.305158000	0.721530000
6	-4.178368000	0.621930000	0.721522000
6	0.770672000	0.731392000	-4.145042000
6	-4.152333000	0.850450000	-0.624682000
6	-0.583408000	0.915552000	-4.139693000
1	-1.412009000	-0.475145000	5.048226000
1	5.087630000	-0.136992000	-1.298185000
1	1.280740000	-0.723940000	5.054721000
1	5.049717000	-0.469157000	1.388602000
1	-5.030509000	0.620383000	1.385171000
1	1.448068000	0.763299000	-4.985921000
1	-4.979692000	1.071781000	-1.282485000
1	-1.234109000	1.127089000	-4.975352000
6	-2.436168000	0.108311000	2.443384000
6	2.476247000	0.259540000	-2.371227000
6	-2.344687000	0.886590000	-2.357834000
6	2.408889000	-0.367047000	2.453155000
1	-3.218391000	0.046844000	3.192357000
1	3.249582000	0.266604000	-3.131386000
1	-3.092980000	1.100473000	-3.112659000
1	3.161829000	-0.566484000	3.207451000
8	0.343873000	2.705514000	0.965544000
9	-0.210075000	-1.818565000	-0.219777000
6	-0.538321000	3.775343000	1.088177000
6	-1.387699000	3.938972000	2.189685000
6	-2.241108000	5.045591000	2.242989000
6	-2.264098000	6.002216000	1.213826000
6	-1.396955000	5.814393000	0.121769000
6	-0.539450000	4.715802000	0.052769000
1	0.240242000	2.016882000	1.663902000
1	-1.387575000	3.207221000	2.991612000
1	-2.902523000	5.163029000	3.098111000
1	-1.398366000	6.538455000	-0.689361000
1	0.126359000	4.567675000	-0.790096000
6	-3.169585000	7.217154000	1.294934000
6	-2.566654000	8.366954000	2.131292000
1	-4.137314000	6.927771000	1.727149000
1	-3.379881000	7.583764000	0.281622000
1	-3.248107000	9.224270000	2.171711000
1	-1.618213000	8.704496000	1.701581000
1	-2.366755000	8.041799000	3.157541000

²TS1_{OH}:

26	0.028953000	0.022886000	-0.049535000
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7	0.083054000	0.067827000	1.967320000
7	2.030695000	0.040372000	-0.113714000
7	-2.014363000	-0.047451000	0.007451000
7	-0.035543000	-0.166100000	-2.063096000
6	-1.005731000	0.055865000	2.819936000
6	2.828274000	-0.083089000	-1.239701000
6	1.208302000	0.122819000	2.764884000
6	2.890493000	0.067766000	0.974411000
6	-2.803513000	-0.031224000	1.139673000
6	1.046415000	-0.205906000	-2.929116000
6	-2.872497000	-0.099475000	-1.074302000
6	-1.175340000	-0.194532000	-2.856306000
6	-0.545587000	0.107978000	4.193993000
6	4.221412000	-0.110861000	-0.848816000
6	0.818141000	0.151298000	4.160505000
6	4.259357000	-0.014211000	0.513257000
6	-4.202817000	-0.069109000	0.757748000
6	0.574815000	-0.279033000	-4.293909000
6	-4.245666000	-0.109187000	-0.605846000
6	-0.791485000	-0.269588000	-4.248892000
1	-1.196069000	0.107559000	5.056389000
1	5.048179000	-0.207201000	-1.537893000
1	1.509465000	0.191013000	4.989497000
1	5.123050000	-0.016733000	1.162214000
1	-5.027835000	-0.068211000	1.455089000
1	1.216034000	-0.330037000	-5.162044000
1	-5.112750000	-0.148809000	-1.249269000
1	-1.488820000	-0.311857000	-5.072919000
6	-2.340003000	0.011778000	2.445383000
6	2.379577000	-0.181151000	-2.548197000
6	-2.486970000	-0.161509000	-2.404459000
6	2.517407000	0.127564000	2.307641000
1	-3.080016000	0.011304000	3.238674000
1	3.127149000	-0.252094000	-3.330882000
1	-3.271969000	-0.199325000	-3.152298000
1	3.308887000	0.152592000	3.049036000
8	-0.273869000	1.742541000	-0.118503000
6	0.602504000	3.440381000	-0.356291000
6	0.498386000	3.602867000	-1.778225000
6	1.624170000	3.544670000	-2.580604000
6	2.914894000	3.385854000	-2.019493000
6	3.034193000	3.294287000	-0.615155000
6	1.915845000	3.338636000	0.204269000
1	-0.193854000	3.824639000	0.267859000
1	-0.485523000	3.732950000	-2.214527000
1	1.523954000	3.625754000	-3.659505000
1	4.020279000	3.178557000	-0.175708000
1	2.019648000	3.270555000	1.281388000
6	4.143308000	3.365050000	-2.903914000
6	4.719971000	4.777341000	-3.162145000
1	3.894189000	2.899378000	-3.866359000
1	4.916567000	2.739731000	-2.440113000
1	5.605115000	4.723385000	-3.806715000
1	5.010564000	5.258793000	-2.221546000
1	3.978942000	5.419145000	-3.652085000
8	0.010447000	-1.811494000	0.103183000

