

Electronic Supplementary Information for

Theoretical Investigation on the Elusive Structure-Activity Relationship of the Bioinspired High-Valent Nickel-Halogen Complexes in the Oxidative Fluorination Reactions

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Part I. The Calculated data on the oxidants **1_F** and **1_{Cl}**

Table S1. Benchmark of the performance of the employed B3LYP functional with six other functionals (PBE0, B3LYP*, TPSSh, B3LYP-D3(BJ), M06, and B97D3). Calculations were done at the UB3LYP/B2 level.

	b3lyp	ΔE	pbe1pbe	ΔE	b3lyp-star	ΔE	tpssh	ΔE
² 1_F	-2812.209399	0.0	-2810.447218	0.0	-2810.345562	0.0	-2812.278146	0.0
⁴ 1_F	-2812.189000	12.8	-2810.432076	9.5	-2810.315022	19.2	-2812.243017	22.0
	b3lyp-d3bj	ΔE	m06	ΔE	b97d3	ΔE		
² 1_F	-2812.339660	0.0	-2811.226569	0.0	-2812.052309	0.0		
⁴ 1_F	-2812.318557	13.2	-2811.202656	15.0	-2812.007612	28.0		

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

Table S2. Various SCF and free energies of the oxidant **1_F** on the different spin states. Calculations were done at the UB3LYP/B2 level in solvent.

	OPT/B2	ΔE	OPT +ZPE	ΔE	G	ΔG
² 1_F	-2812.209399 ^a	0.0	-2811.815548	0.0	-2811.857437	0.0
⁴ 1_F	-2812.189000	12.8	-2811.796861	11.7	-2811.839565	11.2
⁶ 1_F	-2812.099867	68.7	-2811.711516	65.3	-2811.753505	65.2

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

Table S3. Various SCF and free energies of the oxidant **1_{Cl}** on the different spin states. Calculations were done at the UB3LYP/B2 level in solvent.

	OPT/B2	ΔE	OPT +ZPE	ΔE	G	ΔG
² 1_{Cl}	-3172.570627 ^a	0.0	-3172.177651	0.0	-3172.219806	0.0
⁴ 1_{Cl}	-3172.550249	12.8	-3172.159021	11.7	-3172.202570	10.8
⁶ 1_{Cl}	-3172.455174	72.4	-3172.068354	68.6	-3172.111891	67.7

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

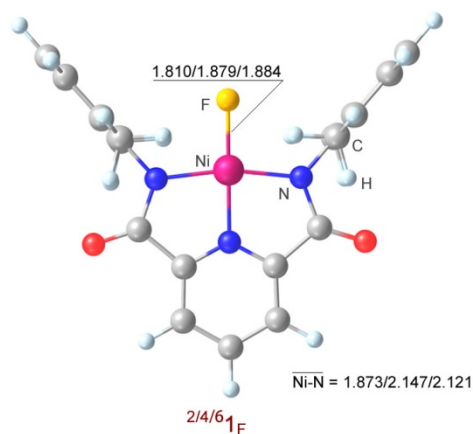


Fig. S1 The optimized structures of the oxidant 1_F on the doublet/quartet/sextet spin states. Lengths are in Å units. Calculations were done at the UB3LYP/B2 level in solvent.

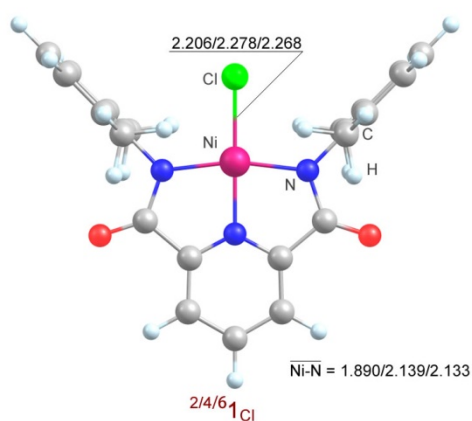


Fig. S2 The optimized structures of the oxidant 1_{Cl} on the doublet/quartet/sextet spin states. Lengths are in Å units. Calculations were done at the UB3LYP/B2 level in solvent.

Table S4. Mulliken charges and spin densities of the oxidant **1_F** on the different spin states. Calculations were done at the UB3LYP/B2 level.

	Spin density			Charge		
	Ni	L	F	Ni	L	F
² 1_F	0.76	0.25	-0.01	1.07	-0.60	-0.47
⁴ 1_F	1.80	1.15	0.05	1.13	-0.49	-0.63
⁶ 1_F	1.83	3.13	0.04	1.06	-0.43	-0.63

Table S5. Mulliken charges and spin densities of the oxidant **1_{Cl}** on the different spin states. Calculations were done at the UB3LYP/B2 level.

	Spin density			Charge		
	Ni	L	Cl	Ni	L	Cl
² 1_{Cl}	0.79	0.23	-0.02	0.72	-0.35	-0.36
⁴ 1_{Cl}	1.67	1.27	0.06	0.97	-0.38	-0.59
⁶ 1_{Cl}	1.72	3.19	0.08	0.89	-0.31	-0.57

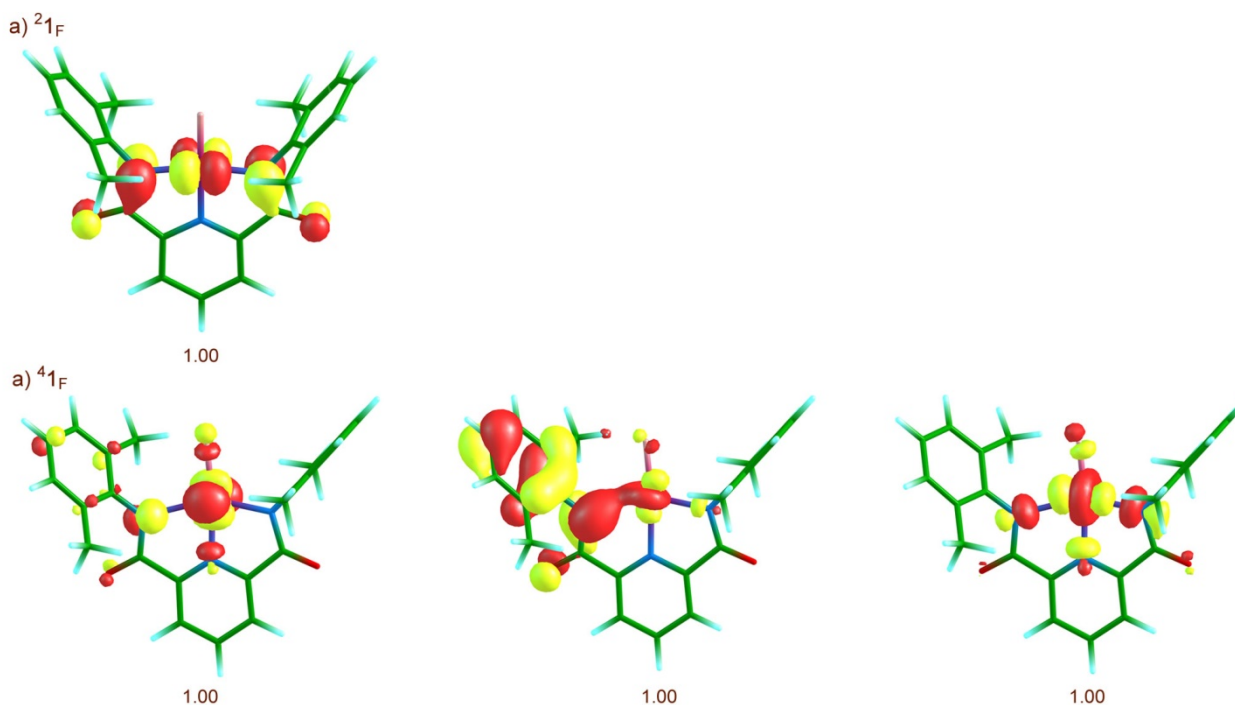


Fig. S3 Singly-occupied natural orbitals (SNOs) of the oxidant 1_F on the doublet and quartet spin states. Calculations were done at the UB3LYP/B2 level. Positive values represent alpha-electron occupations and negative ones represent beta-electron occupations.

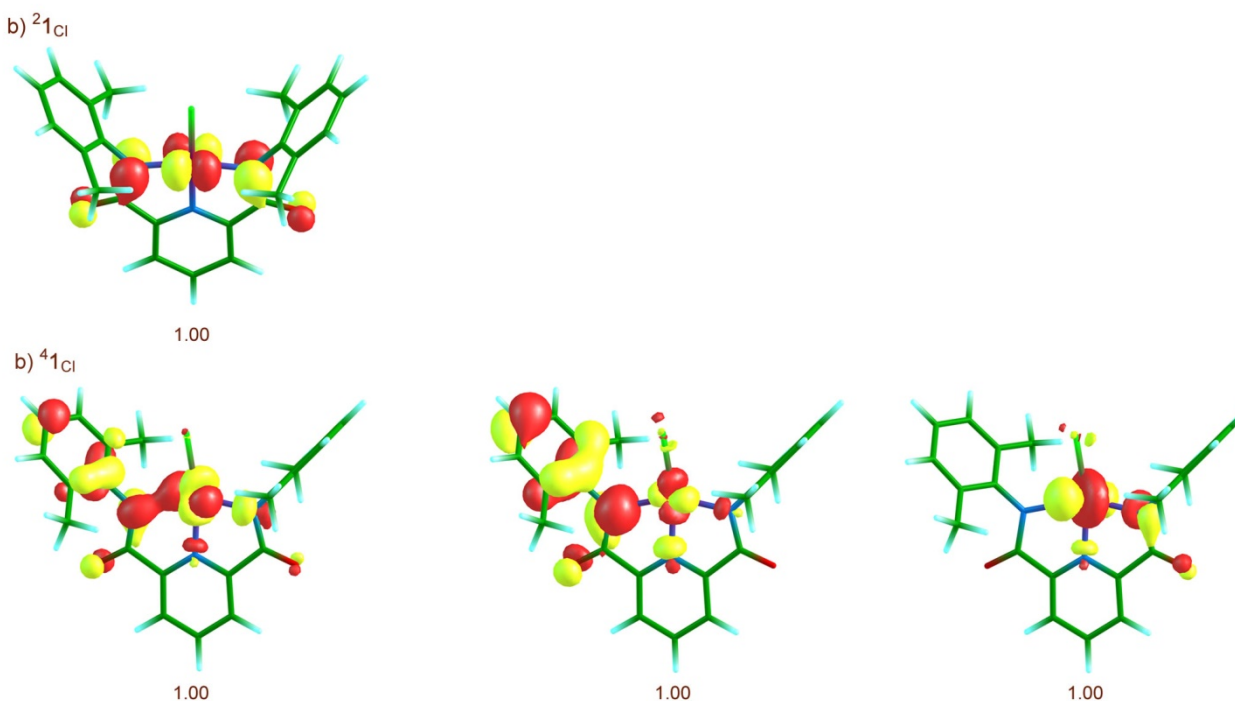


Fig. S4 Singly-occupied natural orbitals (SNOs) of the oxidant 1_{Cl} on the doublet and quartet spin states. Calculations were done at the UB3LYP/B2 level. Positive values represent alpha-electron occupations and negative ones represent beta-electron occupations.

Part II. C-H bond activation of CHD by the oxidants **1_F** and **1_{Cl}**

Table S6. Various SCF and free energies of the reaction intermediates in C-H bond activation of CHD by the oxidant **1_F** on the doublet and quartet spin states. Calculations were done at the UB3LYP/B2 level in solvent.

	OPT/B2	ΔE	OPT +ZPE	ΔE	G	ΔG
² RC_F	-3045.647076 ^a	0.0	-3045.131220	0.0	-3045.185054	0.0
⁴ RC_F	-3045.622942	15.1	-3045.109208	13.8	-3045.164155	13.1
² TS_F	-3045.617893	18.3	-3045.109937	13.4	-3045.160271	15.6
⁴ TS_F	-3045.611871	22.1	-3045.102119	18.3	-3045.152237	20.6
² IM_F	-3045.632639	9.1	-3045.120966	6.4	-3045.172701	7.8
⁴ IM_F	-3045.632237	9.3	-3045.120718	6.6	-3045.173168	7.5

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

Table S7. Various SCF and free energies of the reaction intermediates in C-H bond activation of CHD by the oxidant **1_{Cl}** on the doublet and quartet spin states. Calculations were done at the UB3LYP/B2 level in solvent.

	OPT/B2	ΔE	OPT +ZPE	ΔE	G	ΔG
² RC_{Cl}	-3406.008250 ^a	0.0	-3405.493367	0.0	-3405.548591	0.0
⁴ RC_{Cl}	-3405.990503	11.1	-3405.477227	10.1	-3405.533948	9.2
² TS_{Cl}	-3405.971390	23.1	-3405.464740	18.0	-3405.516050	20.4
⁴ TS_{Cl}	-3405.970910	23.4	-3405.464467	18.1	-3405.515828	20.6
² IM_{Cl}	-3405.974169	21.4	-3405.465677	17.4	-3405.518382	19.0
⁴ IM_{Cl}	-3405.973946	21.5	-3405.465447	17.5	-3405.518748	18.7

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

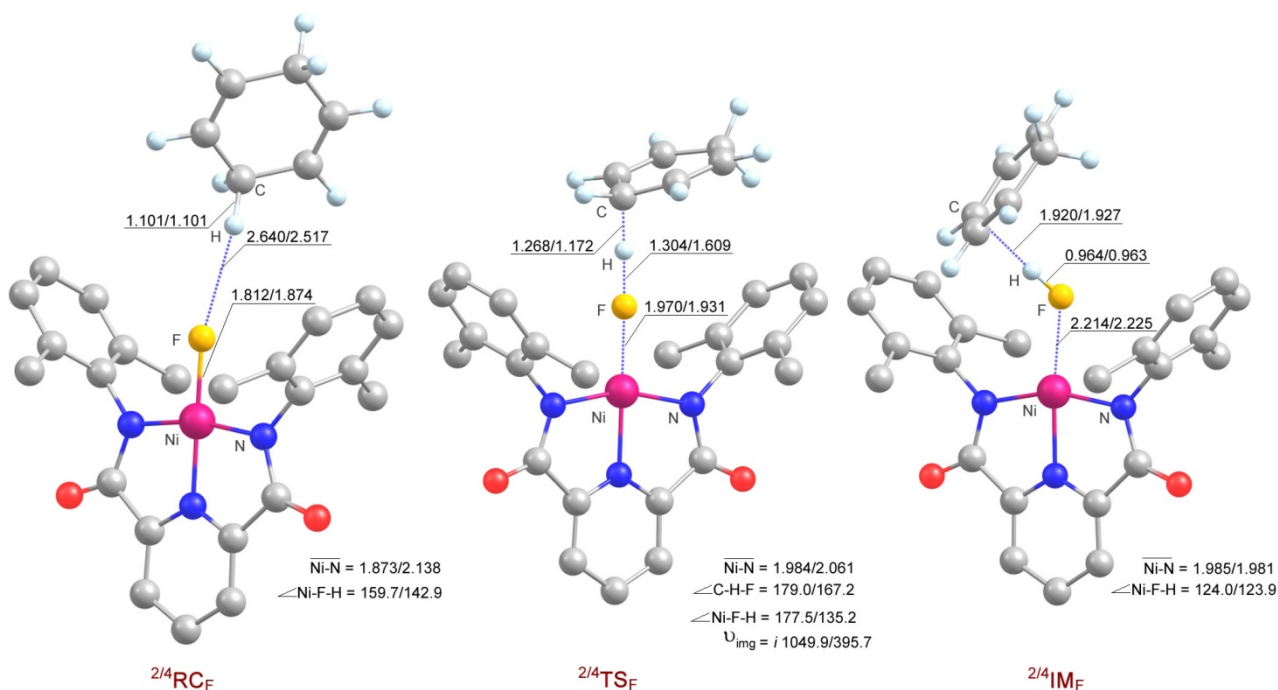


Fig. S5 The optimized structures of the reaction intermediates in C-H bond activation of CHD by the oxidant **1_F** on the doublet/quartet spin states. Lengths are in Å units, bond angles are in degree units and imaginary frequencies are in cm^{-1} units. Hydrogen atoms of the ligand are omitted for clarity. Calculations were done at the UB3LYP/B2 level in solvent.

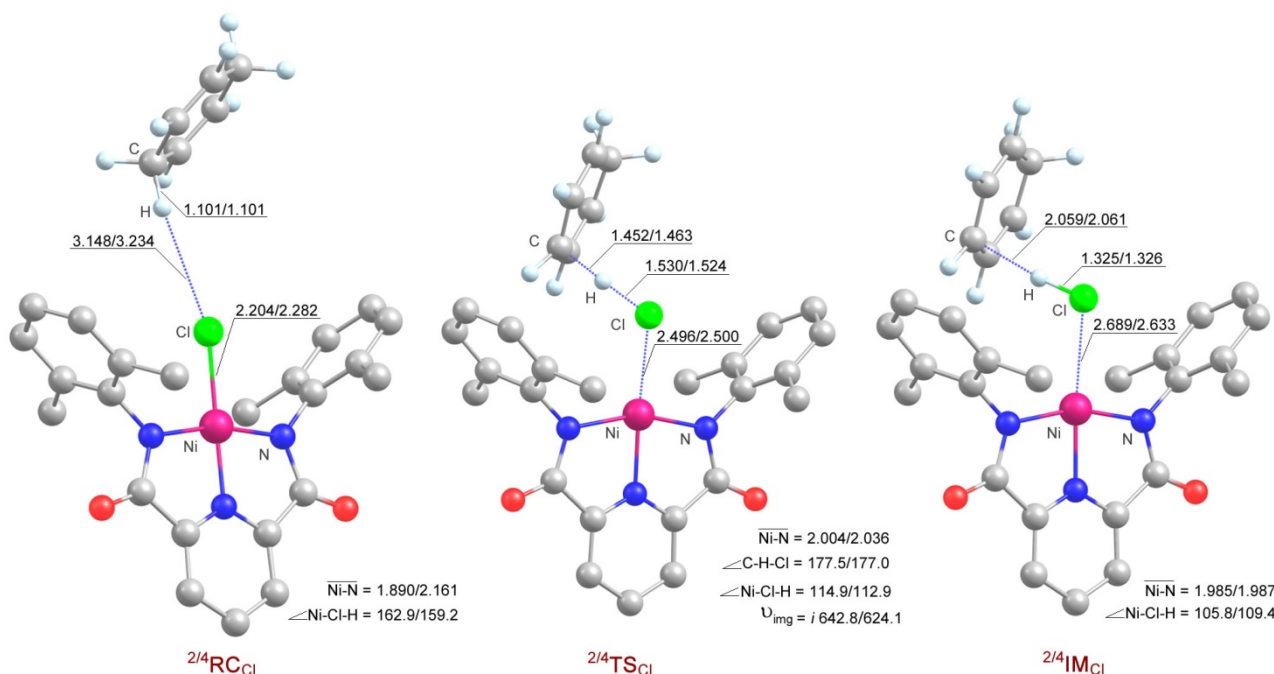


Fig. S6 The optimized structures of the reaction intermediates in C-H bond activation of CHD by the oxidant **1_{Cl}** on the doublet/quartet spin states. Lengths are in Å units, bond angles are in degree units and imaginary frequencies are in cm^{-1} units. Hydrogen atoms of the ligand are omitted for clarity. Calculations were done at the UB3LYP/B2 level in solvent.

Table S8. Mulliken charges and spin densities of the reaction intermediates in C-H bond activation of CHD by the oxidant **1_F** on the doublet/quartet spin states. Calculations were done at the UB3LYP/B2 level in solvent.

	Spin density					Charge				
	Ni	L	F	H	Sub-H	Ni	L	F	H	Sub-H
² RC_F	0.76	0.25	-0.01	0.00	0.00	0.97	-0.52	-0.44	0.17	-0.18
⁴ RC_F	1.71	1.23	0.05	0.00	0.00	1.04	-0.42	-0.60	0.18	-0.19
² TS_F	1.53	0.25	-0.06	-0.07	-0.64	0.93	-1.09	-0.35	0.32	0.19
⁴ TS_F	1.80	0.38	0.08	0.08	0.66	1.20	-1.30	-0.50	0.28	0.32
² IM_F	1.60	0.37	0.02	-0.05	-0.95	1.05	-1.18	-0.33	0.43	0.03
⁴ IM_F	1.58	0.41	0.00	0.05	0.96	1.04	-1.17	-0.33	0.44	0.03

Table S9. Mulliken charges and spin densities of the reaction intermediates in C-H bond activation of CHD by the oxidant **1_{Cl}** on the doublet/quartet spin states. Calculations were done at the UB3LYP/B2 level in solvent.

	Spin density					Charge				
	Ni	L	Cl	H	Sub-H	Ni	L	Cl	H	Sub-H
² RC_{Cl}	0.79	0.23	-0.02	0.00	0.00	0.74	-0.35	-0.39	0.16	-0.15
⁴ RC_{Cl}	1.79	1.16	0.05	0.00	0.00	1.10	-0.51	-0.59	0.16	-0.16
² TS_{Cl}	1.57	0.37	-0.11	-0.05	-0.79	0.87	-1.08	-0.22	0.10	0.32
⁴ TS_{Cl}	1.77	0.21	0.17	0.05	0.80	1.14	-1.30	-0.23	0.10	0.29
² IM_{Cl}	1.58	0.39	0.00	-0.03	-0.95	0.87	-0.98	-0.12	0.15	0.09
⁴ IM_{Cl}	1.59	0.39	0.05	0.03	0.95	0.92	-1.04	-0.11	0.15	0.09

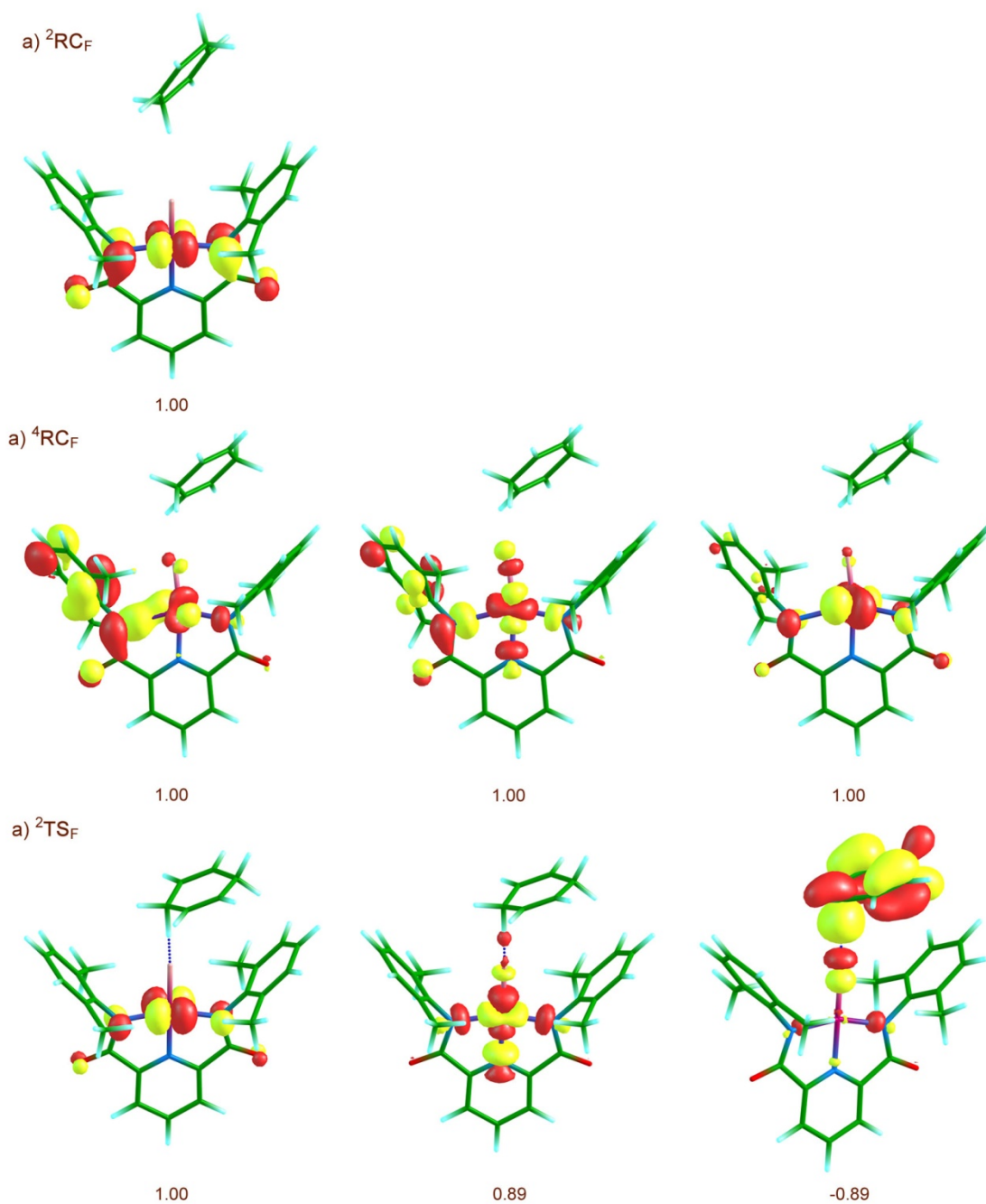


Fig. S7 Singly-occupied natural orbitals (SNOs) of the reaction intermediates in C-H bond activation of CHD by the oxidant 1_F on the doublet/quartet spin states. Calculations were done at the UB3LYP/B2 level in solvent. Positive values represent alpha-electron occupations and negative ones represent beta-electron occupations. (To be continued.)

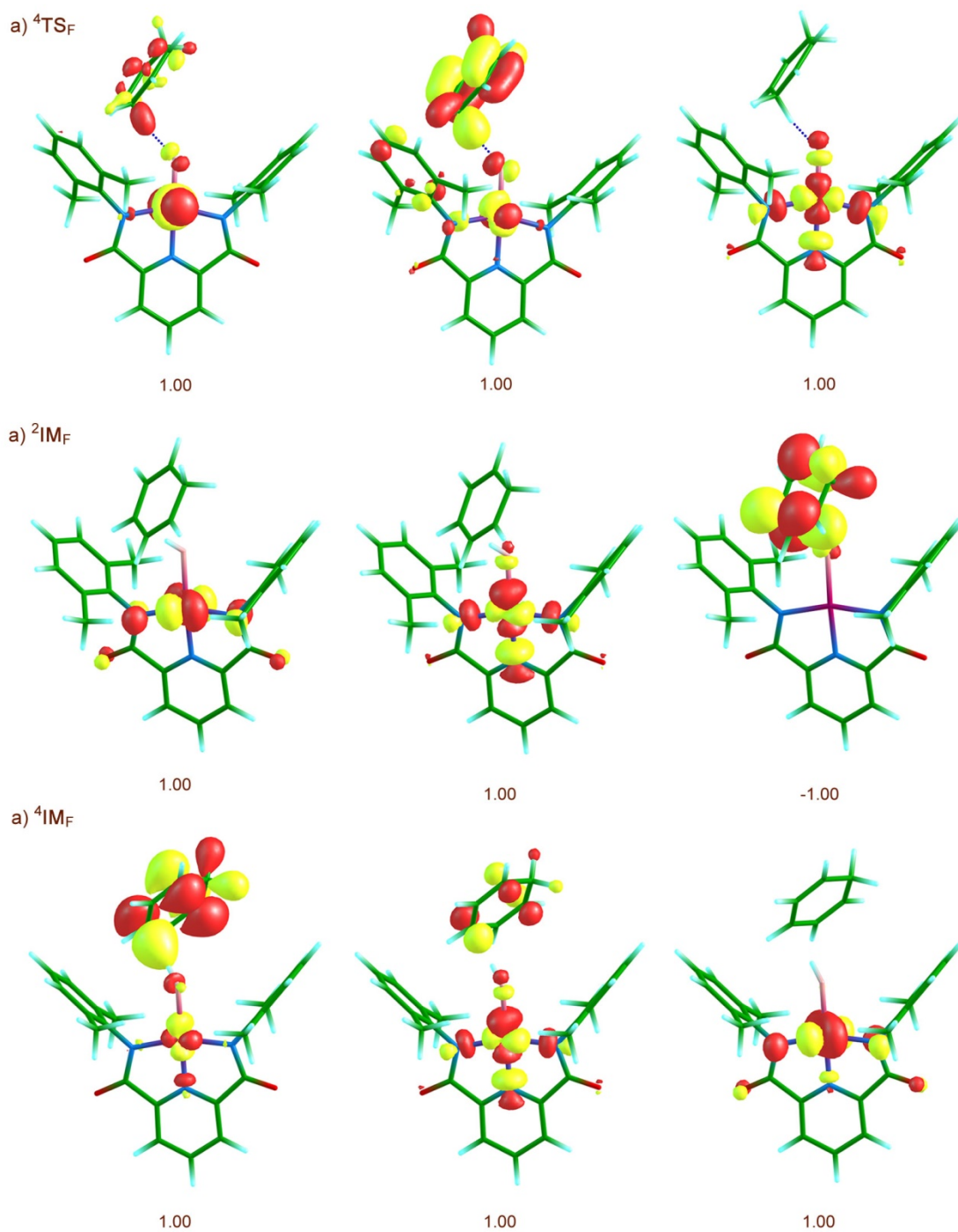


Fig. S7 Singly-occupied natural orbitals (SNOs) of the reaction intermediates in C-H bond activation of CHD by the oxidant $\mathbf{1}_F$ on the doublet/quartet spin states. Calculations were done at the UB3LYP/B2 level in solvent. Positive values represent alpha-electron occupations and negative ones represent beta-electron occupations.

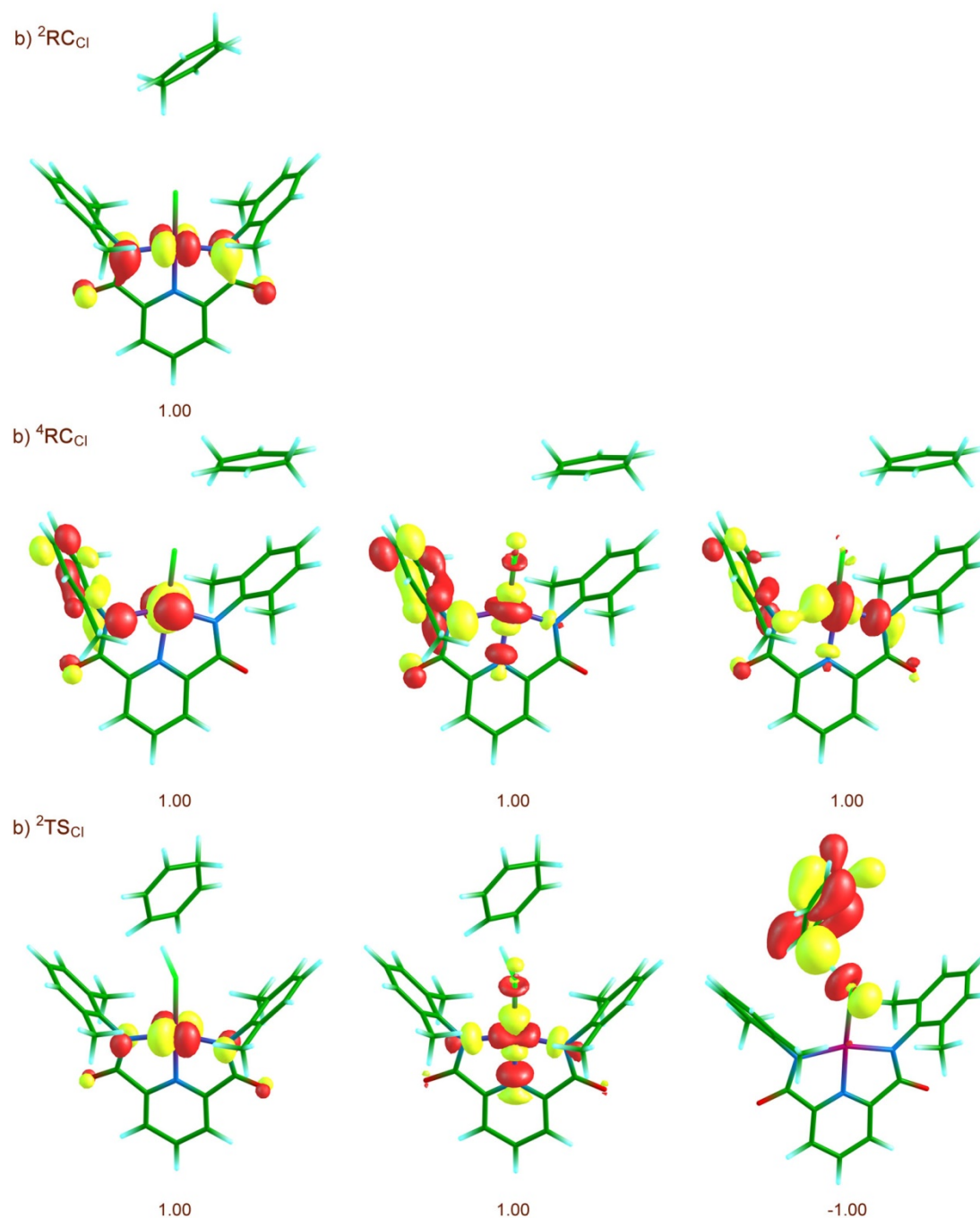


Fig. S8 Singly-occupied natural orbitals (SNOs) of the reaction intermediates in C-H bond activation of CHD by the oxidant $\mathbf{1}_{\text{Cl}}$ on the doublet/quartet spin states. Calculations were done at the UB3LYP/B2 level in solvent. Positive values represent alpha-electron occupations and negative ones represent beta-electron occupations. (To be continued.)

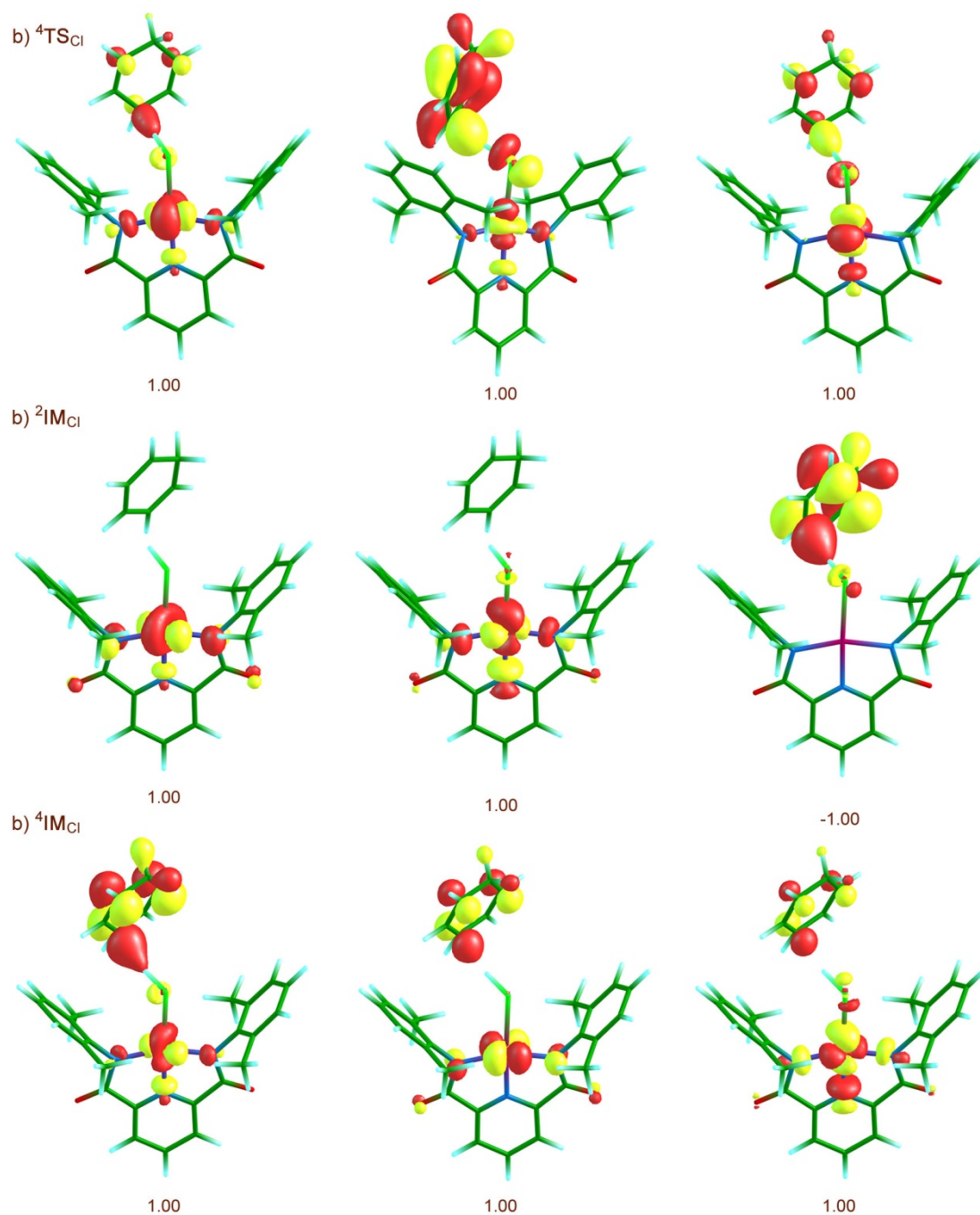


Fig. S8 Singly-occupied natural orbitals (SNOs) of the reaction intermediates in C-H bond activation of CHD by the oxidant 1_{Cl} on the doublet/quartet spin states. Calculations were done at the UB3LYP/B2 level in solvent. Positive values represent alpha-electron occupations and negative ones represent beta-electron occupations.

Part III. Desaturation vs. Halogenation of the CHD-H radical

Part III-1: desaturation vs. halogenation by the oxidant 1_F

Table S10. Various SCF and free energies of the reaction intermediates in the CHD-H radical halogenation by 1_F . Calculations were done at the UB3LYP/B2 level in solvent.

	OPT/B2	ΔE	OPT +ZPE	ΔE	G	ΔG
$^3\text{IM}'$	-3045.041082 ^a	0.0	-3044.538431	0.0	-3044.591009	0.0
$^3\text{TS}_2$	-3045.040149	0.6	-3044.536712	1.1	-3044.587071	2.5
$^3\text{PC}_F$	-3045.043726	-1.7	-3044.538324	0.1	-3044.588769	1.4

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

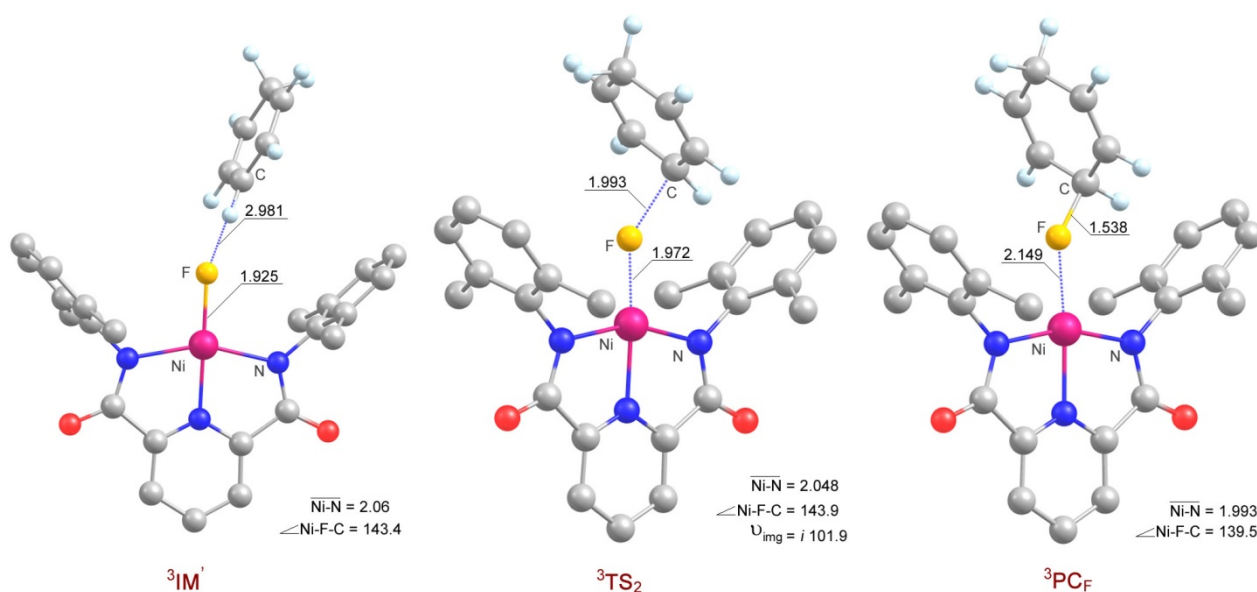


Fig. S9 The optimized structures of the reaction intermediates in the CHD-H radical halogenation by 1_F . Lengths are in Å units, bond angles are in degree units and the imaginary frequencies are in cm⁻¹ units. Hydrogen atoms of the ligand are omitted for clarity. Calculations were done at the UB3LYP/B2 level in solvent.

Table S11. Mulliken charges and spin densities of the reaction intermediates in the CHD-H radical halogenation by **1_F**. Calculations were done at the UB3LYP/B2 level in solvent.

	Spin density				Charge			
	Ni	L	F	Sub-H	Ni	L	F	Sub-H
³ IM'	1.79	0.17	0.03	0.00	1.19	-1.53	-0.60	0.95
³ TS₂	1.78	0.19	0.02	0.02	1.24	-1.48	-0.38	0.62
³ PC_F	1.60	0.38	0.01	0.01	1.07	-1.22	-0.13	0.27

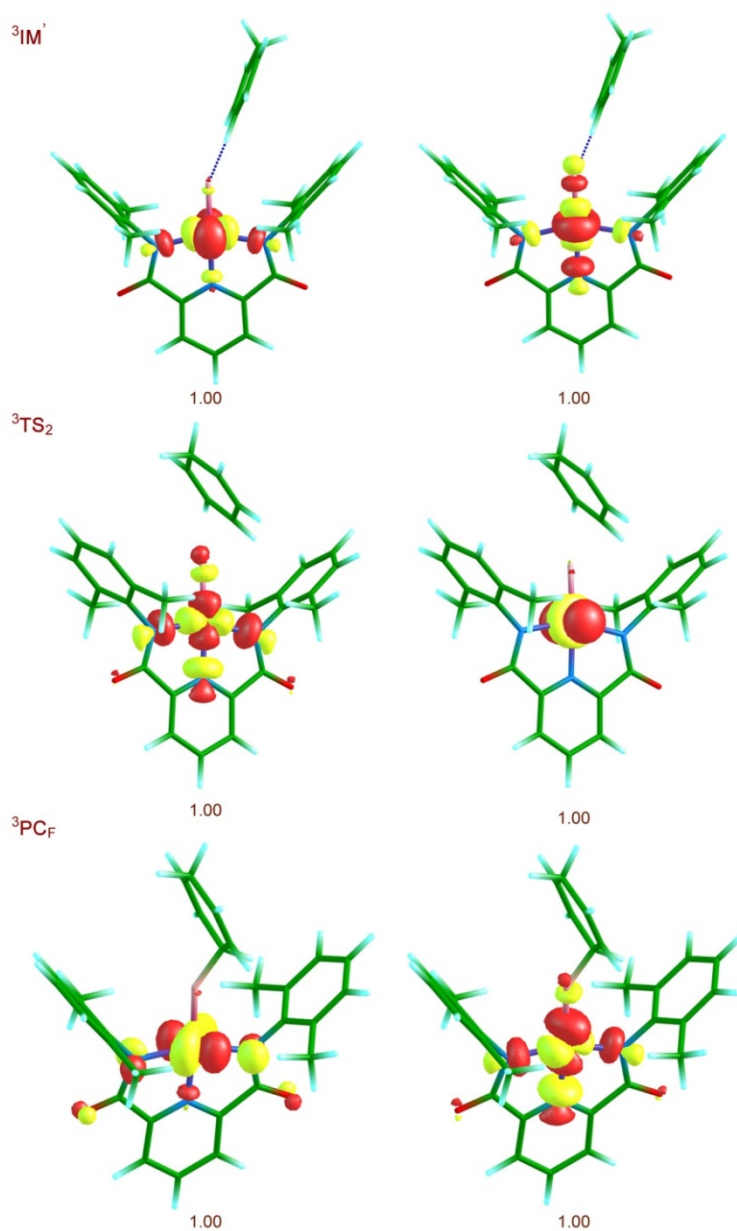


Fig. S10 Singly-occupied natural orbitals (SNOs) of the reaction intermediates in the CHD-H radical halogenation by **1_F**. Positive values represent alpha-electron occupations.

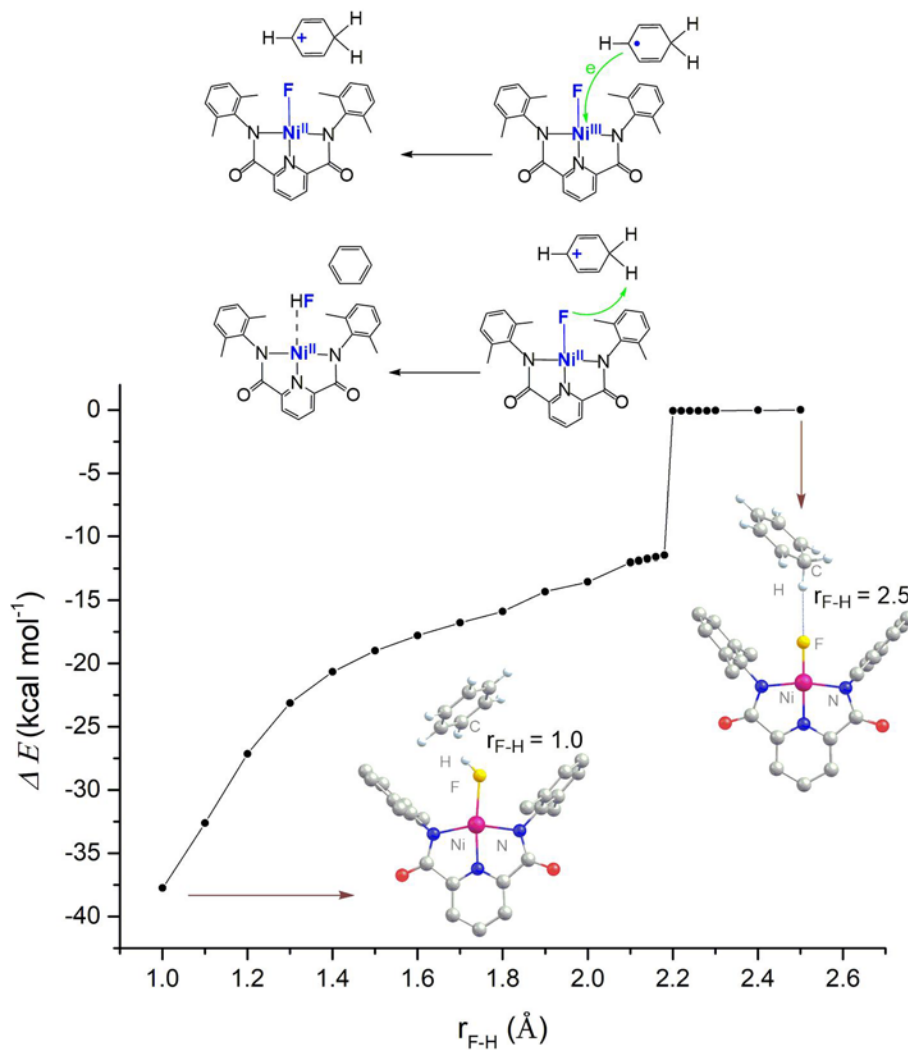


Fig. S11 The SCF energy plot of the relaxed scan along the F-H distance. Lengths are in Å units. Calculations were done at the UB3LYP/B2 level in solvent. Energies are in kcal mol⁻¹.

Part III-2: desaturation vs. halogenation by AgF

Table S12. Various SCF and free energies of the reaction intermediates in the CHD-H radical desaturation by the inorganic salt AgF in the absence of **1_F**. Calculations were done at the UB3LYP/B2 level in solvent.

	OPT/B2	ΔE	OPT +ZPE	ΔE	G	ΔG
²IM0	-478.488577 ^a	0.0	-478.377427	0.0	-478.404545	0.0
²TS0_H	-478.450723	23.8	-478.344725	20.5	-478.371476	20.8
²PC0_H	-478.493489	-3.1	-478.382113	-2.9	-478.414803	-6.4

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

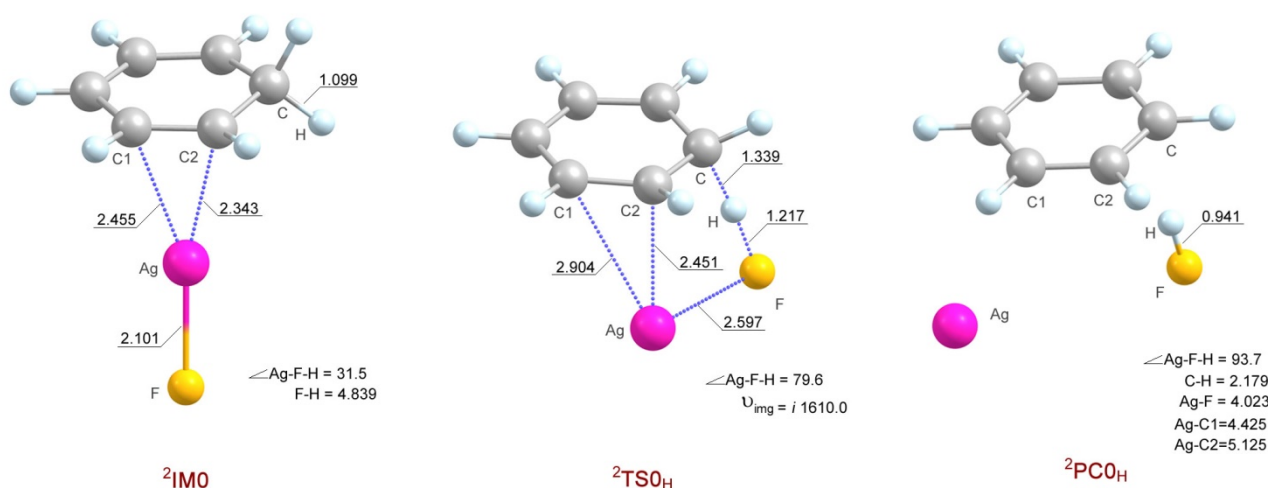


Fig. S12 Optimized structures of the reaction intermediates in the CHD-H radical desaturation by the inorganic salt AgF in the absence of **1_F**. Calculations were done at the UB3LYP/B2 level in solvent. Lengths are in Å units, bond angles are in degree units and the imaginary frequencies are in cm⁻¹ units.

Table S13. Mulliken charges and spin densities of the reaction intermediates in the CHD-H radical desaturation by the inorganic salt AgF in the absence of **1_F**. Calculations were done at the UB3LYP/B2 level in solvent.

	Spin density				Charge			
	Ag	F	H	Sub-H	Ag	F	H	Sub-H
²IM0	0.08	0.00	0.04	0.88	0.38	-0.76	0.18	0.20
²TS0_H	0.38	0.04	0.05	0.52	0.35	-0.59	0.37	-0.13
²PC0_H	0.99	0.00	0.00	0.01	0.03	-0.43	0.41	-0.01

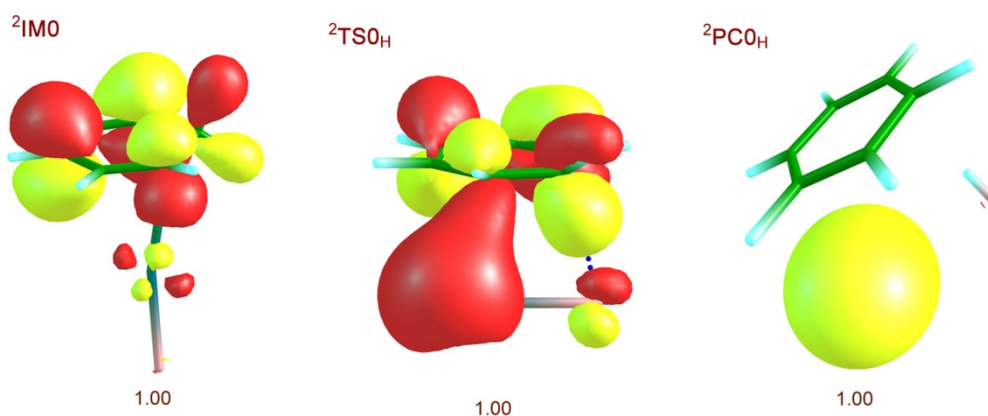


Fig. S13 Singly-occupied natural orbitals (SNOs) of the reaction intermediates in the CHD-H radical desaturation by the inorganic salt AgF in the absence of **1_F**. Calculations were done at the UB3LYP/B2 level in solvent. Positive values represent alpha-electron occupations.