1	-0.088306000	-2.232302000	-0.777263000
²A_{SH}(face-on):			
26	0.009414000	-0.006375000	-0.000649000
7	0.003650000	0.006599000	2.038464000
7	2.020293000	-0.027933000	-0.002531000
7	-2.010553000	-0.162129000	0.020768000
7	0.013354000	-0.143900000	-1.992174000
6	-1.100922000	0.027274000	2.866347000
6	2.857949000	-0.028413000	-1.106404000
6	1.111658000	0.056857000	2.860632000
6	2.843597000	0.032674000	1.114205000
6	-2.836089000	-0.125288000	1.131875000
6	1.118466000	-0.162124000	-2.830987000
6	-2.838934000	-0.295566000	-1.078418000
6	-1.100209000	-0.300940000	-2.812786000
6	-0.673317000	0.095602000	4.249956000
6	4.235554000	0.028537000	-0.672175000
6	0.691064000	0.111177000	4.246843000
6	4.226465000	0.065166000	0.693404000
6	-4.217920000	-0.230372000	0.712227000
6	0.685977000	-0.307017000	-4.201153000
6	-4.219871000	-0.338605000	-0.648467000
6	-0.677881000	-0.394113000	-4.189173000
1	-1.343107000	0.122934000	5.096617000
1	5.086877000	0.035960000	-1.336567000
1	1.364459000	0.155238000	5.090621000
1	5.068558000	0.109717000	1.368667000
1	-5.062381000	-0.227147000	1.385107000
1	1.352078000	-0.352988000	-5.049652000
1	-5.065256000	-0.441141000	-1.312922000
1	-1.348920000	-0.524609000	-5.025649000
6	-2.422039000	-0.027513000	2.450720000
6	2.442037000	-0.090409000	-2.427159000
6	-2.419088000	-0.365499000	-2.397379000
6	2.430517000	0.067054000	2.436190000
1	-3.190292000	-0.010718000	3.215654000
1	3.204970000	-0.106218000	-3.196746000
1	-3.179386000	-0.486324000	-3.161482000
1	3.201528000	0.110961000	3.198095000
8	-0.083560000	1.782527000	0.115995000
6	-0.075191000	3.107418000	-0.652351000
6	-0.668787000	2.978195000	-2.007935000
6	0.068428000	3.183495000	-3.147203000
6	1.443069000	3.555766000	-3.096993000
6	2.045637000	3.743718000	-1.822648000
6	1.335855000	3.573193000	-0.658452000
1	-0.706653000	3.718293000	0.005209000
1	-1.712848000	2.690200000	-2.066758000
1	-0.397793000	3.046881000	-4.119037000
1	3.091656000	4.036602000	-1.778020000
1	1.802097000	3.728572000	0.308048000
6	2.222635000	3.785551000	-4.370937000
6	2.034142000	5.212217000	-4.943658000
1	1.908393000	3.055084000	-5.128593000
1	3.291438000	3.613919000	-4.187492000

1	2.592681000	5.328190000	-5.879361000
1	2.388492000	5.969795000	-4.235779000
1	0.976537000	5.413999000	-5.149730000
16	0.007041000	-2.381286000	0.143992000
1	1.206995000	-2.594343000	-0.505494000

²TS1_{SH}(face-on):

26	-0.000897000	-0.006823000	0.003740000
7	-0.001176000	-0.005552000	2.038373000
7	2.011879000	-0.008324000	-0.003389000
7	-2.018855000	-0.198739000	0.030149000
7	0.001945000	-0.180884000	-1.986942000
6	-1.103881000	-0.000494000	2.871619000
6	2.846520000	-0.000726000	-1.108904000
6	1.108485000	0.053172000	2.859237000
6	2.838745000	0.053806000	1.109152000
6	-2.843518000	-0.171857000	1.142277000
6	1.104069000	-0.183260000	-2.829098000
6	-2.848152000	-0.343198000	-1.065813000
6	-1.110997000	-0.349178000	-2.805407000
6	-0.673028000	0.067024000	4.254126000
6	4.226476000	0.067809000	-0.680847000
6	0.690738000	0.098287000	4.246608000
6	4.221341000	0.099884000	0.684577000
6	-4.225894000	-0.292626000	0.727185000
6	0.673077000	-0.344471000	-4.199498000
6	-4.229045000	-0.401046000	-0.633659000
6	-0.689372000	-0.448369000	-4.184312000
1	-1.340414000	0.081182000	5.103185000
1	5.075300000	0.081788000	-1.348854000
1	1.366095000	0.145664000	5.088112000
1	5.065229000	0.147788000	1.357105000
1	-5.068380000	-0.300389000	1.402841000
1	1.339344000	-0.387396000	-5.048875000
1	-5.074317000	-0.514626000	-1.296462000
1	-1.360169000	-0.590342000	-5.019044000
6	-2.425331000	-0.072012000	2.459963000
6	2.427381000	-0.077483000	-2.428326000
6	-2.428574000	-0.418028000	-2.385459000
6	2.426336000	0.078498000	2.431744000
1	-3.190486000	-0.067202000	3.228694000
1	3.189223000	-0.085082000	-3.200270000
1	-3.189715000	-0.546668000	-3.147467000
1	3.197826000	0.124741000	3.192751000
8	-0.128828000	1.731383000	0.137137000
6	-0.112217000	3.333438000	-0.739462000
6	-0.624679000	3.116367000	-2.071609000
6	0.213785000	3.154475000	-3.169196000
6	1.591566000	3.448444000	-3.031565000
6	2.098297000	3.736169000	-1.739832000
6	1.276216000	3.719342000	-0.629231000
1	-0.802223000	3.737256000	-0.004289000
1	-1.678108000	2.886395000	-2.188614000
1	-0.182706000	2.943763000	-4.157866000
1	3.151880000	3.977016000	-1.629074000
1	1.668919000	3.944174000	0.355510000

6	2.488132000	3.499087000	-4.247277000
6	2.513683000	4.893154000	-4.917493000
1	2.148746000	2.757307000	-4.980093000
1	3.510168000	3.220646000	-3.962691000
1	3.150564000	4.879882000	-5.808299000
1	2.904323000	5.652743000	-4.229541000
1	1.506492000	5.198754000	-5.222179000
16	0.079292000	-2.428175000	0.192191000
1	1.146262000	-2.623197000	-0.662798000

²Cpdl(CF₃COO):

26	-0.005990000	0.022370000	-0.015646000
7	-0.009886000	-0.044875000	2.008798000
7	2.022288000	0.003493000	-0.012999000
7	-2.027189000	-0.103027000	-0.024658000
7	-0.001315000	-0.055773000	-2.039473000
6	-1.111133000	-0.118552000	2.835052000
6	2.855083000	-0.020819000	-1.111012000
6	1.089629000	-0.024979000	2.840919000
6	2.848638000	0.021518000	1.091546000
6	-2.860137000	-0.154025000	1.075956000
6	1.104041000	-0.055244000	-2.868154000
6	-2.855623000	-0.075836000	-1.126710000
6	-1.099998000	-0.029888000	-2.872786000
6	-0.695527000	-0.136377000	4.221824000
6	4.240283000	-0.010878000	-0.688773000
6	0.668540000	-0.076575000	4.225418000
6	4.236110000	0.017384000	0.676551000
6	-4.245089000	-0.168294000	0.652864000
6	0.687548000	-0.039425000	-4.254996000
6	-4.241951000	-0.114302000	-0.711120000
6	-0.677269000	-0.017851000	-4.257188000
1	-1.366524000	-0.191901000	5.066246000
1	5.088781000	-0.028634000	-1.356606000
1	1.336756000	-0.074680000	5.073651000
1	5.080981000	0.026296000	1.349126000
1	-5.092845000	-0.212926000	1.320112000
1	1.359546000	-0.043874000	-5.100196000
1	-5.086483000	-0.110620000	-1.383910000
1	-1.346115000	-0.005284000	-5.104682000
6	-2.433144000	-0.166319000	2.399474000
6	2.426162000	-0.047009000	-2.436035000
6	-2.424209000	-0.026519000	-2.448057000
6	2.413505000	0.018158000	2.413257000
1	-3.201811000	-0.215268000	3.164096000
1	3.194605000	-0.055771000	-3.202347000
1	-3.189458000	-0.004455000	-3.216944000
1	3.178510000	0.028641000	3.183023000
8	-0.057303000	1.683812000	-0.027173000
8	0.155086000	-1.970970000	0.091974000
6	-0.419049000	-2.935612000	-0.569292000
8	-1.329584000	-2.891901000	-1.418438000
6	0.182396000	-4.303457000	-0.182046000
9	1.551357000	-4.347825000	-0.440662000
9	-0.391811000	-5.350129000	-0.876392000
9	0.017108000	-4.576118000	1.173914000

⁴Cpdl(CF₃COO):

26	0.000000000	0.000000000	0.000000000
7	0.000000000	0.000000000	2.025565000
7	2.028367000	0.000000000	-0.000630000
7	-2.019956000	-0.144333000	-0.000956000
7	0.002133000	-0.145273000	-2.020122000
6	-1.099176000	-0.056384000	2.855927000
6	2.859578000	-0.053057000	-1.098830000
6	1.100625000	0.057702000	2.854450000
6	2.856297000	0.062351000	1.101116000
6	-2.850613000	-0.166456000	1.102346000
6	1.106096000	-0.162036000	-2.850489000
6	-2.850386000	-0.161433000	-1.101706000
6	-1.098088000	-0.157254000	-2.851720000
6	-0.681183000	-0.024291000	4.241724000
6	4.245305000	-0.016274000	-0.679820000
6	0.682272000	0.048224000	4.240706000
6	4.243075000	0.057281000	0.683819000
6	-4.236054000	-0.207591000	0.682626000
6	0.687234000	-0.196146000	-4.236288000
6	-4.235622000	-0.198907000	-0.682403000
6	-0.677726000	-0.187293000	-4.236569000
1	-1.350268000	-0.057946000	5.088813000
1	5.092852000	-0.048346000	-1.348327000
1	1.351811000	0.084478000	5.087122000
1	5.088911000	0.096349000	1.354100000
1	-5.082278000	-0.237883000	1.352617000
1	1.357878000	-0.222444000	-5.082165000
1	-5.081237000	-0.225392000	-1.353318000
1	-1.348029000	-0.209074000	-5.082725000
6	-2.421386000	-0.130830000	2.424718000
6	2.428779000	-0.127213000	-2.421426000
6	-2.421585000	-0.152039000	-2.424790000
6	2.423350000	0.098865000	2.423045000
1	-3.188328000	-0.161470000	3.192021000
1	3.196032000	-0.154309000	-3.188502000
1	-3.188248000	-0.162611000	-3.192512000
1	3.189465000	0.141992000	3.190565000
8	-0.066808000	1.659596000	-0.066579000
8	0.179813000	-1.987089000	0.173426000
6	-0.386376000	-2.978436000	-0.454345000
8	-1.298650000	-2.971385000	-1.302721000
6	0.228411000	-4.327037000	-0.023061000
9	1.597306000	-4.367295000	-0.282694000
9	-0.337141000	-5.401465000	-0.681170000
9	0.067861000	-4.556029000	1.341519000