Table S14. Various SCF and free energies of the reaction intermediates in the CHD-H radical halogenation by the inorganic salt AgF in the absence of **1F**. Calculations were done at the UB3LYP/B2 level in solvent.

	OPT/B2	ΔE	OPT +ZPE	ΔE	G	ΔG
$^2\text{IM0}$	-478.488577 ^a	0.0	-478.377427	0.0	-478.404545	0.0
$^2\text{TS0}_F$	-478.430452	36.5	-478.318887	36.7	-478.346254	36.6
$^2\text{PC0}_F$	-478.449850	24.3	-478.335578	26.3	-478.365325	24.6

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

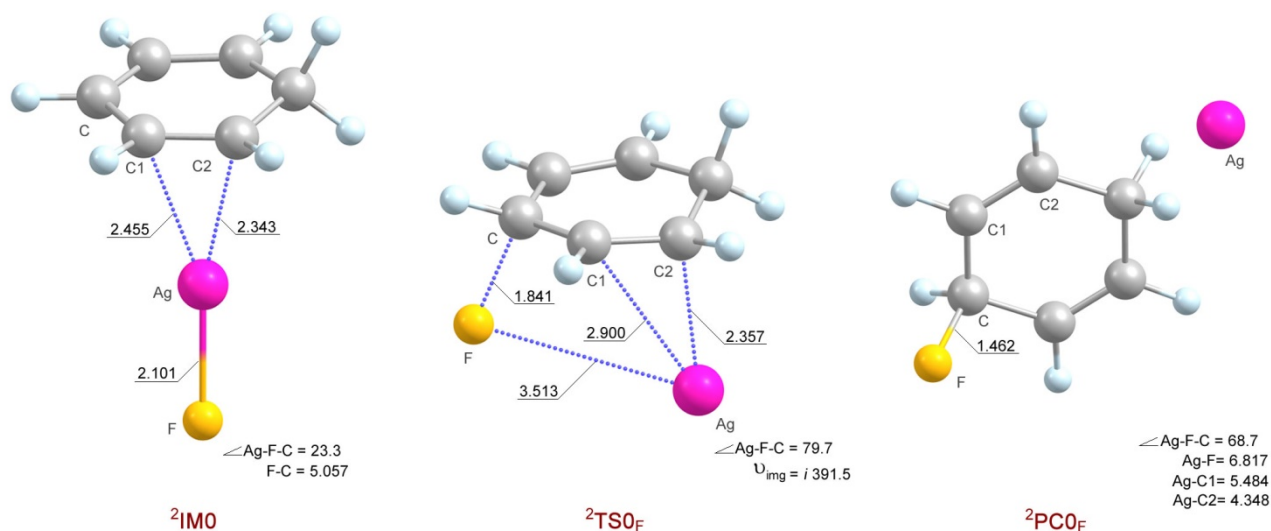


Fig. S14 Optimized structures of the reaction intermediates in the CHD-H radical halogenation by the inorganic salt AgF in the absence of **1F**. Calculations were done at the UB3LYP/B2 level in solvent. Lengths are in Å units, bond angles are in degree units and the imaginary frequencies are in cm⁻¹ units.

Table S15. Mulliken charges and spin densities of the reaction intermediates in the CHD-H radical halogenation by the inorganic salt AgF in the absence of **1_F**. Calculations were done at the UB3LYP/6-31+G** level in solvent.

	Spin density			Charge		
	Ag	F	Sub-H	Ag	F	Sub-H
² IM0	0.08	0.00	0.92	0.38	-0.76	0.38
² TS0_F	0.57	0.08	0.34	0.18	-0.58	0.40
² PC0_F	0.99	0.00	0.01	0.02	-0.36	0.34

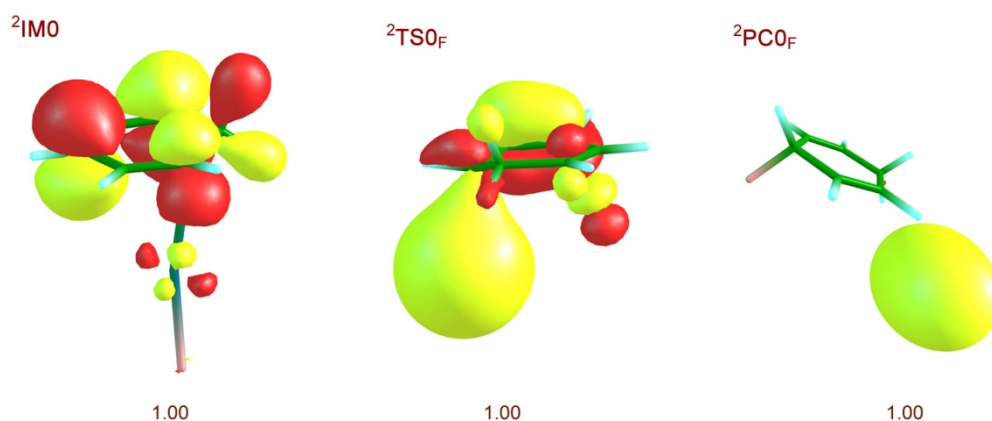


Fig. S15 Singly-occupied natural orbitals (SNOs) of the reaction intermediates in the CHD-H radical halogenation by the inorganic salt AgF in the absence of **1_F**. Calculations were done at the UB3LYP/B2 level in solvent. Positive values represent alpha-electron occupations.

Part IV: The nature of the AgF-binging Ni(III)-F oxidant $\mathbf{1}_{\text{F-Ag-F}}$

Table S16. Various SCF and free energies of $\mathbf{1}_{\text{F-Ag-F}}$ on the different spin states. Calculations were done at the UB3LYP/B2 level in solvent.

	OPT/B2	ΔE	OPT +ZPE	ΔE	G	ΔG
$^2\mathbf{2}$	-3057.883095 ^a	0.0	-3057.487409	0.0	-3057.534426	0.0
$^4\mathbf{2}$	-3057.860430	14.2	-3057.466808	12.9	-3057.516019	11.6
$^6\mathbf{2}$	-3057.774551	68.1	-3057.384497	64.6	-3057.432460	64.0

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

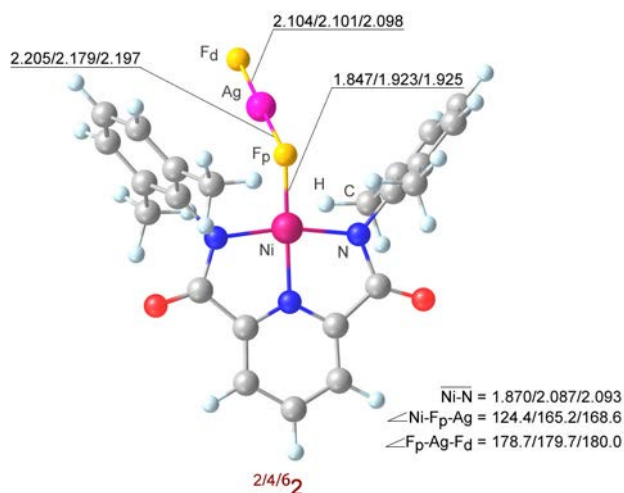


Fig. S16 The optimized structures of $\mathbf{1}_{\text{F-Ag-F}}$ on the doublet/quartet/sextet spin states. Lengths are in Å units, bond angles are in degree units. Calculations were done at the UB3LYP/B2 level in solvent.

Table S17. Mulliken charges and spin densities of $\mathbf{1}_{\text{F-Ag-F}}$ on the different spin states. Calculations were done at the UB3LYP/B2 level in solvent.

	Spin density					Charge				
	Ni	L	F _p	F _d	Ag	Ni	L	F _p	F _d	Ag
$^2\mathbf{2}$	0.74	0.27	-0.01	0.00	0.00	1.02	-0.44	-0.41	-0.74	0.56
$^4\mathbf{2}$	1.70	1.26	0.03	0.00	0.01	0.97	-0.30	-0.48	-0.76	0.56
$^6\mathbf{2}$	1.83	3.14	0.02	0.00	0.01	0.99	-0.29	-0.50	-0.75	0.55

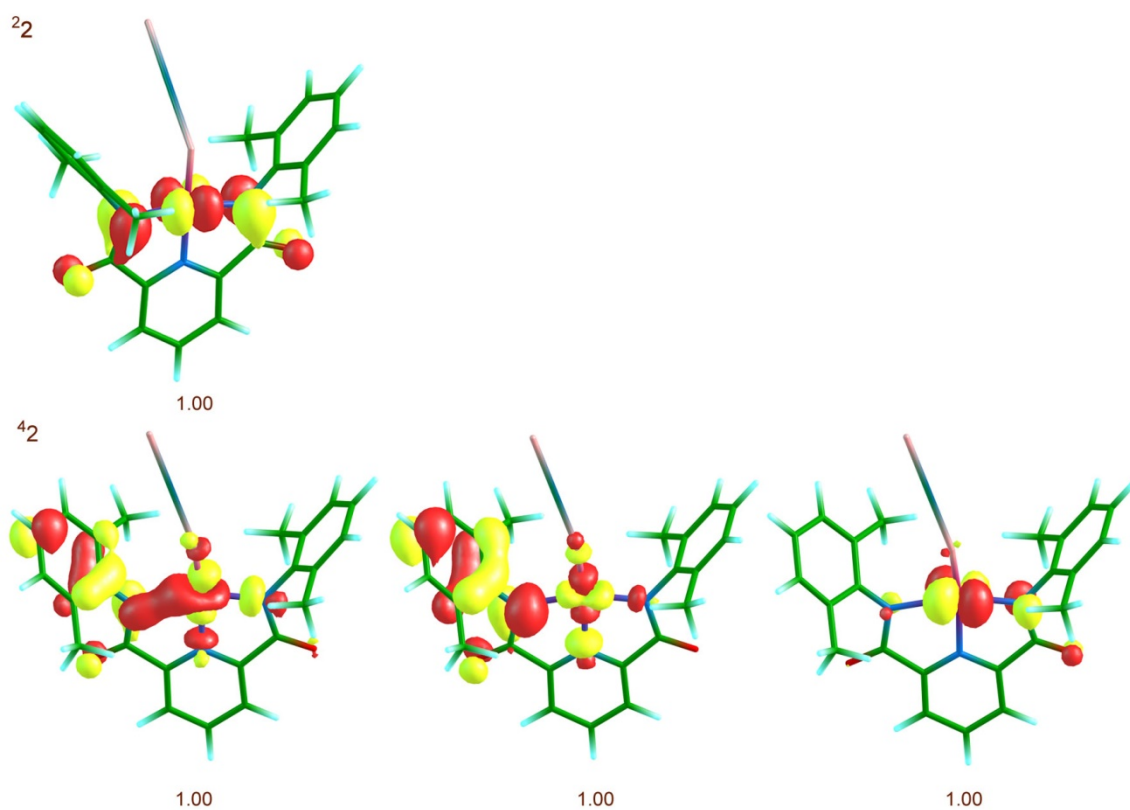


Fig. S17 Singly-occupied natural orbitals (SNOs) of $\mathbf{1}_{\text{F-Ag-F}}$ on the different spin states. Calculations were done at the UB3LYP/B2 level in solvent. Positive values represent alpha-electron occupations.

Part V: C-H bond activation of CHD by the proximal fluorine of $\mathbf{1}_{\text{F-Ag-F}}$

Table S18. Various SCF and free energies of the reaction intermediates in C-H bond activation of CHD by the proximal fluorine F_p of $\mathbf{1}_{\text{F-Ag-F}}$ on different spin states. Calculations were done at the UB3LYP/B2 level in solvent.

	OPT/B2	ΔE	OPT +ZPE	ΔE	G	ΔG
$^2\mathbf{RC}_p$	-3291.320966 ^a	0.0	-3290.803150	0.0	-3290.861761	0.0
$^4\mathbf{RC}_p$	-3291.304015	10.6	-3290.788022	9.5	-3290.849066	8.0
$^2\mathbf{TS}_{pH}$	-3291.287526	21.0	-3290.777423	16.1	-3290.832069	18.6
$^4\mathbf{TS}_{pH}$	-3291.284245	23.0	-3290.773509	18.6	-3290.828403	20.9
$^2\mathbf{IM}_p$	-3291.308120	8.1	-3290.792504	6.7	-3290.847315	9.1
$^4\mathbf{IM}_p$	-3291.292585	17.8	-3290.779493	14.8	-3290.836345	15.9

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

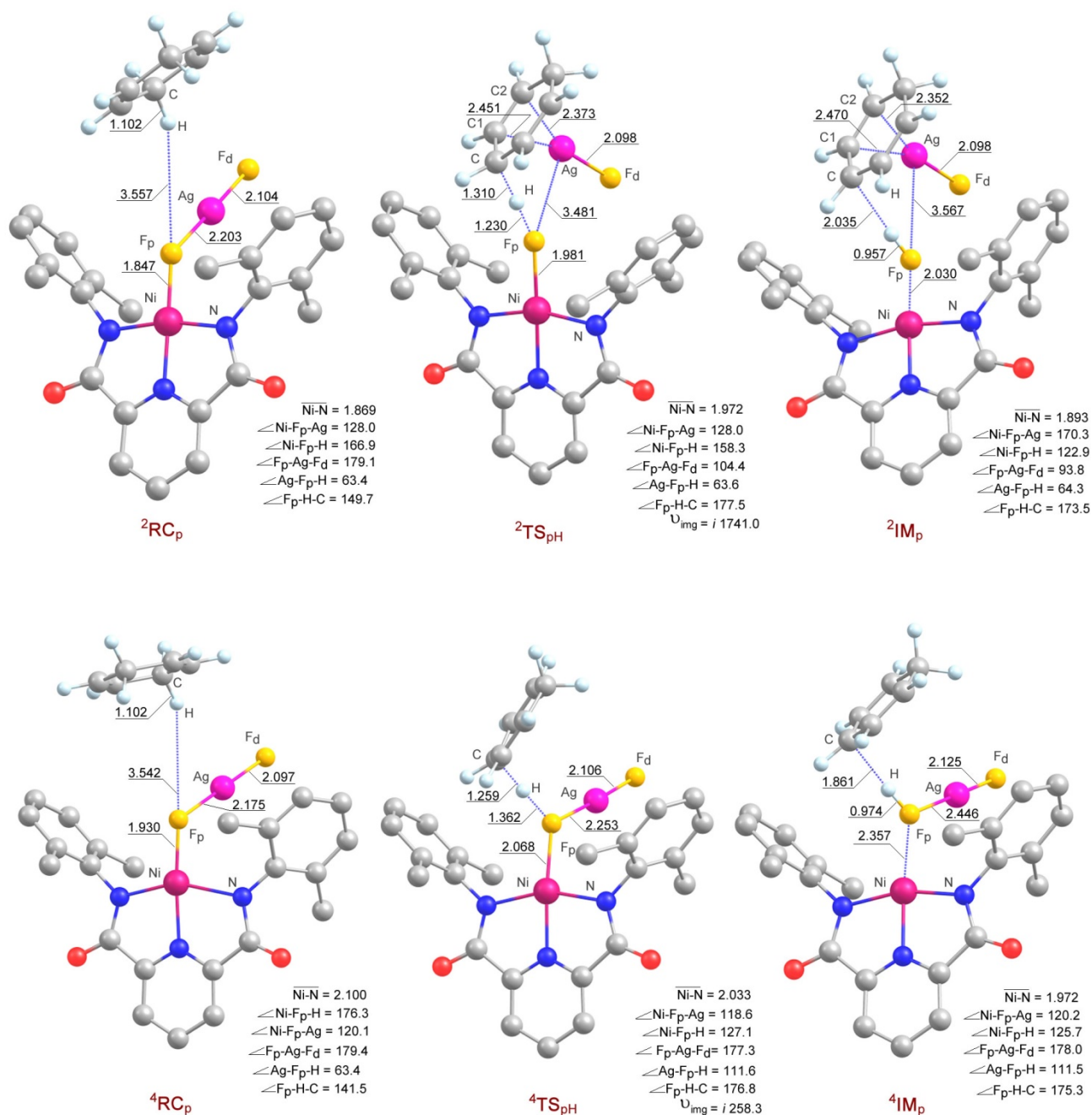


Fig. S18 The optimized structures of the reaction intermediates in C-H bond activation of CHD by the proximal fluorine F_p of **1**F-Ag-F on the doublet/quartet/sextet spin states. Calculations were done at the UB3LYP/B2 level in solvent. Lengths are in Å units, bond angles are in degree units and imaginary frequencies are in cm⁻¹ units. Hydrogen atoms of the ligand are omitted for clarity.

Table S19. Mulliken charges and spin densities of the reaction intermediates in C-H bond activation of CHD by the proximal fluorine F_p of **1**_{F-Ag-F} on different spin states. Calculations were done at the UB3LYP/B2 level in solvent.

	Spin density							Charge						
	Ni	L	F _p	F _d	Ag	H	Sub-H	Ni	L	F _p	F _d	Ag	H	Sub-H
² RC _p	0.74	0.27	-0.01	0.00	0.00	0.00	0.00	1.00	-0.41	-0.40	-0.74	0.56	0.15	-0.16
⁴ RC _p	1.80	1.16	0.03	0.00	0.01	0.00	0.00	1.15	-0.41	-0.54	-0.74	0.55	0.15	-0.16
² TS _{pH}	1.49	0.25	-0.07	0.00	-0.05	-0.05	-0.57	1.01	-1.07	-0.33	-0.75	0.40	0.34	0.40
⁴ TS _{pH}	1.77	0.22	0.06	0.00	0.01	0.12	0.81	1.29	-1.43	-0.44	-0.74	0.61	0.33	0.39
² IM _p	1.59	0.39	0.02	0.00	-0.07	-0.03	-0.91	1.07	-1.20	-0.30	-0.76	0.39	0.42	0.38
⁴ IM _p	1.57	0.43	-0.01	0.00	0.00	0.06	0.95	1.12	-1.21	-0.35	-0.75	0.70	0.43	0.05

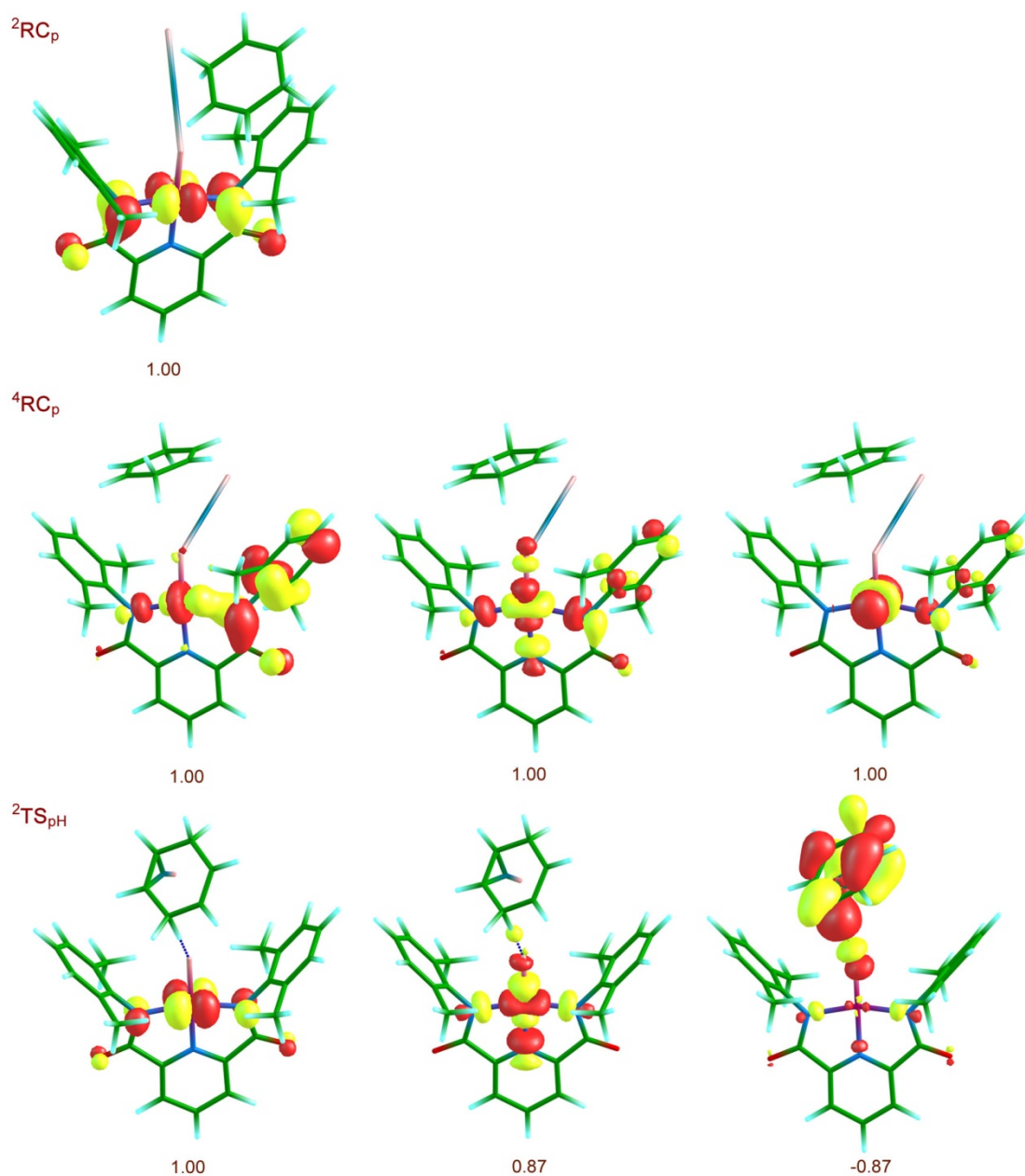


Fig. S19 Singly-occupied natural orbitals (SNOs) of the reaction intermediates in C-H bond activation of CHD by the proximal fluorine F_p of $\mathbf{1}_{F-Ag-F}$ on different spin states. Calculations were done at the UB3LYP/B2 level in solvent. Positive values represent alpha-electron occupancies. (To be continued.)

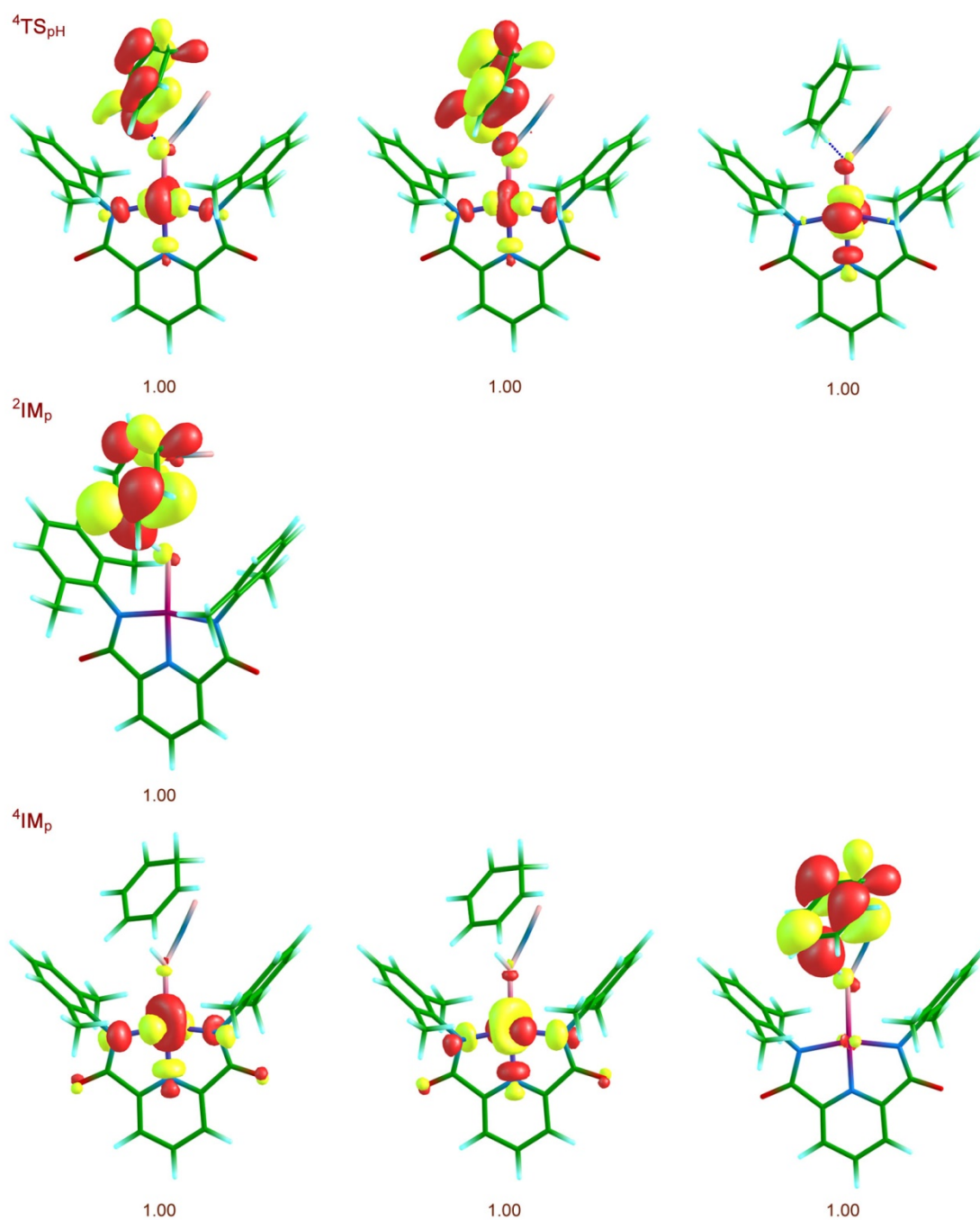


Fig. S19 Singly-occupied natural orbitals (SNOs) of the reaction intermediates in C-H bond activation of CHD by the proximal fluorine F_p of $\mathbf{1}_{F-Ag-F}$ on different spin states. Calculations were done at the UB3LYP/B2 level in solvent. Positive values represent alpha-electron occupations.

Table S20. Various SCF and free energies of the reaction intermediates in halogenation of CHD-H radical by the proximal fluorine F_p of 1_{F-Ag-F} on different spin states. Calculations were done at the UB3LYP/B2 level in solvent.

	OPT/B2	ΔE	OPT +ZPE	ΔE	G	ΔG
$^3IM'_p$	-3290.718991 ^a	0.0	-3290.214213	0.0	-3290.269331	0.0
$^3TS2_{pF}$	-3290.707537	7.2	-3290.201229	8.1	-3290.254555	9.3
$^3PC_{pF}$	-3290.716502	1.6	-3290.208357	3.7	-3290.261485	4.9

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

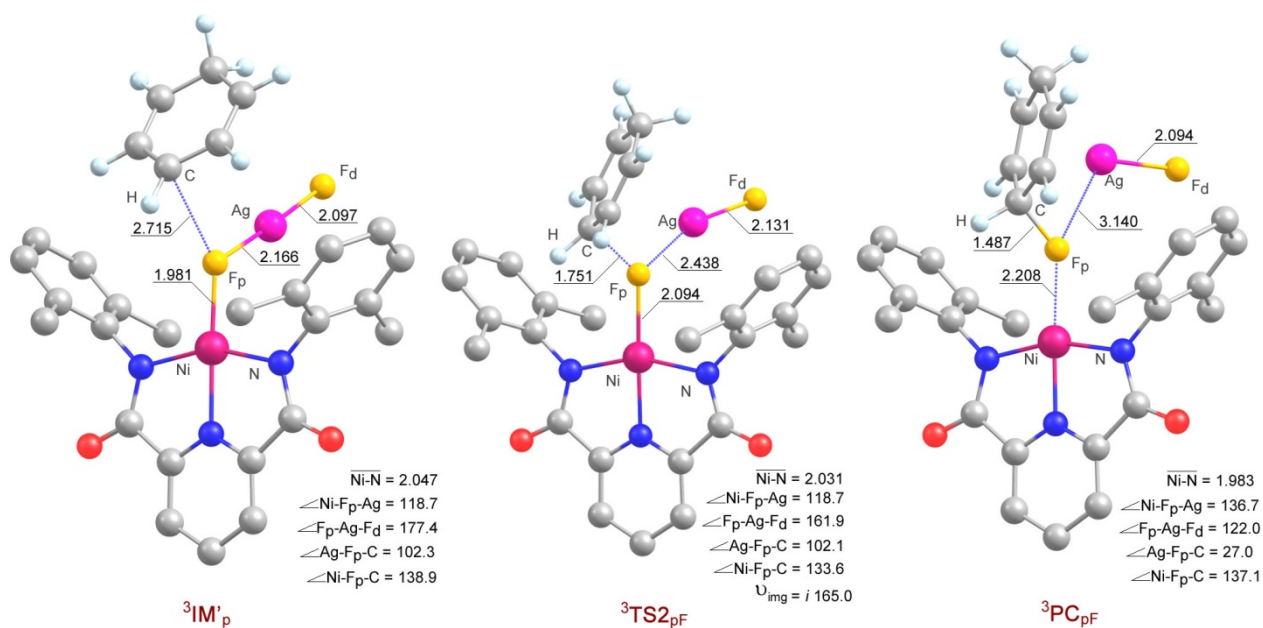


Fig. S20 The optimized structures of the reaction intermediates in halogenation of CHD-H radical by the proximal fluorine F_p of 1_{F-Ag-F} on different spin states. Calculations were done at the UB3LYP/B2 level in solvent. Lengths are in Å units, bond angles are in degree units and the imaginary frequencies are in cm⁻¹ units. Hydrogen atoms of the ligand are omitted for clarity.

Table S21. Mulliken charges and spin densities of the reaction intermediates in halogenation of CHD-H radical by the proximal fluorine F_p of $\mathbf{1}_{F-Ag-F}$ on the triplet spin state. Calculations were done at the UB3LYP/B2 level in solvent.

	Spin density						Charge					
	Ni	L	F_p	F_d	Ag	Sub-H	Ni	L	F_p	F_d	Ag	Sub-H
${}^3\mathbf{IM}'_p$	1.78	0.19	0.02	0.00	0.01	0.00	1.25	-1.50	-0.49	-0.74	0.51	0.97
${}^3\mathbf{TS}_{pF}$	1.76	0.22	0.01	0.00	0.00	0.01	1.32	-1.44	-0.28	-0.75	0.51	0.64
${}^3\mathbf{PC}_{pF}$	1.58	0.40	0.01	0.00	0.00	0.01	1.09	-1.19	-0.13	-0.76	0.28	0.71

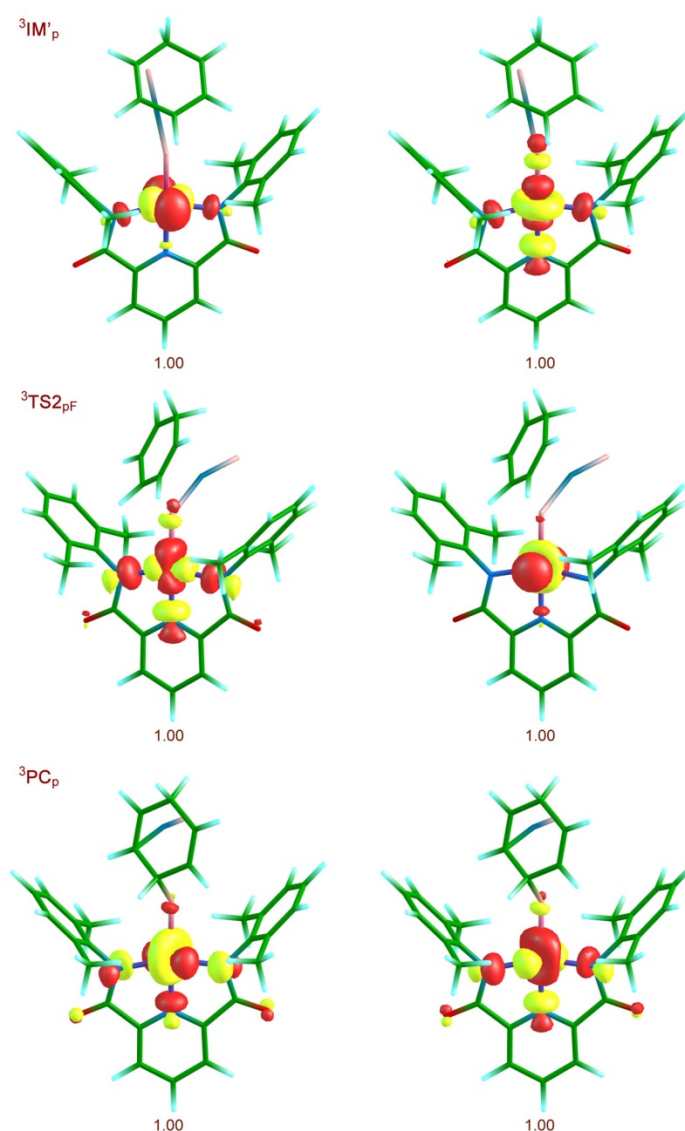


Fig. S21 Singly-occupied natural orbitals (SNOs) of the reaction intermediates in halogenation of CHD-H radical by the proximal fluorine F_p of $\mathbf{1}_{F-Ag-F}$ on the triplet spin state. Calculations were done at the UB3LYP/B2 level in solvent. Positive values represent alpha-electron occupations.

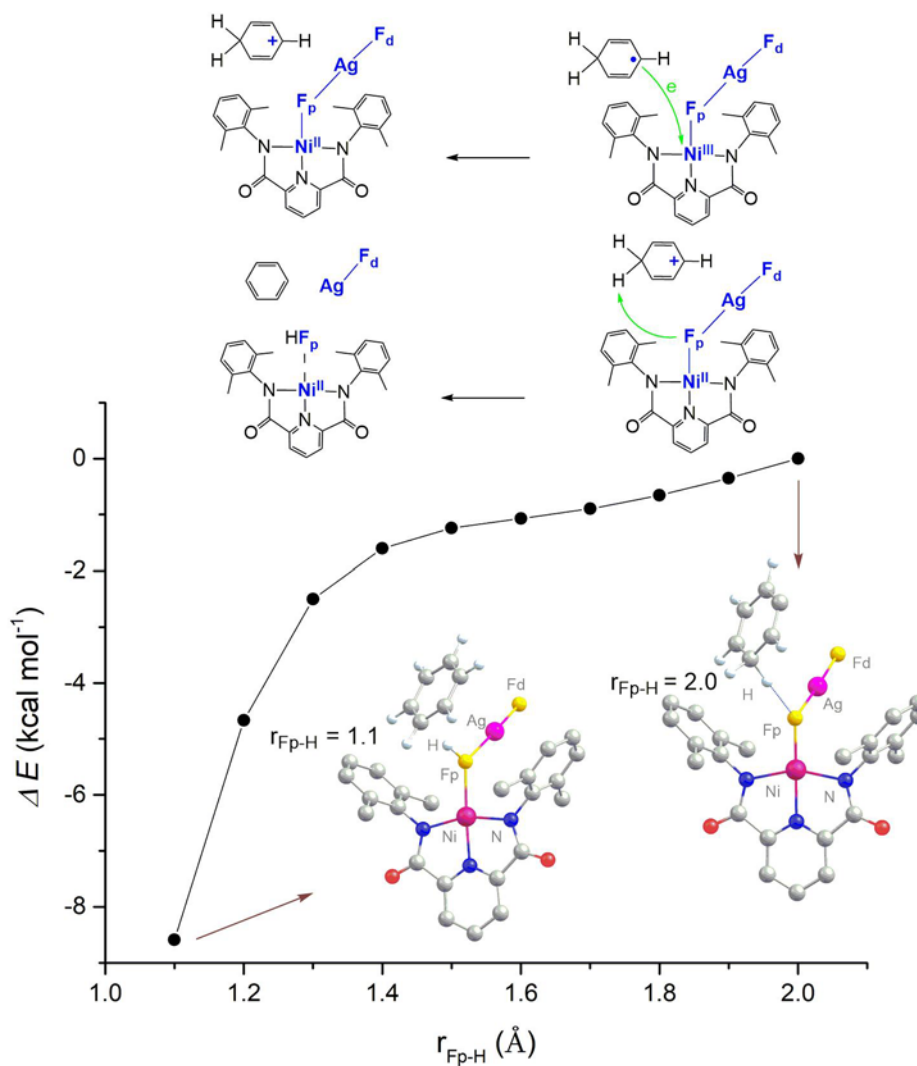


Fig. S22 The energy plot of the relaxed scan alongside of the $\text{F}_p\text{-H}$ distance for desaturation of CHD-H radical by the proximal fluorine F_p of $\mathbf{1}_{\text{F-Ag-F}}$ on the triplet spin state. Calculations were done at the UB3LYP/B2 level in solvent. Energies are in kcal mol^{-1} .

Part VI: C-H bond activation of CHD by the distal fluorine of 1_{F-Ag-F}

Table S22. Various SCF and free energies of the reaction intermediates in C-H bond activation of CHD by the distal fluorine F_d of 1_{F-Ag-F} on different spin states. Calculations were done at the UB3LYP/B2 level in solvent.

	OPT/B2	ΔE	OPT +ZPE	ΔE	G	ΔG
2RC_d	-3291.320815 ^a	0.0	-3290.802918	0.0	-3290.862326	0.0
4RC_d	-3291.302833	11.3	-3290.786596	10.2	-3290.845888	10.3
$^2TS_{dH}$	-3291.303647	10.8	-3290.791828	7.0	-3290.846643	9.8
$^4TS_{dH}$	-3291.290354	19.1	-3290.778076	15.6	-3290.832194	18.9
2IM_d	-3291.330423	-6.0	-3290.815641	-8.0	-3290.872063	-6.1
4IM_d	-3291.319336	0.9	-3290.805998	-1.9	-3290.862714	-0.2

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

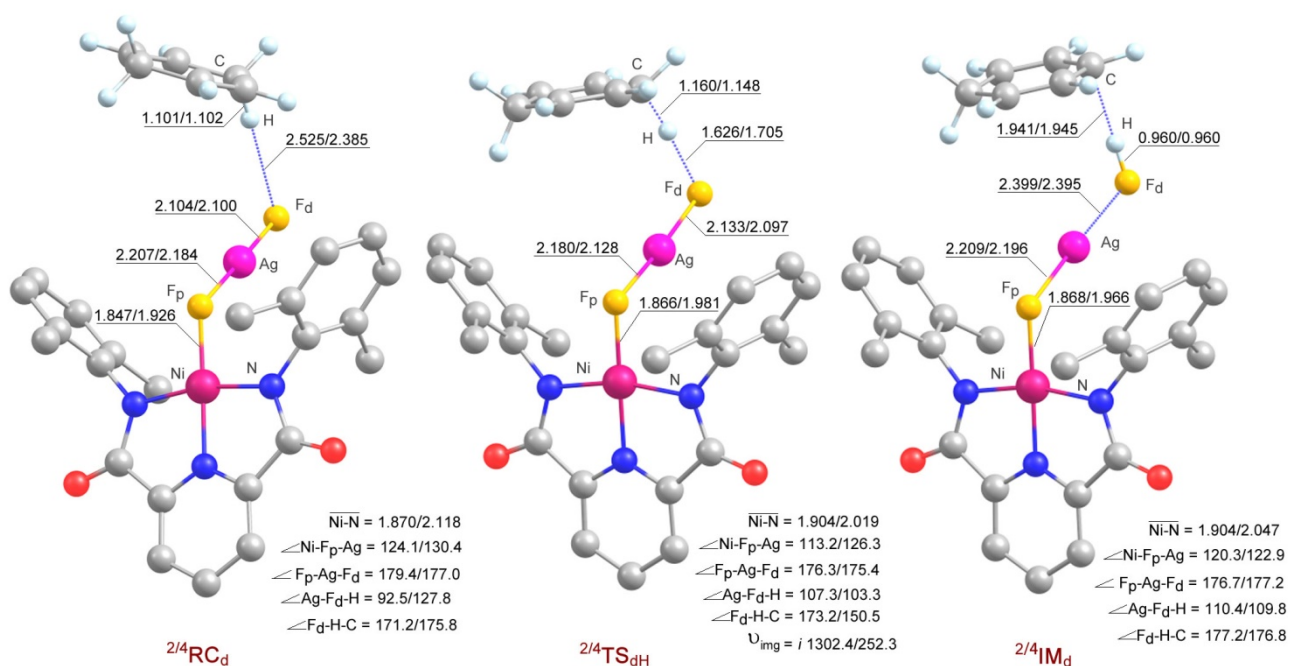


Fig. S23 The optimized structures of the reaction intermediates in C-H bond activation of CHD by the distal fluorine F_d of 1_{F-Ag-F} on different spin states. Calculations were done at the UB3LYP/B2 level in solvent. Lengths are in Å units, bond angles are in degree units and imaginary frequencies are in cm⁻¹ units. Hydrogen atoms of the ligand are omitted for clarity.

Table S23. Mulliken spin densities and charges of the reaction intermediates in C-H bond activation of CHD by the distal fluorine F_d of **1**_{F-Ag-F} on different spin states. Calculations were done at the UB3LYP/B2 level in solvent.

	Spin density							Charge						
	Ni	L	F _p	F _d	Ag	H	Sub-H	Ni	L	F _p	F _d	Ag	H	Sub-H
² RC _d	0.74	0.27	-0.01	0.00	0.00	0.00	0.00	0.99	-0.41	-0.40	-0.72	0.56	0.19	-0.20
⁴ RC _d	1.80	1.17	0.03	0.00	0.00	0.00	0.00	1.15	-0.44	-0.54	-0.72	0.57	0.20	-0.22
² TS _{dH}	0.07	0.22	0.01	0.06	0.01	0.06	0.57	0.52	-0.53	-0.46	-0.62	0.58	0.29	0.22
⁴ TS _{dH}	1.64	0.35	0.06	0.10	0.17	0.06	0.63	1.05	-1.26	-0.48	-0.59	0.54	0.28	0.45
² IM _d	0.00	0.00	0.00	0.00	0.00	0.03	0.97	0.56	-0.92	-0.45	-0.40	0.75	0.42	0.03
⁴ IM _d	1.78	0.19	0.03	0.00	0.01	0.04	0.97	1.24	-1.51	-0.55	-0.40	0.75	0.42	0.04

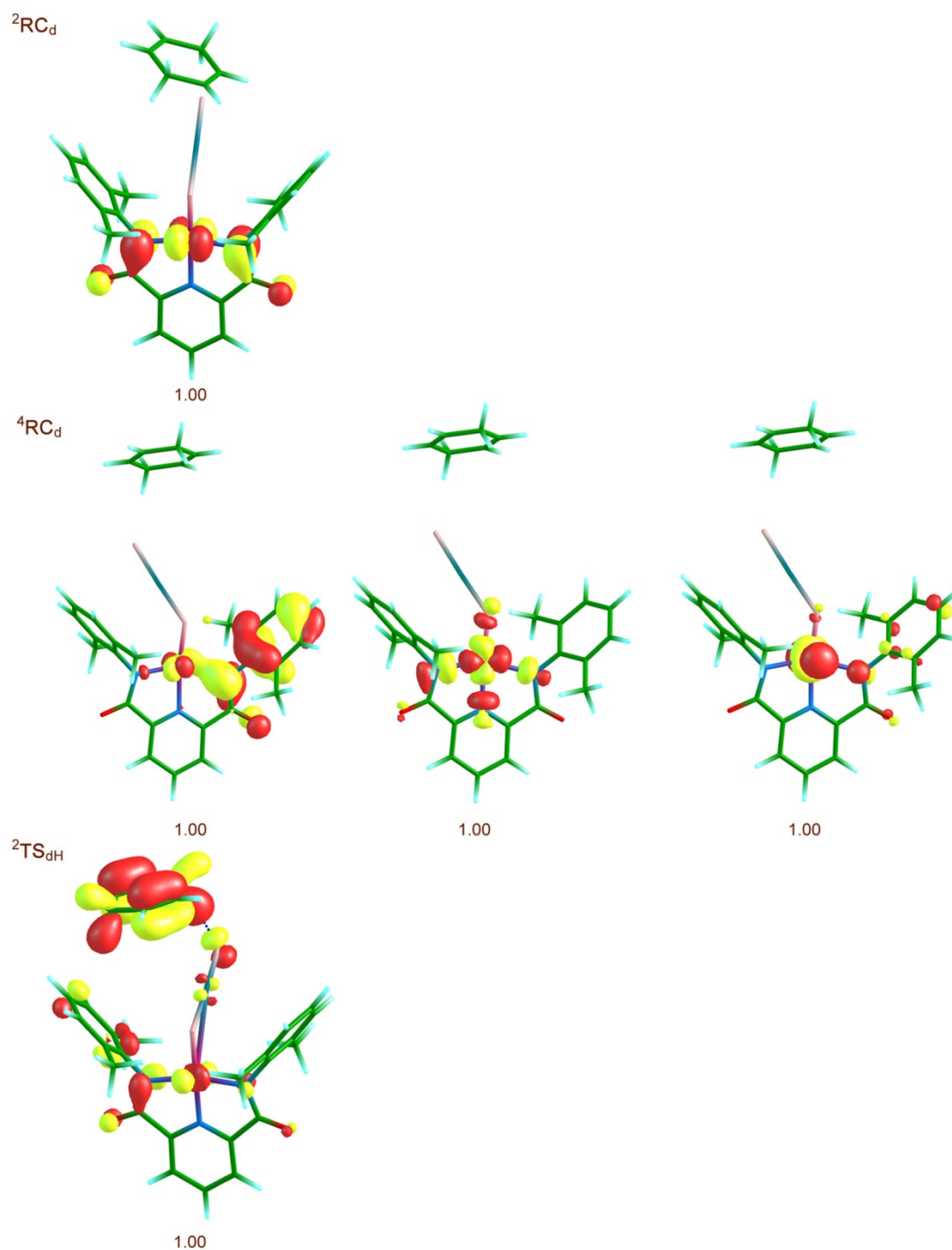


Fig. S24 Singly-occupied natural orbitals (SNOs) of complex the reaction intermediates in C-H bond activation of CHD by the distal fluorine F_d of 1_{F-Ag-F} on different spin states. Calculations were done at the UB3LYP/B2 level in solvent. Positive values represent alpha-electron occupations. (To be continued.)

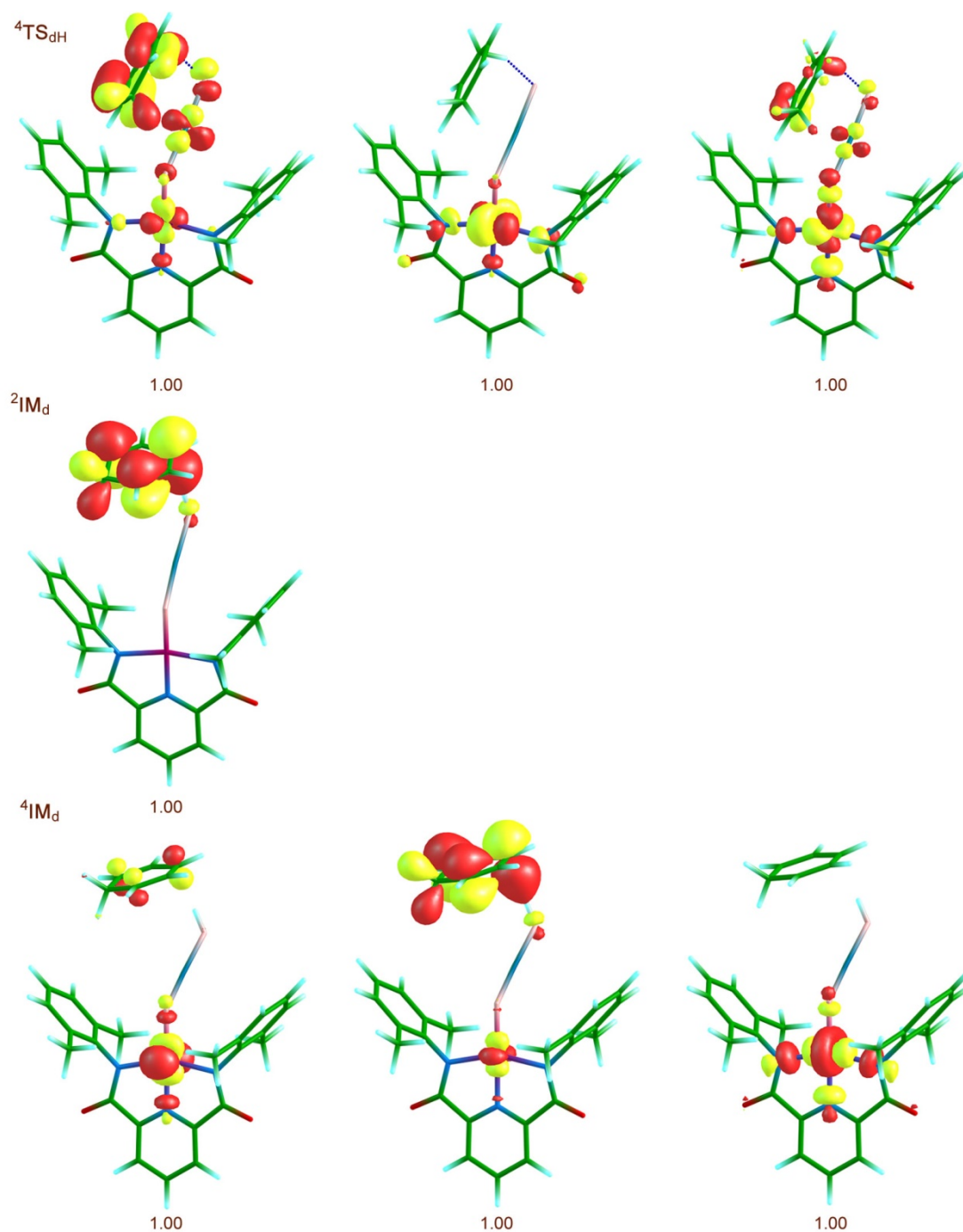


Fig. S24 Singly-occupied natural orbitals (SNOs) of complex the reaction intermediates in C-H bond activation of CHD by the distal fluorine F_d of 1_{F-Ag-F} on different spin states. Calculations were done at the UB3LYP/B2 level in solvent. Positive values represent alpha-electron occupations.

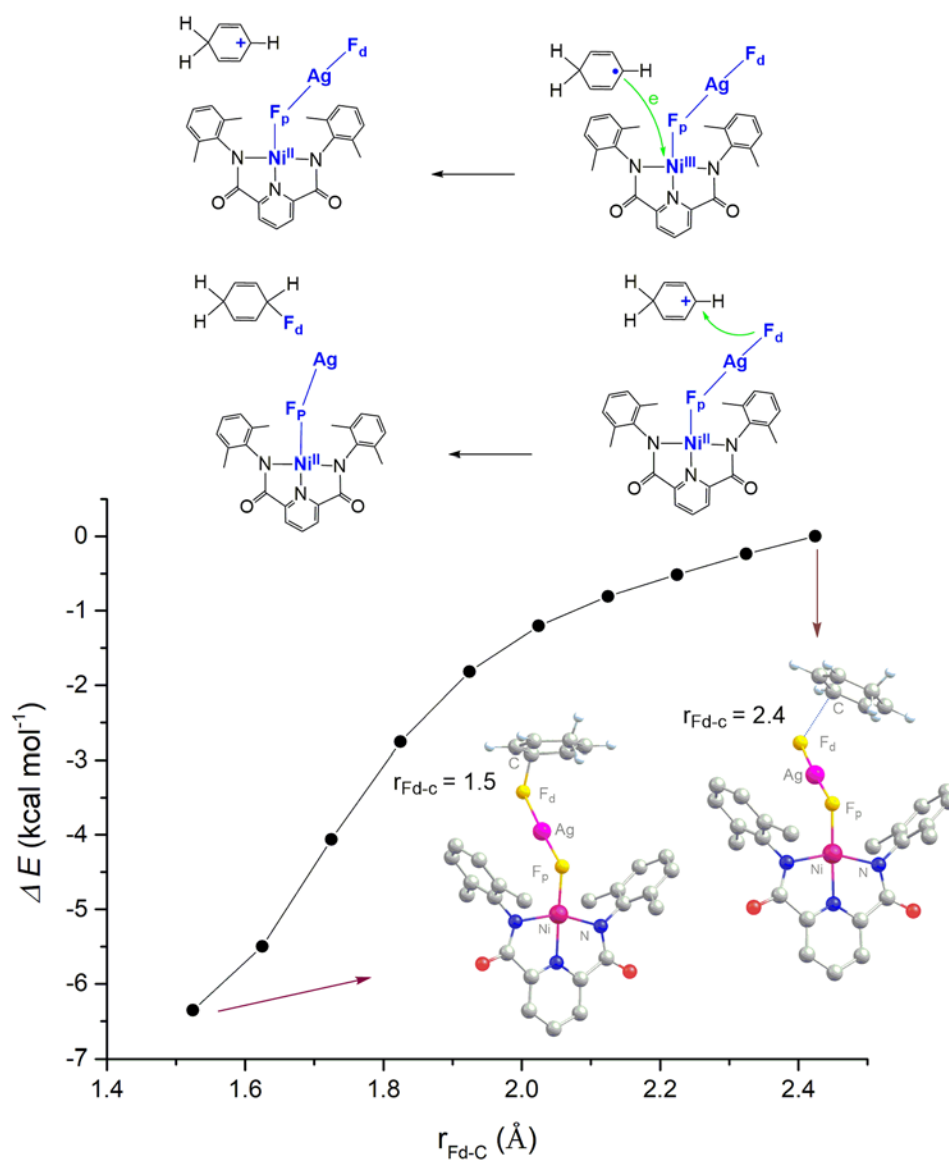


Fig. S25 The energy plot of the relaxed scan alongside of the F_d -C distance for halogenation of CHD-H radical by the distal fluorine F_d of $1_{\text{F-Ag-F}}$ on the triplet spin state. Lengths are in \AA units. Energies are in kcal mol^{-1} . Calculations were done at the UB3LYP/B2 level in solvent.