²TS1_{CF₃COO}:

26	0.006155000	-0.001211000	0.000056000
7	0.006981000	-0.003990000	2.002234000
7	2.028278000	-0.008352000	-0.000161000
7	-2.013386000	-0.103676000	-0.014596000
7	0.002385000	-0.059803000	-2.037612000
6	-1.101112000	-0.108988000	2.833014000
6	2.852039000	-0.043709000	-1.110276000

6	1.115740000	-0.021009000	2.841326000
6	2.863826000	-0.004769000	1.101390000
6	-2.846495000	-0.166850000	1.087980000
6	1.110477000	-0.052063000	-2.864287000
6	-2.839743000	-0.082223000	-1.122386000
6	-1.101901000	-0.016705000	-2.868345000
6	-0.678097000	-0.149535000	4.214641000
6	4.238618000	-0.049078000	-0.693328000
6	0.687369000	-0.093077000	4.219656000
6	4.246282000	-0.022880000	0.672923000
6	-4.229615000	-0.192414000	0.660595000
6	0.689066000	-0.012252000	-4.251910000
6	-4.224668000	-0.134390000	-0.703875000
6	-0.674625000	0.015055000	-4.253123000
1	-1.347980000	-0.225306000	5.058610000
1	5.081778000	-0.077415000	-1.367916000
1	1.354814000	-0.114213000	5.068456000
1	5.096671000	-0.027196000	1.339001000
1	-5.077752000	-0.248503000	1.326781000
1	1.361099000	-0.007643000	-5.097563000
1	-5.068533000	-0.138254000	-1.378020000
1	-1.344059000	0.041802000	-5.100115000
6	-2.422299000	-0.174301000	2.409644000
6	2.429102000	-0.062946000	-2.434459000
6	-2.420491000	-0.024547000	-2.444689000
6	2.439031000	-0.001986000	2.423977000
1	-3.186144000	-0.241308000	3.177366000
1	3.199278000	-0.078294000	-3.198700000
1	-3.190016000	-0.007210000	-3.209194000
1	3.203547000	-0.013150000	3.193937000
8	-0.062614000	1.689891000	-0.288640000
6	0.112676000	3.107843000	1.151628000
6	1.365120000	3.672872000	0.782956000
6	1.420600000	4.895278000	0.126613000
6	0.245053000	5.620243000	-0.155071000
6	-0.996587000	5.081927000	0.253472000
6	-1.066314000	3.862750000	0.910291000
1	0.085332000	2.293834000	1.865918000
1	2.271832000	3.119508000	0.991633000
1	2.379194000	5.310671000	-0.169906000
1	-1.902445000	5.643912000	0.056144000
1	-2.022201000	3.454972000	1.218249000
6	0.307100000	6.930281000	-0.909227000
6	0.214452000	6.741071000	-2.439163000
1	1.242303000	7.450734000	-0.671425000
1	-0.510099000	7.581473000	-0.581739000
1	0.262079000	7.709208000	-2.950529000
1	-0.724154000	6.250726000	-2.714330000
1	1.034760000	6.119123000	-2.805616000
8	0.131953000	-1.950789000	0.106133000
6	-0.409621000	-2.912735000	-0.595274000
8	-1.269013000	-2.866961000	-1.490943000
6	0.153606000	-4.279937000	-0.154773000
9	1.543397000	-4.320611000	-0.261057000
9	-0.343886000	-5.320889000	-0.917435000
9	-0.161009000	-4.559240000	1.175252000

²Cpdl(CH₃COO):

26	0.020571000	0.026871000	-0.048187000
7	0.015070000	-0.045667000	1.974414000
7	2.046434000	0.020530000	-0.040822000
7	-1.999003000	-0.098537000	-0.062615000
7	0.022064000	-0.061381000	-2.069605000
6	-1.086782000	-0.168061000	2.794934000
6	2.877957000	-0.041641000	-1.136076000
6	1.111453000	0.026136000	2.808951000
6	2.870206000	0.094358000	1.065936000
6	-2.831296000	-0.198580000	1.034206000
6	1.134246000	-0.110464000	-2.894979000
6	-2.828993000	-0.015776000	-1.169546000
6	-1.070113000	0.005208000	-2.903551000
6	-0.673944000	-0.173111000	4.183144000
6	4.262816000	0.001272000	-0.713037000
6	0.686738000	-0.046019000	4.191978000
6	4.257702000	0.092119000	0.650512000
6	-4.216952000	-0.197665000	0.607476000
6	0.718941000	-0.094856000	-4.282531000
6	-4.214815000	-0.072678000	-0.750481000
6	-0.644416000	-0.011995000	-4.287673000
1	-1.344907000	-0.259330000	5.025180000
1	5.112135000	-0.032527000	-1.379471000
1	1.350842000	-0.011770000	5.043080000
1	5.102160000	0.143232000	1.322026000
1	-5.064220000	-0.277601000	1.272232000
1	1.391208000	-0.132932000	-5.127061000
1	-5.060298000	-0.038098000	-1.421410000
1	-1.310871000	0.024473000	-5.136750000
6	-2.405742000	-0.245977000	2.355937000
6	2.451634000	-0.113919000	-2.461364000
6	-2.397718000	0.060855000	-2.481687000
6	2.433886000	0.114484000	2.385376000
1	-3.174033000	-0.330931000	3.118123000
1	3.222286000	-0.151796000	-3.224962000
1	-3.158650000	0.123274000	-3.252843000
1	3.195834000	0.168618000	3.156691000
8	-0.035627000	1.690513000	-0.057562000
8	0.234256000	-1.957358000	0.022916000
6	-0.589433000	-2.922766000	-0.323623000
8	-1.770604000	-2.780046000	-0.738388000
6	0.010101000	-4.321533000	-0.199343000
1	0.802750000	-4.443583000	-0.946373000
1	-0.759457000	-5.078152000	-0.359505000
1	0.464021000	-4.445051000	0.788255000

⁴Cpdl(CH₃COO):

26	0.024576000	0.023935000	-0.053500000
7	0.017861000	-0.059687000	1.968734000
7	2.051096000	0.027529000	-0.044162000
7	-1.991575000	-0.105287000	-0.066577000
7	0.027907000	-0.053114000	-2.074344000
6	-1.083944000	-0.177628000	2.788833000
6	2.883894000	-0.031011000	-1.138916000

6	1.114698000	0.020022000	2.805243000
6	2.873053000	0.096193000	1.063193000
6	-2.827337000	-0.201912000	1.029466000
6	1.142836000	-0.100099000	-2.898919000
6	-2.823757000	-0.020963000	-1.176948000
6	-1.063332000	0.002704000	-2.908485000
6	-0.672444000	-0.175200000	4.177718000
6	4.267952000	0.009506000	-0.714290000
6	0.687814000	-0.045796000	4.187831000
6	4.261149000	0.094944000	0.649967000
6	-4.212131000	-0.197172000	0.599957000
6	0.727674000	-0.090681000	-4.286522000
6	-4.208998000	-0.074250000	-0.757117000
6	-0.636831000	-0.018176000	-4.292735000
1	-1.344644000	-0.257938000	5.019073000
1	5.118000000	-0.022679000	-1.379949000
1	1.350741000	-0.005811000	5.039637000
1	5.104505000	0.142103000	1.323159000
1	-5.060288000	-0.274720000	1.263753000
1	1.400798000	-0.126456000	-5.130579000
1	-5.054317000	-0.038091000	-1.428280000
1	-1.303273000	0.010658000	-5.142162000
6	-2.403995000	-0.252919000	2.349965000
6	2.459143000	-0.099969000	-2.465117000
6	-2.393783000	0.050530000	-2.486471000
6	2.436075000	0.112043000	2.383308000
1	-3.172683000	-0.334579000	3.111822000
1	3.230450000	-0.135341000	-3.228184000
1	-3.155061000	0.105351000	-3.257839000
1	3.197714000	0.167772000	3.154714000
8	-0.054960000	1.688820000	-0.053993000
8	0.253057000	-1.956335000	-0.017581000
6	-0.600853000	-2.917280000	-0.291030000
8	-1.812885000	-2.771416000	-0.608052000
6	-0.004040000	-4.319695000	-0.208159000
1	0.758561000	-4.435828000	-0.986265000
1	-0.782939000	-5.071418000	-0.343652000
1	0.487475000	-4.454609000	0.760094000

²TS1_{CH3COO}:

26	-0.056873000	0.013036000	0.044212000
7	-0.031997000	0.038241000	2.038680000
7	1.972161000	0.087369000	0.016042000
7	-2.059860000	-0.130448000	0.068078000
7	-0.069979000	-0.085451000	-1.983336000
6	-1.118784000	-0.145183000	2.889296000
6	2.784836000	0.015816000	-1.101452000
6	1.089881000	0.140731000	2.857496000
6	2.810466000	0.218182000	1.105153000
6	-2.874796000	-0.255849000	1.178413000
6	1.030360000	-0.124099000	-2.819387000
6	-2.896390000	-0.101180000	-1.035134000
6	-1.186330000	-0.059608000	-2.795919000
6	-0.667871000	-0.130107000	4.260532000
6	4.172895000	0.111316000	-0.698287000
6	0.686005000	0.054948000	4.241298000

6	4.188800000	0.244622000	0.660545000
6	-4.259854000	-0.303995000	0.762146000
6	0.588571000	-0.140643000	-4.199348000
6	-4.272418000	-0.196469000	-0.599277000
6	-0.775288000	-0.089973000	-4.184252000
1	-1.314590000	-0.249373000	5.117549000
1	5.010696000	0.080292000	-1.379483000
1	1.364877000	0.111326000	5.079583000
1	5.042243000	0.339039000	1.315566000
1	-5.097632000	-0.408175000	1.435585000
1	1.249514000	-0.179745000	-5.053016000
1	-5.123456000	-0.203308000	-1.264131000
1	-1.455486000	-0.087823000	-5.022826000
6	-2.439330000	-0.284963000	2.495039000
6	2.355655000	-0.099895000	-2.414720000
6	-2.500293000	-0.040185000	-2.359996000
6	2.402279000	0.262028000	2.430314000
1	-3.185941000	-0.406280000	3.271892000
1	3.115384000	-0.141875000	-3.187752000
1	-3.278383000	-0.031226000	-3.114840000
1	3.170097000	0.346412000	3.191383000
8	-0.134462000	1.710087000	-0.251393000
6	-0.495761000	3.079217000	1.111352000
6	0.523045000	4.010906000	0.742601000
6	0.213355000	5.112356000	-0.036684000
6	-1.120781000	5.371170000	-0.437428000
6	-2.142979000	4.497471000	-0.003916000
6	-1.850344000	3.389383000	0.775866000
1	-0.300085000	2.368267000	1.903154000
1	1.546313000	3.811089000	1.039963000
1	0.997825000	5.796653000	-0.346130000
1	-3.170528000	4.706881000	-0.286943000
1	-2.636965000	2.718613000	1.099855000
6	-1.439081000	6.539601000	-1.343378000
6	-1.338519000	6.166838000	-2.843167000
1	-0.750296000	7.368524000	-1.133330000
1	-2.452814000	6.905406000	-1.134470000
1	-1.575739000	7.032672000	-3.472451000
1	-2.035269000	5.357590000	-3.092518000
1	-0.327558000	5.825060000	-3.092003000
8	0.153706000	-1.871695000	0.090576000
6	-0.486563000	-2.914194000	-0.458765000
8	-1.490143000	-2.851564000	-1.193795000
6	0.175503000	-4.237710000	-0.100175000
1	1.084071000	-4.360831000	-0.698468000
1	-0.504597000	-5.063228000	-0.314879000
1	0.469336000	-4.246394000	0.951237000