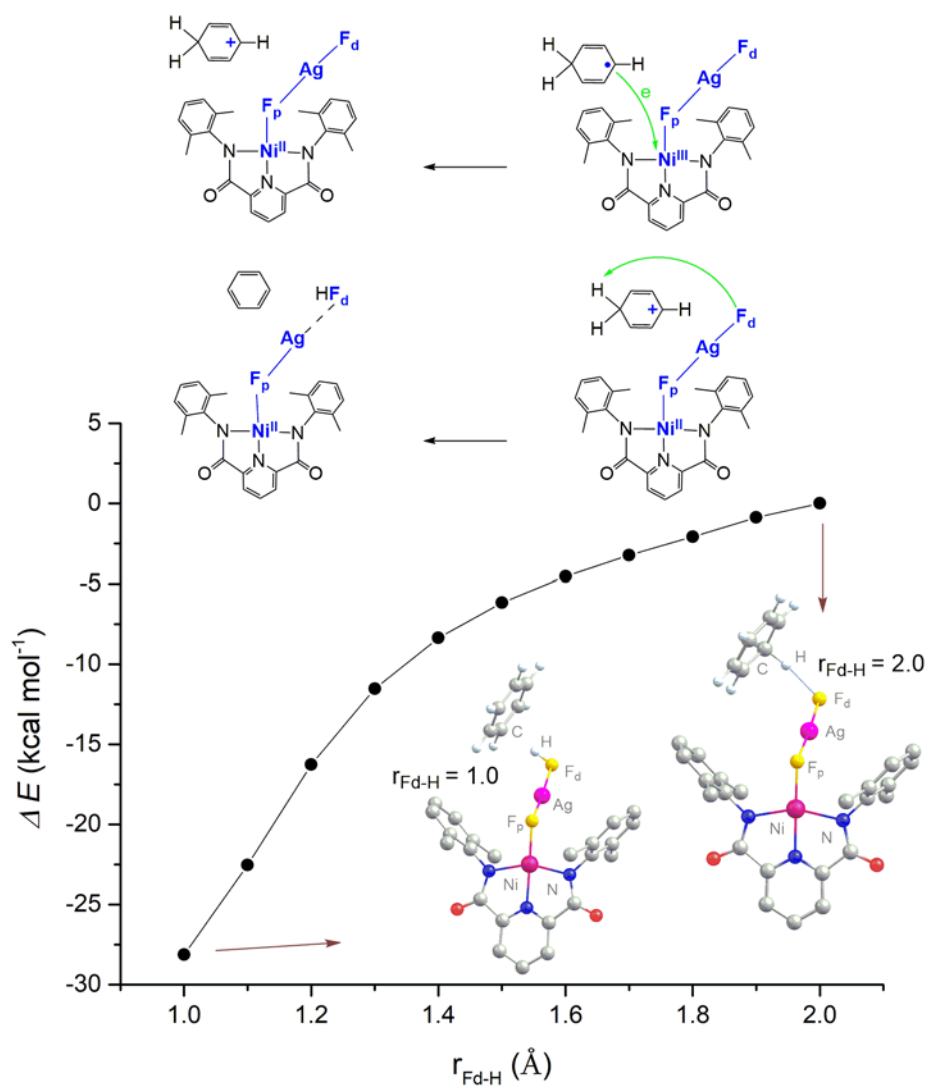


Fig. S26 The energy plot of the relaxed scan alongside of the $\text{F}_d\text{-H}$ distance for desaturation of CHD-H radical by the distal fluorine F_d of $\mathbf{1}_{\text{F-Ag-F}}$ on the triplet spin state. Lengths are in \AA units. Energies are in kcal mol^{-1} . Calculations were done at the UB3LYP/B2 level in solvent.

Part VII: Difluorination of PPh₃ by two separated 1_FS

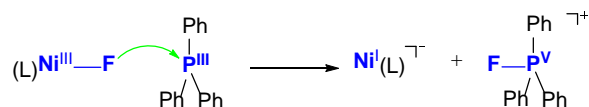


Table S24. Various SCF and free energies of the reaction intermediates in the first fluorination of PPh₃ by 1_F. Calculations were done at the UB3LYP/B2 level in solvent.

	OPT/B2	ΔE	OPT +ZPE	ΔE	G	ΔG
² RC _{PF}	-3848.549523 ^a	0.0	-3847.882209	0.0	-3847.947776	0.0
⁴ RC _{PF}	-3848.530335	12.0	-3847.863734	11.6	-3847.924101	14.9
² TS _{1PF}	-3848.503788	28.7	-3847.835470	29.3	-3847.890057	36.2
⁴ TS _{1PF}	-3848.502630	29.4	-3847.837327	28.2	-3847.901648	28.9
² IM _{1PF}	-3848.540422	5.7	-3847.872661	6.0	-3847.934706	8.2
⁴ IM _{1PF}	-3848.518692	19.3	-3847.852603	18.6	-3847.915817	20.1

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

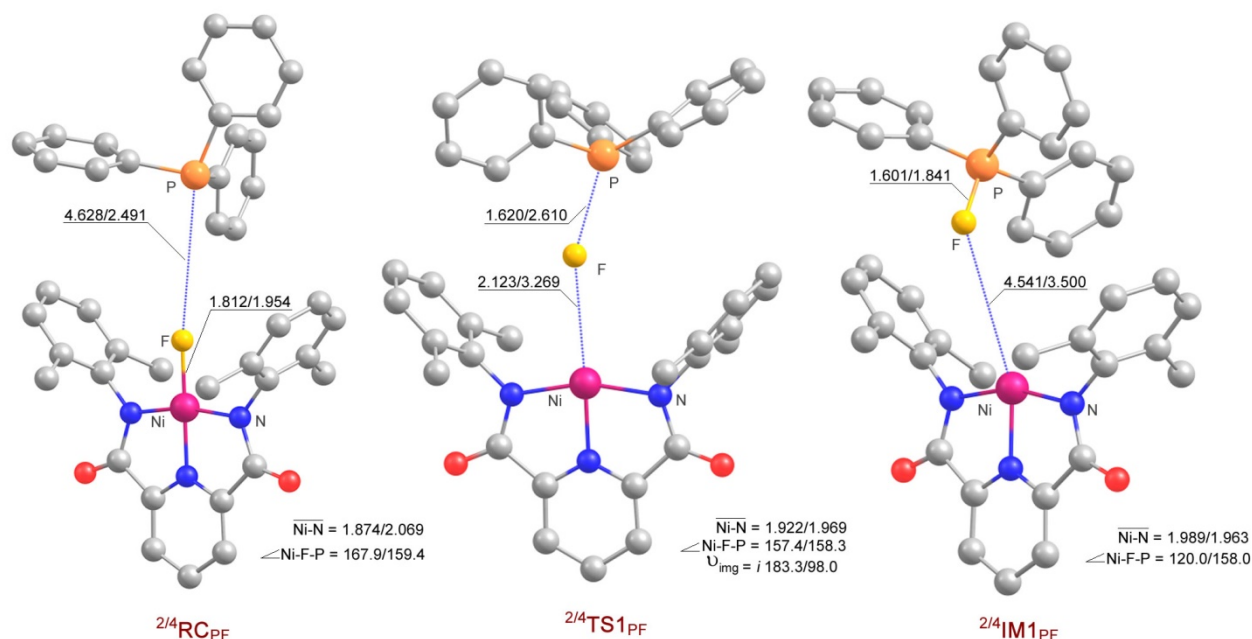
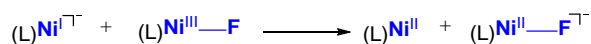


Fig. S27 The optimized structures of the reaction intermediates in the first fluorination of PPh₃ by 1_F on the doublet/quartet spin states. Calculations were done at the UB3LYP/B2 level in solvent. Lengths are in Å units, bond angles are in degree units and imaginary frequencies are in cm⁻¹ units. Hydrogen atoms are omitted for clarity.

Table S25. Mulliken charges and spin densities of the reaction intermediates *i* in the first fluorination of PPh₃ by **1_F** on the doublet/quartet spin states. Calculations were done at the UB3LYP/B2 level in solvent.

	Spin density					Charge				
	Ni	L	F	P	Sub-P	Ni	L	F	P	Sub-P
² RC _{PF}	0.76	0.25	-0.01	0.00	0.00	0.96	-0.51	-0.40	-0.56	0.51
⁴ RC _{PF}	1.80	0.18	0.07	0.83	0.13	1.19	-1.32	-0.45	-0.20	0.77
² TS1 _{PF}	0.06	0.00	-0.11	0.84	0.21	0.32	-0.44	0.06	-0.46	0.52
⁴ TS1 _{PF}	1.58	0.42	0.15	0.72	0.14	1.09	-1.07	-0.65	-0.14	0.77
² IM1 _{PF}	0.82	0.14	0.00	0.01	0.02	0.28	-1.22	-0.23	0.06	1.11
⁴ IM1 _{PF}	1.56	0.44	0.05	0.82	0.13	1.07	-1.03	-0.35	-0.53	0.84

Table S26. Energy variation of the conversion of the complex containing the Ni^I and the Ni^{III}-F species to the complex containing the Ni^{II} and the Ni^{II}-F species. Calculations were done at the UB3LYP/B2 level in solvent.



(L)Ni ^I	(L)Ni ^{III} F	(L)Ni ^{II}	(L)Ni ^{II} F	ΔE ^a
-2712.099228	-2811.815548	-2711.965441	-2812.006016	-35.6

a. $\Delta E = (E((\text{L})\text{Ni}^{\text{II}}) + E((\text{L})\text{Ni}^{\text{II}}-\text{F}) - (E((\text{L})\text{Ni}^{\text{III}}-\text{F}) + E((\text{L})\text{Ni}^{\text{I}})))$. Absolute energies are in au units and the relative ones are in kcal mol⁻¹ units.

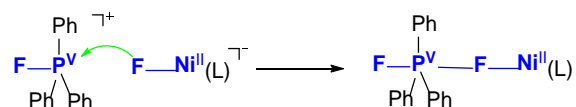


Table S27. Various SCF and free energies of the reaction intermediates in the second fluorination of the intermediate $[FPPH_3]^+$ by 1e-reduced $\mathbf{1}_F$ on the singlet/triplet spin states. Calculations were done at the UB3LYP/B2 level in solvent.

	OPT/B2	ΔE	OPT +ZPE	ΔE	G	ΔG
$^1\mathbf{IM}'_{PF}$	-3948.452013 ^a	0.0	-3947.780401	0.0	-3947.842734	0.0
$^3\mathbf{IM}'_{PF}$	-3948.437640	9.0	-3947.767300	8.2	-3947.828070	9.2
$^1\mathbf{TS2}_{PF}$	-3948.430580	13.4	-3947.757660	14.3	-3947.812094	19.2
$^3\mathbf{TS2}_{PF}$	-3948.428576	14.7	-3947.757006	14.7	-3947.813988	18.0
$^1\mathbf{IM2}_{PF}$	-3948.432154	12.5	-3947.758934	13.5	-3947.814023	18.0
$^3\mathbf{IM2}_{PF}$	-3948.436457	9.8	-3947.764098	10.2	-3947.820959	13.7

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

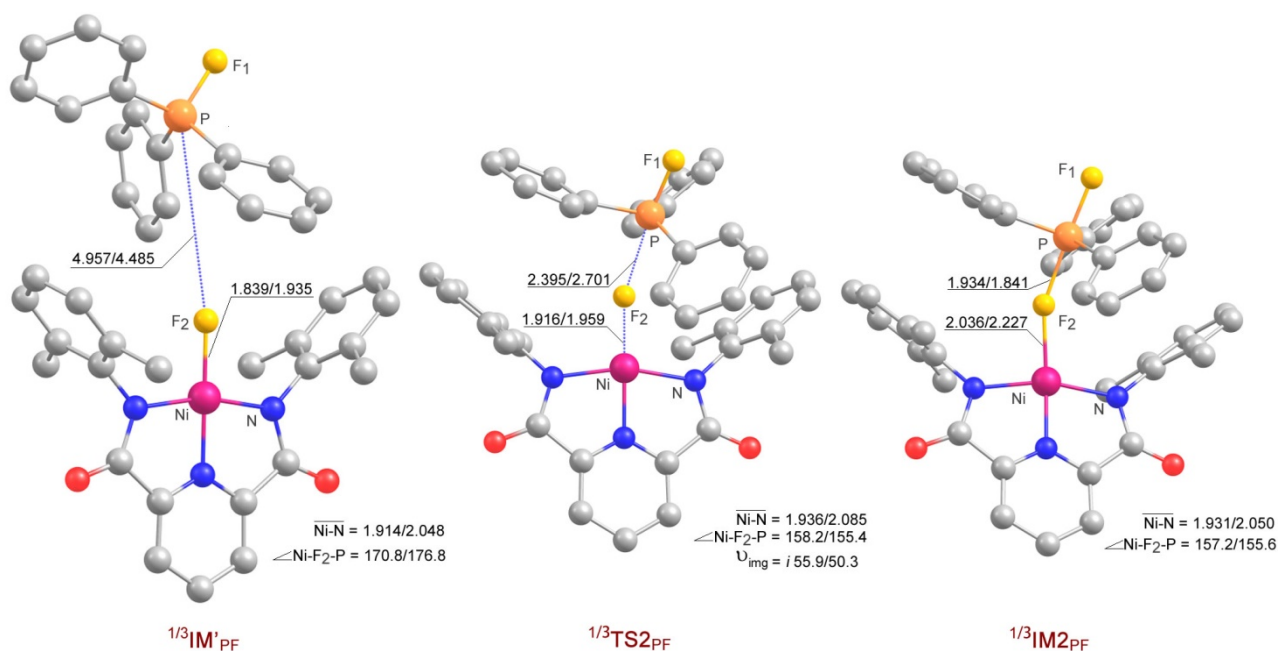


Fig. S28 The optimized structures of the reaction intermediates in the second fluorination of the intermediate $[FPPH_3]^+$ by 1e-reduced $\mathbf{1}_F$ on the singlet/triplet spin states. Calculations were done at the UB3LYP/B2 level in solvent. Lengths are in Å units, bond angles are in degree units and imaginary frequencies are in cm⁻¹ units. Hydrogen atoms of the ligand are omitted for clarity.

Table S28. Mulliken charges and spin densities of the reaction intermediates in the second fluorination of the intermediate $[\text{FPPh}_3]^+$ by 1e-reduced $\mathbf{1}_F$ on the singlet/triplet spin states. Calculations were done at the UB3LYP/B2 level in solvent.

	Spin density						Charge					
	Ni	L	F ₁	F ₂	P	Sub-P	Ni	L	F ₁	F ₂	P	Sub-P
$^1\text{IM}'_{\text{PF}}$	0.00	0.00	0.00	0.00	0.00	0.00	-0.24	1.68	-0.67	0.16	0.16	-1.10
$^3\text{IM}'_{\text{PF}}$	0.00	1.88	0.00	0.00	0.00	0.11	-0.27	1.78	-0.68	0.16	0.16	-1.15
$^1\text{TS2}_{\text{PF}}$	0.00	0.00	0.00	0.00	0.00	0.00	-0.35	1.29	-0.64	0.17	0.14	-0.61
$^3\text{TS2}_{\text{PF}}$	0.00	1.98	0.00	0.00	0.00	0.02	-0.31	1.72	-0.65	0.17	0.14	-1.08
$^1\text{IM2}_{\text{PF}}$	0.00	0.00	0.00	0.00	0.00	0.00	-0.43	1.33	-0.69	0.17	0.14	-0.53
$^3\text{IM2}_{\text{PF}}$	0.00	2.01	0.00	0.00	0.00	-0.01	-0.44	1.42	-0.65	0.17	0.14	-0.64

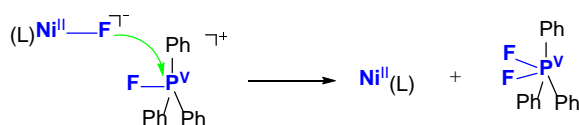


Table S29. Various SCF and free energies of the reaction intermediates in the second fluorination to form a *cis*-F₂PPh₃ product on the singlet/triplet spin states. Calculations were done at the UB3LYP/B2 level in solvent.

	OPT/B2	ΔE	OPT +ZPE	ΔE	G	ΔG
$^1\text{IM}'_{\text{PF-cis}}$	-3948.452957 ^a	0.0	-3947.781379	0.0	-3947.844051	0.0
$^3\text{IM}'_{\text{PF-cis}}$	-3948.441404	7.2	-3947.771249	6.4	-3947.834924	5.7
$^1\text{TS2}_{\text{PF-cis}}$	-3948.408485	27.9	-3947.736459	28.2	-3947.794563	31.1
$^3\text{TS2}_{\text{PF-cis}}$	-3948.414866	23.9	-3947.743406	23.8	-3947.802043	26.4
$^1\text{IM2}_{\text{PF-cis}}$	-3948.412291	25.5	-3947.741030	25.3	-3947.802149	26.3
$^3\text{IM2}_{\text{PF-cis}}$	-3948.417002	22.6	-3947.746414	21.9	-3947.809381	21.8

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

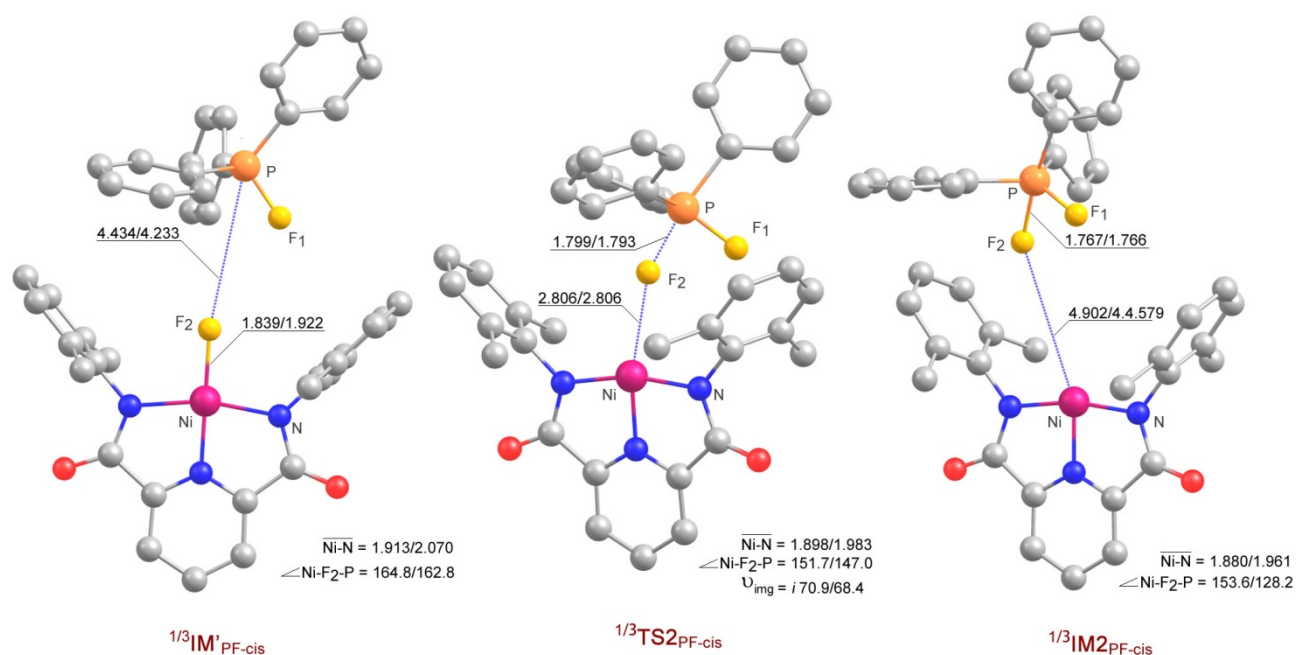


Fig. S29 The optimized structures of the reaction intermediates in the second fluorination to form a *cis*-F₂PPh₃ product on the singlet/triplet spin states. Calculations were done at the UB3LYP/B2 level in solvent. Lengths are in Å units, bond angles are in degree units and imaginary frequencies are in cm⁻¹ units. Hydrogen atoms of the ligand are omitted for clarity.

Table S30. Mulliken charges and spin densities of the reaction intermediates in the second fluorination to form a *cis*-F₂PPh₃ product on the singlet/triplet spin states. Calculations were done at the UB3LYP/B2 level in solvent.

	Spin density						Charge					
	Ni	L	F ₁	F ₂	P	Sub-P	Ni	L	F ₁	F ₂	P	Sub-P
¹ IM'PF-cis	0.00	0.00	0.00	0.00	0.00	0.00	0.53	-1.02	-0.44	-0.18	-0.25	1.36
³ IM'PF-cis	1.80	0.17	0.04	0.00	0.00	0.00	1.18	-1.51	-0.59	-0.20	-0.06	1.18
¹ TS2PF-cis	0.00	0.00	0.00	0.00	0.00	0.00	0.65	-0.58	-0.40	-0.26	-0.21	0.81
³ TS2PF-cis	1.58	0.41	0.00	0.00	0.02	0.00	1.07	-1.02	-0.44	-0.25	-0.09	0.73
¹ IM2PF-cis	0.00	0.00	0.00	0.00	0.00	0.00	0.55	-0.53	-0.44	-0.30	0.09	0.63
³ IM2PF-cis	1.55	0.44	0.00	0.00	0.00	0.00	1.03	-1.01	-0.41	-0.27	-0.09	0.75

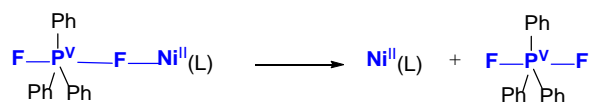


Table S31. Various SCF and free energies of the reaction intermediates of F₂PPh₃ desorption from the nickel complex. Calculations were done at the UB3LYP/B2 level in solvent.

	OPT/B2	ΔE	OPT +ZPE	ΔE	G	ΔG
³ IM ₂ PF	-3948.436457 ^a	0.0	-3947.764098	0.0	-3947.820959	0.0
¹ IM ₂ PF	-3948.432154	2.7	-3947.758934	3.2	-3947.814023	4.4
¹ TS ₃ PF	-3948.429478	4.4	-3947.756287	4.9	-3947.811647	5.8
¹ PC _{PF}	-3948.442998	-4.1	-3947.771100	-4.4	-3947.835482	-9.1
³ PC _{PF}	-3948.447580	-7.0	-3947.776769	-8.0	-3947.842573	-13.6

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

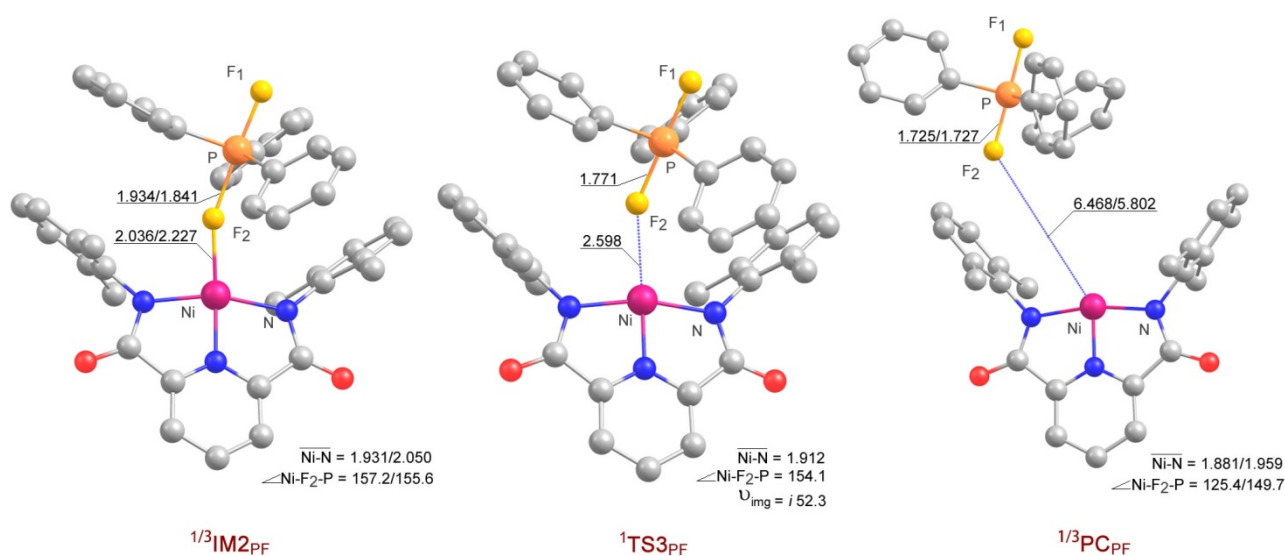


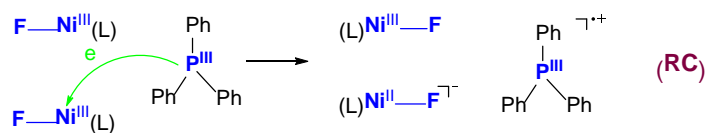
Fig. S30 The optimized structures of the reaction intermediates of F₂PPh₃ desorption from the nickel complex. Calculations were done at the UB3LYP/B2 level in solvent. Lengths are in Å units, bond angles are in degree units and imaginary frequencies are in cm⁻¹ units. Hydrogen atoms of the ligand are omitted for clarity.

Table S32. Mulliken charges and spin densities of the reaction intermediates of F₂PPh₃ desorption from the nickel complex. Calculations were done at the UB3LYP/B2 level in solvent.

	Spin density						Charge					
	Ni	L	F1	F2	P	Sub-P	Ni	L	F1	F2	P	Sub-P
¹ IM _{2PF}	0.00	0.00	0.00	0.00	0.00	0.00	-0.43	1.33	⁻ 0.69	0.17	0.14	-0.53
³ IM _{2PF}	0.00	2.01	0.00	0.00	0.00	-0.01	-0.44	1.42	⁻ 0.65	0.17	0.14	-0.64
¹ TS _{3PF}	0.00	0.00	0.00	0.00	0.00	0.00	-0.46	1.43	⁻ 0.60	0.18	0.15	-0.69
¹ PC _{PF}	0.00	0.00	0.00	0.00	0.00	0.00	-0.48	1.56	⁻ 0.57	0.17	0.16	-0.84
³ PC _{PF}	0.00	1.87	0.02	0.00	0.00	0.11	-0.47	1.89	⁻ 0.72	0.16	0.16	-1.02

Part VIII: Difluorination of PPh₃ by the cooperation of two 1_FS

Table S33. Energy comparison of the complex of 2 Ni(III)-F oxidants plus PPh₃ and the reagent complex (RC) with one 1_F, one Ni(II)-F complex and an 1e-oxidized species (PPh₃)^{•+}. Calculations were done at the UB3LYP/B2//B1 level in solvent.



2(L)Ni ^{III} F + P ^{III} Ph ₃	RC	ΔE ^a
-6660.728374	-6660.742755	-9.0

a. ΔE = E(RC) - [E(2Ni^{III}F(L)) + E(PPh₃)]. Absolute energies are in au units and the relative ones are in kcal mol⁻¹ units.

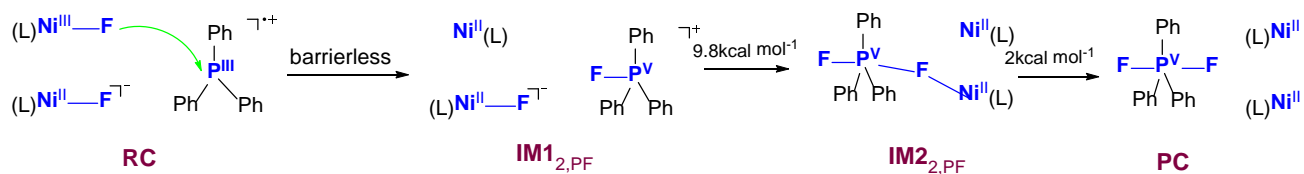


Table S34. Various SCF and free energies of the reaction intermediates of difluorination of PPh₃ by the cooperation of two 1_Fs. Calculations were done at the UB3LYP/B2//B1 level in solvent.

	OPT/B1	ΔE	OPT +ZPE	ΔE	SPE/B2	ΔE	SPE+ZPE	ΔE	G	ΔG
³ RC _{2,PF}	-6660.609047 ^a	0.0	-6659.541893	0.0	-6660.742755	0.0	-6659.675601	0.0	-6659.624998	0.0
¹ RC _{2,PF}	-6660.609046	0.0	-6659.541890	0.0	-6660.742729	0.0	-6659.675573	0.0	-6659.624168	0.5
³ TS _{2,PF}	-6660.603157	3.7	-6659.537026	3.1	-6660.735888	4.3	-6659.669757	3.7	-6659.618724	3.9
¹ IM1 _{2,PF}	-6660.661345	-32.8	-6659.592741	-31.9	-6660.797042	-34.1	-6659.728438	-33.2	-6659.676303	-32.2
³ IM1 _{2,PF}	-6660.666293	-35.9	-6659.598513	-35.5	-6660.801494	-36.9	-6659.733714	-36.5	-6659.683296	-36.6
¹ IM1' _{2,PF}	-6660.661601	-33.0	-6659.592917	-32.0	-6660.795612	-33.2	-6659.726928	-32.2	-6659.676885	-32.6
³ IM1' _{2,PF}	-6660.666141	-35.8	-6659.598289	-35.4	-6660.799970	-35.9	-6659.732118	-35.5	-6659.682313	-36.0
¹ TS2 _{2,PF}	-6660.650274	-25.9	-6659.581318	-24.7	-6660.780547	-23.7	-6659.711592	-22.6	-6659.662316	-23.4
³ TS2 _{2,PF}	-6660.654229	-28.4	-6659.586427	-27.9	-6660.784378	-26.1	-6659.716576	-25.7	-6659.668597	-27.4
¹ IM2 _{2,PF}	-6660.653418	-27.8	-6659.584140	-26.5	-6660.781587	-24.4	-6659.712308	-23.0	-6659.664908	-25.0
³ IM2 _{2,PF}	-6660.658045	-30.7	-6659.590080	-30.2	-6660.786337	-27.3	-6659.718372	-26.8	-6659.673293	-30.3
¹ TS3 _{2,PF}	-6660.647967	-24.4	-6659.579110	-23.4	-6660.778900	-22.7	-6659.710042	-21.6	-6659.661512	-22.9
³ TS3 _{2,PF}	-6660.6525761	-27.3	-6659.584481	-26.7	-6660.783183	-25.4	-6659.715088	-24.8	-6659.667299	-26.5
¹ PC _{2,PF}	-6660.656243	-29.6	-6659.586757	-28.2	-6660.789835	-29.5	-6659.720349	-28.1	-6659.672506	-29.8
³ PC _{2,PF}	-6660.664449	-34.8	-6659.596024	-34.0	-6660.797866	-34.6	-6659.729441	-33.8	-6659.683202	-36.5

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

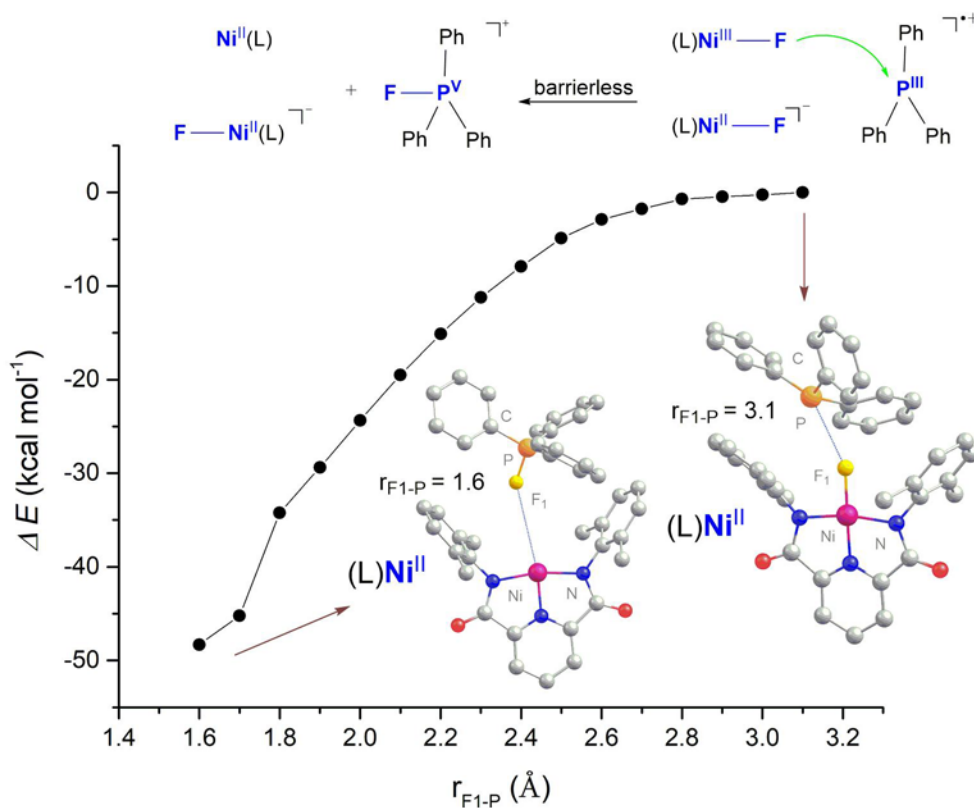


Fig. S31 The energy plot of the relaxed scan alongside of the F-P distance on the singlet spin state for the first F-atom transfer from the Ni(III)-F dimer to PPh₃. Lengths are in \AA units. Energies are in kcal mol^{-1} . Calculations were done at the UB3LYP/B1 level in solvent.

Table S35. Mulliken spin densities and charges of the reaction intermediates of difluorination of PPh₃ by the cooperation of two **1**F_s. Calculations were done at the UB3LYP/B1 level in solvent.

	Spin density								Charge							
	Ni ₁	L ₁	F ₁	Ni ₂	L ₂	F ₂	P	Sub-P	Ni ₁	L ₁	F ₁	Ni ₂	L ₂	F ₂	P	Sub-P
¹ RC _{2,PF}	0.01	0.18	0.00	-0.69	-0.32	0.01	0.50	0.31	0.60	-0.86	-0.50	0.86	-0.34	-0.46	0.53	0.18
³ RC _{2,PF}	0.01	0.18	0.00	0.69	0.32	-0.01	0.51	0.31	0.60	-0.86	-0.50	0.86	-0.34	-0.47	0.53	0.18
³ TS _{2,PF}	1.02	0.21	0.01	0.00	0.00	0.00	0.54	0.23	0.86	-0.35	-0.40	0.58	-1.02	-0.49	0.63	0.19
¹ IM1 _{2,PF}	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.74	-0.72	-0.31	0.58	-1.02	-0.49	0.93	0.30
³ IM1 _{2,PF}	1.64	0.36	0.00	0.00	0.00	0.00	0.00	0.00	0.86	-0.84	-0.31	0.58	-1.02	-0.49	0.93	0.30
¹ IM1' _{2,PF}	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.74	-0.78	-0.31	0.59	-0.95	-0.49	0.93	0.27
³ IM1' _{2,PF}	1.64	0.36	0.00	0.00	0.00	0.00	0.00	0.00	0.87	-0.90	-0.31	0.59	-0.95	-0.49	0.93	0.27
¹ TS2 _{2,PF}	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.74	-0.79	-0.35	0.61	-0.88	-0.48	0.96	0.19
³ TS2 _{2,PF}	1.64	0.36	0.00	0.00	0.00	0.00	0.00	0.00	0.87	-0.91	-0.35	0.61	-0.89	-0.48	0.96	0.19
¹ IM2 _{2,PF}	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.74	-0.78	-0.41	0.63	-0.80	-0.47	1.06	0.01
³ IM2 _{2,PF}	1.64	0.36	0.00	-0.01	0.01	0.00	0.00	0.00	0.87	-0.90	-0.41	0.65	-0.81	-0.47	1.06	0.01
¹ TS3 _{2,PF}	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.74	-0.78	-0.44	0.70	-0.75	-0.45	1.08	-0.10
³ TS3 _{2,PF}	1.64	0.36	0.00	0.00	0.00	0.00	0.00	0.00	0.87	-0.90	-0.44	0.69	-0.75	-0.45	1.08	-0.10
¹ PC _{2,PF}	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.74	-0.78	-0.45	0.74	-0.72	-0.45	1.07	-0.15
³ PC _{2,PF}	-0.01	0.01	0.00	1.64	0.35	0.00	0.00	0.00	0.81	-0.85	-0.45	0.86	-0.85	-0.45	1.06	-0.14

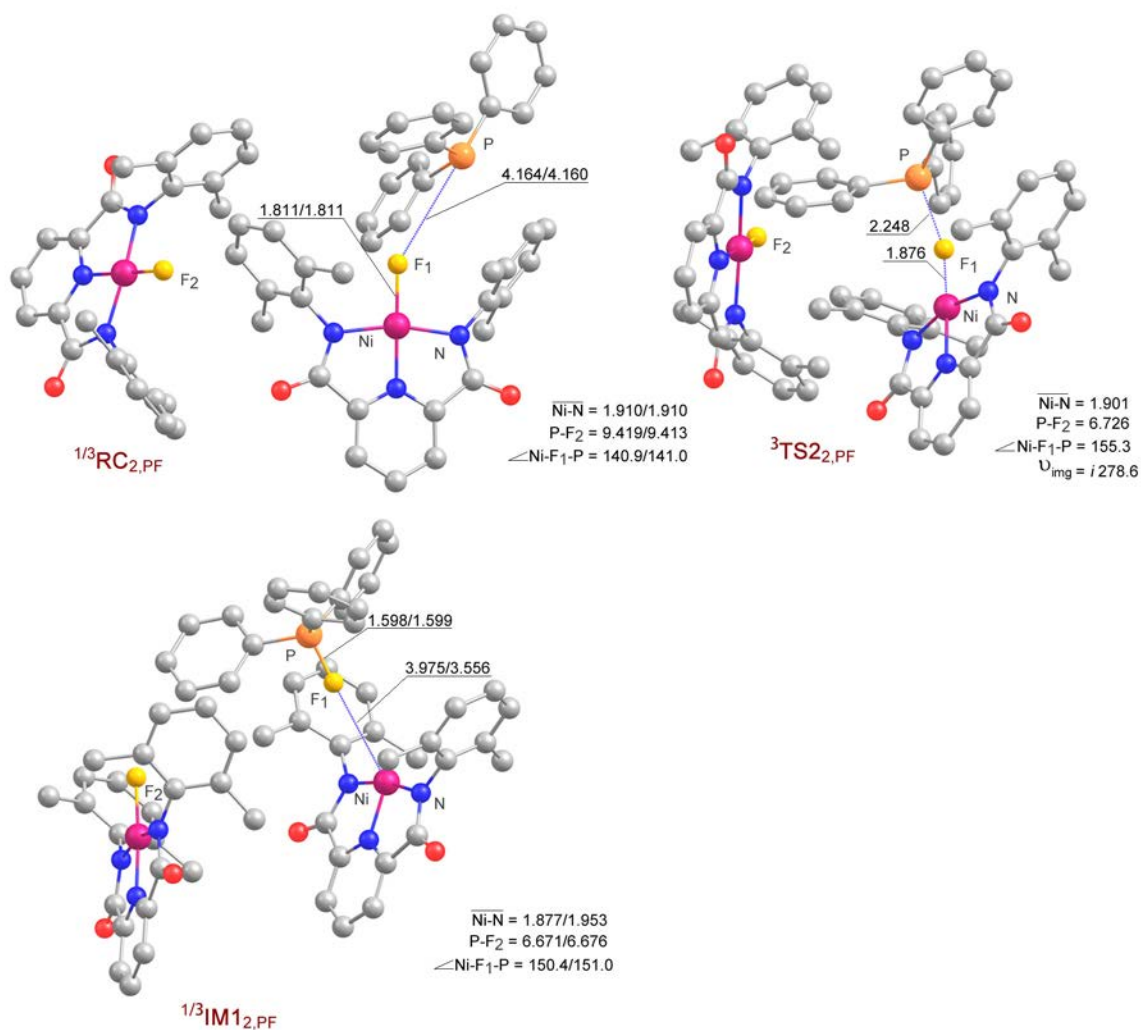


Fig. S32 Optimized structures of the reaction intermediates of difluorination of PPh₃ by the cooperation of two **1**F_s on the singlet/triplet spin states. Calculations were done at the UB3LYP/B1 level in solvent. Lengths are in Å units, bond angles are in degree units and imaginary frequencies are in cm⁻¹ units. Hydrogen atoms of the ligand are omitted for clarity. (To be continued.)

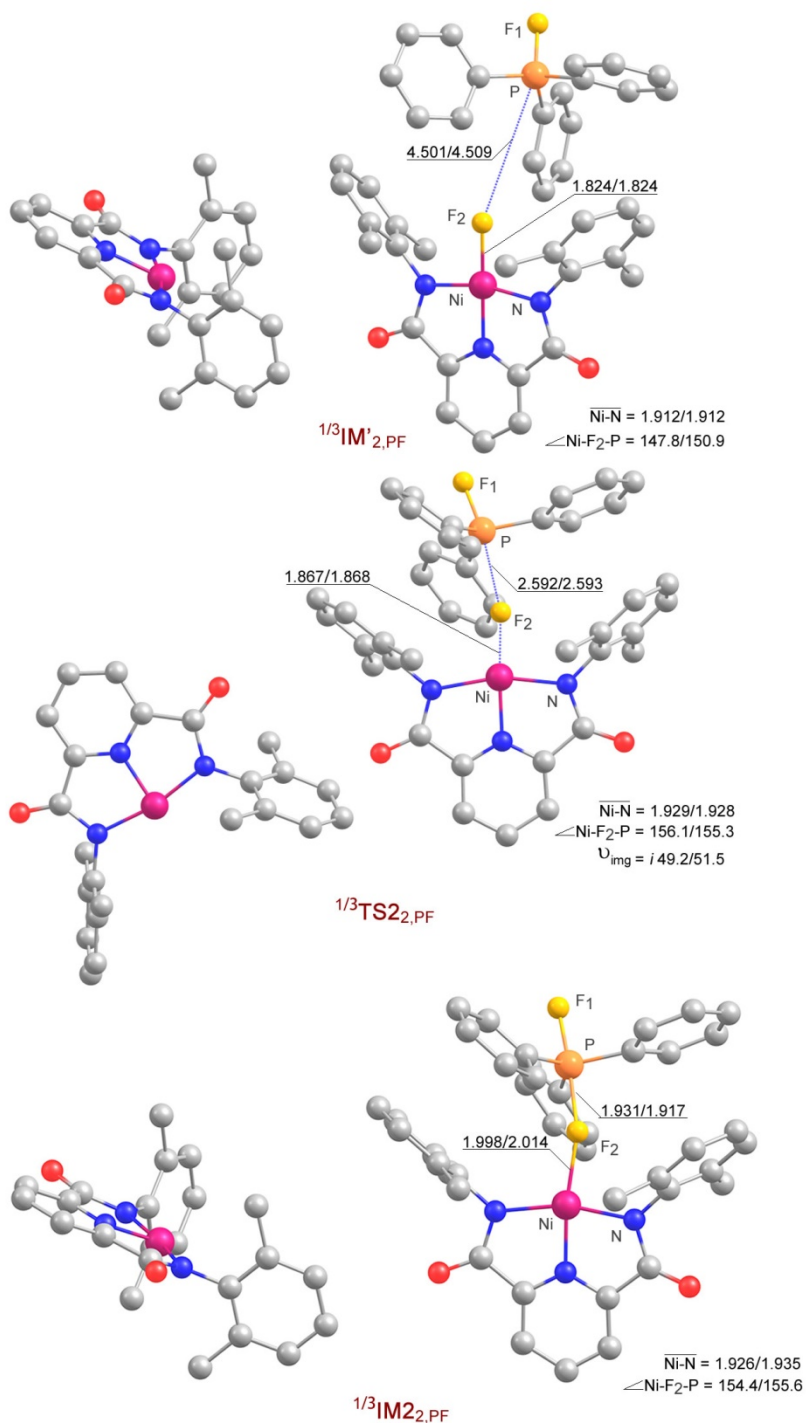


Fig. S33 Optimized structures of the reaction intermediates of difluorination of PPh_3 by the cooperation of two $\mathbf{1}_{\text{FS}}$ on the singlet/triplet spin states. Calculations were done at the UB3LYP/B2//B1 level in solvent. Lengths are in Å units, bond angles are in degree units and imaginary frequencies are in cm^{-1} units. Hydrogen atoms of the ligand are omitted for clarity. (To be continued.)

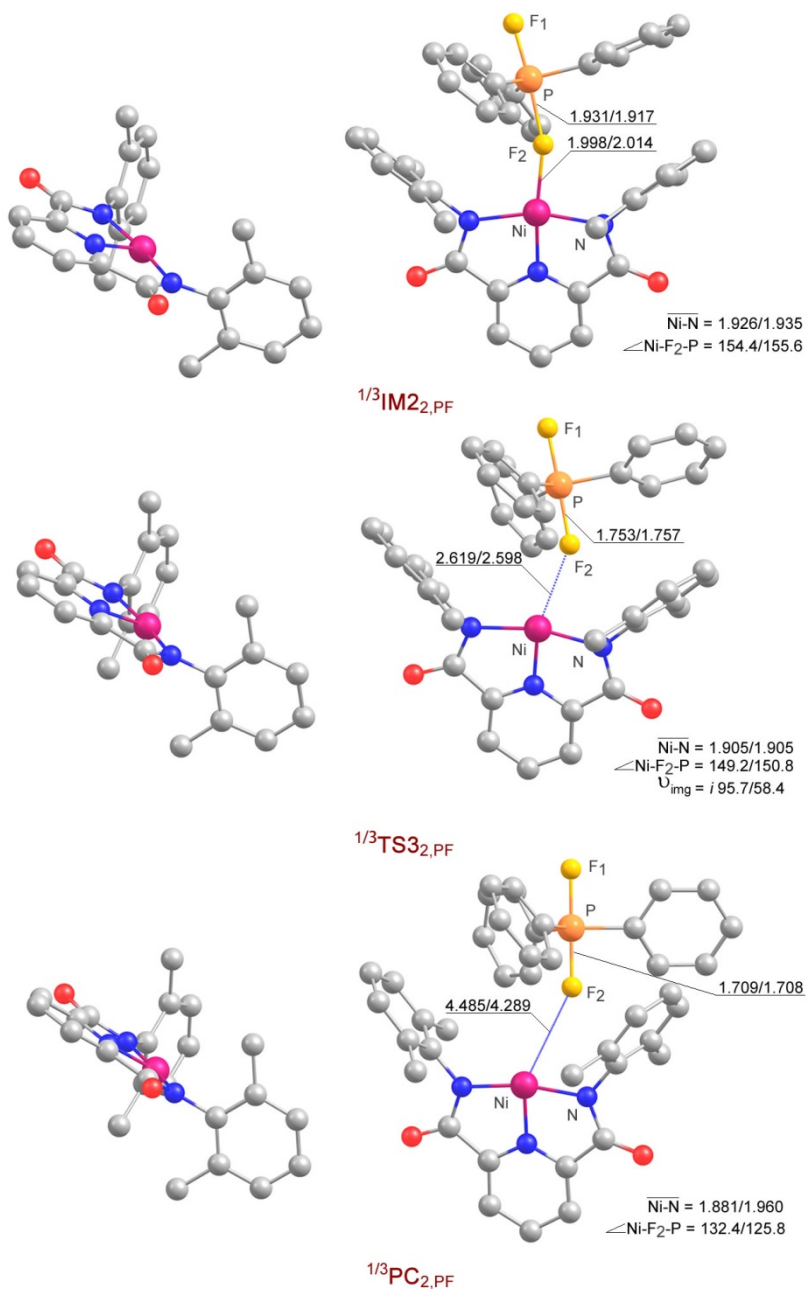


Fig. S34 Optimized structures of the reaction intermediates of difluorination of PPh_3 by the cooperation of two $\mathbf{1}_{\text{FS}}$. Calculations were done at the UB3LYP/B2//B1 level in solvent. Lengths are in Å units, bond angles are in degree units and imaginary frequencies are in cm^{-1} units. Hydrogen atoms of the ligand are omitted for clarity.