²TS1_{OH}:

26	0.000954000	-0.001218000	-0.002688000
7	-0.000525000	-0.004129000	1.992948000
7	2.014623000	0.001762000	-0.007764000
7	-2.028737000	-0.076526000	-0.016995000
7	-0.013557000	-0.033774000	-2.042410000
6	-1.109022000	-0.146100000	2.821077000
6	2.832469000	-0.067886000	-1.121409000

6	1.109565000	0.025100000	2.826335000
6	2.848272000	0.057032000	1.091549000
6	-2.856814000	-0.151977000	1.088967000
6	1.094547000	-0.080072000	-2.866275000
6	-2.857692000	0.016668000	-1.125255000
6	-1.121337000	0.043951000	-2.869618000
6	-0.679144000	-0.178374000	4.201411000
6	4.221320000	-0.051995000	-0.704055000
6	0.682640000	-0.065580000	4.205048000
6	4.231612000	0.032387000	0.657970000
6	-4.240645000	-0.117347000	0.664863000
6	0.670601000	-0.044989000	-4.251904000
6	-4.240614000	-0.006689000	-0.697607000
6	-0.692755000	0.038681000	-4.253805000
1	-1.344957000	-0.277501000	5.046464000
1	5.062932000	-0.098402000	-1.379924000
1	1.351454000	-0.059564000	5.053452000
1	5.082814000	0.064103000	1.322448000
1	-5.087898000	-0.167671000	1.333068000
1	1.341056000	-0.074842000	-5.098535000
1	-5.088562000	0.048145000	-1.365066000
1	-1.360367000	0.086850000	-5.101977000
6	-2.430496000	-0.210498000	2.408829000
6	2.414702000	-0.116790000	-2.442019000
6	-2.441705000	0.081868000	-2.447387000
6	2.431889000	0.086718000	2.414007000
1	-3.190568000	-0.292303000	3.178388000
1	3.183150000	-0.160721000	-3.206451000
1	-3.210303000	0.142280000	-3.210528000
1	3.196289000	0.114240000	3.182901000
8	-0.056213000	1.729600000	-0.265067000
8	0.061497000	-1.831906000	-0.039340000
6	-0.349516000	3.088988000	1.174840000
6	0.799365000	3.900183000	0.950132000
6	0.691092000	5.092136000	0.249231000
6	-0.562676000	5.555560000	-0.207675000
6	-1.714919000	4.790937000	0.082000000
6	-1.621592000	3.595622000	0.779610000
1	-0.296185000	2.292838000	1.904665000
1	1.765035000	3.549079000	1.296202000
1	1.577983000	5.686538000	0.049593000
1	-2.685244000	5.156367000	-0.242394000
1	-2.509526000	3.012717000	0.995437000
6	-0.666639000	6.829896000	-1.016990000
6	-0.538850000	6.579658000	-2.538084000
1	0.117198000	7.530937000	-0.703200000
1	-1.628845000	7.318265000	-0.813824000
1	-0.621375000	7.520805000	-3.093015000
1	-1.325211000	5.903546000	-2.889435000
1	0.426457000	6.121321000	-2.779383000
1	-0.656878000	-2.225035000	-0.577733000

²TS1_{SH}(side-on):

26	0.001184000	-0.005491000	-0.003129000
7	0.000812000	-0.001758000	1.992043000
7	2.019965000	-0.006014000	0.002577000

7	-2.012707000	-0.165680000	-0.012262000
7	0.003988000	-0.136976000	-2.028930000
6	-1.106722000	-0.137110000	2.826048000
6	2.846787000	-0.073987000	-1.107196000
6	1.108037000	0.081213000	2.831114000
6	2.850915000	0.105966000	1.101815000
6	-2.844270000	-0.241926000	1.091548000
6	1.115295000	-0.175173000	-2.850868000
6	-2.840585000	-0.150271000	-1.125293000
6	-1.100605000	-0.122667000	-2.862846000
6	-0.680693000	-0.113304000	4.206254000
6	4.231422000	-0.004136000	-0.687193000
6	0.678636000	0.027509000	4.209553000
6	4.234224000	0.112933000	0.672722000
6	-4.225703000	-0.279158000	0.662079000
6	0.696074000	-0.195731000	-4.237635000
6	-4.222993000	-0.216339000	-0.702948000
6	-0.668479000	-0.157182000	-4.245356000
1	-1.347016000	-0.197753000	5.052399000
1	5.076357000	-0.040283000	-1.359410000
1	1.344461000	0.076385000	5.058933000
1	5.081447000	0.187196000	1.338571000
1	-5.073042000	-0.343688000	1.328826000
1	1.371144000	-0.230987000	-5.080044000
1	-5.068111000	-0.221914000	-1.375750000
1	-1.335126000	-0.157933000	-5.095534000
6	-2.424255000	-0.246175000	2.413766000
6	2.434606000	-0.162513000	-2.426398000
6	-2.422852000	-0.117702000	-2.446982000
6	2.429644000	0.161174000	2.421951000
1	-3.184831000	-0.326732000	3.182779000
1	3.205307000	-0.203140000	-3.188593000
1	-3.189848000	-0.114081000	-3.214049000
1	3.190304000	0.230202000	3.191940000
8	-0.056774000	1.714620000	-0.268117000
16	0.151880000	-2.411604000	0.009899000
6	-0.409284000	3.088270000	1.035736000
6	0.681367000	3.978361000	0.761400000
6	0.477890000	5.136738000	0.031456000
6	-0.814808000	5.501748000	-0.414895000
6	-1.908885000	4.664477000	-0.086793000
6	-1.726421000	3.502407000	0.643409000
1	-0.307177000	2.377152000	1.847782000
1	1.674134000	3.705419000	1.101251000
1	1.316974000	5.787359000	-0.197790000
1	-2.906447000	4.951011000	-0.408573000
1	-2.569563000	2.866031000	0.891372000
6	-1.018488000	6.744857000	-1.253253000
6	-0.897392000	6.465188000	-2.771996000
1	-0.280299000	7.507054000	-0.969538000
1	-2.009260000	7.170051000	-1.046477000
1	-1.047511000	7.386992000	-3.347243000
1	-1.645202000	5.731747000	-3.094709000
1	0.091012000	6.063253000	-3.018181000
1	-0.828969000	-2.664417000	-0.926452000

²TS1_{Cl}:

26	0.147408000	0.000000000	-0.307492000
7	0.000000000	-1.151188000	1.310111000
7	0.000000000	-1.634544000	-1.491786000
7	0.193241000	1.639106000	0.864803000
7	0.206208000	1.178884000	-1.962990000
6	-0.091646000	-0.729519000	2.636896000
6	0.000983000	-1.656367000	-2.876490000
6	-0.133055000	-2.539363000	1.338974000
6	-0.086552000	-2.950696000	-1.081117000
6	0.118527000	1.683352000	2.245462000
6	0.175043000	0.762303000	-3.279195000
6	0.313795000	2.952931000	0.437683000
6	0.322968000	2.554331000	-1.989020000
6	-0.252855000	-1.874529000	3.500611000
6	-0.085294000	-3.025446000	-3.341533000
6	-0.274824000	-2.985244000	2.704513000
6	-0.135911000	-3.823857000	-2.235373000
6	0.207881000	3.054851000	2.697993000
6	0.272133000	1.911151000	-4.157832000
6	0.330445000	3.836025000	1.584077000
6	0.364929000	3.015973000	-3.362538000
1	-0.344414000	-1.819714000	4.575650000
1	-0.107631000	-3.316964000	-4.381537000
1	-0.389778000	-4.018048000	2.999827000
1	-0.210420000	-4.900501000	-2.186178000
1	0.170857000	3.362028000	3.733092000
1	0.265819000	1.858310000	-5.236578000
1	0.412781000	4.911633000	1.525132000
1	0.448592000	4.051768000	-3.657834000
6	-0.021171000	0.581117000	3.075502000
6	0.075183000	-0.551533000	-3.708205000
6	0.380488000	3.380489000	-0.877976000
6	-0.145209000	-3.376976000	0.237103000
1	-0.088685000	0.758110000	4.143287000
1	0.059370000	-0.729268000	-4.778038000
1	0.467530000	4.447629000	-1.051672000
1	-0.236557000	-4.442296000	0.418663000
8	1.880704000	-0.015583000	-0.476142000
17	-2.184354000	0.197467000	-0.413430000
6	3.031493000	-0.641882000	0.754883000
6	3.890637000	-1.484924000	-0.045583000
6	5.164032000	-1.077001000	-0.382392000
6	5.688875000	0.155517000	0.090699000
6	4.884368000	0.962492000	0.931494000
6	3.606053000	0.572504000	1.285938000
1	2.255663000	-1.128154000	1.339717000
1	3.494581000	-2.427936000	-0.404996000
1	5.788803000	-1.708295000	-1.007955000
1	5.290570000	1.896973000	1.307539000
1	2.997180000	1.190477000	1.934982000
6	7.070947000	0.603878000	-0.325112000
6	7.107826000	1.177562000	-1.762943000
1	7.764789000	-0.246182000	-0.264480000
1	7.438341000	1.363439000	0.375710000
1	8.126904000	1.481386000	-2.027489000

1	6.453689000	2.051537000	-1.851900000
1	6.772523000	0.432737000	-2.492888000

⁴CpdI(NCCH₃):