PART IX. Cartesian coordinates

D) The Calculated data on the oxidants **1_F** and **1_{Cl}**

²**1_F**

Ni	0.084108000	0.034799000	0.027763000	H	-2.369711000	2.345164000	-4.649417000
N	0.093744000	-0.009572000	1.910516000	C	-2.391934000	0.202867000	-4.889500000
N	1.925763000	0.126958000	0.223231000	H	-3.136130000	0.221138000	-5.680749000
N	0.480564000	0.133239000	-1.810046000	C	-1.868454000	-1.015457000	-4.450828000
C	-1.064921000	-0.101737000	2.736080000	H	-2.205671000	-1.944695000	-4.902439000
C	-1.569049000	-1.376439000	3.070394000	C	-0.909895000	-1.062201000	-3.430036000
C	-0.892837000	-2.633904000	2.579832000	C	-0.346344000	-2.381030000	-2.958754000
H	0.134395000	-2.711204000	2.954368000	H	0.734162000	-2.441457000	-3.133009000
H	-1.439231000	-3.520241000	2.912352000	H	-0.818825000	-3.213035000	-3.487239000
H	-0.836972000	-2.656693000	1.485869000	H	-0.505453000	-2.523012000	-1.884197000
C	-2.715859000	-1.444932000	3.872133000	F	-1.712915000	-0.082862000	-0.163156000
H	-3.116308000	-2.419103000	4.140221000	⁴ 1_F			
C	-3.345783000	-0.283504000	4.325043000	Ni	-0.247782000	0.409313000	0.125936000
H	-4.235265000	-0.354429000	4.944724000	N	-0.014653000	0.060933000	2.113177000
C	-2.834042000	0.969010000	3.978442000	N	1.740135000	0.067711000	0.170632000
H	-3.326304000	1.872115000	4.329499000	N	0.480071000	0.505193000	-2.151602000
C	-1.689402000	1.083114000	3.178583000	C	-1.077811000	0.060369000	3.058177000
C	-1.139910000	2.438021000	2.802540000	C	-1.723790000	-1.152987000	3.381949000
H	-1.083540000	2.558209000	1.714927000	C	-1.265328000	-2.455413000	2.769885000
H	-0.126160000	2.583509000	3.193213000	H	-0.230688000	-2.686932000	3.047239000
H	-1.771743000	3.235261000	3.202422000	H	-1.897976000	-3.283830000	3.100423000
C	1.337997000	0.028399000	2.501450000	H	-1.298474000	-2.415025000	1.674924000
O	1.582123000	-0.000889000	3.707553000	C	-2.801148000	-1.124185000	4.278415000
C	2.423325000	0.111798000	1.460422000	H	-3.302711000	-2.054682000	4.533032000
C	3.801787000	0.168316000	1.645484000	C	-3.235902000	0.077801000	4.842203000
H	4.214907000	0.155868000	2.647328000	H	-4.073244000	0.084501000	5.534538000
C	4.616589000	0.239642000	0.507485000	C	-2.590980000	1.271397000	4.509279000
H	5.694422000	0.284021000	0.621238000	H	-2.927581000	2.208872000	4.945221000
C	4.053996000	0.255577000	-0.775947000	C	-1.509666000	1.283048000	3.616996000
H	4.664506000	0.312041000	-1.669587000	C	-0.819560000	2.578511000	3.260074000
C	2.667370000	0.196721000	-0.882825000	H	-0.864079000	2.772060000	2.181892000
C	1.819735000	0.205492000	-2.127724000	H	0.241526000	2.557951000	3.533280000
O	2.306893000	0.272450000	-3.256114000	H	-1.286297000	3.421796000	3.776674000
C	-0.484209000	0.155734000	-2.859746000	C	1.237057000	-0.174625000	2.526927000
C	-1.003405000	1.396671000	-3.285869000	O	1.641656000	-0.397179000	3.689779000
C	-0.540652000	2.690195000	-2.659603000	C	2.244516000	-0.155955000	1.392353000
H	-0.711564000	2.694791000	-1.577374000	C	3.613479000	-0.358275000	1.574371000
H	-1.073389000	3.540598000	-3.092880000	H	3.993815000	-0.538388000	2.572500000
H	0.532542000	2.850920000	-2.814181000	C	4.450962000	-0.318781000	0.457105000
C	-1.960536000	1.397638000	-4.308872000	H	5.519364000	-0.470777000	0.570008000

C	3.907219000	-0.085115000	-0.808735000	H	-0.092070000	3.089840000	4.336121000
H	4.521362000	-0.050907000	-1.700284000	C	1.293282000	-0.283050000	2.534220000
C	2.528795000	0.104912000	-0.911446000	O	1.620623000	-0.582725000	3.710616000
C	1.844261000	0.334672000	-2.228864000	C	2.201837000	-0.056256000	1.450118000
O	2.502107000	0.462839000	-3.265910000	C	3.607065000	-0.019793000	1.592096000
C	-0.359399000	0.253609000	-3.181231000	H	4.032033000	-0.179042000	2.577802000
C	-1.423215000	1.213810000	-3.422950000	C	4.412518000	0.223940000	0.493915000
C	-1.510918000	2.474004000	-2.612285000	H	5.491769000	0.260301000	0.596935000
H	-1.784198000	2.233771000	-1.578553000	C	3.806718000	0.424408000	-0.781062000
H	-2.266588000	3.143175000	-3.030375000	H	4.398787000	0.611995000	-1.669146000
H	-0.551397000	3.000095000	-2.588176000	C	2.431943000	0.361235000	-0.880743000
C	-2.308825000	0.977399000	-4.464808000	C	1.726918000	0.510444000	-2.179851000
H	-3.084375000	1.706000000	-4.679262000	O	2.298780000	0.858932000	-3.220315000
C	-2.209422000	-0.180535000	-5.248427000	C	-0.398246000	0.032393000	-3.197632000
H	-2.921433000	-0.351981000	-6.049904000	C	-1.638256000	0.760036000	-3.396925000
C	-1.202201000	-1.129715000	-5.000420000	C	-2.015093000	1.895102000	-2.487993000
H	-1.166551000	-2.034878000	-5.598951000	H	-2.225970000	1.513532000	-1.483072000
C	-0.265314000	-0.946902000	-3.995251000	H	-2.904341000	2.405044000	-2.866617000
C	0.750887000	-2.024810000	-3.722171000	H	-1.203682000	2.625632000	-2.405765000
H	1.731577000	-1.758103000	-4.128083000	C	-2.420906000	0.452489000	-4.501871000
H	0.434947000	-2.962502000	-4.184647000	H	-3.328542000	1.019751000	-4.684386000
H	0.878670000	-2.202519000	-2.649806000	C	-2.050198000	-0.566256000	-5.389717000
F	-2.098387000	0.635135000	-0.111826000	H	-2.685419000	-0.801402000	-6.238494000
⁶ I _F				C	-0.866626000	-1.294399000	-5.185461000
Ni	-0.307914000	-0.049442000	0.012732000	H	-0.618624000	-2.106383000	-5.862693000
N	-0.091709000	-0.285873000	2.150491000	C	-0.016594000	-1.017754000	-4.124163000
N	1.631173000	0.130628000	0.198440000	C	1.195446000	-1.887862000	-3.906004000
N	0.341336000	0.341721000	-2.102450000	H	2.105576000	-1.398056000	-4.264911000
C	-1.049519000	0.016901000	3.073759000	H	1.079538000	-2.830455000	-4.446205000
C	-2.226548000	-0.820530000	3.123041000	H	1.345862000	-2.120369000	-2.847359000
C	-2.326070000	-2.056590000	2.271507000	F	-2.156145000	-0.283910000	-0.272514000
H	-1.477760000	-2.726986000	2.448567000	² I _{Cl}			
H	-3.246478000	-2.600628000	2.499724000	Ni	0.007687000	0.029858000	0.018184000
H	-2.324755000	-1.788171000	1.210003000	N	0.036717000	-0.022425000	1.917572000
C	-3.220009000	-0.525934000	4.051520000	N	1.867922000	0.109070000	0.214630000
H	-4.087611000	-1.175658000	4.121128000	N	0.425524000	0.134116000	-1.832212000
C	-3.110580000	0.578544000	4.904397000	C	-1.081715000	-0.102062000	2.803944000
H	-3.904150000	0.798279000	5.612484000	C	-1.553351000	-1.370357000	3.201622000
C	-1.983152000	1.409786000	4.840583000	C	-0.902240000	-2.635961000	2.699374000
H	-1.931393000	2.287661000	5.478486000	H	0.148497000	-2.697200000	3.004530000
C	-0.936887000	1.154682000	3.960754000	H	-1.417959000	-3.516280000	3.091355000
C	0.198990000	2.146169000	3.867829000	H	-0.922023000	-2.685799000	1.605114000
H	0.471208000	2.354624000	2.828657000	C	-2.647733000	-1.425278000	4.074565000
H	1.096357000	1.777333000	4.372445000	H	-3.023571000	-2.394651000	4.390979000

C	-3.256452000	-0.256454000	4.537763000	C	-1.115385000	0.004360000	3.033811000
H	-4.105249000	-0.316804000	5.212989000	C	-1.687465000	-1.177320000	3.552216000
C	-2.775016000	0.989768000	4.129957000	C	-1.162794000	-2.532922000	3.144504000
H	-3.249630000	1.898824000	4.489603000	H	-0.118205000	-2.666363000	3.447797000
C	-1.683042000	1.089799000	3.257845000	H	-1.752828000	-3.330988000	3.603469000
C	-1.168378000	2.438075000	2.815917000	H	-1.198617000	-2.661201000	2.056637000
H	-1.194073000	2.535108000	1.724934000	C	-2.758834000	-1.065258000	4.449150000
H	-0.129283000	2.594338000	3.127212000	H	-3.206246000	-1.969932000	4.853503000
H	-1.772815000	3.241021000	3.245508000	C	-3.256441000	0.185040000	4.824370000
C	1.292263000	0.009259000	2.491411000	H	-4.088678000	0.254826000	5.519397000
O	1.546630000	-0.018759000	3.695622000	C	-2.681170000	1.344948000	4.300673000
C	2.369052000	0.088153000	1.448504000	H	-3.066162000	2.319672000	4.590157000
C	3.747636000	0.137985000	1.635087000	C	-1.607569000	1.275065000	3.401756000
H	4.158334000	0.121190000	2.637801000	C	-0.991717000	2.534163000	2.839142000
C	4.563565000	0.209059000	0.498472000	H	-1.060892000	2.559513000	1.745243000
H	5.641525000	0.248456000	0.611881000	H	0.072804000	2.608960000	3.088866000
C	3.998849000	0.231034000	-0.783441000	H	-1.495332000	3.421222000	3.233121000
H	4.606811000	0.286919000	-1.678776000	C	1.212642000	-0.212644000	2.537837000
C	2.611695000	0.178640000	-0.888001000	O	1.593313000	-0.310859000	3.718682000
C	1.772200000	0.194275000	-2.132361000	C	2.236611000	-0.225880000	1.422578000
O	2.268404000	0.267191000	-3.256656000	C	3.611542000	-0.325301000	1.635344000
C	-0.488767000	0.161834000	-2.930524000	H	3.986892000	-0.434550000	2.645706000
C	-0.993866000	1.403436000	-3.368954000	C	4.463082000	-0.272855000	0.528878000
C	-0.589237000	2.690816000	-2.692944000	H	5.536958000	-0.351800000	0.662316000
H	-0.855978000	2.682082000	-1.630236000	C	3.926840000	-0.101897000	-0.749811000
H	-1.083996000	3.544751000	-3.162650000	H	4.553236000	-0.034936000	-1.631020000
H	0.492866000	2.853840000	-2.750236000	C	2.540577000	-0.007755000	-0.880614000
C	-1.885433000	1.410929000	-4.449637000	C	1.866964000	0.218835000	-2.204240000
H	-2.283202000	2.359441000	-4.800520000	O	2.534396000	0.335878000	-3.236789000
C	-2.265148000	0.221263000	-5.075402000	C	-0.329114000	0.285360000	-3.171827000
H	-2.958645000	0.244245000	-5.911205000	C	-1.335998000	1.318018000	-3.356505000
C	-1.754500000	-0.998217000	-4.624379000	C	-1.348797000	2.533412000	-2.474335000
H	-2.050984000	-1.923622000	-5.110905000	H	-1.586039000	2.267822000	-1.439570000
C	-0.860499000	-1.050696000	-3.546949000	H	-2.095879000	3.249279000	-2.824332000
C	-0.314299000	-2.370801000	-3.060234000	H	-0.370651000	3.024965000	-2.464088000
H	0.775556000	-2.418226000	-3.165293000	C	-2.219516000	1.203159000	-4.417959000
H	-0.743183000	-3.198979000	-3.630146000	H	-2.949690000	1.987049000	-4.592801000
H	-0.541895000	-2.529074000	-2.000371000	C	-2.176586000	0.092277000	-5.274538000
Cl	-2.182512000	-0.106026000	-0.214376000	H	-2.887843000	0.014239000	-6.091102000
⁴¹ Ca				C	-1.229630000	-0.929097000	-5.080448000
Ni	-0.273464000	-0.073106000	0.111332000	H	-1.241274000	-1.794995000	-5.735344000
N	-0.054075000	-0.076574000	2.085325000	C	-0.295507000	-0.866385000	-4.058686000
N	1.737192000	-0.089586000	0.186828000	C	0.650664000	-2.017201000	-3.841225000
N	0.510072000	0.429792000	-2.122892000	H	1.653403000	-1.780578000	-4.209994000

H	0.291879000	-2.902209000	-4.371369000	C	3.586573000	-0.035511000	1.649278000
H	0.744311000	-2.270929000	-2.780624000	H	3.995274000	-0.089949000	2.651566000
Cl	-2.483915000	-0.414025000	-0.322558000	C	4.422984000	0.166919000	0.512892000
⁶¹ Cl				H	5.497597000	0.249720000	0.632586000
Ni	-0.286002000	-0.238440000	-0.061671000	C	3.838743000	0.283338000	-0.739115000
N	-0.051892000	-0.388004000	2.245028000	H	4.436828000	0.468294000	-1.625309000
N	1.644094000	-0.078598000	0.229430000	C	2.443806000	0.167551000	-0.883866000
N	0.334332000	0.206062000	-2.038087000	C	1.761531000	0.333065000	-2.137566000
C	-1.052206000	-0.040131000	3.099254000	O	2.302417000	0.687233000	-3.210659000
C	-2.127424000	-0.986396000	3.304714000	C	-0.409229000	0.070371000	-3.175339000
C	-1.997644000	-2.394402000	2.798325000	C	-1.578482000	0.905964000	-3.321739000
H	-1.210812000	-2.922728000	3.351370000	C	-1.913825000	1.966113000	-2.305340000
H	-2.933890000	-2.940701000	2.936560000	H	-2.277203000	1.515228000	-1.376202000
H	-1.724652000	-2.417248000	1.741629000	H	-2.699277000	2.621999000	-2.689010000
C	-3.201271000	-0.615050000	4.105064000	H	-1.042219000	2.578553000	-2.056564000
H	-3.998312000	-1.328823000	4.290116000	C	-2.338052000	0.793406000	-4.480608000
C	-3.253273000	0.653332000	4.696067000	H	-3.189111000	1.453141000	-4.621359000
H	-4.107036000	0.930376000	5.307099000	C	-2.016539000	-0.143684000	-5.470626000
C	-2.205215000	1.570570000	4.510698000	H	-2.634486000	-0.226230000	-6.359664000
H	-2.274690000	2.555919000	4.961922000	C	-0.907682000	-0.985601000	-5.311044000
C	-1.090181000	1.254529000	3.746536000	H	-0.698697000	-1.740948000	-6.063197000
C	-0.019577000	2.291204000	3.519571000	C	-0.079023000	-0.897171000	-4.197533000
H	0.260018000	2.360918000	2.463507000	C	1.035051000	-1.904345000	-4.034160000
H	0.887917000	2.054773000	4.083592000	H	1.994845000	-1.491751000	-4.356896000
H	-0.372336000	3.273506000	3.841823000	H	0.824648000	-2.791241000	-4.637301000
C	1.289057000	-0.274565000	2.608597000	H	1.148453000	-2.221594000	-2.993789000
O	1.663687000	-0.380425000	3.785588000	Cl	-2.305921000	-1.168200000	-0.509200000
C	2.225366000	-0.143240000	1.469002000				

II) C-H bond activation of CHD by the oxidants **1_F** and **1_{Cl}**

² RC _F				H	-3.071189000	-2.021360000	4.248418000
Ni	0.300899000	0.043062000	0.072087000	C	-2.919940000	0.109284000	4.539507000
N	0.394720000	-0.077549000	1.947906000	H	-3.777443000	0.157904000	5.204765000
N	2.143944000	-0.138349000	0.170682000	C	-2.216940000	1.273177000	4.220107000
N	0.618927000	0.161735000	-1.780646000	H	-2.528709000	2.227010000	4.637513000
C	-0.721561000	-0.015141000	2.832761000	C	-1.109872000	1.233497000	3.362404000
C	-1.421349000	-1.201448000	3.138753000	C	-0.354183000	2.493850000	3.016726000
C	-0.995843000	-2.528118000	2.557575000	H	-0.324888000	2.658012000	1.933845000
H	0.022255000	-2.794312000	2.864153000	H	0.685242000	2.447107000	3.361566000
H	-1.665981000	-3.326171000	2.887439000	H	-0.823194000	3.364581000	3.482034000
H	-1.004140000	-2.504945000	1.462254000	C	1.658486000	-0.243773000	2.472423000
C	-2.522485000	-1.116490000	4.000814000	O	1.954013000	-0.355982000	3.661945000

C	2.692860000	-0.276164000	1.378104000	N	-0.045003000	0.078647000	1.992967000
C	4.072553000	-0.422125000	1.491392000	N	1.795495000	-0.063131000	0.209001000
H	4.527240000	-0.534760000	2.468715000	N	0.437469000	0.380303000	-1.920137000
C	4.833608000	-0.417482000	0.314665000	C	-1.138912000	0.177966000	2.896230000
H	5.911002000	-0.529882000	0.372189000	C	-1.912679000	-0.970281000	3.179023000
C	4.218346000	-0.267486000	-0.935485000	C	-1.569753000	-2.301466000	2.554184000
H	4.787584000	-0.258710000	-1.857677000	H	-0.569392000	-2.638024000	2.849750000
C	2.833955000	-0.126535000	-0.970351000	H	-2.288088000	-3.068423000	2.856621000
C	1.937552000	0.055343000	-2.167015000	H	-1.571419000	-2.240946000	1.459767000
O	2.374646000	0.098554000	-3.316903000	C	-2.998232000	-0.850371000	4.056741000
C	-0.380658000	0.371654000	-2.775604000	H	-3.594841000	-1.730470000	4.283931000
C	-0.703881000	1.691726000	-3.155038000	C	-3.318959000	0.378118000	4.640947000
C	0.000875000	2.874191000	-2.535042000	H	-4.157962000	0.453509000	5.327317000
H	-0.103876000	2.875402000	-1.444371000	C	-2.550926000	1.507665000	4.344743000
H	-0.409022000	3.812013000	-2.918646000	H	-2.799413000	2.465025000	4.796278000
H	1.075044000	2.862368000	-2.753028000	C	-1.457632000	1.428698000	3.471988000
C	-1.698126000	1.877034000	-4.124518000	C	-0.632101000	2.653767000	3.159138000
H	-1.958412000	2.887486000	-4.428698000	H	-0.609196000	2.855804000	2.082074000
C	-2.354064000	0.785361000	-4.698031000	H	0.408659000	2.529567000	3.479361000
H	-3.123758000	0.946645000	-5.447586000	H	-1.038567000	3.534342000	3.664200000
C	-2.022614000	-0.513419000	-4.305447000	C	1.184081000	-0.196021000	2.505117000
H	-2.534788000	-1.362014000	-4.751327000	O	1.482337000	-0.377062000	3.699518000
C	-1.034858000	-0.744012000	-3.338847000	C	2.257912000	-0.281055000	1.438027000
C	-0.680066000	-2.148804000	-2.915131000	C	3.611364000	-0.561510000	1.625269000
H	0.369917000	-2.380354000	-3.127784000	H	4.000461000	-0.739709000	2.620873000
H	-1.299269000	-2.878854000	-3.442730000	C	4.434505000	-0.604372000	0.491654000
H	-0.826814000	-2.289672000	-1.838471000	H	5.492283000	-0.819583000	0.604991000
F	-1.499429000	0.228793000	-0.016130000	C	3.907524000	-0.376835000	-0.787086000
H	-3.868759000	1.391642000	-0.089367000	H	4.527679000	-0.411440000	-1.675123000
C	-4.799833000	1.926187000	-0.334036000	C	2.544001000	-0.102503000	-0.891546000
H	-4.553662000	2.496930000	-1.244058000	C	1.755839000	0.159660000	-2.160924000
C	-5.897362000	0.936662000	-0.634553000	O	2.334566000	0.149145000	-3.262837000
H	-5.705920000	0.217479000	-1.429540000	C	-0.420680000	0.620056000	-3.031812000
C	-7.066556000	0.904601000	0.018113000	C	-0.646323000	1.944680000	-3.464640000
H	-7.813880000	0.160113000	-0.252388000	C	0.049369000	3.104241000	-2.792157000
C	-7.425781000	1.855580000	1.132560000	H	-0.179993000	3.141223000	-1.720817000
H	-7.678406000	1.287393000	2.042148000	H	-0.257120000	4.053396000	-3.240526000
H	-8.354309000	2.392947000	0.881434000	H	1.139004000	3.024435000	-2.878849000
C	-6.327537000	2.844371000	1.434990000	C	-1.529878000	2.162405000	-4.531244000
H	-6.517868000	3.561802000	2.231871000	H	-1.707954000	3.179740000	-4.871375000
C	-5.158794000	2.875384000	0.781404000	C	-2.178399000	1.095366000	-5.157639000
H	-4.410827000	3.618630000	1.053678000	H	-2.860797000	1.279959000	-5.982843000
² TS _F				C	-1.947273000	-0.209911000	-4.716869000
Ni	-0.101392000	0.336250000	0.004533000	H	-2.450905000	-1.042855000	-5.201533000

C	-1.070854000	-0.468144000	-3.653552000	C	2.246734000	-0.564265000	1.404338000
C	-0.828591000	-1.882155000	-3.181437000	C	3.552402000	-1.050969000	1.475883000
H	0.224386000	-2.167061000	-3.288029000	H	3.988517000	-1.315621000	2.431986000
H	-1.430679000	-2.591613000	-3.755933000	C	4.268321000	-1.181182000	0.277270000
H	-1.080763000	-1.998005000	-2.120916000	H	5.286340000	-1.557051000	0.300583000
F	-2.016573000	0.744449000	-0.210837000	C	3.688655000	-0.832093000	-0.950811000
H	-3.276476000	1.019742000	-0.408201000	H	4.230432000	-0.926543000	-1.884594000
C	-4.497781000	1.288862000	-0.621655000	C	2.378399000	-0.352705000	-0.938421000
H	-4.407937000	1.408368000	-1.706368000	C	1.546108000	0.088916000	-2.129183000
C	-5.206572000	0.092575000	-0.170865000	O	2.035027000	0.042029000	-3.272804000
H	-5.175066000	-0.792541000	-0.800391000	C	-0.576370000	0.930018000	-2.823837000
C	-5.849156000	0.057681000	1.024802000	C	-0.717364000	2.308523000	-3.093849000
H	-6.343332000	-0.852180000	1.354876000	C	0.093258000	3.332716000	-2.334693000
C	-5.910147000	1.246109000	1.928022000	H	-0.117443000	3.298220000	-1.259378000
H	-5.352095000	1.017515000	2.860294000	H	-0.128202000	4.342459000	-2.691497000
H	-6.939104000	1.404133000	2.290174000	H	1.169052000	3.159351000	-2.450490000
C	-5.364518000	2.503755000	1.334231000	C	-1.620699000	2.710644000	-4.088569000
H	-5.496083000	3.424770000	1.895836000	H	-1.733767000	3.770669000	-4.302577000
C	-4.726033000	2.517920000	0.135991000	C	-2.367110000	1.772583000	-4.804884000
H	-4.334567000	3.449424000	-0.263830000	H	-3.063039000	2.099566000	-5.572588000
² IM _F				C	-2.215136000	0.411689000	-4.528900000
Ni	-0.097398000	0.451341000	0.178012000	H	-2.794484000	-0.321931000	-5.084328000
N	0.081435000	0.154477000	2.148969000	C	-1.324107000	-0.030220000	-3.540520000
N	1.732707000	-0.245472000	0.219517000	C	-1.171085000	-1.504194000	-3.248915000
N	0.300520000	0.508449000	-1.779209000	H	-0.155187000	-1.851751000	-3.468169000
C	-0.910955000	0.400077000	3.145170000	H	-1.867306000	-2.093084000	-3.852448000
C	-1.791878000	-0.636795000	3.521239000	H	-1.360696000	-1.725151000	-2.192226000
C	-1.662252000	-2.015581000	2.918291000	F	-2.057293000	1.481748000	0.206200000
H	-0.690089000	-2.465585000	3.149534000	H	-2.841548000	1.162925000	-0.255146000
H	-2.442016000	-2.680658000	3.299763000	C	-4.443538000	0.652073000	-1.183209000
H	-1.743753000	-1.983314000	1.825571000	H	-3.850080000	0.682711000	-2.093734000
C	-2.791502000	-0.361024000	4.465112000	C	-4.624895000	-0.585204000	-0.491807000
H	-3.473211000	-1.154999000	4.760546000	H	-4.074818000	-1.460705000	-0.827028000
C	-2.920494000	0.911869000	5.025656000	C	-5.470064000	-0.682415000	0.580243000
H	-3.700557000	1.110450000	5.755571000	H	-5.591395000	-1.630828000	1.096579000
C	-2.042683000	1.928434000	4.642357000	C	-6.255561000	0.492887000	1.084479000
H	-2.139951000	2.920690000	5.076309000	H	-6.000161000	0.687794000	2.143209000
C	-1.029600000	1.691453000	3.702223000	H	-7.329180000	0.236504000	1.134256000
C	-0.084564000	2.796897000	3.294143000	C	-6.063159000	1.743148000	0.276503000
H	-0.127872000	2.983101000	2.214638000	H	-6.631784000	2.623336000	0.564192000
H	0.955808000	2.543722000	3.528124000	C	-5.206935000	1.794497000	-0.789435000
H	-0.330992000	3.728394000	3.811318000	H	-5.096464000	2.719165000	-1.350058000
C	1.282173000	-0.335736000	2.555157000	⁴ RC _F			
O	1.639571000	-0.596849000	3.718865000	Ni	-0.138913000	-0.093106000	0.150555000

N	0.088259000	-0.212402000	2.126124000	C	-1.166471000	-0.890429000	-3.439493000
N	1.832034000	0.292327000	0.244917000	C	-1.137483000	-2.181133000	-2.673938000
N	0.652121000	-0.057294000	-2.129366000	H	-0.127480000	-2.599615000	-2.628740000
C	-0.948646000	-0.534980000	3.048834000	H	-1.801746000	-2.914066000	-3.137858000
C	-1.244658000	-1.891939000	3.301153000	H	-1.471035000	-2.007531000	-1.644482000
C	-0.442162000	-2.991036000	2.645828000	F	-1.967526000	-0.287079000	-0.214552000
H	0.621033000	-2.922628000	2.902784000	H	-4.119412000	0.999919000	-0.444474000
H	-0.804278000	-3.974341000	2.958602000	C	-5.054088000	1.572827000	-0.549900000
H	-0.506021000	-2.935427000	1.552631000	H	-5.376344000	1.385484000	-1.587157000
C	-2.300388000	-2.199358000	4.171001000	C	-6.091642000	1.045115000	0.408944000
H	-2.533607000	-3.242192000	4.371823000	H	-6.341920000	-0.011793000	0.328705000
C	-3.049724000	-1.188703000	4.777344000	C	-6.700303000	1.799370000	1.333556000
H	-3.865959000	-1.442130000	5.448275000	H	-7.438677000	1.348761000	1.995183000
C	-2.747403000	0.149523000	4.514603000	C	-6.422504000	3.269717000	1.524842000
H	-3.331166000	0.938611000	4.982343000	H	-6.100834000	3.457612000	2.561807000
C	-1.699782000	0.497897000	3.650567000	H	-7.357218000	3.843985000	1.422287000
C	-1.386368000	1.947397000	3.365717000	C	-5.387289000	3.799447000	0.563939000
H	-1.429198000	2.161395000	2.291505000	H	-5.136586000	4.856125000	0.645268000
H	-0.378037000	2.213453000	3.702639000	C	-4.779324000	3.043485000	-0.359792000
H	-2.097092000	2.604864000	3.873906000	H	-4.040240000	3.494640000	-1.020419000
C	1.316776000	0.088595000	2.597062000	⁴ TS _F			
O	1.691256000	0.134541000	3.783969000	Ni	-0.178962000	0.176511000	0.293877000
C	2.316412000	0.370308000	1.492409000	N	0.182320000	-0.131095000	2.323564000
C	3.661291000	0.658774000	1.724078000	N	1.814406000	0.142993000	0.324884000
H	4.024118000	0.718224000	2.743195000	N	0.280694000	0.393570000	-1.748928000
C	4.500983000	0.854390000	0.624430000	C	-0.813645000	-0.235026000	3.330846000
H	5.551359000	1.082295000	0.773344000	C	-1.439964000	-1.480227000	3.559952000
C	3.985374000	0.742606000	-0.669115000	C	-1.013642000	-2.704435000	2.784723000
H	4.606369000	0.870042000	-1.547468000	H	0.042813000	-2.941012000	2.955986000
C	2.628182000	0.453159000	-0.819446000	H	-1.608330000	-3.575524000	3.074421000
C	1.983457000	0.289145000	-2.167405000	H	-1.130091000	-2.553447000	1.704906000
O	2.662008000	0.342064000	-3.197694000	C	-2.461811000	-1.559089000	4.516711000
C	-0.211883000	0.166047000	-3.142663000	H	-2.944857000	-2.516494000	4.697756000
C	-0.254904000	1.414409000	-3.887871000	C	-2.862754000	-0.430215000	5.235556000
C	0.620815000	2.589169000	-3.540024000	H	-3.656694000	-0.505469000	5.973700000
H	0.722700000	2.714100000	-2.457458000	C	-2.238900000	0.797148000	4.997229000
H	0.192589000	3.507594000	-3.947883000	H	-2.550202000	1.679445000	5.551781000
H	1.628018000	2.469670000	-3.950817000	C	-1.213635000	0.914844000	4.048380000
C	-1.195345000	1.539031000	-4.898309000	C	-0.554503000	2.249035000	3.790052000
H	-1.259290000	2.472313000	-5.449625000	H	-0.634844000	2.535134000	2.734769000
C	-2.082745000	0.493924000	-5.210576000	H	0.514509000	2.221635000	4.029920000
H	-2.800467000	0.623157000	-6.014981000	H	-1.017287000	3.034966000	4.393792000
C	-2.061017000	-0.704810000	-4.482924000	C	1.474384000	-0.183658000	2.680679000
H	-2.751156000	-1.501924000	-4.741249000	O	1.957038000	-0.345519000	3.826418000

C	2.420055000	-0.026434000	1.503004000	N	0.053805000	-0.077901000	2.149885000
C	3.813628000	-0.047758000	1.574315000	N	1.811730000	0.114094000	0.286506000
H	4.303632000	-0.184413000	2.530980000	N	0.277047000	0.391432000	-1.758822000
C	4.538358000	0.111365000	0.387190000	C	-1.000826000	-0.151661000	3.109240000
H	5.623646000	0.099836000	0.412238000	C	-1.520304000	-1.409821000	3.482457000
C	3.873024000	0.283906000	-0.832584000	C	-0.939212000	-2.683846000	2.916247000
H	4.410020000	0.407564000	-1.765489000	H	0.117050000	-2.798188000	3.185112000
C	2.477923000	0.293814000	-0.823951000	H	-1.480085000	-3.557042000	3.291557000
C	1.591903000	0.463603000	-2.043105000	H	-0.989650000	-2.694696000	1.821257000
O	2.120272000	0.623918000	-3.165655000	C	-2.590721000	-1.453725000	4.387190000
C	-0.681316000	0.575929000	-2.759778000	H	-2.996919000	-2.419150000	4.679228000
C	-0.961483000	1.875353000	-3.261325000	C	-3.137209000	-0.280856000	4.913411000
C	-0.191563000	3.073217000	-2.764259000	H	-3.966669000	-0.331301000	5.613522000
H	-0.231734000	3.145545000	-1.671369000	C	-2.613014000	0.957007000	4.534390000
H	-0.596543000	3.997095000	-3.185867000	H	-3.035092000	1.872437000	4.942078000
H	0.866279000	3.004569000	-3.040739000	C	-1.543399000	1.042097000	3.631580000
C	-1.977078000	2.025039000	-4.210079000	C	-0.983729000	2.385255000	3.226055000
H	-2.204070000	3.016732000	-4.592916000	H	-1.049308000	2.535303000	2.141957000
C	-2.709070000	0.921175000	-4.665614000	H	0.075138000	2.477693000	3.493223000
H	-3.495088000	1.055656000	-5.403161000	H	-1.528893000	3.196520000	3.716503000
C	-2.417721000	-0.357472000	-4.174631000	C	1.333995000	-0.136463000	2.604451000
H	-2.977271000	-1.215380000	-4.538500000	O	1.715053000	-0.259736000	3.783023000
C	-1.414902000	-0.549906000	-3.220155000	C	2.360714000	-0.025066000	1.490212000
C	-1.105765000	-1.932067000	-2.699758000	C	3.750618000	-0.044473000	1.610200000
H	-0.045506000	-2.177977000	-2.821706000	H	4.216750000	-0.157151000	2.582042000
H	-1.696946000	-2.685116000	-3.228065000	C	4.509585000	0.086599000	0.438314000
H	-1.328504000	-2.016563000	-1.629692000	H	5.593253000	0.073941000	0.499030000
F	-2.098915000	0.389995000	0.317292000	C	3.889615000	0.237031000	-0.810440000
H	-3.207424000	0.887437000	-0.738621000	H	4.464241000	0.343452000	-1.723028000
C	-4.169571000	1.254521000	-1.299529000	C	2.494869000	0.247894000	-0.846729000
H	-3.816078000	1.126577000	-2.337211000	C	1.602746000	0.407201000	-2.065388000
C	-5.237585000	0.318394000	-0.920253000	O	2.116542000	0.533109000	-3.191761000
H	-5.160214000	-0.708759000	-1.265928000	C	-0.652885000	0.564814000	-2.827688000
C	-6.275997000	0.693151000	-0.126934000	C	-0.950613000	1.865117000	-3.292923000
H	-7.037779000	-0.027375000	0.157557000	C	-0.264427000	3.073908000	-2.702406000
C	-6.425809000	2.089280000	0.370702000	H	-0.383181000	3.109122000	-1.613502000
H	-6.435255000	2.088486000	1.478140000	H	-0.674756000	3.996320000	-3.122497000
H	-7.437313000	2.467070000	0.134803000	H	0.812684000	3.059980000	-2.904083000
C	-5.397822000	3.050081000	-0.118831000	C	-1.898270000	2.013367000	-4.315474000
H	-5.503227000	4.091757000	0.171410000	H	-2.132724000	3.011279000	-4.678087000
C	-4.365619000	2.658848000	-0.911768000	C	-2.541627000	0.903152000	-4.867689000
H	-3.634779000	3.386835000	-1.252636000	H	-3.274672000	1.034377000	-5.658867000
⁴ IM _F				C	-2.239569000	-0.376023000	-4.395924000
Ni	-0.138604000	0.110255000	0.174791000	H	-2.736630000	-1.242846000	-4.824570000

C	-1.296095000	-0.566657000	-3.375578000	C	2.603938000	0.029736000	1.376857000
C	-0.974253000	-1.957834000	-2.881446000	C	3.988169000	0.045077000	1.524354000
H	0.097726000	-2.172206000	-2.951016000	H	4.426403000	0.027914000	2.515438000
H	-1.510559000	-2.708823000	-3.468253000	C	4.773125000	0.082473000	0.364610000
H	-1.255814000	-2.087447000	-1.829475000	H	5.854635000	0.094767000	0.447352000
F	-2.335777000	-0.235279000	0.111677000	C	4.173469000	0.104946000	-0.901218000
H	-2.961633000	0.358503000	-0.317152000	H	4.757582000	0.135026000	-1.813591000
C	-4.290112000	1.448480000	-1.190375000	C	2.782975000	0.088101000	-0.966650000
H	-3.713587000	1.328335000	-2.104104000	C	1.909201000	0.112152000	-2.187701000
C	-5.380658000	0.568148000	-0.911484000	O	2.375229000	0.154806000	-3.325848000
H	-5.552750000	-0.280282000	-1.568897000	C	-0.372694000	0.121863000	-2.922488000
C	-6.201160000	0.772418000	0.164437000	C	-0.857113000	1.370820000	-3.363811000
H	-7.022585000	0.089319000	0.363165000	C	-0.400608000	2.655110000	-2.715848000
C	-6.011068000	1.927998000	1.103557000	H	-0.626883000	2.661196000	-1.643692000
H	-5.855613000	1.553112000	2.132771000	H	-0.894374000	3.515652000	-3.174616000
H	-6.951019000	2.502379000	1.190889000	H	0.681960000	2.794724000	-2.815317000
C	-4.884503000	2.842648000	0.719556000	C	-1.776374000	1.388263000	-4.420828000
H	-4.713039000	3.720582000	1.336572000	H	-2.158887000	2.342583000	-4.773324000
C	-4.088978000	2.598694000	-0.367128000	C	-2.203233000	0.201385000	-5.020789000
H	-3.284144000	3.286700000	-0.612806000	H	-2.917687000	0.232293000	-5.838660000
² RC _{Cl}				C	-1.712347000	-1.025299000	-4.567731000
Ni	0.202792000	0.016868000	0.013274000	H	-2.045179000	-1.948595000	-5.034623000
N	0.283555000	-0.016655000	1.911480000	C	-0.791908000	-1.088062000	-3.513349000
N	2.069523000	0.050914000	0.157189000	C	-0.266517000	-2.415822000	-3.024927000
N	0.570549000	0.084297000	-1.849502000	H	0.819861000	-2.489590000	-3.149983000
C	-0.812822000	-0.055677000	2.827390000	H	-0.725095000	-3.239317000	-3.578451000
C	-1.311096000	-1.306067000	3.249053000	H	-0.477323000	-2.559285000	-1.959322000
C	-0.710435000	-2.594134000	2.741585000	Cl	-1.992691000	-0.074988000	-0.161410000
H	0.347194000	-2.681686000	3.015450000	H	-4.994819000	0.633171000	-0.794905000
H	-1.238000000	-3.456305000	3.157713000	C	-6.079957000	0.802859000	-0.880726000
H	-0.764798000	-2.653514000	1.648800000	H	-6.181692000	1.485929000	-1.739172000
C	-2.384070000	-1.321090000	4.149650000	C	-6.779655000	-0.499723000	-1.177076000
H	-2.780056000	-2.276267000	4.484422000	H	-6.462099000	-1.035722000	-2.070195000
C	-2.946318000	-0.130959000	4.616979000	C	-7.748370000	-1.012373000	-0.407204000
H	-3.779183000	-0.160385000	5.313937000	H	-8.209292000	-1.959946000	-0.681949000
C	-2.438543000	1.096901000	4.186411000	C	-8.256458000	-0.346893000	0.847349000
H	-2.876663000	2.022703000	4.549959000	H	-8.144821000	-1.030109000	1.704512000
C	-1.366622000	1.157386000	3.286304000	H	-9.343234000	-0.183250000	0.770258000
C	-0.823230000	2.486013000	2.820279000	C	-7.561389000	0.959226000	1.140152000
H	-0.878267000	2.577530000	1.729721000	H	-7.881306000	1.497055000	2.031350000
H	0.229224000	2.611439000	3.099430000	C	-6.592970000	1.471660000	0.369754000
H	-1.388952000	3.310538000	3.261796000	H	-6.134525000	2.421012000	0.642520000
C	1.554720000	-0.009930000	2.450532000	² TS _{Cl}			
O	1.842201000	-0.032376000	3.646953000	Ni	-0.328273000	-0.227521000	0.105084000

N	-0.101989000	-0.391784000	2.102978000	C	-1.108914000	-1.140831000	-3.547276000
N	1.590102000	0.194415000	0.255580000	C	-0.464981000	-2.415331000	-3.055561000
N	0.096985000	0.139851000	-1.841001000	H	0.627684000	-2.365339000	-3.121860000
C	-1.108292000	-0.707242000	3.065187000	H	-0.802258000	-3.272446000	-3.645263000
C	-1.349556000	-2.055265000	3.405545000	H	-0.709639000	-2.606618000	-2.004270000
C	-0.524662000	-3.163775000	2.795715000	Cl	-2.714963000	-0.944084000	-0.047354000
H	0.538256000	-3.055124000	3.039462000	H	-3.662806000	0.092498000	-0.654507000
H	-0.857442000	-4.140058000	3.159222000	C	-4.600170000	1.031152000	-1.246922000
H	-0.599536000	-3.162095000	1.701934000	H	-3.906293000	1.211851000	-2.069586000
C	-2.372985000	-2.346527000	4.318788000	C	-5.746693000	0.187895000	-1.507283000
H	-2.564291000	-3.383169000	4.585693000	H	-5.707325000	-0.496185000	-2.350240000
C	-3.142958000	-1.328207000	4.885557000	C	-6.839812000	0.215660000	-0.697315000
H	-3.932853000	-1.569266000	5.591753000	H	-7.684026000	-0.439395000	-0.894290000
C	-2.892795000	0.001621000	4.539043000	C	-6.939588000	1.143753000	0.471141000
H	-3.489663000	0.797637000	4.977955000	H	-7.052295000	0.557032000	1.402072000
C	-1.877875000	0.332210000	3.629696000	H	-7.886643000	1.708497000	0.423914000
C	-1.616052000	1.773000000	3.259624000	C	-5.788680000	2.088315000	0.610759000
H	-1.721383000	1.933467000	2.180230000	H	-5.844232000	2.838031000	1.395262000
H	-0.597800000	2.078758000	3.525881000	C	-4.707617000	2.038528000	-0.214840000
H	-2.314608000	2.438934000	3.774072000	H	-3.889942000	2.742249000	-0.087562000
C	1.153304000	-0.167432000	2.568482000	² IM _{Cl}			
O	1.544547000	-0.211948000	3.750786000	Ni	-0.293957000	-0.218624000	0.069451000
C	2.138329000	0.176723000	1.468498000	N	-0.114634000	-0.390076000	2.051522000
C	3.494278000	0.468579000	1.619118000	N	1.590448000	0.280757000	0.251316000
H	3.949946000	0.457948000	2.602255000	N	0.129853000	0.115799000	-1.856951000
C	4.230972000	0.772836000	0.466387000	C	-1.127149000	-0.767003000	2.985721000
H	5.288156000	1.004189000	0.550654000	C	-1.321777000	-2.131832000	3.286300000
C	3.617614000	0.784422000	-0.793567000	C	-0.438364000	-3.191775000	2.671470000
H	4.169733000	1.020242000	-1.695733000	H	0.612025000	-3.050991000	2.950827000
C	2.256972000	0.482837000	-0.859679000	H	-0.744783000	-4.189234000	2.998605000
C	1.392855000	0.445804000	-2.104606000	H	-0.478920000	-3.163717000	1.576295000
O	1.906539000	0.684807000	-3.214769000	C	-2.352566000	-2.485682000	4.168749000
C	-0.799802000	0.100287000	-2.950026000	H	-2.509322000	-3.535365000	4.405152000
C	-1.390969000	1.295385000	-3.415457000	C	-3.172749000	-1.512444000	4.743927000
C	-1.051495000	2.623419000	-2.780754000	H	-3.967705000	-1.801918000	5.425777000
H	-1.228010000	2.608425000	-1.699147000	C	-2.966477000	-0.165215000	4.438175000
H	-1.652827000	3.426543000	-3.215986000	H	-3.602186000	0.595511000	4.884835000
H	0.005245000	2.875723000	-2.925158000	C	-1.946472000	0.227887000	3.560094000
C	-2.297515000	1.227346000	-4.483570000	C	-1.730705000	1.686848000	3.234595000
H	-2.755567000	2.144018000	-4.847493000	H	-1.816125000	1.873082000	2.157673000
C	-2.614788000	0.005522000	-5.081813000	H	-0.731479000	2.022165000	3.534974000
H	-3.319131000	-0.031397000	-5.908394000	H	-2.466056000	2.311911000	3.748822000
C	-2.021127000	-1.168076000	-4.612118000	C	1.119003000	-0.105856000	2.549691000
H	-2.262651000	-2.120925000	-5.077023000	O	1.479190000	-0.138461000	3.740499000

C	2.114432000	0.285860000	1.473998000	N	-0.029863000	0.233803000	2.045732000
C	3.455735000	0.629397000	1.645194000	N	1.730202000	-0.233752000	0.153687000
H	3.897651000	0.639110000	2.634623000	N	0.740496000	0.531263000	-2.219476000
C	4.198310000	0.955577000	0.501570000	C	-1.066317000	0.534172000	2.973411000
H	5.244545000	1.226626000	0.601917000	C	-1.963984000	-0.479167000	3.375163000
C	3.608381000	0.935152000	-0.770079000	C	-1.812921000	-1.890582000	2.860290000
H	4.169291000	1.182760000	-1.663633000	H	-0.854890000	-2.327241000	3.164484000
C	2.261458000	0.582090000	-0.856988000	H	-2.613296000	-2.530715000	3.241839000
C	1.413914000	0.486618000	-2.111422000	H	-1.843304000	-1.919865000	1.765061000
O	1.923416000	0.735470000	-3.219255000	C	-3.000699000	-0.147539000	4.258218000
C	-0.754860000	0.007137000	-2.972767000	H	-3.696379000	-0.921982000	4.572186000
C	-1.406590000	1.159246000	-3.463955000	C	-3.150843000	1.157390000	4.734291000
C	-1.142128000	2.515728000	-2.854555000	H	-3.960682000	1.399098000	5.417267000
H	-1.333526000	2.515342000	-1.775347000	C	-2.256231000	2.150081000	4.327566000
H	-1.776170000	3.278398000	-3.315196000	H	-2.369525000	3.166301000	4.697386000
H	-0.097335000	2.817314000	-2.990553000	C	-1.206473000	1.857386000	3.445636000
C	-2.303735000	1.020596000	-4.532756000	C	-0.241594000	2.936131000	3.013370000
H	-2.809295000	1.903459000	-4.916710000	H	-0.254565000	3.074699000	1.925801000
C	-2.552525000	-0.228489000	-5.106368000	H	0.789691000	2.685989000	3.287006000
H	-3.250899000	-0.319976000	-5.933747000	H	-0.494393000	3.892206000	3.480244000
C	-1.898505000	-1.358765000	-4.611618000	C	1.124998000	-0.274668000	2.498985000
H	-2.086814000	-2.332393000	-5.057551000	O	1.443785000	-0.530668000	3.680437000
C	-0.993499000	-1.260943000	-3.544805000	C	2.127448000	-0.547020000	1.395342000
C	-0.283688000	-2.488961000	-3.025928000	C	3.392351000	-1.088461000	1.628547000
H	0.804912000	-2.382630000	-3.092559000	H	3.684584000	-1.330138000	2.643308000
H	-0.574010000	-3.374563000	-3.598079000	C	4.240628000	-1.301322000	0.539912000
H	-0.518568000	-2.673091000	-1.971144000	H	5.229097000	-1.722620000	0.691440000
Cl	-2.820169000	-1.119930000	-0.124237000	C	3.810260000	-0.969306000	-0.746945000
H	-3.533464000	-0.103504000	-0.589202000	H	4.436015000	-1.118200000	-1.618456000
C	-4.794880000	1.368615000	-1.283925000	C	2.532637000	-0.430104000	-0.901238000
H	-4.065088000	1.448261000	-2.084539000	C	1.984467000	-0.049456000	-2.247461000
C	-5.941110000	0.532656000	-1.445921000	O	2.684442000	-0.155101000	-3.260607000
H	-6.019297000	-0.086249000	-2.336266000	C	-0.078260000	0.592893000	-3.292504000
C	-6.930803000	0.493737000	-0.502505000	C	-0.731994000	1.864158000	-3.554406000
H	-7.793430000	-0.152672000	-0.640979000	C	-0.403410000	3.073995000	-2.726995000
C	-6.876752000	1.328132000	0.744889000	H	-0.758022000	2.952263000	-1.698633000
H	-6.920323000	0.674464000	1.636254000	H	-0.877271000	3.963231000	-3.149014000
H	-7.798477000	1.930884000	0.836341000	H	0.677261000	3.241432000	-2.680530000
C	-5.670825000	2.219349000	0.824691000	C	-1.590202000	1.959718000	-4.638880000
H	-5.583003000	2.874739000	1.687158000	H	-2.053788000	2.913600000	-4.870523000
C	-4.705185000	2.223895000	-0.144631000	C	-1.858299000	0.844264000	-5.446855000
H	-3.848442000	2.886154000	-0.049030000	H	-2.545883000	0.937125000	-6.282030000
⁴ RC _{Cl}				C	-1.252283000	-0.396540000	-5.182451000
Ni	-0.154491000	0.502671000	0.043536000	H	-1.500384000	-1.251833000	-5.803674000

C	-0.359175000	-0.557563000	-4.134555000	C	2.194176000	0.465083000	1.494144000
C	0.216711000	-1.918410000	-3.845977000	C	3.554987000	0.760999000	1.577903000
H	1.252819000	-1.989838000	-4.191146000	H	4.022401000	0.897308000	2.545845000
H	-0.366584000	-2.688582000	-4.355504000	C	4.279215000	0.871946000	0.384032000
H	0.213614000	-2.141903000	-2.774612000	H	5.339703000	1.101600000	0.418189000
Cl	-2.354400000	0.905885000	-0.412054000	C	3.648915000	0.688189000	-0.853275000
H	-5.565707000	0.516601000	-0.404948000	H	4.189734000	0.767096000	-1.788860000
C	-6.654326000	0.349533000	-0.423543000	C	2.284640000	0.396267000	-0.856478000
H	-7.052611000	1.210589000	-0.983939000	C	1.421268000	0.160824000	-2.081303000
C	-6.963700000	-0.928672000	-1.161681000	O	1.949338000	0.218637000	-3.214316000
H	-6.601248000	-1.004614000	-2.185765000	C	-0.762777000	-0.319964000	-2.864032000
C	-7.646162000	-1.948196000	-0.624330000	C	-1.336273000	0.780690000	-3.538988000
H	-7.832120000	-2.842961000	-1.216529000	C	-0.975605000	2.195721000	-3.151729000
C	-8.188513000	-1.938883000	0.783044000	H	-1.133258000	2.373816000	-2.081605000
H	-7.789311000	-2.799482000	1.343354000	H	-1.575846000	2.917683000	-3.712768000
H	-9.277117000	-2.107773000	0.765565000	H	0.081280000	2.405489000	-3.352488000
C	-7.880390000	-0.660024000	1.520993000	C	-2.238839000	0.536736000	-4.584134000
H	-8.242632000	-0.584231000	2.545140000	H	-2.682212000	1.380367000	-5.107963000
C	-7.197716000	0.359132000	0.983207000	C	-2.571760000	-0.767365000	-4.958410000
H	-7.011379000	1.253618000	1.575646000	H	-3.271971000	-0.940668000	-5.771122000
⁴ TS _{Cl}				C	-1.998649000	-1.846978000	-4.282462000
Ni	-0.310092000	-0.106127000	0.235931000	H	-2.252158000	-2.863943000	-4.572445000
N	-0.017447000	0.009625000	2.276527000	C	-1.091170000	-1.642942000	-3.232948000
N	1.626341000	0.299877000	0.298844000	C	-0.464536000	-2.818358000	-2.520782000
N	0.134279000	-0.099415000	-1.779660000	H	0.628494000	-2.796925000	-2.596594000
C	-1.000157000	-0.185911000	3.289174000	H	-0.816503000	-3.762429000	-2.946329000
C	-1.202761000	-1.476218000	3.825242000	H	-0.706530000	-2.815417000	-1.451683000
C	-0.352873000	-2.639492000	3.371128000	Cl	-2.730737000	-0.731049000	0.267053000
H	0.707106000	-2.474110000	3.595076000	H	-3.598700000	0.209545000	-0.560518000
H	-0.663465000	-3.564245000	3.865683000	C	-4.493296000	1.081602000	-1.323508000
H	-0.426893000	-2.789330000	2.287598000	H	-3.643539000	1.562861000	-1.807949000
C	-2.209617000	-1.658893000	4.784001000	C	-5.240713000	0.108283000	-2.087672000
H	-2.370038000	-2.650558000	5.200552000	H	-4.761559000	-0.352501000	-2.946646000
C	-3.002962000	-0.589625000	5.206887000	C	-6.499983000	-0.256262000	-1.720439000
H	-3.779900000	-0.746371000	5.950282000	H	-7.040969000	-1.006002000	-2.291332000
C	-2.793297000	0.681765000	4.667246000	C	-7.195087000	0.357698000	-0.547275000
H	-3.409111000	1.516892000	4.992876000	H	-7.437092000	-0.427781000	0.193014000
C	-1.796117000	0.902629000	3.706523000	H	-8.192337000	0.722310000	-0.848584000
C	-1.579653000	2.278900000	3.123463000	C	-6.430183000	1.456072000	0.120008000
H	-1.700476000	2.272730000	2.033648000	H	-6.919002000	1.991083000	0.929562000
H	-0.567616000	2.647504000	3.326009000	C	-5.171786000	1.800477000	-0.268314000
H	-2.291924000	2.995502000	3.542344000	H	-4.644999000	2.606019000	0.235288000
C	1.239441000	0.297012000	2.662015000	⁴ IM _{Cl}			
O	1.677769000	0.430984000	3.826815000	Ni	-0.228107000	-0.062169000	0.236620000

N	0.006856000	-0.014447000	2.223406000	C	-0.719241000	-0.361001000	-2.797220000
N	1.685801000	0.354548000	0.313498000	C	-1.322748000	0.701274000	-3.504774000
N	0.178196000	-0.081413000	-1.722239000	C	-1.000765000	2.137593000	-3.166053000
C	-0.989653000	-0.245884000	3.220294000	H	-1.169188000	2.347571000	-2.103523000
C	-1.194352000	-1.555034000	3.705571000	H	-1.617818000	2.822924000	-3.753933000
C	-0.338564000	-2.701114000	3.219668000	H	0.050631000	2.369180000	-3.371178000
H	0.719744000	-2.540205000	3.454659000	C	-2.223703000	0.396656000	-4.535160000
H	-0.649259000	-3.641022000	3.684275000	H	-2.691619000	1.209353000	-5.085575000
H	-0.405671000	-2.818560000	2.131804000	C	-2.524442000	-0.927907000	-4.860684000
C	-2.209734000	-1.771815000	4.648274000	H	-3.224545000	-1.147715000	-5.662079000
H	-2.373581000	-2.777701000	5.027280000	C	-1.920793000	-1.968297000	-4.151140000
C	-3.005575000	-0.718072000	5.103186000	H	-2.150181000	-3.000901000	-4.402936000
H	-3.788688000	-0.901397000	5.833800000	C	-1.012979000	-1.704583000	-3.115376000
C	-2.791106000	0.572358000	4.613342000	C	-0.353844000	-2.838353000	-2.365710000
H	-3.409283000	1.395064000	4.964560000	H	0.737661000	-2.798535000	-2.455767000
C	-1.786226000	0.828767000	3.669807000	H	-0.691121000	-3.804622000	-2.751048000
C	-1.566541000	2.225958000	3.140339000	H	-0.582276000	-2.800198000	-1.294160000
H	-1.680230000	2.261622000	2.050444000	Cl	-2.793676000	-0.655934000	0.255972000
H	-0.556769000	2.588097000	3.364342000	H	-3.447534000	0.185619000	-0.533979000
H	-2.282539000	2.925023000	3.581425000	C	-4.755106000	1.387135000	-1.580320000
C	1.259309000	0.297012000	2.652638000	H	-3.870428000	1.788441000	-2.065516000
O	1.648402000	0.413363000	3.829148000	C	-5.456286000	0.293311000	-2.171521000
C	2.239583000	0.505252000	1.513578000	H	-5.036695000	-0.182157000	-3.054228000
C	3.597669000	0.809746000	1.610175000	C	-6.630702000	-0.166548000	-1.640982000
H	4.064133000	0.936402000	2.580055000	H	-7.147482000	-1.004612000	-2.101207000
C	4.325167000	0.939633000	0.418769000	C	-7.251260000	0.452062000	-0.421541000
H	5.383541000	1.176712000	0.461044000	H	-7.367297000	-0.312386000	0.369613000
C	3.705739000	0.761074000	-0.826105000	H	-8.295116000	0.744869000	-0.635644000
H	4.256141000	0.849496000	-1.755382000	C	-6.487873000	1.628723000	0.115148000
C	2.343668000	0.459116000	-0.837664000	H	-6.897734000	2.145157000	0.979131000
C	1.469031000	0.199634000	-2.049112000	C	-5.317032000	2.054306000	-0.449807000
O	1.966796000	0.246686000	-3.188731000	H	-4.796090000	2.911783000	-0.031279000

III) Desaturation vs. Halogenation of the CHD-H radical

III-1) desaturation vs. halogenation by the oxidant 1_F

³ IM'				H	0.590597000	-3.156305000	2.630679000
Ni	-0.094611000	-0.083869000	-0.090362000	H	-0.878357000	-4.148217000	2.615035000
N	0.145346000	-0.376637000	1.977711000	H	-0.526500000	-3.035536000	1.278274000
N	1.862990000	0.251165000	0.133588000	C	-2.287247000	-2.388393000	3.951472000
N	0.486611000	0.331268000	-2.066157000	H	-2.553809000	-3.432118000	4.101810000
C	-0.885062000	-0.715770000	2.894721000	C	-2.995576000	-1.386139000	4.619115000
C	-1.230678000	-2.072286000	3.085284000	H	-3.812064000	-1.645837000	5.287641000
C	-0.472925000	-3.163262000	2.365902000	C	-2.647945000	-0.047705000	4.419957000

H	-3.196505000	0.737059000	4.936059000	H	-8.141775000	1.423335000	1.079126000
C	-1.596829000	0.306485000	3.561768000	C	-6.195068000	2.182958000	1.413362000
C	-1.229119000	1.756636000	3.353546000	H	-6.445907000	3.225892000	1.582437000
H	-1.282754000	2.033727000	2.294194000	C	-4.947882000	1.816468000	0.977608000
H	-0.203312000	1.961066000	3.680845000	H	-4.181286000	2.560536000	0.792202000
H	-1.900832000	2.413100000	3.914300000	³ TS ₂			
C	1.391301000	-0.214617000	2.444391000	Ni	-0.295350000	0.138652000	0.163654000
O	1.802883000	-0.329320000	3.625283000	N	0.133752000	-0.255591000	2.159910000
C	2.388216000	0.149367000	1.357380000	N	1.691013000	0.116731000	0.124391000
C	3.752792000	0.368652000	1.551874000	N	0.062374000	0.505057000	-1.851989000
H	4.177372000	0.286369000	2.545333000	C	-0.817462000	-0.452751000	3.197432000
C	4.535096000	0.691218000	0.436453000	C	-1.327929000	-1.748163000	3.438638000
H	5.599789000	0.866754000	0.556996000	C	-0.819132000	-2.931322000	2.649493000
C	3.954066000	0.787414000	-0.833711000	H	0.255426000	-3.082885000	2.802639000
H	4.537229000	1.033312000	-1.713172000	H	-1.336934000	-3.848075000	2.945564000
C	2.582753000	0.554774000	-0.949712000	H	-0.965956000	-2.786532000	1.572724000
C	1.785325000	0.611835000	-2.241611000	C	-2.314909000	-1.914886000	4.420984000
O	2.384103000	0.900967000	-3.306858000	H	-2.711347000	-2.909826000	4.609338000
C	-0.375512000	0.364945000	-3.194819000	C	-2.791841000	-0.825373000	5.154138000
C	-1.002688000	1.576408000	-3.562508000	H	-3.558785000	-0.969142000	5.910266000
C	-0.715033000	2.849130000	-2.801342000	C	-2.278370000	0.450499000	4.907890000
H	-0.943297000	2.736252000	-1.734942000	H	-2.646449000	1.301364000	5.476330000
H	-1.309288000	3.679875000	-3.192929000	C	-1.290167000	0.656365000	3.934208000
H	0.343043000	3.126966000	-2.868797000	C	-0.740036000	2.038885000	3.675021000
C	-1.897730000	1.576548000	-4.641876000	H	-0.873135000	2.331895000	2.627175000
H	-2.381271000	2.507863000	-4.928106000	H	0.335365000	2.086323000	3.881045000
C	-2.173958000	0.403250000	-5.348536000	H	-1.239187000	2.780804000	4.304770000
H	-2.870297000	0.418167000	-6.182711000	C	1.438999000	-0.327514000	2.467843000
C	-1.550730000	-0.789590000	-4.973789000	O	1.959729000	-0.548538000	3.586450000
H	-1.762884000	-1.706238000	-5.519412000	C	2.342766000	-0.107002000	1.267425000
C	-0.649856000	-0.828018000	-3.899737000	C	3.737939000	-0.125301000	1.279887000
C	0.015867000	-2.123674000	-3.499615000	H	4.269946000	-0.305898000	2.206366000
H	1.107091000	-2.056029000	-3.577018000	C	4.410513000	0.094015000	0.071195000
H	-0.319298000	-2.946834000	-4.137320000	H	5.495968000	0.085160000	0.049966000
H	-0.209555000	-2.382930000	-2.458409000	C	3.694818000	0.323924000	-1.110398000
F	-1.989343000	-0.354924000	-0.298481000	H	4.192805000	0.494882000	-2.057403000
C	-4.655223000	0.447812000	0.767805000	C	2.300953000	0.328467000	-1.043804000
H	-3.656243000	0.165042000	0.415156000	C	1.355036000	0.558131000	-2.210080000
C	-5.614173000	-0.568483000	0.991890000	O	1.837777000	0.765656000	-3.348668000
H	-5.344264000	-1.604040000	0.817196000	C	-0.929096000	0.710119000	-2.850268000
C	-6.869505000	-0.230727000	1.427567000	C	-1.385586000	2.018071000	-3.126146000
H	-7.623800000	-0.990886000	1.607326000	C	-0.787623000	3.205771000	-2.409546000
C	-7.235202000	1.173828000	1.663913000	H	-0.886369000	3.106647000	-1.322209000
H	-7.622280000	1.287873000	2.694926000	H	-1.280532000	4.133232000	-2.714945000

H	0.283214000	3.305082000	-2.620934000	C	-0.799130000	2.003101000	3.621079000
C	-2.404728000	2.194131000	-4.072971000	H	-0.934235000	2.298402000	2.574070000
H	-2.758533000	3.199707000	-4.288778000	H	0.274693000	2.066523000	3.830687000
C	-2.967051000	1.101160000	-4.737234000	H	-1.311092000	2.734959000	4.251973000
H	-3.756307000	1.252772000	-5.468693000	C	1.434559000	-0.325604000	2.464031000
C	-2.508731000	-0.187907000	-4.454467000	O	1.907203000	-0.539340000	3.596324000
H	-2.942917000	-1.042178000	-4.968894000	C	2.369311000	-0.079988000	1.294396000
C	-1.491191000	-0.402846000	-3.513667000	C	3.764065000	-0.057741000	1.318839000
C	-1.003459000	-1.800883000	-3.214063000	H	4.299255000	-0.228225000	2.245564000
H	0.063165000	-1.911988000	-3.440231000	C	4.435516000	0.191016000	0.113658000
H	-1.553888000	-2.539672000	-3.803721000	H	5.520624000	0.215197000	0.100154000
H	-1.126944000	-2.048939000	-2.153264000	C	3.724013000	0.408961000	-1.074335000
F	-2.260487000	0.304229000	0.158275000	H	4.228099000	0.602096000	-2.013966000
C	-3.914715000	-0.093212000	1.197298000	C	2.330486000	0.370483000	-1.015800000
H	-3.257195000	-0.237642000	2.044455000	C	1.358061000	0.573707000	-2.163698000
C	-4.395049000	-1.253776000	0.499490000	O	1.796755000	0.799455000	-3.307671000
H	-3.902218000	-2.204506000	0.670243000	C	-0.941884000	0.638886000	-2.783079000
C	-5.442583000	-1.148868000	-0.354676000	C	-1.485582000	1.918658000	-3.023586000
H	-5.809431000	-2.022166000	-0.886759000	C	-0.983164000	3.124183000	-2.264860000
C	-6.142589000	0.139017000	-0.584503000	H	-1.098137000	2.991842000	-1.182695000
H	-7.225246000	0.009427000	-0.419604000	H	-1.530673000	4.023924000	-2.559349000
H	-6.091911000	0.395374000	-1.657802000	H	0.082788000	3.300280000	-2.449237000
C	-5.646504000	1.284567000	0.217511000	C	-2.503566000	2.049245000	-3.979107000
H	-6.166037000	2.233061000	0.113838000	H	-2.926970000	3.032500000	-4.169926000
C	-4.597674000	1.164310000	1.068092000	C	-2.975635000	0.939407000	-4.683668000
H	-4.254980000	2.005823000	1.659970000	H	-3.765264000	1.055915000	-5.421015000
³ PC _F				C	-2.428960000	-0.321531000	-4.433947000
Ni	-0.232386000	0.100380000	0.171240000	H	-2.794591000	-1.188477000	-4.979141000
N	0.123222000	-0.279667000	2.111977000	C	-1.409751000	-0.491947000	-3.486187000
N	1.729114000	0.131765000	0.147232000	C	-0.827654000	-1.860109000	-3.220137000
N	0.059602000	0.477323000	-1.779174000	H	0.243636000	-1.893321000	-3.449285000
C	-0.841586000	-0.491145000	3.141493000	H	-1.327135000	-2.619412000	-3.828375000
C	-1.333374000	-1.793873000	3.375079000	H	-0.933344000	-2.141251000	-2.165811000
C	-0.802896000	-2.969793000	2.589584000	F	-2.373193000	0.075318000	-0.015908000
H	0.273653000	-3.103362000	2.745186000	C	-3.626002000	-0.003855000	0.873309000
H	-1.305778000	-3.893891000	2.887759000	H	-3.162865000	-0.196097000	1.840737000
H	-0.950699000	-2.831148000	1.512218000	C	-4.414777000	-1.147651000	0.353432000
C	-2.326383000	-1.973713000	4.348799000	H	-3.982636000	-2.137803000	0.467470000
H	-2.711502000	-2.973645000	4.533118000	C	-5.611828000	-0.978459000	-0.228338000
C	-2.822526000	-0.891106000	5.078754000	H	-6.160956000	-1.842916000	-0.594297000
H	-3.593718000	-1.045788000	5.828291000	C	-6.264397000	0.360159000	-0.383748000
C	-2.323837000	0.391629000	4.839706000	H	-7.266950000	0.338605000	0.070499000
H	-2.707717000	1.236513000	5.406271000	H	-6.459699000	0.554076000	-1.450365000
C	-1.330565000	0.612269000	3.874715000	C	-5.472871000	1.491535000	0.195406000

H	-5.917612000	2.482836000	0.147661000	C	2.452049000	0.204681000	-0.867465000
C	-4.275606000	1.326417000	0.777906000	C	1.646923000	0.297321000	-2.151896000
H	-3.740537000	2.169224000	1.206289000	O	2.237338000	0.378740000	-3.244679000
³ PC _H				C	-0.554598000	0.350367000	-3.073782000
Ni	-0.248348000	0.141718000	-0.024041000	C	-1.007260000	1.609876000	-3.521406000
N	-0.193709000	-0.021672000	1.964342000	C	-0.551832000	2.879142000	-2.840939000
N	1.691145000	0.125564000	0.220836000	H	-0.809634000	2.876171000	-1.775343000
N	0.304777000	0.276552000	-1.935813000	H	-1.016528000	3.754886000	-3.302412000
C	-1.296334000	-0.091858000	2.868995000	H	0.535686000	3.000561000	-2.901778000
C	-1.790526000	-1.351482000	3.272402000	C	-1.892009000	1.659636000	-4.608171000
C	-1.149177000	-2.626791000	2.779065000	H	-2.245141000	2.626430000	-4.958864000
H	-0.108818000	-2.707576000	3.114143000	C	-2.321452000	0.490401000	-5.240063000
H	-1.691724000	-3.501452000	3.148297000	H	-3.007786000	0.544705000	-6.080721000
H	-1.133130000	-2.669439000	1.684027000	C	-1.865992000	-0.749151000	-4.784918000
C	-2.885608000	-1.395283000	4.147225000	H	-2.199024000	-1.661735000	-5.273449000
H	-3.270478000	-2.361367000	4.464659000	C	-0.980766000	-0.839780000	-3.701233000
C	-3.482676000	-0.221202000	4.612555000	C	-0.497647000	-2.185125000	-3.213187000
H	-4.330376000	-0.271541000	5.290335000	H	0.591915000	-2.274170000	-3.290907000
C	-2.988614000	1.017625000	4.197699000	H	-0.945637000	-2.993396000	-3.797908000
H	-3.452347000	1.933587000	4.555634000	H	-0.752642000	-2.343338000	-2.158756000
C	-1.894145000	1.103052000	3.324973000	F	-2.416770000	0.147125000	-0.507374000
C	-1.359566000	2.447558000	2.891121000	C	-6.272339000	-0.385843000	-1.501408000
H	-1.375996000	2.553252000	1.800128000	H	-6.772472000	-0.393557000	-2.465623000
H	-0.318564000	2.585730000	3.204825000	C	-5.733862000	-1.570045000	-0.985828000
H	-1.953660000	3.258167000	3.322059000	H	-5.817357000	-2.495695000	-1.547554000
C	1.055078000	-0.052676000	2.505148000	C	-5.089314000	-1.561264000	0.256490000
O	1.353123000	-0.135226000	3.710445000	H	-4.674949000	-2.479587000	0.662312000
C	2.155794000	0.027758000	1.463028000	C	-4.978417000	-0.363781000	0.981981000
C	3.533935000	0.007305000	1.679796000	H	-3.176858000	-0.052519000	0.030800000
H	3.931303000	-0.072187000	2.684845000	H	-4.509790000	-0.362793000	1.962795000
C	4.372693000	0.091167000	0.559260000	C	-5.522082000	0.822005000	0.460778000
H	5.449477000	0.077501000	0.695078000	H	-5.440888000	1.746795000	1.024456000
C	3.840829000	0.190913000	-0.734386000	C	-6.165736000	0.809909000	-0.780669000
H	4.477245000	0.254883000	-1.609186000	H	-6.584037000	1.727143000	-1.184583000

III-2) desaturation vs. halogenation by AgF

² IM0				C	5.313748000	0.036851000	-0.130347000
Ag	3.229080000	-0.185683000	0.917571000	H	5.077141000	-0.597768000	-0.981641000
F	1.199998000	-0.219785000	1.463482000	C	5.642328000	1.484452000	-0.411144000
C	6.189680000	0.223161000	2.160422000	H	4.798247000	1.998959000	-0.892959000
H	6.432731000	-0.259075000	3.100653000	H	6.437123000	1.515520000	-1.182194000
C	5.650995000	-0.550260000	1.086823000	C	6.103177000	2.241218000	0.801640000
H	5.578065000	-1.629636000	1.198880000	H	6.258236000	3.311383000	0.696436000

C	6.378544000	1.619100000	1.992957000	C	5.313748000	0.036851000	-0.130347000
H	6.747839000	2.204368000	2.830897000	H	5.077141000	-0.597768000	-0.981641000
² TS0 _H				C	5.642328000	1.484452000	-0.411144000
Ag	3.029024000	-0.757907000	0.852102000	H	4.798247000	1.998959000	-0.892959000
F	2.733181000	1.690786000	0.038606000	H	6.437123000	1.515520000	-1.182194000
C	6.445087000	0.246434000	2.205508000	C	6.103177000	2.241218000	0.801640000
H	6.909127000	-0.121025000	3.115584000	H	6.258236000	3.311383000	0.696436000
C	5.898984000	-0.650987000	1.287342000	C	6.378544000	1.619100000	1.992957000
H	5.978159000	-1.721010000	1.463330000	H	6.747839000	2.204368000	2.830897000
C	5.292016000	-0.195766000	0.095464000	² TS0 _F			
H	5.120571000	-0.907638000	-0.709907000	Ag	2.924634000	0.027509000	-0.344287000
C	5.233755000	1.243510000	-0.202638000	F	3.929657000	0.161231000	3.019953000
H	3.936913000	1.560657000	-0.090422000	C	5.571766000	0.174054000	2.185890000
H	5.338603000	1.513032000	-1.260436000	H	6.001392000	-0.314570000	3.052740000
C	5.894092000	2.121454000	0.752782000	C	5.418391000	-0.600386000	0.997908000
H	5.930332000	3.186330000	0.534205000	H	5.326830000	-1.679079000	1.090301000
C	6.424813000	1.647782000	1.929367000	C	5.280306000	-0.000352000	-0.259439000
H	6.872279000	2.337150000	2.640589000	H	5.345888000	-0.643828000	-1.135014000
³ PC0 _H				C	5.755584000	1.426299000	-0.450673000
Ag	2.255775000	-0.437497000	3.243125000	H	5.159906000	1.967572000	-1.192103000
F	2.805062000	1.473114000	-0.254647000	H	6.771353000	1.385536000	-0.890957000
C	6.126546000	0.146516000	2.089880000	C	5.840535000	2.202709000	0.831050000
H	6.210678000	-0.306444000	3.073421000	H	6.012763000	3.273991000	0.755546000
C	6.035796000	-0.665419000	0.952796000	C	5.791856000	1.612131000	2.042192000
H	6.049038000	-1.746612000	1.054568000	H	5.906069000	2.199988000	2.948368000
C	5.927495000	-0.083963000	-0.314856000	³ PC0 _F			
H	5.859619000	-0.711552000	-1.198699000	Ag	2.353240000	0.819870000	-2.913921000
C	5.908129000	1.313274000	-0.445731000	F	4.745205000	0.043893000	3.423140000
H	3.743318000	1.405957000	-0.214017000	C	5.834157000	0.217856000	2.462749000
H	5.850284000	1.766168000	-1.432180000	H	6.706947000	-0.126391000	3.028286000
C	5.998139000	2.124970000	0.695517000	C	5.548485000	-0.663751000	1.289863000
H	5.986123000	3.206314000	0.593734000	H	5.488714000	-1.731093000	1.488373000
C	6.106459000	1.539984000	1.962566000	C	5.370973000	-0.184300000	0.051264000
H	6.174473000	2.167994000	2.845999000	H	5.162924000	-0.869037000	-0.768280000
³ IM0				C	5.455567000	1.274290000	-0.286858000
Ag	3.229080000	-0.185683000	0.917571000	H	4.516193000	1.593035000	-0.768673000
F	1.199998000	-0.219785000	1.463482000	H	6.219882000	1.432621000	-1.063481000
C	6.189680000	0.223161000	2.160422000	C	5.745658000	2.148998000	0.896021000
H	6.432731000	-0.259075000	3.100653000	H	5.823469000	3.218613000	0.712459000
C	5.650995000	-0.550260000	1.086823000	C	5.922643000	1.673982000	2.136615000
H	5.578065000	-1.629636000	1.198880000	H	6.142875000	2.344219000	2.963921000

IV) The nature of the AgF-binding Ni(III)-F oxidant 1_{F-Ag-F}

2				C	-0.795723000	-0.215598000	-5.221724000
Ni	1.263787000	0.851906000	-0.773002000	H	-1.153492000	-1.135181000	-5.676994000
N	1.304395000	0.800370000	1.105911000	C	0.182559000	-0.286519000	-4.221369000
N	3.106505000	0.789847000	-0.617272000	C	0.745752000	-1.617636000	-3.785168000
N	1.621403000	0.876227000	-2.619108000	H	1.814939000	-1.694106000	-4.014749000
C	0.157248000	0.762974000	1.950848000	H	0.233770000	-2.437588000	-4.294980000
C	-0.334838000	-0.486764000	2.387636000	H	0.637429000	-1.766260000	-2.705314000
C	0.346886000	-1.775568000	1.995175000	F	-0.573023000	0.972385000	-0.932821000
H	1.358743000	-1.836421000	2.412510000	F	-3.273667000	-2.381849000	-1.079953000
H	-0.218336000	-2.636528000	2.360627000	Ag	-1.936264000	-0.759131000	-1.006911000
H	0.441222000	-1.865361000	0.907531000	42			
C	-1.470902000	-0.498830000	3.207353000	Ni	1.034885000	0.869803000	-0.899274000
H	-1.863139000	-1.451614000	3.552710000	N	1.361537000	0.459732000	1.320746000
C	-2.100669000	0.690677000	3.579787000	N	2.996516000	1.111081000	-0.640441000
H	-2.981982000	0.662467000	4.214293000	N	1.583401000	0.913413000	-2.809204000
C	-1.599177000	1.916309000	3.135444000	C	0.316134000	0.489076000	2.181909000
H	-2.089671000	2.840876000	3.427875000	C	-0.641180000	-0.603404000	2.096018000
C	-0.466461000	1.975977000	2.313761000	C	-0.416991000	-1.752222000	1.153261000
C	0.076750000	3.302737000	1.841528000	H	0.616045000	-2.108314000	1.190015000
H	0.096593000	3.360292000	0.747896000	H	-1.084495000	-2.580204000	1.402455000
H	1.103702000	3.462995000	2.189313000	H	-0.623666000	-1.456221000	0.118756000
H	-0.537956000	4.125508000	2.215439000	C	-1.721497000	-0.608419000	2.963986000
C	2.561725000	0.749304000	1.672979000	H	-2.418906000	-1.439810000	2.943096000
O	2.824822000	0.709916000	2.873192000	C	-1.920330000	0.439631000	3.875953000
C	3.627330000	0.750314000	0.609748000	H	-2.782730000	0.422923000	4.535191000
C	5.009936000	0.713926000	0.765792000	C	-1.022385000	1.520082000	3.935540000
H	5.441734000	0.681308000	1.759307000	H	-1.221642000	2.337939000	4.621179000
C	5.803544000	0.720255000	-0.389170000	C	0.097537000	1.577873000	3.121611000
H	6.884035000	0.692537000	-0.297972000	C	0.982202000	2.795847000	3.163594000
C	5.216239000	0.761656000	-1.660820000	H	1.300626000	3.103612000	2.163031000
H	5.809993000	0.767289000	-2.567429000	H	1.886171000	2.608700000	3.751107000
C	3.827008000	0.796460000	-1.739362000	H	0.445368000	3.630406000	3.620047000
C	2.956693000	0.846611000	-2.966724000	C	2.659089000	0.751499000	1.706400000
O	3.419785000	0.862638000	-4.105476000	O	3.091518000	0.632360000	2.854004000
C	0.634415000	0.921053000	-3.646389000	C	3.576705000	1.080340000	0.562382000
C	0.123436000	2.173919000	-4.048775000	C	4.946155000	1.307804000	0.701753000
C	0.621100000	3.455059000	-3.424543000	H	5.402460000	1.281565000	1.684004000
H	0.459631000	3.461372000	-2.341137000	C	5.692236000	1.558011000	-0.454560000
H	0.103634000	4.318000000	-3.851324000	H	6.758725000	1.743661000	-0.380514000
H	1.696243000	3.591273000	-3.588551000	C	5.069019000	1.550036000	-1.706853000
C	-0.853385000	2.197443000	-5.052188000	H	5.622550000	1.714324000	-2.623709000
H	-1.255413000	3.153534000	-5.376623000	C	3.695360000	1.312298000	-1.762151000
C	-1.312139000	1.014185000	-5.635699000	C	2.885222000	1.203069000	-3.039607000
H	-2.071735000	1.050527000	-6.411459000	O	3.450018000	1.353297000	-4.137819000

C	0.713897000	0.705833000	-3.919123000	C	0.297122000	1.685689000	3.242316000
C	0.104201000	1.809666000	-4.553938000	C	1.398880000	2.711287000	3.320880000
C	0.395227000	3.220149000	-4.100171000	H	1.747842000	3.015237000	2.329473000
H	0.166867000	3.352652000	-3.036320000	H	2.263621000	2.320748000	3.865337000
H	-0.198599000	3.940618000	-4.669312000	H	1.040565000	3.602148000	3.841573000
H	1.453262000	3.473041000	-4.232515000	C	2.592155000	0.496551000	1.647899000
C	-0.780546000	1.567695000	-5.614064000	O	2.983940000	0.211825000	2.783848000
H	-1.253834000	2.411358000	-6.110360000	C	3.515063000	0.729688000	0.505311000
C	-1.060477000	0.265810000	-6.036231000	C	4.882347000	0.819087000	0.661412000
H	-1.749383000	0.095455000	-6.858973000	H	5.321341000	0.699186000	1.645131000
C	-0.453826000	-0.816127000	-5.394298000	C	5.682583000	1.084719000	-0.489580000
H	-0.670598000	-1.830778000	-5.719274000	H	6.759812000	1.167402000	-0.393041000
C	0.437736000	-0.616094000	-4.331187000	C	5.073414000	1.240141000	-1.720747000
C	1.087760000	-1.790819000	-3.639173000	H	5.654278000	1.448324000	-2.613612000
H	2.180796000	-1.742901000	-3.703473000	C	3.667657000	1.122810000	-1.838990000
H	0.762533000	-2.733477000	-4.087799000	C	2.937848000	1.257139000	-3.061094000
H	0.836320000	-1.815644000	-2.572116000	O	3.418453000	1.584707000	-4.176239000
F	-0.886866000	0.956339000	-0.914161000	C	0.750546000	0.714069000	-3.965804000
F	-5.059771000	0.516949000	-0.067103000	C	-0.471075000	1.435000000	-4.238497000
Ag	-3.009938000	0.728543000	-0.479343000	C	-0.800255000	2.697344000	-3.488643000
δ^2				H	-0.909348000	2.502308000	-2.418118000
Ni	0.969396000	0.877289000	-0.861122000	H	-1.731148000	3.129434000	-3.864390000
N	1.237519000	0.507226000	1.292436000	H	-0.004571000	3.441034000	-3.609371000
N	2.910456000	0.867805000	-0.705942000	C	-1.272892000	1.016202000	-5.294843000
N	1.508121000	1.123685000	-2.907809000	H	-2.172392000	1.576593000	-5.530836000
C	0.260796000	0.652578000	2.223573000	C	-0.927284000	-0.097941000	-6.068430000
C	-0.879486000	-0.239845000	2.132291000	H	-1.574372000	-0.416861000	-6.880176000
C	-0.881225000	-1.382921000	1.155046000	C	0.250761000	-0.807971000	-5.796836000
H	0.005339000	-2.013225000	1.280841000	H	0.488100000	-1.691429000	-6.382134000
H	-1.769055000	-2.001467000	1.305799000	C	1.114525000	-0.424972000	-4.777248000
H	-0.885569000	-1.016281000	0.124813000	C	2.316227000	-1.285566000	-4.468428000
C	-1.913817000	-0.093713000	3.045695000	H	3.241517000	-0.822899000	-4.822637000
H	-2.752565000	-0.782214000	3.016003000	H	2.213050000	-2.257445000	-4.956710000
C	-1.881833000	0.915409000	4.018295000	H	2.427155000	-1.457576000	-3.393489000
H	-2.710378000	1.023636000	4.712291000	F	-0.944365000	1.088525000	-0.836792000
C	-0.789235000	1.794182000	4.099039000	F	-5.141387000	1.353132000	0.038530000
H	-0.802019000	2.591489000	4.836438000	Ag	-3.091142000	1.223871000	-0.389064000

V) C-H bond activation of CHD by the proximal fluorine of 1_F-Ag-F

${}^3\text{RC}_p$				N	2.210737000	-0.098082000	-2.471669000
Ni	1.881347000	-0.025742000	-0.622509000	C	0.811513000	0.101432000	2.112713000
N	1.943776000	-0.020095000	1.255436000	C	0.166744000	-1.067728000	2.570612000
N	3.716828000	-0.206616000	-0.487709000	C	0.671349000	-2.437550000	2.185625000

H	1.686700000	-2.610951000	2.560494000	F	-3.048541000	-2.760494000	-1.155541000
H	0.023872000	-3.215958000	2.597000000	Ag	-1.522935000	-1.324722000	-0.959816000
H	0.704969000	-2.561370000	1.097579000	H	-3.398372000	4.709129000	-4.026926000
C	-0.950577000	-0.922466000	3.403296000	C	-4.071918000	4.516433000	-3.176599000
H	-1.458011000	-1.811883000	3.767116000	H	-4.789281000	5.352235000	-3.203923000
C	-1.415876000	0.343310000	3.766342000	C	-4.798321000	3.211071000	-3.384299000
H	-2.284780000	0.437829000	4.411464000	H	-5.380249000	3.112897000	-4.299473000
C	-0.765718000	1.487952000	3.299286000	C	-4.759415000	2.194933000	-2.512517000
H	-1.128757000	2.472048000	3.583554000	H	-5.309651000	1.280186000	-2.727255000
C	0.354787000	1.389874000	2.464562000	C	-3.983864000	2.234656000	-1.220012000
C	1.054843000	2.629547000	1.962489000	H	-3.270589000	1.394899000	-1.185496000
H	1.051018000	2.675888000	0.867736000	H	-4.661249000	2.048480000	-0.371256000
H	2.103194000	2.657496000	2.280518000	C	-3.252267000	3.537205000	-1.015317000
H	0.563862000	3.529094000	2.342333000	H	-2.667538000	3.633970000	-0.101882000
C	3.202282000	-0.136862000	1.809382000	C	-3.291405000	4.553737000	-1.886626000
O	3.479613000	-0.148628000	3.006989000	H	-2.738002000	5.467026000	-1.673289000
C	4.250237000	-0.248330000	0.733905000	² TS _{pH}			
C	5.628596000	-0.381558000	0.874385000	Ni	1.622828000	0.352584000	-0.814303000
H	6.071126000	-0.415807000	1.863112000	N	1.544535000	0.134729000	1.166000000
C	6.404039000	-0.468811000	-0.289655000	N	3.456307000	-0.197210000	-0.502416000
H	7.480783000	-0.573312000	-0.210455000	N	2.248000000	0.331198000	-2.697766000
C	5.803383000	-0.425108000	-1.554987000	C	0.402547000	0.336399000	1.992145000
H	6.382854000	-0.494304000	-2.468204000	C	-0.443626000	-0.755263000	2.287715000
C	4.419451000	-0.291034000	-1.618026000	C	-0.119746000	-2.140372000	1.781257000
C	3.535625000	-0.231049000	-2.835312000	H	0.833621000	-2.500490000	2.184744000
O	3.980446000	-0.294158000	-3.979607000	H	-0.898946000	-2.851010000	2.069700000
C	1.209768000	-0.060095000	-3.485314000	H	-0.028239000	-2.156363000	0.689471000
C	0.746665000	1.192121000	-3.943171000	C	-1.585467000	-0.527218000	3.068371000
C	1.307186000	2.478575000	-3.387222000	H	-2.241048000	-1.362229000	3.303038000
H	1.160903000	2.541015000	-2.303342000	C	-1.887531000	0.750668000	3.545495000
H	0.820669000	3.342067000	-3.847819000	H	-2.776001000	0.911264000	4.150051000
H	2.384776000	2.560114000	-3.570319000	C	-1.041812000	1.821095000	3.243692000
C	-0.242479000	1.208367000	-4.934538000	H	-1.273151000	2.816193000	3.615741000
H	-0.607276000	2.163703000	-5.302106000	C	0.110167000	1.633925000	2.467176000
C	-0.761140000	0.018684000	-5.451113000	C	1.024540000	2.793855000	2.152666000
H	-1.530211000	0.049467000	-6.217718000	H	1.133527000	2.936457000	1.071373000
C	-0.294576000	-1.210416000	-4.979992000	H	2.032023000	2.629717000	2.551757000
H	-0.701236000	-2.134967000	-5.380894000	H	0.636781000	3.721154000	2.583384000
C	0.695136000	-1.274304000	-3.990408000	C	2.712147000	-0.237995000	1.755786000
C	1.201959000	-2.605832000	-3.490394000	O	2.922309000	-0.420976000	2.967318000
H	2.261267000	-2.748367000	-3.733770000	C	3.831560000	-0.434862000	0.752444000
H	0.640407000	-3.426016000	-3.944600000	C	5.143144000	-0.830084000	1.013927000
H	1.107641000	-2.689041000	-2.402131000	H	5.462241000	-1.026926000	2.030755000
F	0.052129000	0.201299000	-0.748737000	C	6.017188000	-0.962479000	-0.073890000

H	7.044280000	-1.268228000	0.097963000	N	2.190678000	0.209623000	-2.637418000
C	5.580441000	-0.709013000	-1.381470000	C	0.419262000	0.129778000	1.932776000
H	6.240667000	-0.811076000	-2.234820000	C	-0.376004000	-1.026422000	2.093043000
C	4.253944000	-0.318324000	-1.561073000	C	0.045893000	-2.347205000	1.493819000
C	3.555973000	-0.006104000	-2.869757000	H	1.038240000	-2.647049000	1.848443000
O	4.180802000	-0.077925000	-3.941323000	H	-0.663709000	-3.135644000	1.758938000
C	1.473815000	0.637537000	-3.854020000	H	0.103198000	-2.296450000	0.400821000
C	1.411335000	1.970145000	-4.317215000	C	-1.560086000	-0.928629000	2.837482000
C	2.186193000	3.065363000	-3.624064000	H	-2.177498000	-1.813773000	2.968225000
H	1.914186000	3.139401000	-2.564875000	C	-1.949076000	0.282479000	3.413806000
H	1.994675000	4.033366000	-4.095224000	H	-2.869412000	0.341817000	3.988294000
H	3.265623000	2.878738000	-3.660594000	C	-1.150039000	1.416691000	3.252134000
C	0.617401000	2.254846000	-5.436934000	H	-1.449818000	2.359560000	3.702860000
H	0.565245000	3.277648000	-5.802102000	C	0.040031000	1.361443000	2.512702000
C	-0.101398000	1.246883000	-6.083979000	C	0.899567000	2.592763000	2.349460000
H	-0.712788000	1.483413000	-6.950537000	H	1.119590000	2.793325000	1.294944000
C	-0.033447000	-0.065866000	-5.611241000	H	1.863437000	2.472733000	2.857049000
H	-0.592644000	-0.852193000	-6.112309000	H	0.402624000	3.470757000	2.770995000
C	0.749284000	-0.391288000	-4.494887000	C	2.804204000	-0.043411000	1.762842000
C	0.820104000	-1.813064000	-3.991240000	O	3.038617000	-0.115719000	2.983875000
H	1.843509000	-2.203225000	-4.033075000	C	3.924970000	-0.063617000	0.753357000
H	0.183086000	-2.468874000	-4.590915000	C	5.292018000	-0.163586000	0.996739000
H	0.496982000	-1.884341000	-2.946399000	H	5.651330000	-0.239473000	2.016373000
F	-0.230660000	0.981200000	-1.124905000	C	6.163395000	-0.161487000	-0.099709000
F	-2.557280000	-2.837101000	-1.536460000	H	7.233610000	-0.237785000	0.062611000
Ag	-3.168466000	-0.885837000	-1.065763000	C	5.663152000	-0.062426000	-1.404128000
H	-4.908333000	0.914781000	-3.029823000	H	6.313782000	-0.059038000	-2.270863000
C	-4.778502000	1.688695000	-2.255874000	C	4.285123000	0.033984000	-1.576761000
H	-5.767659000	2.176821000	-2.221061000	C	3.519618000	0.148033000	-2.871861000
C	-4.503889000	1.069667000	-0.910743000	O	4.112012000	0.173421000	-3.967373000
H	-5.318140000	0.525719000	-0.435884000	C	1.291096000	0.344475000	-3.735424000
C	-3.383854000	1.389643000	-0.179003000	C	1.020099000	1.627056000	-4.260016000
H	-3.294230000	1.057831000	0.853338000	C	1.702372000	2.851879000	-3.698758000
C	-2.355829000	2.306966000	-0.697641000	H	1.559302000	2.929060000	-2.615200000
H	-1.273055000	1.607452000	-0.935486000	H	1.311408000	3.761113000	-4.163553000
H	-1.852361000	2.904385000	0.070154000	H	2.784027000	2.820904000	-3.873492000
C	-2.655584000	2.989422000	-1.944810000	C	0.109928000	1.739158000	-5.320266000
H	-1.961249000	3.749857000	-2.291456000	H	-0.103931000	2.721972000	-5.733069000
C	-3.750757000	2.683366000	-2.692982000	C	-0.520994000	0.610198000	-5.847874000
H	-3.927075000	3.198635000	-3.633161000	H	-1.225198000	0.713477000	-6.668917000
² IM _p				C	-0.244702000	-0.651806000	-5.316934000
Ni	1.680569000	0.146407000	-0.780452000	H	-0.733610000	-1.531551000	-5.727830000
N	1.605855000	0.056801000	1.146003000	C	0.660713000	-0.805732000	-4.257698000
N	3.481192000	0.030540000	-0.506213000	C	0.962296000	-2.175402000	-3.696844000

H	2.028485000	-2.415108000	-3.777789000	C	4.082821000	-0.210082000	0.644021000
H	0.398932000	-2.944975000	-4.231463000	C	5.435712000	-0.477574000	0.858866000
H	0.703834000	-2.241419000	-2.633854000	H	5.821391000	-0.494136000	1.871179000
F	-0.321134000	0.159044000	-1.121327000	C	6.252276000	-0.720776000	-0.249675000
F	-3.591844000	-2.387100000	-2.101811000	H	7.307625000	-0.931828000	-0.111167000
Ag	-3.824569000	-0.383338000	-1.523720000	C	5.708848000	-0.699205000	-1.538221000
H	-4.544374000	2.105525000	-3.398673000	H	6.310779000	-0.891607000	-2.418136000
C	-4.295844000	2.673713000	-2.488746000	C	4.347618000	-0.425599000	-1.671405000
H	-5.032119000	3.498933000	-2.497986000	C	3.629397000	-0.400383000	-2.990625000
C	-4.525103000	1.845095000	-1.248270000	O	4.246437000	-0.524433000	-4.050589000
H	-5.548458000	1.552616000	-1.022031000	C	1.411065000	-0.410197000	-3.900231000
C	-3.549685000	1.727141000	-0.270157000	C	0.461132000	0.619654000	-4.288168000
H	-3.794340000	1.269101000	0.685184000	C	0.522398000	1.990029000	-3.675842000
C	-2.254023000	2.332506000	-0.431560000	H	0.204804000	1.955997000	-2.628650000
H	-0.883272000	0.901213000	-0.896939000	H	-0.136755000	2.674888000	-4.214104000
H	-1.569275000	2.334460000	0.412580000	H	1.539857000	2.392198000	-3.700005000
C	-1.978447000	3.095338000	-1.595404000	C	-0.437272000	0.342757000	-5.307987000
H	-1.007677000	3.572426000	-1.696709000	H	-1.121811000	1.117280000	-5.639165000
C	-2.914199000	3.245324000	-2.590532000	C	-0.462446000	-0.915309000	-5.926879000
H	-2.677774000	3.831347000	-3.473749000	H	-1.184233000	-1.114476000	-6.713082000
⁴ RC _p				C	0.431464000	-1.926691000	-5.533254000
Ni	1.639582000	0.233525000	-0.739996000	H	0.366693000	-2.904102000	-6.001499000
N	1.834498000	0.263191000	1.276467000	C	1.378454000	-1.712261000	-4.544368000
N	3.586768000	-0.186269000	-0.598345000	C	2.264013000	-2.848936000	-4.105290000
N	2.278359000	-0.113331000	-2.900662000	H	3.260857000	-2.767741000	-4.549495000
C	0.768379000	0.495684000	2.189524000	H	1.829832000	-3.801794000	-4.416036000
C	-0.016788000	-0.592676000	2.629435000	H	2.390452000	-2.871685000	-3.018724000
C	0.294215000	-1.999090000	2.175064000	F	-0.256070000	0.512026000	-0.973322000
H	1.308811000	-2.299711000	2.459858000	F	-2.785918000	-2.751474000	-2.070510000
H	-0.407644000	-2.713127000	2.614854000	Ag	-1.545783000	-1.151506000	-1.522549000
H	0.231554000	-2.088767000	1.083673000	H	-2.867079000	5.456638000	-2.032188000
C	-1.091688000	-0.341696000	3.493567000	C	-3.838397000	4.984825000	-1.813465000
H	-1.699573000	-1.174783000	3.838198000	H	-4.553152000	5.823280000	-1.813025000
C	-1.388738000	0.957276000	3.913113000	C	-4.192931000	4.010497000	-2.908775000
H	-2.225598000	1.136495000	4.582620000	H	-4.236562000	4.405557000	-3.922628000
C	-0.607152000	2.025235000	3.465624000	C	-4.450837000	2.714122000	-2.691826000
H	-0.837327000	3.037623000	3.788762000	H	-4.701874000	2.067704000	-3.531417000
C	0.475601000	1.814468000	2.600399000	C	-4.417278000	2.074124000	-1.326793000
C	1.312754000	2.974579000	2.116178000	H	-3.707210000	1.230866000	-1.325658000
H	1.315658000	3.035548000	1.021521000	H	-5.391165000	1.607587000	-1.108380000
H	2.357917000	2.874336000	2.430313000	C	-4.058390000	3.047277000	-0.232259000
H	0.930000000	3.920538000	2.509279000	H	-4.012749000	2.651838000	0.781204000
C	3.072771000	0.050315000	1.746959000	C	-3.800455000	4.343612000	-0.448906000
O	3.458245000	0.035207000	2.936025000	H	-3.547922000	4.989557000	0.390580000

⁴ TS _{pH}				C	-0.043708000	-0.740522000	-5.737718000
Ni	1.398367000	0.180934000	-0.815595000	H	-0.394841000	-1.615886000	-6.279137000
N	1.474469000	0.202903000	1.244626000	C	0.797405000	-0.917563000	-4.629612000
N	3.322922000	-0.180256000	-0.523662000	C	1.216896000	-2.303481000	-4.200789000
N	2.054640000	0.078249000	-2.765369000	H	2.294628000	-2.450341000	-4.335834000
C	0.389477000	0.486636000	2.120563000	H	0.694117000	-3.066192000	-4.784666000
C	-0.455896000	-0.559242000	2.551871000	H	1.003690000	-2.477090000	-3.139904000
C	-0.172831000	-1.988666000	2.155523000	F	-0.643773000	0.242102000	-1.137525000
H	0.805976000	-2.318587000	2.521927000	F	-2.781987000	-3.430261000	-2.105136000
H	-0.932303000	-2.662779000	2.561383000	Ag	-1.710893000	-1.670324000	-1.666768000
H	-0.156908000	-2.107650000	1.065906000	H	-3.994745000	2.460021000	-3.574053000
C	-1.557104000	-0.248170000	3.363061000	C	-4.084008000	2.840927000	-2.537435000
H	-2.211301000	-1.050065000	3.696962000	H	-4.942085000	3.531852000	-2.625374000
C	-1.819695000	1.068839000	3.746583000	C	-4.429013000	1.717648000	-1.624509000
H	-2.677150000	1.294777000	4.374549000	H	-5.356542000	1.182888000	-1.807030000
C	-0.972040000	2.094545000	3.319209000	C	-3.627620000	1.371646000	-0.575492000
H	-1.169979000	3.121062000	3.618645000	H	-3.905919000	0.550935000	0.078830000
C	0.137897000	1.822470000	2.506020000	C	-2.363438000	2.050817000	-0.336285000
C	1.048112000	2.938203000	2.049566000	H	-1.513456000	1.207401000	-0.727947000
H	1.116924000	2.977053000	0.956069000	H	-2.004350000	2.055292000	0.700297000
H	2.068781000	2.800402000	2.424203000	C	-2.066302000	3.235728000	-1.127279000
H	0.684566000	3.906575000	2.404762000	H	-1.176455000	3.809188000	-0.885757000
C	2.686748000	-0.028660000	1.780439000	C	-2.854611000	3.599644000	-2.178485000
O	3.001794000	-0.060193000	2.991679000	H	-2.606465000	4.472443000	-2.775362000
C	3.761608000	-0.264361000	0.732963000	⁴ IM _p			
C	5.108341000	-0.534909000	0.977180000	Ni	1.549475000	0.214078000	-0.784146000
H	5.473136000	-0.605515000	1.995076000	N	1.539648000	0.208409000	1.198735000
C	5.954974000	-0.706575000	-0.125863000	N	3.438960000	-0.172468000	-0.486128000
H	7.007804000	-0.918328000	0.033192000	N	2.132029000	0.115057000	-2.675703000
C	5.458296000	-0.605094000	-1.431901000	C	0.427164000	0.460083000	2.058280000
H	6.096867000	-0.731053000	-2.298208000	C	-0.461319000	-0.592304000	2.366438000
C	4.099432000	-0.333882000	-1.596809000	C	-0.219057000	-1.986928000	1.839459000
C	3.366844000	-0.179352000	-2.918857000	H	0.752137000	-2.377048000	2.164026000
O	4.012680000	-0.290128000	-3.985369000	H	-0.995099000	-2.673412000	2.188887000
C	1.248560000	0.223882000	-3.929085000	H	-0.215383000	-2.007015000	0.742757000
C	0.863314000	1.519342000	-4.339379000	C	-1.572845000	-0.318828000	3.176817000
C	1.359884000	2.737949000	-3.597501000	H	-2.260607000	-1.124937000	3.420514000
H	1.039078000	2.729033000	-2.548999000	C	-1.802722000	0.966174000	3.672782000
H	0.982876000	3.654835000	-4.059597000	H	-2.668187000	1.162794000	4.299592000
H	2.454751000	2.784798000	-3.589586000	C	-0.915429000	1.998175000	3.358145000
C	0.021522000	1.656024000	-5.452463000	H	-1.091674000	3.000172000	3.741844000
H	-0.273995000	2.652183000	-5.773508000	C	0.207198000	1.765035000	2.551018000
C	-0.433558000	0.535513000	-6.151361000	C	1.159605000	2.888623000	2.216694000
H	-1.086166000	0.655471000	-7.011902000	H	1.264860000	3.015628000	1.133001000

H	2.163141000	2.693912000	2.611602000	C	-2.312464000	3.372239000	-1.422720000
H	0.807754000	3.833684000	2.639562000	H	-1.473609000	4.063008000	-1.403143000
C	2.743268000	-0.049143000	1.782826000	C	-3.150390000	3.348977000	-2.504306000
O	2.992014000	-0.113115000	2.999523000	H	-2.979718000	4.019171000	-3.342355000
C	3.855322000	-0.271317000	0.772606000	³ IM' _p			
C	5.198408000	-0.550389000	1.027331000	Ni	1.016428000	0.753505000	-0.806956000
H	5.559539000	-0.636233000	2.045483000	N	1.247177000	0.736589000	1.256368000
C	6.051560000	-0.712349000	-0.074035000	N	2.996074000	0.733087000	-0.653773000
H	7.101937000	-0.929983000	0.091578000	N	1.563915000	0.827115000	-2.811405000
C	5.569396000	-0.596988000	-1.386065000	C	0.195747000	0.766754000	2.213564000
H	6.218970000	-0.719351000	-2.244841000	C	-0.346353000	-0.442408000	2.703031000
C	4.213124000	-0.317910000	-1.557196000	C	0.225104000	-1.771369000	2.268690000
C	3.455492000	-0.147096000	-2.862538000	H	1.280122000	-1.865020000	2.550112000
O	4.059167000	-0.249611000	-3.944938000	H	-0.323652000	-2.599194000	2.726809000
C	1.312679000	0.271914000	-3.834948000	H	0.176828000	-1.890711000	1.179628000
C	1.020949000	1.570977000	-4.302482000	C	-1.422634000	-0.387466000	3.600492000
C	1.611749000	2.785203000	-3.625489000	H	-1.842150000	-1.316115000	3.980489000
H	1.310733000	2.843686000	-2.572717000	C	-1.958255000	0.836381000	4.009198000
H	1.287095000	3.702944000	-4.123657000	H	-2.792295000	0.863092000	4.705318000
H	2.707255000	2.760401000	-3.638223000	C	-1.414146000	2.025867000	3.517869000
C	0.172574000	1.712792000	-5.410035000	H	-1.824831000	2.981587000	3.835616000
H	-0.055188000	2.710466000	-5.777496000	C	-0.337111000	2.010313000	2.619691000
C	-0.376779000	0.595455000	-6.042684000	C	0.246557000	3.301268000	2.095529000
H	-1.033367000	0.720822000	-6.899308000	H	0.197187000	3.347459000	1.001058000
C	-0.078186000	-0.684252000	-5.569114000	H	1.303864000	3.402692000	2.365495000
H	-0.502987000	-1.556501000	-6.059972000	H	-0.291170000	4.164075000	2.499086000
C	0.767143000	-0.867720000	-4.465336000	C	2.515565000	0.698467000	1.696442000
C	1.090528000	-2.257098000	-3.968502000	O	2.926357000	0.677480000	2.880818000
H	2.158544000	-2.480261000	-4.073571000	C	3.532469000	0.689418000	0.567554000
H	0.531349000	-3.009789000	-4.530836000	C	4.919484000	0.649978000	0.715345000
H	0.846293000	-2.371272000	-2.906105000	H	5.358895000	0.614676000	1.705223000
F	-0.757967000	0.455842000	-1.203492000	C	5.705726000	0.658022000	-0.443771000
F	-3.266688000	-3.175223000	-2.392504000	H	6.787763000	0.626870000	-0.360163000
Ag	-2.095827000	-1.478453000	-1.876192000	C	5.108825000	0.708202000	-1.709846000
H	-4.230533000	1.770853000	-3.475537000	H	5.697312000	0.718967000	-2.619602000
C	-4.324170000	2.417693000	-2.583057000	C	3.715426000	0.745129000	-1.777839000
H	-5.246220000	2.989627000	-2.791448000	C	2.885907000	0.812171000	-3.049245000
C	-4.512943000	1.571364000	-1.358483000	O	3.476021000	0.854846000	-4.154647000
H	-5.369749000	0.903749000	-1.331908000	C	0.676776000	0.909192000	-3.919895000
C	-3.651848000	1.629066000	-0.296373000	C	0.162534000	2.168197000	-4.301874000
H	-3.825199000	1.004921000	0.576180000	C	0.599424000	3.424184000	-3.584817000
C	-2.512492000	2.494765000	-0.311588000	H	0.367199000	3.376005000	-2.514257000
H	-1.320281000	1.187613000	-0.889055000	H	0.102046000	4.304112000	-4.002938000
H	-1.909891000	2.606700000	0.586528000	H	1.681968000	3.576116000	-3.663432000