26	0.000172000	0.012043000	-0.004376000
7	0.004075000	0.022792000	2.021054000
7	2.025172000	0.011728000	-0.003350000
7	-2.015462000	-0.181826000	0.004767000
7	0.005576000	-0.192297000	-2.019622000
6	-1.094035000	0.028965000	2.854921000
6	2.858250000	0.005541000	-1.113602000
6	1.110815000	0.137065000	2.850952000
6	2.856629000	0.125908000	1.090712000
6	-2.849816000	-0.150758000	1.113606000
6	1.102400000	-0.172325000	-2.855032000
6	-2.848545000	-0.263569000	-1.091020000
6	-1.102789000	-0.272198000	-2.851503000
6	-0.676699000	0.140157000	4.234982000
6	4.239048000	0.110027000	-0.696976000
6	0.688890000	0.207200000	4.232417000
6	4.238237000	0.184510000	0.668167000
6	-4.232149000	-0.224506000	0.695372000
6	0.683459000	-0.250165000	-4.236946000
6	-4.231595000	-0.294074000	-0.669992000
6	-0.682356000	-0.311359000	-4.234725000
1	-1.346219000	0.167376000	5.081615000
1	5.085468000	0.127823000	-1.366819000
1	1.355196000	0.299580000	5.076994000
1	5.083589000	0.275430000	1.333641000
1	-5.079724000	-0.218358000	1.363942000
1	1.351819000	-0.251703000	-5.084924000
1	-5.078356000	-0.355563000	-1.337088000
1	-1.350196000	-0.373216000	-5.080894000
6	-2.422097000	-0.053436000	2.430250000
6	2.429988000	-0.080754000	-2.430882000
6	-2.421488000	-0.304372000	-2.420270000
6	2.428750000	0.183731000	2.418976000
1	-3.187539000	-0.032776000	3.199108000
1	3.193799000	-0.069322000	-3.201556000
1	-3.190756000	-0.361932000	-3.183470000
1	3.196156000	0.279807000	3.180088000
8	-0.078773000	1.653584000	-0.092074000
7	0.104438000	-2.109403000	0.112043000
6	0.170247000	-3.269801000	0.177924000
6	0.254565000	-4.721254000	0.261687000
1	0.069764000	-5.055915000	1.287520000
1	-0.487880000	-5.185524000	-0.394993000
1	1.248859000	-5.063319000	-0.041521000

²TS1_{NCCH₃}:

26	0.026685000	-0.000060000	-0.320542000
7	0.000000000	-1.151195000	1.310099000
7	0.000000000	-1.647311000	-1.477667000
7	-0.156524000	1.651087000	0.835983000
7	-0.121484000	1.172843000	-1.981548000
6	-0.022965000	-0.722231000	2.635962000

6	0.034045000	-1.679404000	-2.865443000
6	-0.023242000	-2.545785000	1.360705000
6	-0.000844000	-2.970605000	-1.061253000
6	-0.126683000	1.701678000	2.220269000
6	-0.040531000	0.747161000	-3.295678000
6	-0.239192000	2.966222000	0.404231000
6	-0.189564000	2.555664000	-2.023658000
6	-0.027514000	-1.864174000	3.518913000
6	0.062450000	-3.051234000	-3.320647000
6	-0.032172000	-2.984523000	2.735486000
6	0.036807000	-3.847313000	-2.209438000
6	-0.196009000	3.076241000	2.664946000
6	-0.063998000	1.891295000	-4.183562000
6	-0.269361000	3.855138000	1.545193000
6	-0.159575000	3.004950000	-3.400186000
1	-0.035308000	-1.803442000	4.597005000
1	0.091623000	-3.351809000	-4.357640000
1	-0.042056000	-4.018197000	3.048373000
1	0.042306000	-4.926172000	-2.159151000
1	-0.191175000	3.388741000	3.698707000
1	-0.015597000	1.832823000	-5.260599000
1	-0.333614000	4.931319000	1.481152000
1	-0.202752000	4.039017000	-3.708595000
6	-0.059271000	0.598523000	3.058693000
6	0.026775000	-0.575397000	-3.706755000
6	-0.265611000	3.388118000	-0.917919000
6	-0.018886000	-3.390687000	0.261735000
1	-0.056861000	0.780313000	4.127875000
1	0.067707000	-0.764413000	-4.773902000
1	-0.326939000	4.455668000	-1.098704000
1	-0.025291000	-4.458525000	0.450827000
8	1.676936000	0.233024000	-0.481788000
6	3.118586000	-0.904042000	0.535983000
6	3.574564000	-1.659088000	-0.584607000
6	4.767800000	-1.334081000	-1.212108000
6	5.562032000	-0.261589000	-0.743067000
6	5.115177000	0.475985000	0.389911000
6	3.930205000	0.163285000	1.023783000
1	2.316199000	-1.287677000	1.151333000
1	2.972167000	-2.484919000	-0.944516000
1	5.098259000	-1.911640000	-2.066684000
1	5.730650000	1.291521000	0.757481000
1	3.597947000	0.728928000	1.886876000
6	6.869364000	0.137160000	-1.392282000
6	7.414282000	-0.792588000	-2.484083000
1	7.620814000	0.247881000	-0.595697000
1	6.746271000	1.151956000	-1.804810000
1	8.380810000	-0.422395000	-2.839573000
1	6.744649000	-0.843562000	-3.349864000
1	7.567954000	-1.810287000	-2.107782000
7	-2.050871000	-0.068548000	-0.347169000
6	-3.213059000	-0.102281000	-0.361571000
6	-4.668266000	-0.142784000	-0.377335000
1	-5.023624000	-0.734945000	-1.226353000
1	-5.046832000	-0.593869000	0.545193000
1	-5.075927000	0.869271000	-0.463270000