C	-0.754748000	2.233420000	-5.360754000	C	-0.337471000	2.102660000	2.743180000
H	-1.149606000	3.201642000	-5.660314000	C	0.305415000	3.408022000	2.336324000
C	-1.159390000	1.078005000	-6.033869000	H	0.295286000	3.542517000	1.248206000
H	-1.870225000	1.143075000	-6.853260000	H	1.355584000	3.447700000	2.647056000
C	-0.642503000	-0.161349000	-5.648308000	H	-0.215147000	4.255623000	2.790773000
H	-0.952583000	-1.063489000	-6.170582000	C	2.428405000	0.904644000	1.656341000
C	0.276412000	-0.265900000	-4.594032000	O	2.844677000	0.927952000	2.836073000
C	0.833190000	-1.610724000	-4.190875000	C	3.435104000	0.911180000	0.520028000
H	1.922058000	-1.643785000	-4.309708000	C	4.823773000	0.952409000	0.647059000
H	0.400094000	-2.409248000	-4.800018000	H	5.279181000	0.980832000	1.629889000
H	0.622704000	-1.831967000	-3.137787000	C	5.590956000	0.958040000	-0.525194000
F	-0.957741000	0.673553000	-0.959267000	H	6.673987000	0.991256000	-0.458111000
F	-2.904853000	-3.089387000	-1.430381000	C	4.975403000	0.922394000	-1.783203000
Ag	-1.905747000	-1.259598000	-1.202722000	H	5.550583000	0.927136000	-2.701451000
C	-3.082497000	2.364132000	-0.961379000	C	3.581526000	0.881136000	-1.829825000
H	-2.197411000	2.978169000	-0.840227000	C	2.723106000	0.837974000	-3.081951000
C	-3.548114000	2.097611000	-2.269700000	O	3.283699000	0.821789000	-4.200929000
H	-3.003813000	2.487361000	-3.122336000	C	0.499534000	0.751372000	-3.913723000
C	-4.675540000	1.337382000	-2.434685000	C	-0.046175000	1.940398000	-4.444019000
H	-5.057522000	1.113213000	-3.426120000	C	0.372621000	3.286008000	-3.900376000
C	-5.408804000	0.802759000	-1.275901000	H	0.191468000	3.358134000	-2.821748000
H	-5.521631000	-0.292663000	-1.381454000	H	-0.175260000	4.093258000	-4.394811000
H	-6.465694000	1.127917000	-1.327259000	H	1.444201000	3.462007000	-4.050022000
C	-4.863737000	1.116834000	0.054770000	C	-0.972956000	1.850024000	-5.492618000
H	-5.386515000	0.727673000	0.923297000	H	-1.395379000	2.762917000	-5.906005000
C	-3.735005000	1.880053000	0.195871000	C	-1.354139000	0.609968000	-6.010610000
H	-3.328247000	2.107620000	1.174991000	H	-2.073824000	0.554831000	-6.822916000
³ TS _{pF}				C	-0.803472000	-0.559220000	-5.479961000
Ni	0.912048000	0.846667000	-0.817477000	H	-1.094201000	-1.526558000	-5.882805000
N	1.151845000	0.869934000	1.228655000	C	0.126214000	-0.508670000	-4.431399000
N	2.883718000	0.875960000	-0.693549000	C	0.730060000	-1.777287000	-3.876532000
N	1.403659000	0.821446000	-2.815571000	H	1.812929000	-1.809268000	-4.044221000
C	0.117419000	0.876623000	2.207009000	H	0.287569000	-2.658284000	-4.349599000
C	-0.476444000	-0.344715000	2.595717000	H	0.575836000	-1.856017000	-2.794290000
C	0.021266000	-1.653979000	2.030894000	F	-1.173974000	0.808360000	-1.007098000
H	1.081010000	-1.812367000	2.260761000	F	-2.645986000	-3.331344000	-2.041153000
H	-0.545387000	-2.494718000	2.440770000	Ag	-2.276924000	-1.327828000	-1.415319000
H	-0.070308000	-1.680943000	0.938365000	C	-2.468349000	1.766704000	-0.319499000
C	-1.529559000	-0.320526000	3.521569000	H	-1.830507000	2.206820000	0.438607000
H	-1.988294000	-1.258392000	3.825648000	C	-2.887068000	2.624564000	-1.417576000
C	-1.991038000	0.885123000	4.055343000	H	-2.252468000	3.463877000	-1.680710000
H	-2.809438000	0.888507000	4.770051000	C	-4.035984000	2.382494000	-2.082321000
C	-1.394695000	2.086377000	3.664767000	H	-4.339525000	3.032209000	-2.898691000
H	-1.749825000	3.027155000	4.078669000	C	-4.952512000	1.264080000	-1.724934000

H	-5.096218000	0.605871000	-2.596947000	H	0.235439000	4.203038000	-4.530288000
H	-5.963635000	1.660327000	-1.538062000	H	1.786246000	3.443961000	-4.134711000
C	-4.523544000	0.458679000	-0.547279000	C	-0.761556000	1.992629000	-5.521447000
H	-5.194122000	-0.324112000	-0.203368000	H	-1.085824000	2.918619000	-5.990338000
C	-3.376815000	0.712978000	0.128785000	C	-1.267002000	0.770458000	-5.970923000
H	-3.118807000	0.169137000	1.032288000	H	-1.983141000	0.743028000	-6.787689000
³ PC _{PF}				C	-0.848459000	-0.416133000	-5.364671000
Ni	1.031106000	0.875555000	-0.821654000	H	-1.239475000	-1.369585000	-5.711452000
N	1.194994000	0.873876000	1.168112000	C	0.075550000	-0.401085000	-4.309977000
N	2.982339000	0.912679000	-0.675877000	C	0.528248000	-1.689431000	-3.664466000
N	1.485958000	0.874123000	-2.766149000	H	1.609421000	-1.834335000	-3.771755000
C	0.132444000	0.839827000	2.120402000	H	0.024468000	-2.548053000	-4.116716000
C	-0.393832000	-0.405811000	2.526880000	H	0.315380000	-1.695657000	-2.589140000
C	0.189183000	-1.696884000	2.003395000	F	-1.161573000	0.788093000	-1.070134000
H	1.246283000	-1.798540000	2.273973000	F	-3.075938000	-3.312590000	-1.942669000
H	-0.348943000	-2.557970000	2.409034000	Ag	-3.377711000	-1.437565000	-1.059403000
H	0.137803000	-1.744941000	0.909480000	C	-2.342245000	1.576483000	-0.625081000
C	-1.467316000	-0.420627000	3.429393000	H	-1.893657000	2.285313000	0.074829000
H	-1.876645000	-1.376050000	3.748377000	C	-2.914255000	2.234997000	-1.830946000
C	-2.012107000	0.768784000	3.919434000	H	-2.240685000	2.865664000	-2.403182000
H	-2.845104000	0.741045000	4.616421000	C	-4.199403000	2.097062000	-2.183508000
C	-1.481608000	1.993636000	3.508188000	H	-4.575065000	2.621302000	-3.058470000
H	-1.902388000	2.921393000	3.888095000	C	-5.187248000	1.276168000	-1.410855000
C	-0.405971000	2.050100000	2.609791000	H	-5.732983000	0.599903000	-2.082193000
C	0.171053000	3.380095000	2.184632000	H	-5.966902000	1.932477000	-0.992853000
H	0.172171000	3.492000000	1.094016000	C	-4.575601000	0.506224000	-0.276245000
H	1.212357000	3.484985000	2.510102000	H	-5.252645000	-0.049785000	0.368997000
H	-0.402250000	4.206581000	2.613382000	C	-3.262178000	0.628227000	0.084203000
C	2.468135000	0.905901000	1.646351000	H	-2.904096000	0.207049000	1.020973000
O	2.828129000	0.912271000	2.837650000	³ PC _{pH}			
C	3.511679000	0.932109000	0.544329000	Ni	1.026309000	0.706206000	-0.884081000
C	4.898574000	0.971212000	0.690007000	N	1.064904000	0.728316000	1.100123000
H	5.347073000	0.987554000	1.676420000	N	2.915232000	1.129817000	-0.634397000
C	5.677550000	0.989053000	-0.475817000	N	1.570849000	0.769714000	-2.790232000
H	6.759581000	1.020149000	-0.395818000	C	-0.033013000	0.508699000	1.986572000
C	5.078954000	0.967721000	-1.743581000	C	-0.403963000	-0.813615000	2.312957000
H	5.668831000	0.981244000	-2.652517000	C	0.381869000	-1.990040000	1.783407000
C	3.685516000	0.929049000	-1.804824000	H	1.434207000	-1.938785000	2.084768000
C	2.815995000	0.900256000	-3.049303000	H	-0.032664000	-2.931245000	2.154782000
O	3.350361000	0.899901000	-4.173499000	H	0.370437000	-2.022683000	0.687216000
C	0.578012000	0.841269000	-3.867421000	C	-1.512322000	-1.014557000	3.148412000
C	0.162435000	2.048841000	-4.468240000	H	-1.802595000	-2.030077000	3.406475000
C	0.702185000	3.375539000	-3.988687000	C	-2.239154000	0.066442000	3.651925000
H	0.518983000	3.519438000	-2.917405000	H	-3.095309000	-0.105169000	4.298575000

C	-1.859764000	1.369390000	3.320938000	H	-1.360581000	2.154698000	-6.055172000
H	-2.422893000	2.213516000	3.711667000	C	-0.971352000	0.034663000	-6.085274000
C	-0.757718000	1.611756000	2.488642000	H	-1.636311000	-0.157049000	-6.922959000
C	-0.353016000	3.025109000	2.142323000	C	-0.267869000	-1.016770000	-5.493245000
H	-0.302294000	3.174458000	1.057653000	H	-0.384695000	-2.028900000	-5.872919000
H	0.639600000	3.265117000	2.540271000	C	0.594918000	-0.789844000	-4.411280000
H	-1.065090000	3.744946000	2.555247000	C	1.356963000	-1.932950000	-3.783007000
C	2.278088000	1.008647000	1.652377000	H	2.440097000	-1.783888000	-3.859885000
O	2.557167000	1.080065000	2.862187000	H	1.110005000	-2.878766000	-4.272885000
C	3.360773000	1.243268000	0.613183000	H	1.127822000	-2.031126000	-2.715299000
C	4.705060000	1.545299000	0.833372000	F	-1.144394000	0.101595000	-1.261015000
H	5.089722000	1.642303000	1.841846000	F	-2.509786000	-4.275952000	-1.831703000
C	5.528188000	1.715682000	-0.289336000	Ag	-1.946789000	-2.234368000	-1.625668000
H	6.578338000	1.952508000	-0.150790000	C	-5.121149000	0.232996000	-2.088947000
C	5.016557000	1.582137000	-1.588386000	H	-5.788323000	-0.427126000	-2.635573000
H	5.643305000	1.707640000	-2.463503000	C	-4.817796000	-0.036263000	-0.750224000
C	3.661942000	1.277336000	-1.724740000	H	-5.250784000	-0.900767000	-0.256217000
C	2.880581000	1.068745000	-3.010771000	C	-3.958056000	0.815283000	-0.043403000
O	3.456952000	1.174456000	-4.107902000	H	-3.722333000	0.616137000	0.998003000
C	0.739984000	0.528075000	-3.926541000	C	-3.399646000	1.934861000	-0.683213000
C	0.036442000	1.600584000	-4.514676000	H	-1.883460000	0.674263000	-1.035918000
C	0.196937000	3.007948000	-3.990371000	H	-2.768116000	2.620707000	-0.124418000
H	-0.078712000	3.074334000	-2.931298000	C	-3.708534000	2.201354000	-2.028222000
H	-0.432134000	3.704793000	-4.551167000	H	-3.280533000	3.070159000	-2.519109000
H	1.235163000	3.350049000	-4.068166000	C	-4.566365000	1.349127000	-2.728610000
C	-0.815721000	1.333462000	-5.595827000	H	-4.804144000	1.552855000	-3.768343000

VI) C-H bond activation of CHD by the distal fluorine of 1_F-Ag-F

² RC _d				C	-1.112221000	1.893082000	3.232754000
Ni	1.630837000	0.768080000	-0.743672000	H	-1.589302000	2.824125000	3.526878000
N	1.724940000	0.735120000	1.134008000	C	-0.004168000	1.935659000	2.377062000
N	3.477125000	0.708084000	-0.640498000	C	0.530204000	3.253068000	1.869911000
N	1.934834000	0.765091000	-2.599887000	H	0.511238000	3.297037000	0.775597000
C	0.602705000	0.714545000	2.012528000	H	1.569768000	3.411150000	2.178931000
C	0.117433000	-0.526498000	2.480265000	H	-0.066042000	4.084231000	2.254991000
C	0.781589000	-1.823829000	2.086044000	C	2.998279000	0.691262000	1.664969000
H	1.802298000	-1.886785000	2.481069000	O	3.296355000	0.666192000	2.857356000
H	0.219385000	-2.677147000	2.473474000	C	4.032802000	0.680234000	0.571430000
H	0.850695000	-1.925712000	0.997616000	C	5.419299000	0.643101000	0.688119000
C	-0.993893000	-0.521520000	3.333339000	H	5.879536000	0.620060000	1.669065000
H	-1.380495000	-1.467491000	3.702896000	C	6.179279000	0.635514000	-0.489231000
C	-1.606482000	0.676179000	3.708125000	H	7.261928000	0.606731000	-0.428801000
H	-2.468832000	0.661212000	4.368613000	C	5.555828000	0.663382000	-1.743882000

H	6.123478000	0.656703000	-2.667060000	C	-0.567977000	0.024664000	2.285154000
C	4.164991000	0.699721000	-1.782892000	C	-0.100295000	-1.398387000	2.103766000
C	3.259685000	0.731785000	-2.985337000	H	0.843797000	-1.577411000	2.629594000
O	3.689926000	0.730920000	-4.137035000	H	-0.843462000	-2.100296000	2.491032000
C	0.918292000	0.780453000	-3.598816000	H	0.070370000	-1.627293000	1.045784000
C	0.379047000	2.019637000	-4.006410000	C	-1.738906000	0.298394000	2.999010000
C	0.876274000	3.316917000	-3.416351000	H	-2.298585000	-0.525617000	3.433746000
H	0.740979000	3.338576000	-2.329584000	C	-2.197748000	1.610858000	3.157637000
H	0.337630000	4.166308000	-3.844127000	H	-3.091256000	1.808527000	3.743032000
H	1.945285000	3.463152000	-3.609012000	C	-1.487824000	2.670950000	2.582069000
C	-0.625790000	2.014087000	-4.981999000	H	-1.841037000	3.690554000	2.711805000
H	-1.049409000	2.959481000	-5.310274000	C	-0.316461000	2.442473000	1.853763000
C	-1.085370000	0.815539000	-5.532767000	C	0.453036000	3.596523000	1.260442000
H	-1.867167000	0.829263000	-6.286923000	H	0.493795000	3.520913000	0.168973000
C	-0.541520000	-0.400474000	-5.113422000	H	1.487854000	3.614389000	1.619523000
H	-0.900660000	-1.332030000	-5.542529000	H	-0.016814000	4.548396000	1.522444000
C	0.466133000	-0.442295000	-4.140945000	C	2.461263000	0.481398000	1.653269000
C	1.058441000	-1.758996000	-3.699531000	O	2.615675000	0.359138000	2.880289000
H	2.119536000	-1.829417000	-3.965790000	C	3.593589000	0.220489000	0.695091000
H	0.537485000	-2.593814000	-4.174974000	C	4.889772000	-0.184311000	1.003805000
H	0.990036000	-1.887431000	-2.613860000	H	5.173855000	-0.339876000	2.038028000
F	-0.209371000	0.885219000	-0.851059000	C	5.790182000	-0.380337000	-0.050950000
F	-2.867978000	-2.508546000	-0.913978000	H	6.807074000	-0.695040000	0.160021000
Ag	-1.561905000	-0.858709000	-0.886775000	C	5.385504000	-0.176826000	-1.376124000
H	-4.896429000	-1.040951000	-1.244034000	H	6.059553000	-0.326323000	-2.211549000
C	-5.671875000	-0.280882000	-1.430097000	C	4.072804000	0.225520000	-1.610921000
H	-6.457912000	-0.816708000	-1.986758000	C	3.410391000	0.482705000	-2.941408000
C	-6.226686000	0.220875000	-0.120690000	O	4.042821000	0.354971000	-4.007341000
H	-6.652848000	-0.524173000	0.549751000	C	1.308124000	1.091009000	-3.919062000
C	-6.216072000	1.509319000	0.245840000	C	1.044676000	2.424052000	-4.302245000
H	-6.633086000	1.798760000	1.209370000	C	1.651189000	3.579849000	-3.543343000
C	-5.649579000	2.614935000	-0.610166000	H	1.331040000	3.577921000	-2.495674000
H	-4.867231000	3.155679000	-0.053763000	H	1.357686000	4.533837000	-3.990297000
H	-6.423465000	3.376296000	-0.798798000	H	2.745861000	3.527538000	-3.540330000
C	-5.093609000	2.114188000	-1.920048000	C	0.216550000	2.654079000	-5.409475000
H	-4.664890000	2.859221000	-2.588724000	H	0.011604000	3.677652000	-5.713578000
C	-5.105791000	0.825165000	-2.284806000	C	-0.341092000	1.590711000	-6.123296000
H	-4.686996000	0.536251000	-3.247684000	H	-0.982311000	1.784673000	-6.978845000
² TS _{dH}				C	-0.070561000	0.277115000	-5.733652000
Ni	1.514558000	0.944102000	-0.939469000	H	-0.502793000	-0.552443000	-6.287888000
N	1.339260000	0.872445000	0.990476000	C	0.753195000	0.005217000	-4.631992000
N	3.239888000	0.413549000	-0.580667000	C	1.046402000	-1.420349000	-4.228534000
N	2.118191000	0.845182000	-2.773680000	H	2.103891000	-1.665760000	-4.380505000
C	0.151664000	1.110164000	1.721003000	H	0.448820000	-2.120548000	-4.818669000

H	0.828630000	-1.590537000	-3.168414000	H	5.478755000	-0.072223000	1.934798000
F	-0.240151000	1.461088000	-1.310310000	C	5.974570000	-0.171791000	-0.183878000
F	-3.026026000	-1.788259000	-1.831987000	H	7.015979000	-0.431157000	-0.022209000
Ag	-1.595563000	-0.226497000	-1.572753000	C	5.485548000	-0.036760000	-1.489324000
H	-4.488546000	-1.172409000	-1.474438000	H	6.117391000	-0.184543000	-2.357417000
C	-5.466737000	-0.615050000	-1.191449000	C	4.144264000	0.296892000	-1.660581000
H	-6.163369000	-1.037298000	-1.930181000	C	3.401618000	0.492040000	-2.959605000
C	-5.791953000	-0.995119000	0.198810000	O	3.983144000	0.350343000	-4.056203000
H	-6.130158000	-2.011756000	0.381337000	C	1.239354000	1.017919000	-3.837159000
C	-5.642166000	-0.133234000	1.235218000	C	0.991104000	2.329452000	-4.295780000
H	-5.864379000	-0.452170000	2.250030000	C	1.679209000	3.510982000	-3.654914000
C	-5.172993000	1.267941000	1.039415000	H	1.466124000	3.559096000	-2.581389000
H	-4.194533000	1.398170000	1.558319000	H	1.352142000	4.447870000	-4.114716000
H	-5.814687000	1.976099000	1.590411000	H	2.768503000	3.444252000	-3.757700000
C	-5.026072000	1.688607000	-0.381703000	C	0.097594000	2.513528000	-5.360454000
H	-4.787585000	2.730611000	-0.577221000	H	-0.097826000	3.521069000	-5.719760000
C	-5.184878000	0.817546000	-1.411943000	C	-0.538156000	1.424538000	-5.961636000
H	-5.069149000	1.161312000	-2.436393000	H	-1.228679000	1.582376000	-6.785746000
² IM _d				C	-0.281733000	0.131659000	-5.499334000
Ni	1.604081000	0.935730000	-0.862862000	H	-0.773278000	-0.718345000	-5.966625000
N	1.548219000	0.921499000	1.074463000	C	0.605149000	-0.092452000	-4.436166000
N	3.360135000	0.480302000	-0.590123000	C	0.882731000	-1.496163000	-3.951783000
N	2.113795000	0.818801000	-2.730729000	H	1.928603000	-1.776803000	-4.121937000
C	0.390197000	1.173276000	1.864166000	H	0.249874000	-2.219193000	-4.474028000
C	-0.405337000	0.092282000	2.302686000	H	0.700965000	-1.592774000	-2.875530000
C	-0.012843000	-1.332742000	1.990713000	F	-0.174624000	1.439865000	-1.135388000
H	0.935511000	-1.598731000	2.471795000	F	-3.439167000	-1.762474000	-1.696626000
H	-0.777343000	-2.031665000	2.341526000	Ag	-1.750852000	-0.095383000	-1.339966000
H	0.125839000	-1.484765000	0.914355000	H	-4.314370000	-1.371871000	-1.638803000
C	-1.562685000	0.366274000	3.046037000	C	-6.052616000	-0.509164000	-1.572965000
H	-2.179224000	-0.460916000	3.389660000	H	-6.359750000	-1.070665000	-2.451308000
C	-1.928356000	1.679905000	3.348997000	C	-6.372967000	-0.993187000	-0.267714000
H	-2.827650000	1.876648000	3.926426000	H	-6.838629000	-1.970302000	-0.168326000
C	-1.131453000	2.739561000	2.908942000	C	-6.101155000	-0.251777000	0.850504000
H	-1.412044000	3.763140000	3.145451000	H	-6.349549000	-0.637618000	1.835514000
C	0.033150000	2.505422000	2.164147000	C	-5.460190000	1.103493000	0.772555000
C	0.892350000	3.656089000	1.697131000	H	-4.520149000	1.108765000	1.355444000
H	0.994353000	3.657591000	0.606293000	H	-6.082339000	1.846243000	1.304218000
H	1.906194000	3.592017000	2.108734000	C	-5.193965000	1.569143000	-0.629652000
H	0.461203000	4.612974000	2.004801000	H	-4.761265000	2.557116000	-0.761408000
C	2.710040000	0.613457000	1.684974000	C	-5.487469000	0.794996000	-1.720693000
O	2.944803000	0.529602000	2.909084000	H	-5.285555000	1.171274000	-2.720258000
C	3.797377000	0.357992000	0.670209000	⁴ RC _d			
C	5.127843000	0.026176000	0.914076000	Ni	1.762417000	0.595612000	-0.795111000

N	1.907756000	0.590610000	1.222044000	C	0.647002000	0.294833000	-4.411294000
N	3.758394000	0.595453000	-0.620474000	C	0.418656000	-1.058409000	-3.801034000
N	2.545636000	0.645523000	-2.988044000	H	1.332616000	-1.659939000	-3.812312000
C	0.806679000	0.600440000	2.124049000	H	-0.360253000	-1.594652000	-4.347661000
C	0.252558000	-0.623076000	2.560327000	H	0.101825000	-0.965916000	-2.757563000
C	0.840682000	-1.939052000	2.109013000	F	-0.123083000	0.803420000	-1.132312000
H	1.880630000	-2.047507000	2.437695000	F	-3.477400000	-1.576138000	0.066583000
H	0.268170000	-2.778627000	2.512858000	Ag	-1.821508000	-0.399822000	-0.468646000
H	0.842687000	-2.021345000	1.015902000	H	-5.785239000	-1.125721000	-0.334535000
C	-0.850455000	-0.591325000	3.425328000	C	-6.830974000	-0.842503000	-0.536791000
H	-1.282124000	-1.528854000	3.767022000	H	-7.386666000	-1.794202000	-0.514944000
C	-1.398009000	0.622240000	3.847920000	C	-7.336596000	0.067370000	0.554392000
H	-2.254131000	0.630602000	4.516931000	H	-7.298134000	-0.318260000	1.572305000
C	-0.842938000	1.824956000	3.404083000	C	-7.813855000	1.299547000	0.333760000
H	-1.268272000	2.770961000	3.730291000	H	-8.158215000	1.902353000	1.172892000
C	0.260523000	1.834479000	2.539636000	C	-7.907230000	1.924220000	-1.036432000
C	0.856911000	3.138341000	2.064826000	H	-7.341266000	2.869548000	-1.055895000
H	0.850808000	3.206133000	0.970739000	H	-8.947066000	2.226244000	-1.240355000
H	1.900978000	3.241221000	2.382089000	C	-7.414773000	1.009829000	-2.130836000
H	0.296691000	3.989104000	2.462610000	H	-7.458660000	1.394124000	-3.148942000
C	3.154568000	0.567439000	1.717158000	C	-6.938043000	-0.222038000	-1.907142000
O	3.509685000	0.549591000	2.915347000	H	-6.599067000	-0.826344000	-2.747569000
C	4.218810000	0.568119000	0.636285000	⁴ TS _{dH}			
C	5.591247000	0.547368000	0.889086000	Ni	1.220238000	0.878424000	-0.879711000
H	5.943156000	0.526458000	1.913427000	N	1.319920000	0.828233000	1.157891000
C	6.470977000	0.553572000	-0.196778000	N	3.177763000	0.778589000	-0.628915000
H	7.542852000	0.537463000	-0.028728000	N	1.830442000	0.813811000	-2.827414000
C	5.968695000	0.583196000	-1.501190000	C	0.218512000	0.829940000	2.058710000
H	6.619548000	0.592348000	-2.367085000	C	-0.410610000	-0.392163000	2.386512000
C	4.584615000	0.604096000	-1.673155000	C	0.104266000	-1.695895000	1.824260000
C	3.925810000	0.658868000	-3.021999000	H	1.146204000	-1.875624000	2.112291000
O	4.596427000	0.607967000	-4.056059000	H	-0.496683000	-2.537149000	2.181005000
C	1.784464000	1.105547000	-4.009460000	H	0.076747000	-1.695643000	0.727948000
C	2.034307000	2.381857000	-4.659091000	C	-1.519809000	-0.372772000	3.243768000
C	3.136473000	3.307387000	-4.215202000	H	-2.004460000	-1.311002000	3.503375000
H	3.233508000	3.332545000	-3.125450000	C	-2.004337000	0.828963000	3.766793000
H	2.932957000	4.323485000	-4.560347000	H	-2.864725000	0.828590000	4.430356000
H	4.103279000	2.996277000	-4.622745000	C	-1.377693000	2.031583000	3.429178000
C	1.162647000	2.786815000	-5.657887000	H	-1.753112000	2.969256000	3.831997000
H	1.311193000	3.752996000	-6.130331000	C	-0.265448000	2.052710000	2.575872000
C	0.079028000	1.985501000	-6.057928000	C	0.405789000	3.357595000	2.219327000
H	-0.577823000	2.329855000	-6.850837000	H	0.428953000	3.511452000	1.134329000
C	-0.164729000	0.750581000	-5.438823000	H	1.446030000	3.379707000	2.563600000
H	-0.992851000	0.135414000	-5.776602000	H	-0.119735000	4.201818000	2.674452000

C	2.566330000	0.774217000	1.679887000	C	-6.127187000	0.509922000	-1.111022000
O	2.890310000	0.737993000	2.885240000	H	-7.046750000	0.286279000	-1.644757000
C	3.649891000	0.748677000	0.616760000	⁴ IM _d			
C	5.026703000	0.687775000	0.835224000	Ni	1.447618000	0.968066000	-0.943152000
H	5.419034000	0.663386000	1.845017000	N	1.479846000	0.916684000	1.135830000
C	5.868316000	0.657977000	-0.284667000	N	3.363645000	0.558116000	-0.607168000
H	6.944100000	0.611513000	-0.146974000	N	2.165160000	0.836108000	-2.885681000
C	5.335590000	0.683417000	-1.580360000	C	0.362879000	1.123914000	1.990265000
H	5.969012000	0.655902000	-2.459189000	C	-0.452754000	0.028602000	2.351701000
C	3.948042000	0.743804000	-1.715865000	C	-0.110445000	-1.367747000	1.887719000
C	3.167850000	0.767641000	-3.018587000	H	0.872741000	-1.683800000	2.254687000
O	3.787846000	0.741461000	-4.102521000	H	-0.852763000	-2.088732000	2.242061000
C	0.985638000	0.844389000	-3.973339000	H	-0.070752000	-1.426769000	0.793171000
C	0.617007000	2.085680000	-4.536727000	C	-1.583636000	0.259535000	3.148174000
C	1.160618000	3.377556000	-3.973613000	H	-2.212278000	-0.581642000	3.431271000
H	0.909661000	3.488121000	-2.912225000	C	-1.908401000	1.547628000	3.580981000
H	0.754023000	4.237879000	-4.512815000	H	-2.787016000	1.711620000	4.199040000
H	2.253555000	3.418232000	-4.044881000	C	-1.096127000	2.623590000	3.214279000
C	-0.265261000	2.097287000	-5.626419000	H	-1.345000000	3.628438000	3.547696000
H	-0.552776000	3.050545000	-6.063836000	C	0.042645000	2.431093000	2.419097000
C	-0.775617000	0.907981000	-6.152848000	C	0.912290000	3.601107000	2.023489000
H	-1.459608000	0.933208000	-6.996819000	H	0.981489000	3.695705000	0.933340000
C	-0.401862000	-0.313311000	-5.587762000	H	1.936780000	3.484037000	2.394740000
H	-0.794272000	-1.241929000	-5.995396000	H	0.511280000	4.537026000	2.423042000
C	0.479619000	-0.365698000	-4.497620000	C	2.675266000	0.659146000	1.689745000
C	0.887229000	-1.692621000	-3.901193000	O	2.965359000	0.574510000	2.906983000
H	1.966714000	-1.859148000	-3.994173000	C	3.772671000	0.450926000	0.658649000
H	0.373172000	-2.517782000	-4.402148000	C	5.110830000	0.165063000	0.933045000
H	0.652965000	-1.740461000	-2.831478000	H	5.447809000	0.077110000	1.959144000
F	-0.726223000	1.143763000	-1.135568000	C	5.984059000	-0.002045000	-0.149234000
F	-3.631548000	-1.674509000	-2.340048000	H	7.030729000	-0.225337000	0.033603000
Ag	-2.130102000	-0.334813000	-1.747968000	C	5.519283000	0.114632000	-1.465381000
H	-4.948497000	-1.256592000	-1.340219000	H	6.176230000	-0.013264000	-2.317558000
C	-5.399754000	-0.626958000	-0.492708000	C	4.167816000	0.402551000	-1.660875000
H	-6.052859000	-1.346802000	0.019578000	C	3.474125000	0.562900000	-3.003850000
C	-4.207620000	-0.273616000	0.294274000	O	4.148062000	0.431002000	-4.053083000
H	-3.702812000	-1.061141000	0.847400000	C	1.394396000	1.005699000	-4.068248000
C	-3.704642000	1.004892000	0.325012000	C	1.247758000	2.293206000	-4.630204000
H	-2.813760000	1.221594000	0.907244000	C	1.952363000	3.481319000	-4.018857000
C	-4.406833000	2.140128000	-0.332637000	H	1.661879000	3.621881000	-2.971030000
H	-3.708195000	2.675215000	-0.999343000	H	1.714109000	4.398443000	-4.565216000
H	-4.624057000	2.905332000	0.436546000	H	3.040652000	3.352506000	-4.029283000
C	-5.661382000	1.777348000	-1.060399000	C	0.434078000	2.450015000	-5.761466000
H	-6.209621000	2.584546000	-1.538521000	H	0.319141000	3.439778000	-6.197400000

C	-0.225615000	1.358120000	-6.330992000	C	0.542751000	3.268467000	2.391929000
H	-0.853054000	1.494722000	-7.207667000	H	0.567613000	3.446057000	1.310330000
C	-0.074471000	0.089656000	-5.765343000	H	1.582627000	3.280791000	2.737702000
H	-0.585865000	-0.763877000	-6.204552000	H	0.018463000	4.104443000	2.863800000
C	0.730391000	-0.105419000	-4.633667000	C	2.700016000	0.715336000	1.790625000
C	0.884256000	-1.480285000	-4.026730000	O	3.045659000	0.650612000	2.994492000
H	1.930344000	-1.807117000	-4.030306000	C	3.777752000	0.743769000	0.719687000
H	0.295999000	-2.218071000	-4.579953000	C	5.154504000	0.709268000	0.944989000
H	0.554630000	-1.494444000	-2.980574000	H	5.537429000	0.658488000	1.957304000
F	-0.436090000	1.430185000	-1.269976000	C	6.005375000	0.741857000	-0.166924000
F	-3.734463000	-1.714533000	-1.819779000	H	7.081111000	0.716671000	-0.022343000
Ag	-2.017216000	-0.079715000	-1.477844000	C	5.480452000	0.805925000	-1.463731000
H	-4.596061000	-1.320614000	-1.662955000	H	6.118485000	0.831364000	-2.339126000
C	-6.309570000	-0.437085000	-1.400460000	C	4.092927000	0.836639000	-1.609970000
H	-6.687509000	-0.952077000	-2.279872000	C	3.339177000	0.903752000	-2.927953000
C	-6.523176000	-0.991222000	-0.101380000	O	3.993992000	0.932509000	-3.997400000
H	-6.976952000	-1.975329000	-0.016939000	C	1.180521000	0.994004000	-3.922035000
C	-6.164340000	-0.308016000	1.029453000	C	0.835335000	2.253194000	-4.461427000
H	-6.331831000	-0.747129000	2.009217000	C	1.385348000	3.523163000	-3.856218000
C	-5.536586000	1.054417000	0.972746000	H	1.119890000	3.606773000	-2.795715000
H	-4.552741000	1.036235000	1.477974000	H	0.995651000	4.402815000	-4.376526000
H	-6.116429000	1.763053000	1.591627000	H	2.479503000	3.552884000	-3.910797000
C	-5.386103000	1.595690000	-0.419451000	C	-0.030561000	2.303772000	-5.563194000
H	-4.969326000	2.592812000	-0.532438000	H	-0.298252000	3.271320000	-5.981646000
C	-5.762490000	0.877652000	-1.523099000	C	-0.549925000	1.134912000	-6.125424000
H	-5.643053000	1.307954000	-2.514104000	H	-1.219707000	1.189711000	-6.979419000
³ PC _{df}				C	-0.203821000	-0.104520000	-5.581692000
Ni	1.341206000	0.856916000	-0.792398000	H	-0.605324000	-1.017597000	-6.015268000
N	1.458284000	0.763180000	1.283427000	C	0.658975000	-0.194324000	-4.479755000
N	3.310224000	0.806289000	-0.529048000	C	1.024011000	-1.538948000	-3.895922000
N	2.006876000	0.922449000	-2.767419000	H	2.105773000	-1.711875000	-3.927491000
C	0.354942000	0.745866000	2.179938000	H	0.534217000	-2.347969000	-4.445528000
C	-0.282868000	-0.479669000	2.474254000	H	0.725204000	-1.610888000	-2.842997000
C	0.235717000	-1.773096000	1.890746000	F	-0.596790000	1.035165000	-1.046635000
H	1.275820000	-1.958599000	2.181882000	F	-3.775816000	-2.140386000	-1.571142000
H	-0.367976000	-2.621179000	2.226599000	Ag	-2.074802000	-0.567873000	-1.263253000
H	0.215571000	-1.752705000	0.794114000	C	-5.201582000	-1.663423000	-1.782474000
C	-1.404182000	-0.475480000	3.316482000	H	-5.706147000	-2.625557000	-1.890187000
H	-1.895419000	-1.417740000	3.548322000	C	-5.587416000	-0.930704000	-0.548551000
C	-1.893083000	0.715995000	3.857857000	H	-5.653417000	-1.509824000	0.368301000
H	-2.762970000	0.704390000	4.509070000	C	-5.841279000	0.387324000	-0.553682000
C	-1.257210000	1.922683000	3.555383000	H	-6.116380000	0.886718000	0.372419000
H	-1.635029000	2.853331000	3.972518000	C	-5.798099000	1.225623000	-1.793593000
C	-0.133170000	1.957526000	2.717774000	H	-5.086178000	2.054195000	-1.656591000

H	-6.767737000	1.728152000	-1.933075000	C	4.386117000	0.372335000	-1.608239000
C	-5.447797000	0.459008000	-3.031137000	C	3.787256000	0.648006000	-2.977481000
H	-5.426784000	1.012350000	-3.967137000	O	4.525749000	0.566211000	-3.987798000
C	-5.193526000	-0.858958000	-3.031754000	C	1.792715000	1.223863000	-4.137942000
H	-4.967128000	-1.384770000	-3.955137000	C	1.820903000	2.525065000	-4.687301000
³ PC _{dH}				C	2.621760000	3.620834000	-4.024553000
Ni	1.647340000	0.986361000	-1.019539000	H	2.311891000	3.766487000	-2.983023000
N	1.540592000	0.751907000	1.053840000	H	2.496335000	4.569413000	-4.554504000
N	3.518793000	0.471415000	-0.598128000	H	3.690783000	3.380462000	-4.005905000
N	2.480137000	0.948512000	-2.924677000	C	1.087055000	2.783416000	-5.853915000
C	0.376210000	0.913257000	1.853219000	H	1.106433000	3.783847000	-6.280118000
C	-0.454343000	-0.200048000	2.112843000	C	0.335896000	1.779404000	-6.470108000
C	-0.080139000	-1.571861000	1.602159000	H	-0.227394000	1.994625000	-7.374135000
H	0.873156000	-1.910253000	2.024054000	C	0.311703000	0.497678000	-5.914951000
H	-0.846651000	-2.306931000	1.863931000	H	-0.272138000	-0.287655000	-6.389606000
H	0.039627000	-1.574412000	0.512176000	C	1.031979000	0.202212000	-4.748656000
C	-1.629349000	-0.010646000	2.854708000	C	0.992226000	-1.184811000	-4.151115000
H	-2.269614000	-0.865763000	3.059017000	H	1.994918000	-1.619699000	-4.071892000
C	-1.983148000	1.253567000	3.332776000	H	0.377974000	-1.853569000	-4.761038000
H	-2.896091000	1.385175000	3.907385000	H	0.575416000	-1.170390000	-3.136059000
C	-1.154672000	2.347035000	3.068804000	F	-0.171885000	1.600083000	-1.436404000
H	-1.424810000	3.333127000	3.439614000	F	-3.911006000	-1.076515000	-1.467649000
C	0.028549000	2.196187000	2.331485000	Ag	-1.904149000	0.247003000	-1.441317000
C	0.918174000	3.384907000	2.053404000	C	-6.992171000	1.620768000	-0.992949000
H	1.050568000	3.542046000	0.976569000	H	-7.441293000	2.362419000	-1.647192000
H	1.919612000	3.244607000	2.476059000	C	-7.508206000	0.320049000	-0.955824000
H	0.493648000	4.297188000	2.482301000	H	-8.356450000	0.053181000	-1.579129000
C	2.690267000	0.407677000	1.654119000	C	-6.932064000	-0.636575000	-0.112894000
O	2.900322000	0.207271000	2.874422000	H	-7.332580000	-1.645432000	-0.077804000
C	3.844231000	0.252800000	0.677894000	C	-5.834480000	-0.290972000	0.692488000
C	5.154473000	-0.092799000	1.011527000	H	-4.560071000	-0.790391000	-0.833249000
H	5.421346000	-0.270479000	2.046595000	H	-5.407814000	-1.023019000	1.373475000
C	6.091866000	-0.199900000	-0.023420000	C	-5.317437000	1.014685000	0.651043000
H	7.119134000	-0.466128000	0.206131000	H	-4.471156000	1.280901000	1.277596000
C	5.714780000	0.030859000	-1.352296000	C	-5.897319000	1.968305000	-0.193267000
H	6.420907000	-0.049999000	-2.170202000	H	-5.498268000	2.977730000	-0.225864000

VII) Difluorination of PPh₃ by two separated 1F_S

² RC _{PF}				C	-1.065911000	0.080927000	3.007950000
Ni	0.274928000	-0.086309000	0.387427000	C	-1.696775000	-1.101191000	3.449428000
N	0.148147000	-0.015521000	2.266209000	C	-1.097885000	-2.456475000	3.160287000
N	2.096575000	-0.201127000	0.718930000	H	-0.120405000	-2.574693000	3.642194000
N	0.805516000	-0.219899000	-1.415177000	H	-1.750760000	-3.252979000	3.526320000

H	-0.944232000	-2.605173000	2.085675000	C	-6.360269000	1.677871000	-0.245393000
C	-2.893665000	-0.983866000	4.168019000	C	-7.222802000	0.609581000	-2.797093000
H	-3.392058000	-1.884731000	4.516217000	C	-6.864612000	-1.955054000	-1.009944000
C	-3.449505000	0.268857000	4.437254000	C	-6.973375000	1.171786000	0.912615000
H	-4.379057000	0.342220000	4.994716000	C	-8.511845000	1.044969000	-2.448266000
C	-2.811663000	1.427074000	3.987459000	C	-4.584697000	-1.518819000	-0.326374000
H	-3.245663000	2.401309000	4.196447000	C	-6.150807000	3.065999000	-0.343216000
C	-1.613437000	1.355442000	3.265029000	C	-7.000688000	0.151718000	-4.109310000
C	-0.927362000	2.609706000	2.780480000	C	-6.780748000	-3.241672000	-0.466576000
H	-0.819934000	2.609396000	1.690163000	C	-7.376587000	2.032045000	1.940053000
H	0.079984000	2.706374000	3.201329000	C	-9.552805000	1.014132000	-3.383330000
H	-1.498556000	3.496542000	3.066815000	C	-4.506505000	-2.800721000	0.226774000
C	1.345787000	-0.062577000	2.946599000	C	-6.564819000	3.927569000	0.676342000
O	1.502708000	-0.020495000	4.166777000	C	-8.042300000	0.107492000	-5.039768000
C	2.502359000	-0.175289000	1.988941000	C	-5.602966000	-3.666968000	0.156164000
C	3.862146000	-0.253365000	2.276152000	C	-7.177603000	3.411316000	1.823697000
H	4.200499000	-0.232950000	3.305519000	C	-9.322964000	0.541891000	-4.679151000
C	4.756879000	-0.357848000	1.202780000	H	-7.786646000	-1.639085000	-1.488139000
H	5.822365000	-0.419745000	1.396684000	H	-7.138343000	0.103972000	1.017428000
C	4.289960000	-0.385033000	-0.118171000	H	-8.708977000	1.410185000	-1.445207000
H	4.963232000	-0.467490000	-0.963435000	H	-3.715245000	-0.866214000	-0.278410000
C	2.916304000	-0.302917000	-0.327979000	H	-5.659981000	3.476374000	-1.222737000
C	2.163092000	-0.317227000	-1.631822000	H	-6.005889000	-0.172187000	-4.406351000
O	2.731607000	-0.407229000	-2.719888000	H	-7.636402000	-3.908609000	-0.528746000
C	-0.076948000	-0.229482000	-2.535439000	H	-7.848069000	1.622637000	2.829352000
C	-0.432390000	0.993959000	-3.141532000	H	-10.543259000	1.356267000	-3.095682000
C	0.116853000	2.304186000	-2.631141000	H	-3.585237000	-3.125441000	0.702269000
H	-0.131376000	2.457313000	-1.575072000	H	-6.398946000	4.996931000	0.579830000
H	-0.290889000	3.141841000	-3.202859000	H	-7.851619000	-0.254587000	-6.046229000
H	1.209345000	2.341148000	-2.711755000	H	-5.537990000	-4.666181000	0.577575000
C	-1.307815000	0.960526000	-4.234817000	H	-7.491476000	4.077739000	2.622083000
H	-1.591217000	1.893893000	-4.714074000	H	-10.132102000	0.517699000	-5.403543000
C	-1.817935000	-0.249828000	-4.709803000	² TS1 _{PF}			
H	-2.496975000	-0.257586000	-5.557794000	Ni	-0.797476000	0.070480000	0.093984000
C	-1.457082000	-1.449850000	-4.093098000	N	-0.801035000	0.007141000	2.050739000
H	-1.856129000	-2.390970000	-4.462256000	N	0.963084000	0.576279000	0.353518000
C	-0.584414000	-1.462284000	-2.997192000	N	-0.274718000	0.144230000	-1.793564000
C	-0.195013000	-2.761126000	-2.333605000	C	-1.828900000	-0.472582000	2.920009000
H	0.882648000	-2.945557000	-2.412665000	C	-1.973908000	-1.865048000	3.106387000
H	-0.714924000	-3.602786000	-2.798409000	C	-1.047257000	-2.842171000	2.421309000
H	-0.440305000	-2.754195000	-1.265866000	H	-0.004811000	-2.675348000	2.716234000
F	-1.503423000	0.041460000	0.062416000	H	-1.311474000	-3.871319000	2.679621000
P	-5.759588000	0.635186000	-1.656637000	H	-1.080180000	-2.745752000	1.330387000
C	-5.770244000	-1.076389000	-0.942902000	C	-2.971598000	-2.327682000	3.975289000

H	-3.089140000	-3.398097000	4.124026000	C	-6.604940000	-1.411374000	0.007955000
C	-3.806568000	-1.435406000	4.650579000	C	-5.608393000	1.717069000	1.172975000
H	-4.577821000	-1.808989000	5.318720000	C	-5.747608000	1.716699000	-2.718167000
C	-3.639591000	-0.060666000	4.471319000	C	-4.460409000	-2.412108000	0.517383000
H	-4.276934000	0.637273000	5.008787000	C	-3.806072000	2.740490000	-0.078303000
C	-2.649234000	0.441693000	3.615521000	C	-5.827308000	-0.678739000	-3.081735000
C	-2.433889000	1.928869000	3.483390000	C	-7.252826000	-2.517794000	0.558438000
H	-2.450839000	2.248713000	2.437855000	C	-5.828224000	2.927430000	1.837097000
H	-1.459548000	2.217822000	3.894206000	C	-6.433053000	1.914910000	-3.918903000
H	-3.207149000	2.481776000	4.022759000	C	-5.112547000	-3.525309000	1.055230000
C	0.366196000	0.364804000	2.632873000	C	-4.033765000	3.951385000	0.580862000
O	0.644973000	0.384642000	3.848095000	C	-6.519180000	-0.474314000	-4.273719000
C	1.401000000	0.736353000	1.606822000	C	-6.507807000	-3.581900000	1.079015000
C	2.704252000	1.168396000	1.839051000	C	-5.048726000	4.048490000	1.537275000
H	3.053846000	1.291471000	2.857413000	C	-6.826817000	0.824335000	-4.702499000
C	3.524336000	1.426208000	0.734115000	H	-7.198244000	-0.605371000	-0.410192000
H	4.544162000	1.764990000	0.885468000	H	-6.226377000	0.859739000	1.416690000
C	3.036756000	1.242667000	-0.565252000	H	-5.464620000	2.580496000	-2.126598000
H	3.648282000	1.424876000	-1.441212000	H	-3.378521000	-2.384760000	0.509689000
C	1.722770000	0.808971000	-0.722076000	H	-3.013687000	2.680037000	-0.817676000
C	1.005620000	0.522081000	-2.012620000	H	-5.587601000	-1.693453000	-2.777297000
O	1.602185000	0.624037000	-3.102432000	H	-8.338215000	-2.549544000	0.574697000
C	-1.047196000	-0.207448000	-2.942559000	H	-6.610743000	2.991478000	2.587552000
C	-1.558740000	0.803265000	-3.786559000	H	-6.667066000	2.927273000	-4.237469000
C	-1.297604000	2.262923000	-3.503925000	H	-4.525234000	-4.346048000	1.455447000
H	-1.445025000	2.503973000	-2.446845000	H	-3.416399000	4.813762000	0.347276000
H	-1.956016000	2.899496000	-4.101396000	H	-6.814816000	-1.330601000	-4.873886000
H	-0.260934000	2.526547000	-3.745010000	H	-7.012244000	-4.447209000	1.498878000
C	-2.284828000	0.425412000	-4.924567000	H	-5.225967000	4.988963000	2.050659000
H	-2.680745000	1.198002000	-5.579200000	H	-7.361245000	0.982336000	-5.634543000
C	-2.503303000	-0.919977000	-5.225249000	² IM1 _{PF}			
H	-3.069810000	-1.196316000	-6.110223000	Ni	0.402509000	-0.670437000	-0.244599000
C	-1.991474000	-1.909336000	-4.383251000	N	0.618170000	-1.399009000	1.628639000
H	-2.151948000	-2.958363000	-4.619803000	N	2.178091000	-0.020502000	0.123203000
C	-1.256422000	-1.573239000	-3.237848000	N	0.757607000	0.268523000	-1.998010000
C	-0.666007000	-2.659124000	-2.368928000	C	-0.314379000	-2.189892000	2.348031000
H	0.419153000	-2.545406000	-2.269851000	C	-0.140629000	-3.591183000	2.450702000
H	-0.868015000	-3.645601000	-2.795545000	C	1.074654000	-4.260950000	1.855206000
H	-1.077658000	-2.641734000	-1.353784000	H	1.991132000	-3.944918000	2.366094000
F	-2.864157000	-0.249340000	-0.275767000	H	0.997601000	-5.349424000	1.933302000
P	-4.362809000	0.090825000	-0.788335000	H	1.198435000	-3.997441000	0.797981000
C	-5.197394000	-1.342406000	-0.017448000	C	-1.115355000	-4.350028000	3.114069000
C	-4.600506000	1.614408000	0.201448000	H	-0.982553000	-5.426949000	3.192064000
C	-5.454481000	0.412170000	-2.261264000	C	-2.246951000	-3.747680000	3.670126000

H	-2.992956000	-4.350111000	4.181503000	C	-4.251202000	-3.297378000	-2.645243000
C	-2.411063000	-2.364521000	3.562083000	C	-6.439039000	-0.679858000	1.410572000
H	-3.287478000	-1.887523000	3.995120000	C	-5.580957000	-0.042357000	-3.297237000
C	-1.458315000	-1.571679000	2.906186000	C	-2.795852000	-2.891718000	-0.721314000
C	-1.640428000	-0.075710000	2.809071000	C	-6.730581000	-3.365577000	2.175085000
H	-1.627394000	0.259881000	1.764688000	C	-8.361751000	-0.358151000	-3.057888000
H	-0.828288000	0.460267000	3.314137000	C	-3.398870000	-4.319736000	-3.064487000
H	-2.586965000	0.232845000	3.262797000	C	-7.121384000	-1.003179000	2.581785000
C	1.796642000	-1.107711000	2.210843000	C	-6.427999000	0.435409000	-4.295086000
O	2.188604000	-1.422093000	3.365427000	C	-1.950203000	-3.909071000	-1.158895000
C	2.712767000	-0.291893000	1.316092000	C	-7.269337000	-2.342868000	2.961239000
C	3.993695000	0.172365000	1.624267000	C	-7.814224000	0.275799000	-4.177006000
H	4.436990000	-0.041278000	2.590288000	C	-2.252119000	-4.623076000	-2.324635000
C	4.676400000	0.915104000	0.649875000	H	-5.614437000	-3.852823000	0.400228000
H	5.674360000	1.288361000	0.859894000	H	-7.955426000	-1.323460000	-1.177550000
C	4.082463000	1.182530000	-0.592390000	H	-5.137080000	-3.061464000	-3.224807000
H	4.595612000	1.756623000	-1.355523000	H	-6.326642000	0.360284000	1.121944000
C	2.797838000	0.685853000	-0.825215000	H	-4.507273000	0.085316000	-3.397207000
C	1.965154000	0.856223000	-2.083734000	H	-2.554450000	-2.348641000	0.187475000
O	2.443863000	1.503560000	-3.052441000	H	-6.843072000	-4.402685000	2.473548000
C	-0.106231000	0.347818000	-3.121964000	H	-9.436214000	-0.479867000	-2.968356000
C	-1.125925000	1.326922000	-3.149546000	H	-3.629604000	-4.872862000	-3.969009000
C	-1.253970000	2.327631000	-2.025687000	H	-7.536210000	-0.211347000	3.196895000
H	-1.401810000	1.825855000	-1.061611000	H	-6.006631000	0.930485000	-5.163872000
H	-2.097597000	3.002570000	-2.198233000	H	-1.058473000	-4.143419000	-0.587647000
H	-0.346701000	2.933977000	-1.923003000	H	-7.803584000	-2.588273000	3.873940000
C	-2.008664000	1.360047000	-4.238946000	H	-8.467834000	0.647856000	-4.959979000
H	-2.787102000	2.119619000	-4.265269000	H	-1.589611000	-5.416366000	-2.656992000
C	-1.896152000	0.442516000	-5.286970000	⁴ RC _{PF}			
H	-2.586450000	0.480758000	-6.125472000	Ni	-0.712551000	0.002199000	0.148432000
C	-0.887056000	-0.523431000	-5.248717000	N	-0.467564000	-0.255108000	2.232600000
H	-0.793414000	-1.240825000	-6.061115000	N	1.276819000	0.006449000	0.322828000
C	0.016100000	-0.585376000	-4.178038000	N	-0.125629000	0.365266000	-1.832337000
C	1.103895000	-1.632328000	-4.150166000	C	-1.490795000	-0.366349000	3.213188000
H	2.099376000	-1.174414000	-4.172140000	C	-1.867965000	-1.635496000	3.707734000
H	1.019667000	-2.305380000	-5.008529000	C	-1.175488000	-2.886846000	3.222542000
H	1.054419000	-2.231615000	-3.233306000	H	-0.115894000	-2.888332000	3.502064000
F	-4.090293000	-0.067561000	-0.513526000	H	-1.640837000	-3.779804000	3.649861000
P	-5.043747000	-1.296102000	-0.895155000	H	-1.215957000	-2.967426000	2.130150000
C	-5.894080000	-1.711607000	0.621488000	C	-2.891505000	-1.712995000	4.662937000
C	-6.135164000	-0.677200000	-2.167770000	H	-3.177821000	-2.687340000	5.052710000
C	-3.948546000	-2.584375000	-1.471181000	C	-3.542127000	-0.563964000	5.118819000
C	-6.037255000	-3.056835000	1.003768000	H	-4.335079000	-0.640889000	5.857894000
C	-7.527139000	-0.834947000	-2.045984000	C	-3.166806000	0.684180000	4.616749000

H	-3.667186000	1.583046000	4.969657000	C	-4.608978000	2.556400000	-0.780092000
C	-2.142194000	0.802503000	3.666546000	C	-5.570913000	-1.449548000	-3.332210000
C	-1.728094000	2.160973000	3.151419000	C	-7.248658000	-3.227216000	0.567959000
H	-1.860796000	2.237985000	2.066015000	C	-6.160632000	2.833237000	1.535965000
H	-0.669351000	2.360433000	3.352547000	C	-7.034765000	0.694965000	-4.379225000
H	-2.318951000	2.951588000	3.622912000	C	-5.383572000	-2.900123000	2.080733000
C	0.804672000	-0.314381000	2.655495000	C	-4.804889000	3.817114000	-0.217258000
O	1.229242000	-0.454552000	3.828235000	C	-6.156284000	-1.555389000	-4.591983000
C	1.813188000	-0.173298000	1.532289000	C	-6.560263000	-3.573490000	1.735590000
C	3.200081000	-0.204950000	1.685411000	C	-5.580184000	3.957436000	0.940050000
H	3.630502000	-0.349735000	2.669143000	C	-6.888588000	-0.484230000	-5.118124000
C	3.994709000	-0.044471000	0.544396000	H	-7.312529000	-1.945109000	-1.153438000
H	5.076637000	-0.066474000	0.632447000	H	-6.430531000	0.700482000	1.445437000
C	3.402136000	0.148799000	-0.708997000	H	-6.589146000	1.724074000	-2.546491000
H	3.991622000	0.281979000	-1.608295000	H	-3.961402000	-1.376598000	1.515642000
C	2.008833000	0.170308000	-0.781824000	H	-3.992850000	2.452423000	-1.668137000
C	1.199675000	0.387566000	-2.045029000	H	-4.993706000	-2.280483000	-2.938045000
O	1.809588000	0.571009000	-3.126178000	H	-8.165157000	-3.743404000	0.299121000
C	-0.969663000	0.593143000	-2.953643000	H	-6.761450000	2.939453000	2.433947000
C	-1.403187000	1.907135000	-3.239815000	H	-7.604689000	1.525603000	-4.784056000
C	-0.946267000	3.067299000	-2.386641000	H	-4.846125000	-3.165956000	2.984933000
H	-1.202713000	2.916784000	-1.331562000	H	-4.346877000	4.687295000	-0.677047000
H	-1.406051000	4.001611000	-2.721683000	H	-6.034165000	-2.468727000	-5.165781000
H	0.142091000	3.190863000	-2.429718000	H	-6.939336000	-4.366126000	2.373795000
C	-2.244873000	2.118247000	-4.341395000	H	-5.727417000	4.940123000	1.377828000
H	-2.577066000	3.128776000	-4.568219000	H	-7.339887000	-0.567173000	-6.102167000
C	-2.650919000	1.053975000	-5.150197000	⁴ TS1 _{PF}			
H	-3.300201000	1.232181000	-6.003056000	Ni	-0.025163000	0.087327000	0.228427000
C	-2.220297000	-0.241142000	-4.853473000	N	0.136327000	0.100163000	2.200764000
H	-2.536709000	-1.072931000	-5.478305000	N	1.918476000	0.100504000	0.357835000
C	-1.383204000	-0.491970000	-3.757147000	N	0.392392000	0.068264000	-1.707085000
C	-0.917769000	-1.895563000	-3.448937000	C	-0.934812000	0.105934000	3.145544000
H	0.171984000	-1.982442000	-3.528026000	C	-1.493676000	-1.119638000	3.566600000
H	-1.365772000	-2.614723000	-4.140729000	C	-0.937925000	-2.432471000	3.067678000
H	-1.184105000	-2.189759000	-2.427231000	H	0.113699000	-2.557690000	3.349795000
F	-2.641730000	-0.273282000	0.000621000	H	-1.501840000	-3.273838000	3.479911000
P	-4.943922000	-0.192951000	-0.947353000	H	-0.980342000	-2.494627000	1.973927000
C	-5.580442000	-1.529564000	0.091047000	C	-2.576897000	-1.094121000	4.456688000
C	-5.206057000	1.425055000	-0.191069000	H	-3.013079000	-2.034110000	4.785950000
C	-5.734096000	-0.271382000	-2.572134000	C	-3.097741000	0.115798000	4.920935000
C	-6.764252000	-2.211877000	-0.257195000	H	-3.938076000	0.119778000	5.609827000
C	-5.973518000	1.566428000	0.979080000	C	-2.535950000	1.320817000	4.492838000
C	-6.457159000	0.810083000	-3.114322000	H	-2.940523000	2.264736000	4.850114000
C	-4.885405000	-1.885090000	1.263343000	C	-1.452437000	1.336831000	3.603031000

C	-0.855460000	2.644905000	3.140762000	C	-6.894899000	-3.066991000	1.306196000
H	-0.888102000	2.734827000	2.048689000	C	-8.272413000	2.856767000	0.721618000
H	0.196839000	2.732923000	3.434053000	C	-6.741011000	1.625210000	-4.592625000
H	-1.398200000	3.491767000	3.569814000	C	-5.311787000	-3.877770000	-0.341022000
C	1.410630000	0.114218000	2.679298000	C	-6.306126000	2.729763000	2.136562000
O	1.770407000	0.126272000	3.869988000	C	-7.432712000	-0.698735000	-4.575772000
C	2.453793000	0.114329000	1.574903000	C	-6.174569000	-4.120512000	0.734381000
C	3.842389000	0.126031000	1.708964000	C	-7.572372000	3.259848000	1.864384000
H	4.300619000	0.137200000	2.691001000	C	-7.328636000	0.529683000	-5.237320000
C	4.611173000	0.122785000	0.535751000	H	-7.325037000	-0.958822000	1.254061000
H	5.694217000	0.131894000	0.607051000	H	-8.265126000	1.609751000	-1.031513000
C	4.003303000	0.107311000	-0.728191000	H	-5.789693000	2.345192000	-2.805579000
H	4.587615000	0.103797000	-1.640828000	H	-4.481362000	-2.400594000	-1.665628000
C	2.608931000	0.096066000	-0.778225000	H	-4.739361000	1.397585000	1.441687000
C	1.720224000	0.072973000	-2.010255000	H	-7.048734000	-1.794901000	-2.767285000
O	2.235201000	0.057226000	-3.142393000	H	-7.563226000	-3.252090000	2.141630000
C	-0.533866000	0.028945000	-2.793385000	H	-9.254607000	3.267847000	0.508924000
C	-0.987480000	1.235618000	-3.367377000	H	-6.653676000	2.578468000	-5.104669000
C	-0.477124000	2.566824000	-2.868960000	H	-4.744723000	-4.692120000	-0.781345000
H	-0.675205000	2.694979000	-1.798423000	H	-5.758688000	3.050305000	3.017762000
H	-0.954972000	3.390852000	-3.406057000	H	-7.891516000	-1.548524000	-5.071937000
H	0.606751000	2.657625000	-3.003335000	H	-6.280544000	-5.126941000	1.128037000
C	-1.921837000	1.173282000	-4.410923000	H	-8.011219000	3.989869000	2.538132000
H	-2.275215000	2.098291000	-4.860087000	H	-7.700774000	0.632853000	-6.252109000?
C	-2.400152000	-0.053758000	-4.876148000	⁴ IM1 _{PF}			
H	-3.123849000	-0.085735000	-5.685981000	Ni	-0.123251000	0.059788000	0.162564000
C	-1.946587000	-1.239353000	-4.293703000	N	0.025067000	0.058993000	2.129446000
H	-2.318160000	-2.196383000	-4.652018000	N	1.816841000	0.065645000	0.297067000
C	-1.012127000	-1.218511000	-3.248520000	N	0.292001000	0.058598000	-1.766988000
C	-0.524715000	-2.505210000	-2.625348000	C	-1.051970000	0.053940000	3.067651000
H	0.557554000	-2.627279000	-2.748178000	C	-1.606223000	-1.177086000	3.479231000
H	-1.016614000	-3.368201000	-3.082652000	C	-1.039664000	-2.484541000	2.978267000
H	-0.723857000	-2.528270000	-1.547492000	H	0.009917000	-2.605951000	3.269566000
F	-3.267511000	0.441693000	0.002195000	H	-1.602959000	-3.330706000	3.381327000
P	-5.679718000	0.141717000	-0.948268000	H	-1.071639000	-2.541904000	1.883974000
C	-5.904054000	-1.524905000	-0.281997000	C	-2.692542000	-1.162034000	4.365752000
C	-6.443381000	1.380953000	0.127528000	H	-3.124983000	-2.106057000	4.688265000
C	-6.374433000	0.262258000	-2.613874000	C	-3.220556000	0.042547000	4.835627000
C	-6.760920000	-1.769757000	0.805868000	H	-4.063251000	0.038287000	5.521573000
C	-7.713268000	1.921181000	-0.150897000	C	-2.662769000	1.252771000	4.417355000
C	-6.255870000	1.493858000	-3.292844000	H	-3.072308000	2.192362000	4.780186000
C	-5.167766000	-2.585024000	-0.844672000	C	-1.576414000	1.279600000	3.531263000
C	-5.734243000	1.797013000	1.269845000	C	-0.980360000	2.593187000	3.083437000
C	-6.953749000	-0.840206000	-3.272487000	H	-1.006894000	2.693494000	1.992089000

H	0.070174000	2.680735000	3.383145000	C	-6.828545000	1.502449000	-4.437650000
H	-1.527106000	3.434878000	3.517442000	C	-5.031390000	-3.758593000	0.304863000
C	1.297766000	0.063316000	2.615302000	C	-5.948156000	2.980563000	2.097496000
O	1.649890000	0.062816000	3.807771000	C	-7.127423000	-0.897830000	-4.403816000
C	2.347160000	0.068432000	1.516143000	C	-6.298541000	-4.011674000	0.839623000
C	3.735405000	0.074117000	1.654266000	C	-7.251372000	3.416647000	1.839185000
H	4.191539000	0.076357000	2.637350000	C	-7.247161000	0.325045000	-5.072715000
C	4.507176000	0.076985000	0.482786000	H	-7.694034000	-0.936794000	0.422676000
H	5.590018000	0.081608000	0.557273000	H	-7.932198000	1.510164000	-0.891247000
C	3.903402000	0.073806000	-0.783434000	H	-5.958882000	2.377423000	-2.682567000
H	4.491050000	0.075812000	-1.693948000	H	-3.728830000	-2.295249000	-0.590206000
C	2.509155000	0.067969000	-0.837646000	H	-4.338829000	1.687792000	1.487384000
C	1.620567000	0.063382000	-2.070688000	H	-6.521677000	-1.908485000	-2.608739000
O	2.134432000	0.064247000	-3.202863000	H	-8.237709000	-3.178481000	1.298920000
C	-0.637968000	0.052598000	-2.850785000	H	-8.972856000	3.205315000	0.551561000
C	-1.115292000	1.278304000	-3.362278000	H	-6.910398000	2.456904000	-4.950163000
C	-0.626691000	2.592185000	-2.799673000	H	-4.285142000	-4.547037000	0.272053000
H	-0.824341000	2.665258000	-1.723773000	H	-5.391723000	3.390399000	2.935356000
H	-1.119563000	3.433102000	-3.295379000	H	-7.446986000	-1.816836000	-4.887466000
H	0.455267000	2.708382000	-2.930225000	H	-6.540164000	-4.998188000	1.224490000
C	-2.050442000	1.251375000	-4.406589000	H	-7.712996000	4.166942000	2.474459000
H	-2.421988000	2.191004000	-4.808112000	H	-7.654583000	0.361468000	-6.078679000
C	-2.506302000	0.040639000	-4.932738000	² (L)Ni ^I			
H	-3.230945000	0.036057000	-5.742241000	Ni	-0.062714000	0.060858000	0.012519000
C	-2.030255000	-1.164215000	-4.410921000	N	0.034216000	-0.068028000	2.022424000
H	-2.385778000	-2.108523000	-4.816051000	N	1.848143000	0.130415000	0.216063000
C	-1.094364000	-1.179146000	-3.367015000	N	0.445216000	0.208445000	-1.932226000
C	-0.582878000	-2.486764000	-2.810189000	C	-1.058251000	-0.199554000	2.918984000
H	0.500965000	-2.583315000	-2.940910000	C	-1.425440000	-1.472787000	3.414850000
H	-1.060674000	-3.333976000	-3.309934000	C	-0.623896000	-2.698157000	3.045649000
H	-0.779358000	-2.568310000	-1.734652000	H	0.405868000	-2.627553000	3.413511000
F	-3.610948000	0.249447000	-0.070248000	H	-1.075836000	-3.601104000	3.466852000
P	-5.275881000	0.186377000	-0.854088000	H	-0.562471000	-2.818289000	1.957326000
C	-5.673020000	-1.460054000	-0.153199000	C	-2.550899000	-1.581037000	4.243838000
C	-6.050588000	1.474807000	0.187476000	H	-2.834070000	-2.559950000	4.624670000
C	-6.201612000	0.231768000	-2.449726000	C	-3.309787000	-0.457308000	4.582349000
C	-6.943759000	-1.720631000	0.384587000	H	-4.180313000	-0.557453000	5.225187000
C	-7.365104000	1.915794000	-0.060902000	C	-2.941904000	0.795158000	4.084352000
C	-6.296432000	1.456436000	-3.150322000	H	-3.528279000	1.674337000	4.342449000
C	-4.716990000	-2.488012000	-0.186363000	C	-1.821871000	0.942952000	3.253660000
C	-5.349258000	2.018378000	1.280780000	C	-1.433894000	2.301769000	2.721102000
C	-6.603125000	-0.949469000	-3.109737000	H	-1.395047000	2.301059000	1.624706000
C	-7.253176000	-2.990237000	0.880724000	H	-0.436013000	2.598733000	3.064626000
C	-7.957748000	2.879212000	0.758657000	H	-2.147017000	3.066196000	3.043931000

C	1.281879000	-0.046210000	2.525594000	C	-2.843984000	1.019237000	3.983382000
O	1.631512000	-0.104946000	3.734467000	H	-3.344256000	1.952905000	4.230536000
C	2.350278000	0.070970000	1.451739000	C	-1.710137000	1.050028000	3.158636000
C	3.733567000	0.119654000	1.640179000	C	-1.192132000	2.361974000	2.617714000
H	4.153402000	0.071920000	2.638645000	H	-1.202005000	2.374518000	1.521172000
C	4.548819000	0.230765000	0.503961000	H	-0.154634000	2.540354000	2.921864000
H	5.627987000	0.270875000	0.618891000	H	-1.801346000	3.197582000	2.974666000
C	3.985072000	0.290454000	-0.779285000	C	1.326870000	-0.096243000	2.508033000
H	4.601616000	0.376133000	-1.666974000	O	1.570694000	-0.073490000	3.742208000
C	2.593330000	0.236009000	-0.886772000	C	2.396672000	-0.054814000	1.479769000
C	1.768913000	0.281081000	-2.162296000	C	3.759448000	0.129816000	1.654096000
O	2.359665000	0.371888000	-3.271396000	H	4.172659000	0.205088000	2.655845000
C	-0.442145000	0.261702000	-3.038890000	C	4.592556000	0.258034000	0.513732000
C	-0.792905000	1.505967000	-3.613881000	H	5.660702000	0.406510000	0.634617000
C	-0.182659000	2.787339000	-3.098116000	C	4.013278000	0.278595000	-0.786136000
H	-0.361422000	2.907241000	-2.022791000	H	4.622149000	0.469705000	-1.664876000
H	-0.602792000	3.654954000	-3.615540000	C	2.649058000	0.090717000	-0.915764000
H	0.903787000	2.797716000	-3.240284000	C	1.814087000	0.179531000	-2.146585000
C	-1.723743000	1.532416000	-4.662008000	O	2.313995000	0.327395000	-3.290468000
H	-1.994508000	2.488958000	-5.103802000	C	-0.451472000	0.173330000	-2.969423000
C	-2.305868000	0.355865000	-5.141447000	C	-0.994095000	1.427439000	-3.331804000
H	-3.026578000	0.392789000	-5.954038000	C	-0.566333000	2.684687000	-2.612098000
C	-1.956106000	-0.867683000	-4.564822000	H	-0.780254000	2.622626000	-1.538449000
H	-2.405711000	-1.787766000	-4.931816000	H	-1.085515000	3.559302000	-3.014831000
C	-1.028150000	-0.934050000	-3.515604000	H	0.512174000	2.854148000	-2.706480000
C	-0.658296000	-2.262540000	-2.900052000	C	-1.938185000	1.486395000	-4.367164000
H	0.410564000	-2.476452000	-3.016783000	H	-2.356557000	2.450444000	-4.647649000
H	-1.221888000	-3.078103000	-3.363035000	C	-2.343591000	0.330473000	-5.038824000
H	-0.858193000	-2.268739000	-1.821302000	H	-3.076144000	0.391223000	-5.839291000
⁴ (L)Ni ^I				C	-1.802772000	-0.904481000	-4.672625000
Ni	0.015059000	-0.173041000	0.007673000	H	-2.115940000	-1.807954000	-5.191044000
N	0.056689000	-0.153844000	1.959704000	C	-0.857252000	-1.002494000	-3.641609000
N	1.900653000	-0.169591000	0.203045000	C	-0.286589000	-2.345161000	-3.250435000
N	0.462201000	0.085761000	-1.882836000	H	0.802160000	-2.369681000	-3.371643000
C	-1.059940000	-0.164426000	2.839974000	H	-0.716149000	-3.143698000	-3.862454000
C	-1.548870000	-1.390761000	3.346452000	H	-0.489099000	-2.572496000	-2.196893000
C	-0.862025000	-2.690853000	3.001789000	⁶ (L)Ni ^I			
H	0.178378000	-2.697235000	3.345240000	Ni	0.123915000	0.871871000	0.072607000
H	-1.378762000	-3.538126000	3.462120000	N	0.093669000	0.311223000	1.927300000
H	-0.835474000	-2.852109000	1.917452000	N	2.064259000	0.886077000	0.280823000
C	-2.684376000	-1.382341000	4.169258000	N	0.496845000	0.506757000	-1.799350000
H	-3.061316000	-2.324674000	4.560472000	C	-1.047853000	0.032536000	2.720567000
C	-3.332943000	-0.187226000	4.490287000	C	-1.505488000	-1.298150000	2.884814000
H	-4.212164000	-0.196169000	5.129007000	C	-0.762674000	-2.450319000	2.252392000

H	0.244499000	-2.550431000	2.671151000	Ni	0.145966000	0.073939000	0.033507000
H	-1.296437000	-3.392021000	2.410834000	N	0.153723000	0.023378000	1.940733000
H	-0.642963000	-2.300366000	1.172985000	N	1.952293000	0.124081000	0.220754000
C	-2.670149000	-1.531253000	3.629461000	N	0.544813000	0.137504000	-1.835704000
H	-3.021990000	-2.553075000	3.753694000	C	-1.035525000	-0.031137000	2.719576000
C	-3.382692000	-0.476413000	4.205568000	C	-1.663021000	-1.279757000	2.930564000
H	-4.284007000	-0.673606000	4.779890000	C	-1.052678000	-2.553345000	2.393950000
C	-2.929192000	0.833421000	4.034494000	H	-0.040258000	-2.706964000	2.783963000
H	-3.478607000	1.659049000	4.481255000	H	-1.659357000	-3.419453000	2.671872000
C	-1.767516000	1.106365000	3.297303000	H	-0.970079000	-2.532398000	1.301279000
C	-1.291825000	2.530780000	3.128320000	C	-2.859275000	-1.313618000	3.659970000
H	-1.313028000	2.842172000	2.076653000	H	-3.348274000	-2.269193000	3.831750000
H	-0.257133000	2.651415000	3.467131000	C	-3.424025000	-0.141199000	4.167493000
H	-1.923058000	3.219815000	3.697451000	H	-4.352247000	-0.183817000	4.730594000
C	1.357221000	0.010311000	2.415509000	C	-2.794060000	1.086331000	3.948924000
O	1.591202000	-0.421777000	3.582460000	H	-3.234006000	1.998687000	4.343659000
C	2.434251000	0.280730000	1.473142000	C	-1.597319000	1.163609000	3.223696000
C	3.848922000	-0.138820000	1.640517000	C	-0.920990000	2.493773000	2.991994000
H	4.253557000	-0.278283000	2.636896000	H	-0.760398000	2.680666000	1.924416000
C	4.643900000	-0.271370000	0.495465000	H	0.063294000	2.529390000	3.472697000
H	5.693936000	-0.533049000	0.594907000	H	-1.524670000	3.310761000	3.396285000
C	4.111739000	-0.000366000	-0.771144000	C	1.373161000	0.054454000	2.519371000
H	4.722804000	-0.028917000	-1.666540000	O	1.655012000	0.035644000	3.731804000
C	2.687515000	0.410070000	-0.864191000	C	2.453810000	0.113695000	1.462553000
C	1.838841000	0.249298000	-2.036995000	C	3.834049000	0.151143000	1.640571000
O	2.322224000	-0.056925000	-3.166630000	H	4.247172000	0.143674000	2.642586000
C	-0.452068000	0.308265000	-2.833201000	C	4.649301000	0.197284000	0.501803000
C	-1.091581000	1.432732000	-3.409147000	H	5.728211000	0.226562000	0.614053000
C	-0.720610000	2.834144000	-2.982071000	C	4.084868000	0.205798000	-0.780631000
H	-0.982434000	3.020896000	-1.933208000	H	4.694585000	0.240131000	-1.676050000
H	-1.241213000	3.575781000	-3.595367000	C	2.697519000	0.167995000	-0.891121000
H	0.357064000	3.008828000	-3.069584000	C	1.857534000	0.169903000	-2.149060000
C	-2.074914000	1.233469000	-4.389274000	O	2.383647000	0.201792000	-3.276891000
H	-2.561190000	2.098719000	-4.834281000	C	-0.460743000	0.108863000	-2.841678000
C	-2.431130000	-0.052282000	-4.802055000	C	-1.159489000	1.298734000	-3.148278000
H	-3.194802000	-0.191927000	-5.562577000	C	-0.801541000	2.603932000	-2.476455000
C	-1.800203000	-1.157846000	-4.226000000	H	-0.963552000	2.559902000	-1.393293000
H	-2.078757000	-2.162261000	-4.537353000	H	-1.407923000	3.421828000	-2.875108000
C	-0.813456000	-0.999614000	-3.242857000	H	0.253955000	2.855646000	-2.627614000
C	-0.163472000	-2.210335000	-2.617775000	C	-2.186999000	1.246578000	-4.100063000
H	0.902060000	-2.260859000	-2.866951000	H	-2.728005000	2.156902000	-4.345729000
H	-0.641940000	-3.131400000	-2.963465000	C	-2.518656000	0.047071000	-4.734028000
H	-0.230874000	-2.176153000	-1.524208000	H	-3.318746000	0.022774000	-5.468734000
¹ (L)Ni ^{II}				C	-1.820523000	-1.121552000	-4.420526000

H	-2.079258000	-2.055559000	-4.912974000	H	-1.159734000	3.519785000	-3.168935000
C	-0.787733000	-1.112872000	-3.473262000	H	0.448533000	2.864581000	-2.817457000
C	-0.040916000	-2.381437000	-3.137467000	C	-1.951787000	1.379030000	-4.450789000
H	1.014452000	-2.308790000	-3.423743000	H	-2.386406000	2.321837000	-4.773913000
H	-0.475957000	-3.237001000	-3.661009000	C	-2.323019000	0.189006000	-5.080393000
H	-0.065977000	-2.587423000	-2.061633000	H	-3.045806000	0.203375000	-5.891541000
³ (L)Ni ^{II}				C	-1.763446000	-1.019999000	-4.660800000
Ni	-0.024099000	0.070371000	0.016331000	H	-2.052108000	-1.948494000	-5.147351000
N	0.041001000	0.016879000	1.978343000	C	-0.829792000	-1.059784000	-3.615474000
N	1.903849000	0.112168000	0.219523000	C	-0.234591000	-2.372665000	-3.164656000
N	0.447435000	0.132074000	-1.890249000	H	0.852626000	-2.388924000	-3.301460000
C	-1.073277000	-0.074428000	2.867009000	H	-0.659138000	-3.205673000	-3.731709000
C	-1.583411000	-1.345855000	3.208206000	H	-0.422342000	-2.552185000	-2.099633000
C	-0.932945000	-2.605474000	2.686475000	⁵ (L)Ni ^{II}			
H	0.110120000	-2.685385000	3.013047000	Ni	0.024999000	-0.351892000	0.028631000
H	-1.466798000	-3.491875000	3.039992000	N	0.061615000	-0.143238000	2.010945000
H	-0.922866000	-2.627568000	1.590325000	N	1.840574000	0.263639000	0.193288000
C	-2.709714000	-1.416304000	4.040297000	N	0.476625000	-0.158221000	-1.979814000
H	-3.108946000	-2.391514000	4.308288000	C	-1.037606000	-0.372888000	2.883583000
C	-3.319414000	-0.257023000	4.525102000	C	-1.310203000	-1.688351000	3.320644000
H	-4.191919000	-0.327990000	5.168748000	C	-0.407821000	-2.830781000	2.918379000
C	-2.804320000	0.993669000	4.177021000	H	0.611987000	-2.687685000	3.293644000
H	-3.277569000	1.897986000	4.551714000	H	-0.783584000	-3.780570000	3.309209000
C	-1.679639000	1.105984000	3.347058000	H	-0.331264000	-2.914334000	1.827788000
C	-1.131114000	2.462352000	2.971992000	C	-2.430158000	-1.912287000	4.133741000
H	-1.121148000	2.603278000	1.884781000	H	-2.643896000	-2.922446000	4.474846000
H	-0.098096000	2.587388000	3.315895000	C	-3.268054000	-0.859036000	4.508118000
H	-1.734084000	3.260197000	3.414223000	H	-4.133072000	-1.047182000	5.138264000
C	1.294636000	0.031433000	2.514258000	C	-2.990758000	0.436848000	4.065680000
O	1.598529000	-0.005368000	3.718613000	H	-3.643093000	1.258099000	4.352960000
C	2.387109000	0.096194000	1.457568000	C	-1.880712000	0.699898000	3.250626000
C	3.769079000	0.133645000	1.645940000	C	-1.594282000	2.102159000	2.768299000
H	4.191125000	0.121289000	2.644066000	H	-1.572471000	2.151234000	1.673113000
C	4.581279000	0.187677000	0.502972000	H	-0.618382000	2.455437000	3.119626000
H	5.660216000	0.217956000	0.617066000	H	-2.357133000	2.799542000	3.125712000
C	4.024338000	0.204219000	-0.784856000	C	1.256691000	0.247255000	2.512469000
H	4.644577000	0.246964000	-1.672516000	O	1.536867000	0.433431000	3.716536000
C	2.633587000	0.164505000	-0.890134000	C	2.312083000	0.448782000	1.436630000
C	1.784640000	0.178853000	-2.152644000	C	3.642599000	0.763851000	1.644895000
O	2.332408000	0.233462000	-3.266905000	H	4.023538000	0.917166000	2.647144000
C	-0.461959000	0.151620000	-2.991214000	C	4.490655000	0.857103000	0.492446000
C	-1.020879000	1.381123000	-3.402175000	H	5.542177000	1.093618000	0.625602000
C	-0.626767000	2.673557000	-2.726680000	C	3.994551000	0.646910000	-0.777727000
H	-0.852785000	2.650964000	-1.654002000	H	4.635453000	0.711957000	-1.650760000

C	2.608466000	0.350719000	-0.943364000	C	2.370006000	0.123042000	1.454620000
C	1.908929000	0.102680000	-2.161363000	C	3.749541000	0.182848000	1.638528000
O	2.417989000	-0.032847000	-3.305541000	H	4.158721000	0.163389000	2.641993000
C	-0.399817000	0.128144000	-2.982377000	C	4.567612000	0.266415000	0.504879000
C	-0.295839000	1.325061000	-3.795786000	H	5.645921000	0.314150000	0.619248000
C	0.690363000	2.431112000	-3.500287000	C	4.001214000	0.288317000	-0.775787000
H	0.822304000	2.580162000	-2.424832000	H	4.608805000	0.351923000	-1.671058000
H	0.329853000	3.369314000	-3.929737000	C	2.613880000	0.225753000	-0.885813000
H	1.675288000	2.216059000	-3.922575000	C	1.791355000	0.235625000	-2.150023000
C	-1.230677000	1.522880000	-4.805797000	O	2.344239000	0.306587000	-3.270335000
H	-1.179865000	2.433404000	-5.396121000	C	-0.459123000	0.162529000	-2.941875000
C	-2.251215000	0.596588000	-5.058729000	C	-0.971989000	1.388766000	-3.416962000
H	-2.956146000	0.773101000	-5.865505000	C	-0.506330000	2.698822000	-2.826959000
C	-2.375525000	-0.544781000	-4.257521000	H	-0.679652000	2.733481000	-1.745536000
H	-3.167514000	-1.259518000	-4.461419000	H	-1.032079000	3.540534000	-3.286850000
C	-1.495956000	-0.792219000	-3.209553000	H	0.569058000	2.846702000	-2.979134000
C	-1.660929000	-2.053440000	-2.398942000	C	-1.919874000	1.368170000	-4.450112000
H	-0.702633000	-2.524621000	-2.168188000	H	-2.319426000	2.309175000	-4.820946000
H	-2.280615000	-2.771906000	-2.941364000	C	-2.354211000	0.161335000	-5.003455000
H	-2.169213000	-1.850998000	-1.446150000	H	-3.090604000	0.160809000	-5.802668000
¹ (L)Ni ^{II} F				C	-1.838505000	-1.044855000	-4.523404000
Ni	0.028818000	0.060226000	0.023159000	H	-2.174396000	-1.986429000	-4.951491000
N	0.077314000	-0.013616000	1.966548000	C	-0.889217000	-1.063945000	-3.491517000
N	1.857079000	0.146497000	0.216984000	C	-0.335578000	-2.372552000	-2.979825000
N	0.476516000	0.160049000	-1.868824000	H	0.746535000	-2.440494000	-3.141197000
C	-1.058244000	-0.110708000	2.819314000	H	-0.807094000	-3.219050000	-3.487302000
C	-1.588539000	-1.382022000	3.125563000	H	-0.500920000	-2.479628000	-1.902005000
C	-0.938853000	-2.635014000	2.588683000	F	-1.792654000	-0.033029000	-0.166343000
H	0.088545000	-2.742682000	2.955608000	³ (L)Ni ^{II} F			
H	-1.500636000	-3.524051000	2.889384000	Ni	-0.168832000	-0.118884000	-0.006141000
H	-0.882361000	-2.614167000	1.494705000	N	0.009724000	-0.091858000	2.057267000
C	-2.727956000	-1.459596000	3.939057000	N	1.807477000	-0.008941000	0.203147000
H	-3.142086000	-2.436157000	4.178884000	N	0.427632000	0.148849000	-1.976282000
C	-3.332554000	-0.304608000	4.440917000	C	-1.065228000	-0.123739000	2.988255000
H	-4.215903000	-0.379749000	5.069453000	C	-1.523889000	-1.359655000	3.496066000
C	-2.797288000	0.947511000	4.129447000	C	-0.848159000	-2.651357000	3.100862000
H	-3.265874000	1.848826000	4.517677000	H	0.200293000	-2.669985000	3.419491000
C	-1.659140000	1.064504000	3.318580000	H	-1.354938000	-3.509103000	3.552448000
C	-1.087628000	2.422566000	2.986608000	H	-0.850695000	-2.785216000	2.012790000
H	-1.039628000	2.580764000	1.903267000	C	-2.622165000	-1.367287000	4.367741000
H	-0.065579000	2.530953000	3.367429000	H	-2.978143000	-2.316796000	4.760998000
H	-1.697887000	3.218184000	3.423562000	C	-3.261700000	-0.179848000	4.732106000
C	1.305058000	0.026500000	2.518202000	H	-4.112704000	-0.201906000	5.407564000
O	1.614107000	-0.008719000	3.730143000	C	-2.801926000	1.035551000	4.219578000

H	-3.296965000	1.963100000	4.497900000	H	0.521813000	-2.650793000	3.287454000
C	-1.705937000	1.083042000	3.346050000	H	-0.887879000	-3.712047000	3.465231000
C	-1.219670000	2.402526000	2.794271000	H	-0.563030000	-2.892645000	1.925559000
H	-1.261843000	2.416704000	1.698754000	C	-2.447045000	-1.800514000	4.348780000
H	-0.176439000	2.595123000	3.069912000	H	-2.669992000	-2.804862000	4.701904000
H	-1.828743000	3.229423000	3.170897000	C	-3.230874000	-0.724213000	4.771969000
C	1.269058000	-0.088044000	2.535562000	H	-4.062996000	-0.887146000	5.451743000
O	1.643437000	-0.111354000	3.730123000	C	-2.939638000	0.562691000	4.311950000
C	2.314638000	-0.024513000	1.437056000	H	-3.549014000	1.403757000	4.635146000
C	3.695354000	0.049558000	1.626489000	C	-1.870956000	0.792291000	3.433870000
H	4.107355000	0.034665000	2.628632000	C	-1.571928000	2.186352000	2.935685000
C	4.511097000	0.150599000	0.492683000	H	-1.597770000	2.231493000	1.840607000
H	5.589094000	0.209173000	0.607627000	H	-0.572296000	2.514698000	3.242162000
C	3.945345000	0.191147000	-0.787713000	H	-2.300112000	2.903795000	3.325273000
H	4.554097000	0.287361000	-1.678986000	C	1.177138000	0.287697000	2.531021000
C	2.555955000	0.111857000	-0.894639000	O	1.514267000	0.503489000	3.722591000
C	1.757879000	0.181937000	-2.184122000	C	2.194563000	0.455917000	1.418499000
O	2.369808000	0.274449000	-3.272889000	C	3.522194000	0.778269000	1.639106000
C	-0.434060000	0.210162000	-3.106043000	H	3.875967000	0.947293000	2.648627000
C	-0.991724000	1.450484000	-3.486587000	C	4.393307000	0.858879000	0.506864000
C	-0.634677000	2.712999000	-2.738036000	H	5.442347000	1.101941000	0.649674000
H	-0.896149000	2.633993000	-1.676186000	C	3.904289000	0.624323000	-0.759216000
H	-1.160875000	3.575549000	-3.157157000	H	4.546229000	0.674997000	-1.632501000
H	0.441426000	2.916866000	-2.781286000	C	2.522761000	0.317613000	-0.936331000
C	-1.885425000	1.489169000	-4.566629000	C	1.900335000	0.061234000	-2.192274000
H	-2.316565000	2.442817000	-4.862569000	O	2.500668000	-0.045988000	-3.302322000
C	-2.225752000	0.325994000	-5.261257000	C	-0.334130000	0.065518000	-3.143734000
H	-2.920474000	0.370434000	-6.095722000	C	-0.273755000	1.327378000	-3.850962000
C	-1.669938000	-0.895707000	-4.873435000	C	0.648323000	2.446912000	-3.428321000
H	-1.934177000	-1.805141000	-5.408284000	H	0.647932000	2.578361000	-2.341547000
C	-0.773086000	-0.973805000	-3.798499000	H	0.324522000	3.387232000	-3.882144000
C	-0.186967000	-2.302405000	-3.382871000	H	1.681108000	2.256381000	-3.731680000
H	0.904656000	-2.308343000	-3.480337000	C	-1.186452000	1.558182000	-4.875650000
H	-0.586474000	-3.113144000	-3.998986000	H	-1.171971000	2.517554000	-5.385846000
H	-0.411700000	-2.526170000	-2.333491000	C	-2.137021000	0.596706000	-5.246489000
F	-2.055793000	-0.376450000	-0.223101000	H	-2.827083000	0.803133000	-6.059420000
⁵ (L)Ni ^{II} F				C	-2.206861000	-0.621129000	-4.559471000
Ni	-0.163356000	-0.350141000	0.042308000	H	-2.940595000	-1.365204000	-4.856730000
N	-0.027167000	-0.106078000	2.086864000	C	-1.344666000	-0.904032000	-3.504217000
N	1.708476000	0.241102000	0.178754000	C	-1.408721000	-2.238749000	-2.811752000
N	0.496126000	-0.254122000	-2.115092000	H	-0.447924000	-2.761873000	-2.863000000
C	-1.080586000	-0.302633000	3.016221000	H	-2.170965000	-2.870946000	-3.275614000
C	-1.370339000	-1.608818000	3.471164000	H	-1.657748000	-2.101727000	-1.754255000
C	-0.532056000	-2.780195000	3.015912000	F	-2.034926000	-0.617453000	-0.173349000

¹ IM _{PF}				H	-11.840331000	2.129831000	-3.732478000
F	-6.773489000	6.131015000	1.549488000	H	-10.338663000	1.198343000	-3.563411000
P	-7.924626000	5.104423000	1.105385000	C	-12.357902000	2.156393000	-1.165024000
C	-7.862923000	5.083117000	-0.678586000	H	-12.761597000	2.982970000	-1.745078000
C	-7.482427000	3.551404000	1.868059000	C	-12.578081000	2.100083000	0.213226000
C	-9.435407000	5.808897000	1.753017000	H	-13.150524000	2.880662000	0.707003000
C	-7.882374000	3.867209000	-1.385084000	C	-12.061525000	1.033890000	0.953218000
C	-8.420227000	2.849348000	2.645240000	H	-12.234141000	0.984619000	2.025775000
C	-9.465191000	6.271216000	3.083561000	C	-11.322710000	0.016047000	0.333241000
C	-7.819040000	6.315698000	-1.362590000	C	-10.780927000	-1.140552000	1.139349000
C	-6.178439000	3.048398000	1.690008000	H	-9.694436000	-1.229904000	1.030166000
C	-10.581717000	5.886889000	0.943109000	H	-11.210364000	-2.093525000	0.809356000
C	-7.856419000	3.898000000	-2.781505000	H	-11.011626000	-1.015614000	2.201172000
C	-8.048821000	1.644839000	3.243957000	C	-10.988255000	-2.002416000	-2.195609000
C	-10.643907000	6.812095000	3.593176000	O	-12.213838000	-2.251532000	-2.166776000
C	-7.786378000	6.324929000	-2.754639000	C	-10.023302000	-2.964434000	-2.840442000
C	-5.820495000	1.848242000	2.299671000	C	-10.321714000	-4.178788000	-3.454197000
C	-11.757045000	6.425092000	1.469597000	H	-11.349938000	-4.518281000	-3.501069000
C	-7.807017000	5.116550000	-3.462930000	C	-9.268312000	-4.925909000	-3.995624000
C	-6.753556000	1.148141000	3.074114000	H	-9.472414000	-5.875765000	-4.479585000
C	-11.787538000	6.886883000	2.788537000	C	-7.952796000	-4.452684000	-3.915798000
H	-7.921689000	2.903097000	-0.884672000	H	-7.116623000	-5.007382000	-4.325457000
H	-9.424972000	3.233444000	2.782606000	C	-7.727506000	-3.229945000	-3.287846000
H	-8.581473000	6.217679000	3.711432000	C	-6.406174000	-2.532105000	-3.089706000
H	-7.803641000	7.254337000	-0.817498000	O	-5.345468000	-3.043024000	-3.512510000
H	-5.450761000	3.586019000	1.090533000	C	-5.420400000	-0.570219000	-2.166074000
H	-10.561558000	5.533050000	-0.081927000	C	-4.717464000	-0.746840000	-0.955041000
H	-7.872356000	2.962804000	-3.330527000	C	-5.147144000	-1.799996000	0.038580000
H	-8.770650000	1.099191000	3.842633000	H	-6.183771000	-1.648723000	0.359537000
H	-10.669746000	7.175063000	4.615445000	H	-4.506400000	-1.781945000	0.924792000
H	-7.745642000	7.270734000	-3.285082000	H	-5.095313000	-2.804515000	-0.396852000
H	-4.816637000	1.458743000	2.168206000	C	-3.603761000	0.065327000	-0.697365000
H	-12.644022000	6.485534000	0.847573000	H	-3.055368000	-0.067679000	0.232271000
H	-7.784019000	5.128044000	-4.548421000	C	-3.191893000	1.033989000	-1.615702000
H	-6.468735000	0.212175000	3.544648000	H	-2.327880000	1.657305000	-1.401293000
H	-12.703426000	7.307804000	3.191858000	C	-3.894279000	1.195288000	-2.812308000
Ni	-8.408299000	-0.925391000	-1.955150000	H	-3.573939000	1.944917000	-3.532098000
N	-10.341511000	-0.927729000	-1.703494000	C	-5.010459000	0.399101000	-3.106482000
N	-8.754949000	-2.537151000	-2.778567000	C	-5.747620000	0.562041000	-4.414506000
N	-6.570242000	-1.366539000	-2.434256000	H	-5.659286000	-0.337452000	-5.035211000
C	-11.106238000	0.086656000	-1.059625000	H	-5.347865000	1.405617000	-4.984395000
C	-11.623396000	1.157455000	-1.819890000	H	-6.818503000	0.727189000	-4.253826000
C	-11.405127000	1.218194000	-3.313145000	F	-8.064097000	0.684281000	-1.134594000
H	-11.863480000	0.360201000	-3.818370000	¹ TS _{2PF}			

F	-7.036725000	4.696053000	1.515767000	H	-10.220426000	1.487960000	-3.399120000
P	-7.743111000	3.496507000	0.644734000	C	-12.966307000	2.494565000	-1.947533000
C	-7.276460000	4.167758000	-0.984850000	H	-13.249706000	3.099031000	-2.805913000
C	-6.955104000	2.140929000	1.573414000	C	-13.622502000	2.666503000	-0.727537000
C	-9.449553000	3.833011000	1.133087000	H	-14.409629000	3.409316000	-0.630709000
C	-8.079922000	3.994066000	-2.124164000	C	-13.259291000	1.882263000	0.368230000
C	-7.645482000	0.955833000	1.873549000	H	-13.765770000	2.015718000	1.320709000
C	-9.887202000	3.410976000	2.400803000	C	-12.245766000	0.919637000	0.265639000
C	-6.157558000	5.020030000	-1.043398000	C	-11.896087000	0.055185000	1.452781000
C	-5.694756000	2.380972000	2.150459000	H	-10.815178000	0.013289000	1.618772000
C	-10.223025000	4.741270000	0.391293000	H	-12.234126000	-0.975912000	1.297622000
C	-7.779931000	4.688045000	-3.296607000	H	-12.369336000	0.434617000	2.362666000
C	-7.089557000	0.033736000	2.761916000	C	-11.100970000	-1.534095000	-1.288016000
C	-11.093544000	3.889977000	2.912752000	O	-12.286994000	-1.920401000	-1.223555000
C	-5.853887000	5.688836000	-2.230378000	C	-10.004316000	-2.505080000	-1.610790000
C	-5.138888000	1.441618000	3.020766000	C	-10.133323000	-3.879896000	-1.789892000
C	-11.427764000	5.213417000	0.913900000	H	-11.103341000	-4.345128000	-1.659646000
C	-6.669411000	5.534600000	-3.353918000	C	-8.995545000	-4.615142000	-2.139870000
C	-5.838869000	0.274508000	3.338017000	H	-9.065854000	-5.688556000	-2.283768000
C	-11.862179000	4.793114000	2.173586000	C	-7.769307000	-3.964666000	-2.313138000
H	-8.926292000	3.322579000	-2.088887000	H	-6.868859000	-4.496766000	-2.596576000
H	-8.609361000	0.761969000	1.424196000	C	-7.716260000	-2.586947000	-2.116034000
H	-9.290036000	2.731662000	2.997833000	C	-6.519711000	-1.700854000	-2.292066000
H	-5.531981000	5.179572000	-0.174118000	O	-5.448775000	-2.173081000	-2.729603000
H	-5.151928000	3.295370000	1.943349000	C	-5.744298000	0.515833000	-2.212242000
H	-9.888350000	5.096068000	-0.576139000	C	-4.638133000	0.593029000	-1.337886000
H	-8.415486000	4.559590000	-4.167189000	C	-4.524085000	-0.324208000	-0.146403000
H	-7.637934000	-0.872205000	3.000793000	H	-5.449107000	-0.353542000	0.433827000
H	-11.425960000	3.560450000	3.892133000	H	-3.711779000	-0.007409000	0.512753000
H	-4.984385000	6.337609000	-2.267835000	H	-4.317303000	-1.350111000	-0.473317000
H	-4.163328000	1.631608000	3.457113000	C	-3.606394000	1.495909000	-1.632538000
H	-12.021911000	5.913448000	0.335275000	H	-2.753937000	1.560629000	-0.960298000
H	-6.439055000	6.069068000	-4.270736000	C	-3.651089000	2.292017000	-2.778289000
H	-5.410032000	-0.446097000	4.027853000	H	-2.842082000	2.984557000	-2.994896000
H	-12.797364000	5.168219000	2.578071000	C	-4.736850000	2.186247000	-3.649279000
Ni	-8.672987000	-0.102227000	-1.385887000	H	-4.768602000	2.791591000	-4.551514000
N	-10.619400000	-0.280110000	-1.141029000	C	-5.792043000	1.302621000	-3.384483000
N	-8.816972000	-1.907029000	-1.773266000	C	-6.925939000	1.157202000	-4.371103000
N	-6.796377000	-0.419875000	-1.963557000	H	-6.999979000	0.128598000	-4.742520000
C	-11.596685000	0.747743000	-0.976248000	H	-6.778523000	1.818940000	-5.229187000
C	-11.953693000	1.535885000	-2.093096000	H	-7.892914000	1.398739000	-3.918739000
C	-11.301918000	1.320621000	-3.438631000	F	-8.549912000	1.680136000	-0.692357000
H	-11.445865000	0.293350000	-3.792547000	¹ IM2 _{PF}			
H	-11.723645000	1.999603000	-4.185131000	F	-6.991951000	4.369671000	1.450875000

P	-7.767032000	3.163875000	0.556654000	C	-12.937071000	2.657981000	-1.921676000
C	-7.315917000	3.983594000	-1.022029000	H	-13.216284000	3.286526000	-2.763842000
C	-6.901691000	1.853427000	1.507450000	C	-13.574831000	2.819385000	-0.690597000
C	-9.394595000	3.640786000	1.229696000	H	-14.341170000	3.579974000	-0.568514000
C	-8.173764000	3.925782000	-2.133174000	C	-13.223935000	1.998848000	0.382333000
C	-7.544878000	0.642077000	1.810938000	H	-13.719669000	2.121352000	1.341723000
C	-9.789034000	3.165739000	2.489616000	C	-12.235269000	1.014941000	0.248274000
C	-6.180575000	4.811512000	-1.071688000	C	-11.900210000	0.111852000	1.410232000
C	-5.645778000	2.125894000	2.077590000	H	-10.820257000	0.043695000	1.571911000
C	-10.136503000	4.654167000	0.604897000	H	-12.260923000	-0.907062000	1.228503000
C	-7.913539000	4.705613000	-3.261463000	H	-12.362185000	0.477262000	2.331329000
C	-6.951933000	-0.269113000	2.688077000	C	-11.147027000	-1.425827000	-1.370686000
C	-10.922034000	3.695754000	3.111399000	O	-12.337516000	-1.791349000	-1.304712000
C	-5.910953000	5.563730000	-2.216274000	C	-10.069437000	-2.405204000	-1.727710000
C	-5.047253000	1.198460000	2.932544000	C	-10.218823000	-3.773092000	-1.938282000
C	-11.267847000	5.178853000	1.234026000	H	-11.193918000	-4.227683000	-1.808340000
C	-6.782297000	5.524127000	-3.307659000	C	-9.094889000	-4.514767000	-2.318137000
C	-5.702765000	0.005761000	3.250448000	H	-9.181408000	-5.583364000	-2.486327000
C	-11.660533000	4.705079000	2.488283000	C	-7.861921000	-3.877055000	-2.490567000
H	-9.050183000	3.292243000	-2.111889000	H	-6.971940000	-4.413811000	-2.797294000
H	-8.512565000	0.415264000	1.384505000	C	-7.787318000	-2.505512000	-2.261828000
H	-9.214185000	2.400694000	2.999235000	C	-6.583827000	-1.629235000	-2.435040000
H	-5.512957000	4.882716000	-0.222620000	O	-5.527923000	-2.099576000	-2.904587000
H	-5.137521000	3.058933000	1.870113000	C	-5.784594000	0.579528000	-2.320595000
H	-9.833845000	5.049849000	-0.357955000	C	-4.649209000	0.615208000	-1.481254000
H	-8.596661000	4.666876000	-4.104443000	C	-4.498066000	-0.345897000	-0.329334000
H	-7.470998000	-1.192004000	2.928166000	H	-5.413028000	-0.422569000	0.261448000
H	-11.219547000	3.322036000	4.086536000	H	-3.683666000	-0.037198000	0.330751000
H	-5.023740000	6.188863000	-2.246121000	H	-4.270846000	-1.351363000	-0.703078000
H	-4.072246000	1.417011000	3.357162000	C	-3.616166000	1.514008000	-1.784154000
H	-11.836331000	5.962116000	0.741962000	H	-2.741676000	1.548806000	-1.138609000
H	-6.579975000	6.125403000	-4.189155000	C	-3.686253000	2.341330000	-2.905814000
H	-5.242337000	-0.705404000	3.929780000	H	-2.875761000	3.030214000	-3.128308000
H	-12.536940000	5.119968000	2.977184000	C	-4.797480000	2.269959000	-3.747502000
Ni	-8.699732000	-0.035546000	-1.456710000	H	-4.846770000	2.896498000	-4.634189000
N	-10.642167000	-0.183196000	-1.197260000	C	-5.855194000	1.393009000	-3.473684000
N	-8.875375000	-1.821503000	-1.890176000	C	-7.011207000	1.275230000	-4.438152000
N	-6.840390000	-0.352765000	-2.068666000	H	-7.099056000	0.254792000	-4.828651000
C	-11.598926000	0.859849000	-1.002680000	H	-6.877121000	1.953395000	-5.285399000
C	-11.951243000	1.677074000	-2.100216000	H	-7.967193000	1.515029000	-3.963144000
C	-11.333863000	1.466466000	-3.463189000	F	-8.570025000	1.761096000	-0.506277000
H	-11.499463000	0.444222000	-3.821772000	³ IM' _{PF}			
H	-11.766836000	2.156709000	-4.192538000	F	-6.752944000	6.573531000	2.053856000
H	-10.250022000	1.621785000	-3.455841000	P	-7.384746000	5.243798000	1.428612000

C	-7.059568000	5.408787000	-0.329709000	H	-13.421672000	3.247734000	-1.439565000
C	-6.518630000	3.923833000	2.282500000	C	-13.281983000	2.344100000	0.512890000
C	-9.127055000	5.284032000	1.814810000	H	-13.940732000	3.068059000	0.984464000
C	-7.445103000	4.385592000	-1.216257000	C	-12.718241000	1.311758000	1.266363000
C	-6.778434000	2.582183000	1.946981000	H	-12.939743000	1.232920000	2.328263000
C	-9.584500000	4.738845000	3.030209000	C	-11.868019000	0.366243000	0.675348000
C	-6.435709000	6.577131000	-0.803475000	C	-11.268599000	-0.748972000	1.499202000
C	-5.601598000	4.250327000	3.297692000	H	-10.173989000	-0.743311000	1.443290000
C	-10.018558000	5.943669000	0.946387000	H	-11.596637000	-1.732555000	1.143771000
C	-7.212140000	4.555933000	-2.581858000	H	-11.558643000	-0.654989000	2.549696000
C	-6.116321000	1.573539000	2.648854000	C	-11.264255000	-1.591185000	-1.816634000
C	-10.929413000	4.863935000	3.373531000	O	-12.467795000	-1.933195000	-1.793757000
C	-6.208916000	6.725166000	-2.172557000	C	-10.252139000	-2.507611000	-2.474323000
C	-4.948988000	3.226194000	3.985483000	C	-10.537005000	-3.721596000	-3.101069000
C	-11.360601000	6.061320000	1.303260000	H	-11.555767000	-4.089250000	-3.133767000
C	-6.599834000	5.718881000	-3.060347000	C	-9.476170000	-4.429493000	-3.679030000
C	-5.208275000	1.890665000	3.664488000	H	-9.665883000	-5.377337000	-4.173269000
C	-11.813619000	5.524490000	2.513475000	C	-8.173347000	-3.918859000	-3.630173000
H	-7.905562000	3.459601000	-0.874347000	H	-7.335987000	-4.442159000	-4.076486000
H	-7.464242000	2.303220000	1.148116000	C	-7.970742000	-2.697532000	-2.986268000
H	-8.901455000	4.223504000	3.697017000	C	-6.645040000	-1.974926000	-2.853853000
H	-6.136625000	7.362818000	-0.119307000	O	-5.615769000	-2.501931000	-3.331968000
H	-5.401233000	5.284607000	3.552752000	C	-5.561466000	-0.031543000	-2.045370000
H	-9.670816000	6.356956000	0.005535000	C	-4.755654000	-0.234209000	-0.903604000
H	-7.507934000	3.772939000	-3.271824000	C	-5.110616000	-1.300215000	0.105615000
H	-6.310624000	0.536664000	2.396160000	H	-6.135700000	-1.178949000	0.473602000
H	-11.287103000	4.442432000	4.307221000	H	-4.429669000	-1.269855000	0.960970000
H	-5.730887000	7.627063000	-2.541146000	H	-5.053782000	-2.301974000	-0.336265000
H	-4.242140000	3.474980000	4.770494000	C	-3.613266000	0.560559000	-0.732017000
H	-12.051791000	6.565718000	0.636136000	H	-2.990370000	0.408562000	0.146466000
H	-6.424742000	5.838859000	-4.125167000	C	-3.266760000	1.535787000	-1.670366000
H	-4.700984000	1.096407000	4.203700000	H	-2.379035000	2.145142000	-1.523453000
H	-12.860935000	5.615631000	2.784461000	C	-4.068236000	1.721746000	-2.799275000
Ni	-8.652905000	-0.312849000	-1.523479000	H	-3.800579000	2.476156000	-3.535485000
N	-10.712183000	-0.464752000	-1.322905000	C	-5.218708000	0.946711000	-3.004066000
N	-8.999068000	-2.052306000	-2.433585000	C	-6.068922000	1.140289000	-4.237258000
N	-6.752127000	-0.792757000	-2.214638000	H	-6.072152000	0.241718000	-4.865321000
C	-11.589556000	0.470330000	-0.705114000	H	-5.696833000	1.972989000	-4.840957000
C	-12.144173000	1.515825000	-1.475346000	H	-7.114386000	1.341039000	-3.976570000
C	-11.837684000	1.628317000	-2.950335000	F	-8.322043000	1.346269000	-0.583932000
H	-12.188293000	0.748435000	-3.502210000	³ TS _{2PF}			
H	-12.318431000	2.511467000	-3.380940000	F	-7.030610000	4.809674000	2.054728000
H	-10.758776000	1.701921000	-3.129742000	P	-7.628086000	3.735739000	0.989672000
C	-12.989230000	2.443119000	-0.849214000	C	-6.929271000	4.450936000	-0.523983000

C	-6.950744000	2.246254000	1.761913000	C	-13.960492000	2.450774000	-0.709664000
C	-9.387953000	4.002629000	1.223534000	H	-14.778200000	3.159306000	-0.608613000
C	-7.456606000	4.187925000	-1.799979000	C	-13.540333000	1.699450000	0.389389000
C	-7.717882000	1.086554000	1.951614000	H	-14.031604000	1.826994000	1.351133000
C	-9.958072000	3.624170000	2.452801000	C	-12.489184000	0.778349000	0.280350000
C	-5.878279000	5.378542000	-0.374071000	C	-12.063381000	-0.032444000	1.480745000
C	-5.648735000	2.327907000	2.289221000	H	-10.977014000	-0.006012000	1.617966000
C	-10.126596000	4.767269000	0.305881000	H	-12.342386000	-1.085564000	1.361500000
C	-6.949910000	4.868494000	-2.907620000	H	-12.534598000	0.345101000	2.392791000
C	-7.185854000	0.020315000	2.678672000	C	-11.159561000	-1.631468000	-1.173790000
C	-11.264782000	4.008011000	2.753239000	O	-12.305546000	-2.127054000	-1.049299000
C	-5.369713000	6.035724000	-1.495043000	C	-10.001344000	-2.563967000	-1.458405000
C	-5.124316000	1.251329000	3.004914000	C	-10.094940000	-3.953748000	-1.545300000
C	-11.432904000	5.143608000	0.618188000	H	-11.042847000	-4.442368000	-1.354352000
C	-5.910916000	5.791228000	-2.760052000	C	-8.945705000	-4.673505000	-1.890599000
C	-5.893170000	0.100860000	3.205699000	H	-8.986598000	-5.756168000	-1.961454000
C	-12.000648000	4.767829000	1.839015000	C	-7.749148000	-4.001789000	-2.164412000
H	-8.236882000	3.446330000	-1.911414000	H	-6.849957000	-4.528512000	-2.460608000
H	-8.711893000	1.018729000	1.530216000	C	-7.734590000	-2.610280000	-2.056818000
H	-9.389773000	3.050668000	3.177277000	C	-6.552440000	-1.724724000	-2.386993000
H	-5.465400000	5.602037000	0.601606000	O	-5.510279000	-2.265182000	-2.830954000
H	-5.048732000	3.221875000	2.158108000	C	-5.752037000	0.478837000	-2.570471000
H	-9.690136000	5.077996000	-0.635910000	C	-4.613496000	0.646097000	-1.749989000
H	-7.366529000	4.668024000	-3.889472000	C	-4.461307000	-0.141588000	-0.472171000
H	-7.784123000	-0.872425000	2.831388000	H	-5.350898000	-0.059893000	0.159347000
H	-11.703762000	3.715779000	3.701790000	H	-3.599204000	0.209544000	0.101718000
H	-4.557622000	6.745466000	-1.372796000	H	-4.318364000	-1.207042000	-0.686256000
H	-4.118641000	1.316229000	3.407783000	C	-3.608098000	1.534291000	-2.158289000
H	-12.003978000	5.732010000	-0.092629000	H	-2.731164000	1.664216000	-1.527917000
H	-5.520306000	6.313927000	-3.628030000	C	-3.711581000	2.239259000	-3.359582000
H	-5.484594000	-0.732245000	3.769607000	H	-2.920893000	2.919274000	-3.665232000
H	-13.016662000	5.066353000	2.077777000	C	-4.839625000	2.064655000	-4.163620000
Ni	-8.730344000	0.027007000	-1.418477000	H	-4.926615000	2.609568000	-5.100696000
N	-10.803827000	-0.335973000	-1.135615000	C	-5.870825000	1.194682000	-3.783040000
N	-8.838294000	-1.951898000	-1.695297000	C	-7.079961000	1.011372000	-4.669713000
N	-6.794333000	-0.416805000	-2.195778000	H	-7.215621000	-0.037499000	-4.956241000
C	-11.854991000	0.609226000	-0.972267000	H	-6.984933000	1.605585000	-5.583239000
C	-12.262881000	1.376624000	-2.088271000	H	-8.001211000	1.319086000	-4.160594000
C	-11.602160000	1.200261000	-3.436168000	F	-8.574460000	1.835663000	-0.681233000
H	-11.589066000	0.149718000	-3.745336000	³ IM2 _{PF}			
H	-12.129703000	1.776278000	-4.202153000	F	-7.275692000	4.419349000	1.397529000
H	-10.559117000	1.539704000	-3.425805000	P	-7.982998000	3.168086000	0.480483000
C	-13.316468000	2.289959000	-1.937821000	C	-7.395276000	3.934151000	-1.082285000
H	-13.638513000	2.871313000	-2.798821000	C	-7.108866000	1.916616000	1.499779000

C	-9.643447000	3.665555000	1.056977000	H	-14.701353000	3.113577000	-0.844356000
C	-8.110485000	3.768750000	-2.281401000	C	-13.506441000	1.621098000	0.156447000
C	-7.745561000	0.718409000	1.862795000	H	-14.012746000	1.744957000	1.110636000
C	-10.033199000	3.360516000	2.369847000	C	-12.468713000	0.684440000	0.054020000
C	-6.281754000	4.793993000	-1.063636000	C	-12.085919000	-0.157553000	1.247290000
C	-5.835297000	2.202955000	2.020325000	H	-11.003477000	-0.155633000	1.411414000
C	-10.457204000	4.483028000	0.260722000	H	-12.382952000	-1.202290000	1.100574000
C	-7.737423000	4.474894000	-3.426954000	H	-12.571572000	0.210693000	2.155341000
C	-7.124062000	-0.170112000	2.743971000	C	-11.180909000	-1.728600000	-1.450109000
C	-11.234647000	3.863405000	2.875408000	O	-12.345855000	-2.180193000	-1.377482000
C	-5.895911000	5.471922000	-2.221515000	C	-10.049869000	-2.690868000	-1.740285000
C	-5.207966000	1.298080000	2.878930000	C	-10.171413000	-4.072144000	-1.894526000
C	-11.652898000	4.989907000	0.776850000	H	-11.134845000	-4.548648000	-1.758599000
C	-6.629839000	5.325705000	-3.401829000	C	-9.025071000	-4.800726000	-2.234315000
C	-5.853551000	0.115305000	3.250895000	H	-9.088039000	-5.877389000	-2.358250000
C	-12.043258000	4.683217000	2.082873000	C	-7.801990000	-4.148777000	-2.432503000
H	-8.963630000	3.104715000	-2.320835000	H	-6.905349000	-4.685483000	-2.718326000
H	-8.732852000	0.485398000	1.484473000	C	-7.760607000	-2.765094000	-2.259164000
H	-9.404361000	2.745461000	3.005054000	C	-6.558037000	-1.877302000	-2.486170000
H	-5.722707000	4.946975000	-0.149791000	O	-5.501094000	-2.397438000	-2.908743000
H	-5.334699000	3.129584000	1.767951000	C	-5.708670000	0.315320000	-2.495371000
H	-10.163540000	4.740933000	-0.750957000	C	-4.623884000	0.410683000	-1.595437000
H	-8.312693000	4.351590000	-4.339379000	C	-4.564376000	-0.454064000	-0.360647000
H	-7.636833000	-1.083096000	3.031057000	H	-5.488417000	-0.394493000	0.220981000
H	-11.530694000	3.620073000	3.891476000	H	-3.733632000	-0.154966000	0.283902000
H	-5.027326000	6.122871000	-2.193729000	H	-4.423063000	-1.506392000	-0.633205000
H	-4.218332000	1.525091000	3.263480000	C	-3.574862000	1.292279000	-1.892834000
H	-12.276104000	5.624706000	0.154466000	H	-2.739335000	1.370632000	-1.200979000
H	-6.338268000	5.868434000	-4.296186000	C	-3.582402000	2.053635000	-3.063435000
H	-5.369702000	-0.579275000	3.931161000	H	-2.760098000	2.729814000	-3.281537000
H	-12.972533000	5.079927000	2.480801000	C	-4.650558000	1.935620000	-3.954623000
Ni	-8.730020000	-0.154831000	-1.575766000	H	-4.655946000	2.516469000	-4.873683000
N	-10.780188000	-0.444837000	-1.345482000	C	-5.722284000	1.071878000	-3.687887000
N	-8.864722000	-2.104646000	-1.911593000	C	-6.847901000	0.922678000	-4.684088000
N	-6.794009000	-0.573920000	-2.229014000	H	-6.935474000	-0.111772000	-5.035639000
C	-11.815751000	0.523934000	-1.188861000	H	-6.682443000	1.564625000	-5.554014000
C	-12.196714000	1.302419000	-2.305382000	H	-7.816873000	1.189521000	-4.247718000
C	-11.530376000	1.115786000	-3.648985000	F	-8.720702000	1.797972000	-0.504061000
H	-11.560687000	0.069644000	-3.972178000	¹ IM' _{PF-cis}			
H	-12.025141000	1.723564000	-4.412023000	Ni	0.553735000	0.358830000	-0.189159000
H	-10.473640000	1.407515000	-3.627085000	N	0.620353000	0.735777000	1.721554000
C	-13.236816000	2.232142000	-2.161311000	N	2.377428000	0.581711000	-0.053934000
H	-13.537899000	2.825737000	-3.021389000	N	0.986545000	0.046157000	-2.063527000
C	-13.894728000	2.391930000	-0.940697000	C	-0.493129000	0.789276000	2.608283000

C	-0.893057000	-0.376176000	3.296509000	H	0.212287000	-2.610178000	-1.534810000
C	-0.139318000	-1.672980000	3.118872000	F	-1.266805000	0.127600000	-0.322177000
H	0.895870000	-1.584836000	3.468440000	P	-5.475681000	-1.135528000	0.276735000
H	-0.617838000	-2.480399000	3.680499000	F	-4.316374000	-0.932103000	1.359301000
H	-0.092006000	-1.966550000	2.064369000	C	-5.016580000	-2.610787000	-0.623644000
C	-1.996859000	-0.305322000	4.158355000	C	-6.979519000	-1.335306000	1.224122000
H	-2.308936000	-1.199115000	4.693549000	C	-5.469827000	0.348571000	-0.717221000
C	-2.694481000	0.891629000	4.336106000	C	-5.115383000	-2.641996000	-2.025430000
H	-3.547871000	0.931648000	5.007819000	C	-7.813412000	-2.447051000	1.012567000
C	-2.290429000	2.036741000	3.645692000	C	-6.688396000	0.929729000	-1.114128000
H	-2.830723000	2.970671000	3.781833000	C	-4.583243000	-3.745033000	0.090324000
C	-1.190198000	2.004881000	2.776840000	C	-7.318941000	-0.357570000	2.180686000
C	-0.750320000	3.252112000	2.047478000	C	-4.237484000	0.904349000	-1.115402000
H	-0.732414000	3.095209000	0.963328000	C	-4.786111000	-3.813499000	-2.709001000
H	0.263664000	3.549128000	2.339581000	C	-8.986624000	-2.576285000	1.757830000
H	-1.423027000	4.086847000	2.264461000	C	-6.672671000	2.070283000	-1.917189000
C	1.850233000	0.960145000	2.224442000	C	-4.249158000	-4.904646000	-0.606600000
O	2.171597000	1.219824000	3.405200000	C	-8.489296000	-0.503568000	2.922271000
C	2.899806000	0.864683000	1.146780000	C	-4.244186000	2.051033000	-1.910147000
C	4.275046000	1.035980000	1.286903000	C	-4.353976000	-4.939635000	-2.002436000
H	4.690613000	1.264591000	2.261484000	C	-9.321990000	-1.609473000	2.709883000
C	5.080033000	0.904820000	0.148565000	C	-5.453367000	2.629822000	-2.312131000
H	6.154768000	1.033423000	0.228966000	H	-5.442013000	-1.767512000	-2.577889000
C	4.504512000	0.608181000	-1.093156000	H	-7.555197000	-3.200510000	0.276603000
H	5.100965000	0.500305000	-1.991682000	H	-7.635548000	0.501914000	-0.803165000
C	3.122270000	0.449366000	-1.159624000	H	-4.499937000	-3.722657000	1.172209000
C	2.294051000	0.128980000	-2.377670000	H	-6.678944000	0.503092000	2.349064000
O	2.835246000	-0.023238000	-3.495066000	H	-3.285749000	0.473592000	-0.806623000
C	0.056542000	-0.245924000	-3.101704000	H	-4.861598000	-3.841663000	-3.791016000
C	-0.534593000	0.812589000	-3.824209000	H	-9.633501000	-3.432130000	1.595046000
C	-0.163430000	2.246788000	-3.530056000	H	-7.609599000	2.521668000	-2.226917000
H	-0.337893000	2.496855000	-2.477511000	H	-3.907935000	-5.778712000	-0.061576000
H	-0.746364000	2.934214000	-4.149714000	H	-8.751580000	0.244113000	3.663659000
H	0.898993000	2.433058000	-3.725282000	H	-3.300811000	2.492214000	-2.214850000
C	-1.465562000	0.507553000	-4.827448000	H	-4.094582000	-5.846771000	-2.539569000
H	-1.923850000	1.318389000	-5.388812000	H	-10.234081000	-1.715950000	3.289079000
C	-1.806637000	-0.816602000	-5.112845000	H	-5.444943000	3.520884000	-2.932613000
H	-2.529656000	-1.038137000	-5.893367000	¹ TS2 _{PF-cis}			
C	-1.212924000	-1.854612000	-4.390886000	Ni	-0.202355000	-0.101154000	-0.223988000
H	-1.473654000	-2.886873000	-4.612119000	N	-0.030167000	-0.067702000	1.704390000
C	-0.277807000	-1.588409000	-3.380399000	N	1.366638000	0.834054000	-0.166662000
C	0.368395000	-2.718102000	-2.613884000	N	0.068112000	0.004404000	-2.132790000
H	1.452496000	-2.740972000	-2.774773000	C	-0.928921000	-0.662198000	2.637368000
H	-0.039953000	-3.683286000	-2.926827000	C	-0.985031000	-2.071853000	2.734777000

C	-0.090091000	-2.953141000	1.894112000	F	-2.980729000	0.120995000	-0.554568000
H	0.950155000	-2.613605000	1.921579000	P	-4.665283000	0.000575000	0.067337000
H	-0.125060000	-3.986404000	2.250702000	F	-4.032148000	0.903462000	1.268992000
H	-0.397274000	-2.958611000	0.841551000	C	-4.478753000	-1.824758000	-0.041246000
C	-1.874132000	-2.648464000	3.652186000	C	-6.350058000	0.031361000	0.931683000
H	-1.916599000	-3.731351000	3.738238000	C	-5.191631000	0.959258000	-1.399989000
C	-2.691444000	-1.853885000	4.458426000	C	-3.739777000	-2.418561000	-1.083449000
H	-3.375133000	-2.315790000	5.165499000	C	-7.471153000	-0.441260000	0.224610000
C	-2.624798000	-0.463268000	4.353565000	C	-5.443577000	0.354154000	-2.637674000
H	-3.260728000	0.157765000	4.979694000	C	-5.081059000	-2.651674000	0.923408000
C	-1.751957000	0.154440000	3.447794000	C	-6.544544000	0.505359000	2.238661000
C	-1.689042000	1.659531000	3.362073000	C	-5.392514000	2.340086000	-1.244008000
H	-1.724212000	2.002704000	2.323722000	C	-3.639261000	-3.807889000	-1.171288000
H	-0.756848000	2.037274000	3.797351000	C	-8.742358000	-0.442736000	0.802045000
H	-2.525248000	2.111855000	3.902234000	C	-5.904024000	1.125858000	-3.709535000
C	1.069547000	0.568988000	2.168059000	C	-4.945359000	-4.040097000	0.850928000
O	1.443427000	0.704417000	3.348030000	C	-7.819064000	0.507290000	2.820612000
C	1.884197000	1.128942000	1.031784000	C	-5.833493000	3.107759000	-2.324113000
C	3.065387000	1.861852000	1.111088000	C	-4.236222000	-4.621883000	-0.203093000
H	3.484494000	2.097533000	2.082328000	C	-8.921299000	0.033959000	2.106017000
C	3.675432000	2.270398000	-0.081139000	C	-6.096705000	2.501341000	-3.557387000
H	4.595120000	2.845319000	-0.046848000	H	-3.241294000	-1.801470000	-1.819792000
C	3.110618000	1.933936000	-1.317578000	H	-7.361256000	-0.815997000	-0.789553000
H	3.565837000	2.225487000	-2.256938000	H	-5.291088000	-0.710840000	-2.776083000
C	1.929669000	1.196851000	-1.325717000	H	-5.649720000	-2.220451000	1.738387000
C	1.168541000	0.685994000	-2.521205000	H	-5.703790000	0.874988000	2.813554000
O	1.583251000	0.887839000	-3.678223000	H	-5.211172000	2.819079000	-0.286221000
C	-0.742256000	-0.617495000	-3.126761000	H	-3.083461000	-4.250435000	-1.992238000
C	-1.656704000	0.154667000	-3.876278000	H	-9.590969000	-0.813435000	0.233963000
C	-1.778913000	1.641359000	-3.651154000	H	-6.105799000	0.647918000	-4.663526000
H	-1.964439000	1.865981000	-2.596179000	H	-5.400911000	-4.662853000	1.614837000
H	-2.599358000	2.056330000	-4.242365000	H	-7.944087000	0.879494000	3.833694000
H	-0.856502000	2.159574000	-3.936988000	H	-5.978843000	4.176573000	-2.198108000
C	-2.437211000	-0.487938000	-4.846754000	H	-4.145166000	-5.702250000	-0.267978000
H	-3.144131000	0.097873000	-5.428215000	H	-9.909586000	0.036153000	2.556841000
C	-2.321072000	-1.861432000	-5.071610000	H	-6.449810000	3.097843000	-4.393337000
H	-2.936176000	-2.344278000	-5.826102000	¹ IM2 _{PF-cis}			
C	-1.409393000	-2.611947000	-4.326012000	Ni	0.045561000	0.492412000	-0.197094000
H	-1.309064000	-3.679240000	-4.507019000	N	0.032427000	0.848161000	1.679874000
C	-0.606491000	-2.006441000	-3.349437000	N	1.847979000	0.422585000	0.027846000
C	0.406435000	-2.822622000	-2.581262000	N	0.469156000	0.122825000	-2.027132000
H	1.420610000	-2.430565000	-2.717630000	C	-1.162372000	1.034026000	2.430200000
H	0.396189000	-3.863751000	-2.915256000	C	-1.757970000	-0.071684000	3.078250000
H	0.207144000	-2.811539000	-1.504388000	C	-1.114660000	-1.436892000	3.026144000

H	-0.135362000	-1.434501000	3.518430000	P	-6.034553000	-1.891488000	-0.031653000
H	-1.742484000	-2.180011000	3.525090000	F	-5.414105000	-1.945462000	1.487614000
H	-0.950483000	-1.763062000	1.993232000	C	-5.988078000	-3.415312000	-1.048003000
C	-2.955057000	0.128385000	3.778907000	C	-7.762524000	-2.104295000	0.718604000
H	-3.420905000	-0.714761000	4.282681000	C	-6.347112000	-0.257153000	-0.820279000
C	-3.553399000	1.389332000	3.833582000	C	-5.785504000	-3.343326000	-2.434300000
H	-4.482848000	1.527372000	4.379149000	C	-8.766802000	-2.866479000	0.099360000
C	-2.955760000	2.472312000	3.184593000	C	-7.566172000	-0.009737000	-1.475176000
H	-3.420423000	3.454098000	3.228955000	C	-6.107217000	-4.665880000	-0.424485000
C	-1.757349000	2.315040000	2.475053000	C	-8.096948000	-1.402378000	1.892784000
C	-1.108046000	3.494934000	1.790542000	C	-5.389979000	0.770607000	-0.747195000
H	-0.989228000	3.323210000	0.714932000	C	-5.724945000	-4.515690000	-3.191997000
H	-0.106517000	3.687614000	2.191709000	C	-10.058805000	-2.932214000	0.636203000
H	-1.707804000	4.398936000	1.926904000	C	-7.810134000	1.230789000	-2.069556000
C	1.243649000	0.876717000	2.275380000	C	-6.015523000	-5.836398000	-1.183228000
O	1.511205000	1.074083000	3.475228000	C	-9.383556000	-1.467976000	2.432527000
C	2.334694000	0.623599000	1.259319000	C	-5.657370000	2.023021000	-1.304951000
C	3.710709000	0.576277000	1.465184000	C	-5.832850000	-5.763041000	-2.567589000
H	4.111214000	0.738149000	2.459215000	C	-10.371314000	-2.235708000	1.805376000
C	4.538265000	0.315745000	0.364908000	C	-6.861886000	2.253618000	-1.976476000
H	5.614138000	0.273269000	0.499771000	H	-5.678370000	-2.380343000	-2.923637000
C	3.989554000	0.108633000	-0.907478000	H	-8.556104000	-3.418383000	-0.810421000
H	4.607986000	-0.096485000	-1.773620000	H	-8.328504000	-0.778321000	-1.532526000
C	2.605698000	0.169849000	-1.047078000	H	-6.271373000	-4.734398000	0.646822000
C	1.783067000	-0.019593000	-2.301569000	H	-7.348928000	-0.797797000	2.395782000
O	2.323046000	-0.268035000	-3.395654000	H	-4.442338000	0.592797000	-0.254957000
C	-0.518222000	-0.032107000	-3.040200000	H	-5.584062000	-4.453327000	-4.266973000
C	-1.051238000	1.117893000	-3.664837000	H	-10.815660000	-3.531288000	0.137557000
C	-0.539641000	2.495780000	-3.315626000	H	-8.747071000	1.398349000	-2.592212000
H	-0.687358000	2.724169000	-2.254074000	H	-6.096516000	-6.801745000	-0.692539000
H	-1.055896000	3.260035000	-3.902899000	H	-9.613412000	-0.920530000	3.342434000
H	0.535073000	2.584337000	-3.510661000	H	-4.917086000	2.813364000	-1.223616000
C	-2.055866000	0.952517000	-4.628074000	H	-5.774557000	-6.673085000	-3.157345000
H	-2.470571000	1.830322000	-5.117231000	H	-11.372139000	-2.288938000	2.224288000
C	-2.523930000	-0.319322000	-4.966221000	H	-7.060687000	3.223514000	-2.422982000
H	-3.303485000	-0.431005000	-5.714829000	³ IM' _{PF-cis}			
C	-1.988832000	-1.447178000	-4.339501000	Ni	0.370865000	0.176198000	-0.252417000
H	-2.353096000	-2.437088000	-4.602318000	N	0.580840000	0.613287000	1.795026000
C	-0.985369000	-1.324762000	-3.368912000	N	2.254029000	0.848478000	-0.178544000
C	-0.414139000	-2.548385000	-2.692971000	N	0.973489000	-0.027823000	-2.260117000
H	0.656232000	-2.656718000	-2.900926000	C	-0.423686000	0.469852000	2.789700000
H	-0.920083000	-3.453551000	-3.039423000	C	-0.598620000	-0.777388000	3.429343000
H	-0.523486000	-2.490093000	-1.604313000	C	0.307987000	-1.940082000	3.100211000
F	-4.329988000	-1.702581000	-0.458335000	H	1.355477000	-1.709970000	3.326574000

H	0.024534000	-2.828707000	3.671790000	F	-4.508374000	-0.846892000	1.566144000
H	0.265249000	-2.190233000	2.033665000	C	-5.142909000	-2.389007000	-0.552185000
C	-1.623527000	-0.916845000	4.376387000	C	-7.162788000	-1.100576000	1.223559000
H	-1.758520000	-1.875316000	4.872547000	C	-5.432787000	0.585975000	-0.530863000
C	-2.464974000	0.153453000	4.689600000	C	-5.070864000	-2.332977000	-1.954940000
H	-3.254564000	0.031373000	5.426281000	C	-8.092977000	-2.066011000	0.800853000
C	-2.286431000	1.380955000	4.046587000	C	-6.580255000	1.335036000	-0.850446000
H	-2.940391000	2.217072000	4.284158000	C	-4.888553000	-3.594530000	0.130978000
C	-1.272875000	1.557567000	3.093864000	C	-7.465171000	-0.234446000	2.292834000
C	-1.089925000	2.889056000	2.404366000	C	-4.151533000	1.008226000	-0.940328000
H	-1.146897000	2.785317000	1.314534000	C	-4.746679000	-3.486750000	-2.670432000
H	-0.109771000	3.325299000	2.628773000	C	-9.326247000	-2.159316000	1.448094000
H	-1.858093000	3.600356000	2.721548000	C	-6.444949000	2.512375000	-1.586442000
C	1.769165000	1.113907000	2.160715000	C	-4.558105000	-4.736124000	-0.596095000
O	2.147127000	1.469641000	3.304433000	C	-8.697458000	-0.344324000	2.934201000
C	2.742692000	1.237849000	1.001908000	C	-4.038555000	2.193352000	-1.667808000
C	4.054116000	1.706377000	1.095487000	C	-4.490033000	-4.682599000	-1.993760000
H	4.448049000	2.021802000	2.054274000	C	-9.626573000	-1.302772000	2.511124000
C	4.824888000	1.750048000	-0.072341000	C	-5.176965000	2.940612000	-1.991925000
H	5.848298000	2.110293000	-0.030125000	H	-5.263905000	-1.405665000	-2.483326000
C	4.285521000	1.328365000	-1.293430000	H	-7.862265000	-2.735995000	-0.020310000
H	4.860886000	1.346792000	-2.211414000	H	-7.564038000	1.006835000	-0.532690000
C	2.966639000	0.871865000	-1.307885000	H	-4.940436000	-3.641511000	1.213997000
C	2.226233000	0.363348000	-2.531921000	H	-6.749378000	0.510754000	2.625677000
O	2.826872000	0.346125000	-3.634803000	H	-3.254471000	0.437197000	-0.694388000
C	0.177272000	-0.525737000	-3.326075000	H	-4.690324000	-3.447344000	-3.753217000
C	-0.540823000	0.370140000	-4.149629000	H	-10.046887000	-2.902683000	1.123297000
C	-0.417412000	1.861862000	-3.948268000	H	-7.326457000	3.093241000	-1.837468000
H	-0.643644000	2.145674000	-2.914073000	H	-4.354404000	-5.665086000	-0.073604000
H	-1.098440000	2.402949000	-4.611535000	H	-8.932160000	0.316507000	3.762296000
H	0.602287000	2.208568000	-4.152514000	H	-3.057451000	2.533250000	-1.983217000
C	-1.363701000	-0.147981000	-5.159971000	H	-4.234066000	-5.575874000	-2.555230000
H	-1.917823000	0.539453000	-5.795197000	H	-10.585838000	-1.381689000	3.013415000
C	-1.478126000	-1.525977000	-5.360056000	H	-5.074779000	3.859520000	-2.561351000
H	-2.119159000	-1.913166000	-6.147570000	³ TS _{2PF-cis}			
C	-0.762678000	-2.402578000	-4.540607000	Ni	-0.332039000	-0.042863000	-0.230263000
H	-0.845980000	-3.476305000	-4.692965000	N	-0.051086000	-0.025405000	1.750187000
C	0.068598000	-1.921169000	-3.519049000	N	1.442261000	0.776492000	-0.181206000
C	0.842200000	-2.878197000	-2.642665000	N	0.062263000	-0.051464000	-2.186077000
H	1.922503000	-2.709700000	-2.720042000	C	-0.919116000	-0.538108000	2.762869000
H	0.639287000	-3.915303000	-2.925355000	C	-0.988787000	-1.935067000	2.959318000
H	0.580546000	-2.754048000	-1.585340000	C	-0.127735000	-2.878058000	2.151605000
F	-1.444620000	-0.452036000	-0.325783000	H	0.934131000	-2.620004000	2.228504000
P	-5.588857000	-0.936342000	0.388569000	H	-0.254839000	-3.907756000	2.497459000

H	-0.382315000	-2.848533000	1.085618000	C	-4.516256000	-1.849360000	-0.101023000
C	-1.860912000	-2.436779000	3.936291000	C	-6.403567000	-0.050426000	0.937498000
H	-1.915621000	-3.511168000	4.094313000	C	-5.335767000	0.975062000	-1.392641000
C	-2.646515000	-1.578500000	4.707989000	C	-3.771466000	-2.424322000	-1.149394000
H	-3.317059000	-1.981251000	5.462294000	C	-7.529911000	-0.529893000	0.243562000
C	-2.565102000	-0.199317000	4.504784000	C	-5.197736000	0.549826000	-2.721341000
H	-3.176538000	0.472821000	5.102171000	C	-5.082995000	-2.695357000	0.869304000
C	-1.708519000	0.342022000	3.535990000	C	-6.574195000	0.375665000	2.263333000
C	-1.635516000	1.836059000	3.333548000	C	-5.948057000	2.209199000	-1.120466000
H	-1.764646000	2.102146000	2.279295000	C	-3.633948000	-3.810292000	-1.240684000
H	-0.663764000	2.231461000	3.650218000	C	-8.784482000	-0.584934000	0.853197000
H	-2.412733000	2.342912000	3.912413000	C	-5.689313000	1.341227000	-3.763227000
C	1.112085000	0.551262000	2.161144000	C	-4.910191000	-4.079576000	0.794199000
O	1.515452000	0.690371000	3.329897000	C	-7.832774000	0.325405000	2.877754000
C	1.979316000	1.021478000	1.010401000	C	-6.403049000	3.013950000	-2.167550000
C	3.244195000	1.605340000	1.086088000	C	-4.198210000	-4.641870000	-0.268293000
H	3.695953000	1.811857000	2.049188000	C	-8.940473000	-0.154894000	2.176620000
C	3.901984000	1.898709000	-0.116740000	C	-6.284987000	2.576183000	-3.490624000
H	4.886235000	2.355554000	-0.090862000	H	-3.289291000	-1.796425000	-1.886741000
C	3.314710000	1.591111000	-1.352145000	H	-7.434970000	-0.867593000	-0.785578000
H	3.821518000	1.786799000	-2.289788000	H	-4.717315000	-0.392998000	-2.954394000
C	2.047470000	1.007579000	-1.342504000	H	-5.653543000	-2.282321000	1.692061000
C	1.248078000	0.521744000	-2.535144000	H	-5.727400000	0.748630000	2.827415000
O	1.718006000	0.646066000	-3.680397000	H	-6.075470000	2.545528000	-0.096064000
C	-0.727968000	-0.591762000	-3.246726000	H	-3.073211000	-4.235982000	-2.067157000
C	-1.509870000	0.262188000	-4.054666000	H	-9.638290000	-0.960223000	0.296044000
C	-1.508490000	1.755432000	-3.832953000	H	-5.595311000	0.994407000	-4.787814000
H	-1.744060000	2.004632000	-2.792657000	H	-5.339938000	-4.714408000	1.563140000
H	-2.243889000	2.243662000	-4.478134000	H	-7.940856000	0.662214000	3.905052000
H	-0.525263000	2.187075000	-4.051807000	H	-6.860848000	3.973604000	-1.946907000
C	-2.284690000	-0.304398000	-5.076498000	H	-4.078649000	-5.719283000	-0.335654000
H	-2.888984000	0.347208000	-5.702693000	H	-9.916033000	-0.194190000	2.652757000
C	-2.290580000	-1.683137000	-5.298690000	H	-6.655573000	3.193368000	-4.303765000
H	-2.897246000	-2.105678000	-6.095008000	³ IM2 _{PF-cis}			
C	-1.511266000	-2.515350000	-4.492620000	Ni	-0.219872000	0.266013000	-0.103344000
H	-1.506536000	-3.588800000	-4.665786000	N	-0.260561000	0.658091000	1.827979000
C	-0.720499000	-1.987339000	-3.461711000	N	1.696711000	0.286555000	0.212924000
C	0.133665000	-2.898061000	-2.611489000	N	0.369349000	-0.112004000	-1.944834000
H	1.188478000	-2.603339000	-2.639174000	C	-1.423587000	0.844570000	2.635310000
H	0.059394000	-3.932452000	-2.958533000	C	-1.970496000	-0.251349000	3.337355000
H	-0.173208000	-2.872416000	-1.559287000	C	-1.313618000	-1.610165000	3.281613000
F	-3.098825000	0.145694000	-0.663327000	H	-0.301932000	-1.584558000	3.702203000
P	-4.745007000	-0.026966000	0.027747000	H	-1.895411000	-2.345088000	3.844757000
F	-4.067811000	0.803981000	1.259370000	H	-1.218846000	-1.966351000	2.249213000

C	-3.138902000	-0.053272000	4.086486000	C	-7.137460000	-1.783042000	0.722354000
H	-3.566426000	-0.892105000	4.630368000	C	-6.584796000	0.078695000	-1.278178000
C	-3.756785000	1.198250000	4.139132000	C	-6.073571000	-3.042721000	-2.849330000
H	-4.662246000	1.335578000	4.723844000	C	-8.172602000	-2.704168000	0.490725000
C	-3.206202000	2.272075000	3.436113000	C	-7.966801000	0.095716000	-1.533192000
H	-3.684570000	3.247742000	3.474693000	C	-5.592314000	-4.209708000	-0.776085000
C	-2.037456000	2.115014000	2.677354000	C	-7.173705000	-1.037139000	1.916214000
C	-1.446669000	3.283893000	1.924505000	C	-5.826022000	1.232083000	-1.545198000
H	-1.387545000	3.080853000	0.848618000	C	-6.082158000	-4.262489000	-3.530358000
H	-0.426563000	3.504118000	2.259112000	C	-9.204593000	-2.880985000	1.420823000
H	-2.052233000	4.182974000	2.068452000	C	-8.571866000	1.234266000	-2.071278000
C	0.961152000	0.750048000	2.424646000	C	-5.570606000	-5.424235000	-1.467994000
O	1.199905000	0.989437000	3.620933000	C	-8.200143000	-1.212988000	2.847304000
C	2.109669000	0.527415000	1.453298000	C	-6.443807000	2.382070000	-2.042347000
C	3.478953000	0.553709000	1.719813000	C	-5.823903000	-5.453409000	-2.842818000
H	3.842391000	0.748008000	2.722120000	C	-9.221167000	-2.138197000	2.603213000
C	4.356172000	0.321912000	0.649760000	C	-7.814853000	2.383428000	-2.316949000
H	5.427106000	0.335781000	0.825761000	H	-6.251458000	-2.120907000	-3.394139000
C	3.873679000	0.073807000	-0.644041000	H	-8.188936000	-3.295971000	-0.418316000
H	4.543507000	-0.104623000	-1.477076000	H	-8.578760000	-0.773599000	-1.321607000
C	2.490829000	0.063803000	-0.829589000	H	-5.416279000	-4.201233000	0.295455000
C	1.719765000	-0.171465000	-2.118909000	H	-6.394500000	-0.311909000	2.127843000
O	2.335243000	-0.383305000	-3.177934000	H	-4.758421000	1.231223000	-1.364723000
C	-0.471182000	-0.316943000	-3.081129000	H	-6.279667000	-4.279918000	-4.598073000
C	-0.988068000	0.804463000	-3.765183000	H	-9.991123000	-3.602184000	1.216847000
C	-0.616301000	2.206209000	-3.342032000	H	-9.636486000	1.223539000	-2.284810000
H	-0.911498000	2.404516000	-2.304706000	H	-5.365335000	-6.344787000	-0.929802000
H	-1.104674000	2.946261000	-3.982046000	H	-8.200979000	-0.628138000	3.762940000
H	0.465866000	2.370183000	-3.397181000	H	-5.848883000	3.271902000	-2.225704000
C	-1.852364000	0.591630000	-4.848671000	H	-5.819700000	-6.399269000	-3.376457000
H	-2.253731000	1.450137000	-5.381681000	H	-10.019361000	-2.277083000	3.326793000
C	-2.198846000	-0.700754000	-5.248633000	H	-8.290104000	3.273666000	-2.718411000
H	-2.869972000	-0.850151000	-6.090011000	¹ TS _{3PF}			
C	-1.681539000	-1.800375000	-4.560257000	F	-7.041057000	4.435893000	1.694196000
H	-1.952309000	-2.807765000	-4.866856000	P	-7.849295000	3.215085000	0.784980000
C	-0.815720000	-1.629389000	-3.470870000	C	-7.381495000	4.076501000	-0.771946000
C	-0.267973000	-2.825382000	-2.728947000	C	-6.906367000	1.916175000	1.688265000
H	0.823610000	-2.881614000	-2.808885000	C	-9.431460000	3.737826000	1.543119000
H	-0.684375000	-3.753795000	-3.129384000	C	-8.235295000	4.021940000	-1.887834000
H	-0.505819000	-2.775911000	-1.660097000	C	-7.456967000	0.634119000	1.865933000
F	-4.364914000	-1.050807000	-1.536078000	C	-9.941111000	3.067191000	2.663074000
P	-5.791378000	-1.421346000	-0.562660000	C	-6.230364000	4.881383000	-0.830382000
F	-4.717198000	-1.252792000	0.667387000	C	-5.673587000	2.216163000	2.294951000
C	-5.840166000	-3.014084000	-1.466100000	C	-10.069623000	4.897384000	1.078272000

C	-7.955060000	4.780453000	-3.027122000	H	-12.290313000	0.681247000	2.074497000
C	-6.803092000	-0.313788000	2.657045000	C	-11.140562000	-1.483241000	-1.426849000
C	-11.082642000	3.551700000	3.308613000	O	-12.328278000	-1.837539000	-1.305918000
C	-5.939475000	5.612453000	-1.984252000	C	-10.055801000	-2.499473000	-1.647352000
C	-5.008904000	1.253515000	3.057968000	C	-10.191393000	-3.884127000	-1.694262000
C	-11.213489000	5.373537000	1.724307000	H	-11.164718000	-4.330377000	-1.526819000
C	-6.806351000	5.574319000	-3.080183000	C	-9.054872000	-4.654839000	-1.965982000
C	-5.576752000	-0.008670000	3.253009000	H	-9.132031000	-5.736476000	-2.006175000
C	-11.720490000	4.704405000	2.842343000	C	-7.822399000	-4.034301000	-2.200003000
H	-9.125555000	3.406250000	-1.862705000	H	-6.926932000	-4.598599000	-2.432737000
H	-8.396587000	0.375683000	1.396259000	C	-7.758487000	-2.644810000	-2.138189000
H	-9.452228000	2.177175000	3.044768000	C	-6.564806000	-1.775468000	-2.416358000
H	-5.567376000	4.948885000	0.022765000	O	-5.490230000	-2.280459000	-2.792927000
H	-5.235053000	3.198941000	2.181930000	C	-5.842632000	0.482896000	-2.567888000
H	-9.677185000	5.437006000	0.222395000	C	-4.719876000	0.643578000	-1.722910000
H	-8.635219000	4.744651000	-3.872841000	C	-4.545545000	-0.194223000	-0.481799000
H	-7.253297000	-1.291756000	2.798963000	H	-5.462615000	-0.240152000	0.109661000
H	-11.468770000	3.026639000	4.177334000	H	-3.748388000	0.208124000	0.148337000
H	-5.040081000	6.219946000	-2.019103000	H	-4.282468000	-1.224258000	-0.749515000
H	-4.051581000	1.497754000	3.508568000	C	-3.729444000	1.566452000	-2.087489000
H	-11.702280000	6.270359000	1.355153000	H	-2.865602000	1.694678000	-1.439716000
H	-6.586955000	6.157857000	-3.969558000	C	-3.830509000	2.306244000	-3.266374000
H	-5.066049000	-0.749301000	3.861490000	H	-3.052115000	3.015029000	-3.535467000
H	-12.605945000	5.079556000	3.347027000	C	-4.933407000	2.124299000	-4.102177000
Ni	-8.719107000	-0.113948000	-1.732579000	H	-5.008132000	2.685431000	-5.030213000
N	-10.635384000	-0.227906000	-1.421815000	C	-5.949606000	1.217434000	-3.771622000
N	-8.859175000	-1.937948000	-1.857500000	C	-7.108924000	1.010986000	-4.717455000
N	-6.860508000	-0.466292000	-2.242635000	H	-7.277959000	-0.051179000	-4.921776000
C	-11.549498000	0.858288000	-1.280545000	H	-6.923848000	1.519087000	-5.667995000
C	-11.843273000	1.663594000	-2.405051000	H	-8.043163000	1.409647000	-4.307405000
C	-11.230657000	1.384900000	-3.758092000	F	-8.657847000	1.959716000	-0.167426000
H	-11.281179000	0.321517000	-4.012131000	¹ PC _{PF}			
H	-11.749822000	1.950443000	-4.536975000	F	-7.128612000	5.763059000	2.555490000
H	-10.173729000	1.671808000	-3.795790000	P	-7.934627000	4.245425000	2.401788000
C	-12.754968000	2.718791000	-2.258971000	C	-7.669065000	4.304550000	0.583682000
H	-12.989803000	3.337020000	-3.121923000	C	-6.670397000	3.444902000	3.476441000
C	-13.374775000	2.969776000	-1.033848000	C	-9.446063000	4.978673000	3.150354000
H	-14.082129000	3.788927000	-0.937377000	C	-8.652712000	3.822706000	-0.294172000
C	-13.085782000	2.159150000	0.065240000	C	-6.430720000	2.062076000	3.388264000
H	-13.568048000	2.350442000	1.020127000	C	-10.270661000	4.203102000	3.982430000
C	-12.173801000	1.100305000	-0.034885000	C	-6.478315000	4.833595000	0.058498000
C	-11.897584000	0.224860000	1.162435000	C	-5.924815000	4.206988000	4.393801000
H	-10.825204000	0.054125000	1.296567000	C	-9.788066000	6.317821000	2.900179000
H	-12.365618000	-0.758607000	1.041088000	C	-8.454061000	3.883215000	-1.675928000

C	-5.455349000	1.460795000	4.188299000	C	-11.317123000	-2.030727000	-2.625724000
C	-11.409641000	4.764277000	4.565684000	O	-12.504142000	-2.273218000	-2.338804000
C	-6.271964000	4.865829000	-1.323252000	C	-10.367951000	-3.135834000	-3.029292000
C	-4.966654000	3.596893000	5.207332000	C	-10.632565000	-4.497552000	-3.147355000
C	-10.944605000	6.865848000	3.461792000	H	-11.628657000	-4.870900000	-2.939705000
C	-7.261629000	4.397824000	-2.193703000	C	-9.586933000	-5.346262000	-3.533699000
C	-4.723372000	2.224330000	5.102182000	H	-9.767845000	-6.411623000	-3.632616000
C	-11.753506000	6.093745000	4.301182000	C	-8.309632000	-4.832092000	-3.792558000
H	-9.572644000	3.402384000	0.094027000	H	-7.484089000	-5.467663000	-4.091368000
H	-7.008038000	1.452209000	2.705001000	C	-8.110335000	-3.461043000	-3.656021000
H	-10.025208000	3.165496000	4.176896000	C	-6.837166000	-2.675274000	-3.872147000
H	-5.713913000	5.218057000	0.723610000	O	-5.780409000	-3.238371000	-4.213164000
H	-6.091500000	5.273548000	4.473941000	C	-6.003041000	-0.409438000	-3.765201000
H	-9.156922000	6.931183000	2.268139000	C	-5.131017000	-0.190312000	-2.674876000
H	-9.230370000	3.520082000	-2.342593000	C	-5.268729000	-0.991913000	-1.402460000
H	-5.275354000	0.393413000	4.099847000	H	-6.278628000	-0.911964000	-0.985155000
H	-12.030424000	4.158855000	5.219638000	H	-4.557327000	-0.645676000	-0.647905000
H	-5.341033000	5.262980000	-1.717167000	H	-5.081949000	-2.056914000	-1.581616000
H	-4.407749000	4.198204000	5.918358000	C	-4.129623000	0.781613000	-2.803225000
H	-11.206668000	7.897949000	3.248192000	H	-3.452127000	0.957150000	-1.971386000
H	-7.104161000	4.433883000	-3.267802000	C	-3.994777000	1.523138000	-3.979335000
H	-3.971330000	1.753488000	5.728755000	H	-3.214162000	2.274317000	-4.062614000
H	-12.645580000	6.524920000	4.746283000	C	-4.866154000	1.298454000	-5.047578000
Ni	-8.832624000	-0.895724000	-3.121601000	H	-4.759854000	1.873802000	-5.963788000
N	-10.683186000	-0.838427000	-2.637838000	C	-5.880303000	0.334880000	-4.960109000
N	-9.134952000	-2.681478000	-3.287139000	C	-6.809131000	0.089203000	-6.126031000
N	-7.052870000	-1.362501000	-3.643961000	H	-6.758131000	-0.951321000	-6.465646000
C	-11.359129000	0.354927000	-2.258411000	H	-6.549713000	0.735370000	-6.969048000
C	-11.854177000	1.215792000	-3.263927000	H	-7.853958000	0.283157000	-5.858319000
C	-11.719955000	0.857198000	-4.725621000	F	-8.765406000	2.743602000	2.225297000
H	-12.199866000	-0.102333000	-4.948224000	³ PC _{PF}			
H	-12.180738000	1.623194000	-5.355218000	F	-6.639628000	5.465313000	3.022065000
H	-10.669021000	0.760864000	-5.021065000	P	-7.616690000	4.400366000	2.075580000
C	-12.488204000	2.404120000	-2.876114000	C	-7.025928000	5.219973000	0.541488000
H	-12.877062000	3.071254000	-3.641291000	C	-6.706959000	2.959839000	2.761477000
C	-12.629464000	2.735220000	-1.526413000	C	-9.120473000	5.023384000	2.926137000
H	-13.124026000	3.659766000	-1.241544000	C	-6.823815000	4.473267000	-0.631083000
C	-12.130256000	1.877399000	-0.543517000	C	-7.385157000	1.762438000	3.042891000
H	-12.237478000	2.136457000	0.506821000	C	-9.077317000	5.358261000	4.289583000
C	-11.486000000	0.681796000	-0.889148000	C	-6.773073000	6.601840000	0.528592000
C	-10.944378000	-0.238250000	0.178588000	C	-5.327819000	3.045248000	3.013354000
H	-9.886524000	-0.467899000	0.008105000	C	-10.324873000	5.172372000	2.218811000
H	-11.480684000	-1.194234000	0.189206000	C	-6.361461000	5.098130000	-1.792352000
H	-11.042789000	0.215767000	1.168125000	C	-6.695404000	0.673611000	3.582732000

C	-10.226270000	5.820072000	4.937149000	H	-13.050318000	2.008794000	0.333712000
C	-6.338744000	7.226967000	-0.643238000	C	-12.041713000	0.552446000	-0.887651000
C	-4.636809000	1.943550000	3.524774000	C	-11.385401000	-0.145104000	0.280110000
C	-11.463197000	5.663147000	2.863796000	H	-10.294401000	-0.160458000	0.174695000
C	-6.125147000	6.476259000	-1.803507000	H	-11.710703000	-1.188702000	0.358888000
C	-5.319516000	0.758755000	3.817569000	H	-11.631092000	0.357480000	1.219576000
C	-11.418866000	5.980718000	4.224915000	C	-11.433571000	-2.251906000	-2.387527000
H	-7.023756000	3.408407000	-0.639112000	O	-12.606425000	-2.589161000	-2.152171000
H	-8.447429000	1.679675000	2.845061000	C	-10.376317000	-3.313792000	-2.648717000
H	-8.152430000	5.257719000	4.845331000	C	-10.533535000	-4.700073000	-2.666626000
H	-6.915355000	7.188847000	1.428238000	H	-11.502053000	-5.148643000	-2.478881000
H	-4.793796000	3.966158000	2.810217000	C	-9.399417000	-5.481389000	-2.934931000
H	-10.374994000	4.909411000	1.168715000	H	-9.490170000	-6.562768000	-2.955971000
H	-6.193406000	4.507250000	-2.687831000	C	-8.150223000	-4.890004000	-3.176269000
H	-7.233265000	-0.241771000	3.811412000	H	-7.268976000	-5.485482000	-3.384281000
H	-10.185009000	6.060940000	5.995327000	C	-8.074190000	-3.497292000	-3.139909000
H	-6.161161000	8.298373000	-0.644970000	C	-6.853233000	-2.618360000	-3.363910000
H	-3.567585000	2.015944000	3.700873000	O	-5.754011000	-3.139794000	-3.618544000
H	-12.384565000	5.789343000	2.302892000	C	-6.067828000	-0.352897000	-3.424766000
H	-5.776471000	6.961991000	-2.710308000	C	-5.227517000	-0.041580000	-2.333469000
H	-4.782813000	-0.092655000	4.226034000	C	-5.408377000	-0.725242000	-0.999066000
H	-12.307837000	6.351085000	4.727245000	H	-6.427381000	-0.593988000	-0.617226000
Ni	-9.015263000	-0.862557000	-2.855533000	H	-4.711256000	-0.322078000	-0.259542000
N	-10.935105000	-0.984780000	-2.448289000	H	-5.234683000	-1.804657000	-1.075083000
N	-9.174157000	-2.796694000	-2.882589000	C	-4.222211000	0.919016000	-2.512876000
N	-7.132317000	-1.288900000	-3.253791000	H	-3.571186000	1.164918000	-1.677465000
C	-11.824336000	0.106846000	-2.209384000	C	-4.049972000	1.560222000	-3.741797000
C	-12.428264000	0.758919000	-3.305961000	H	-3.266118000	2.302540000	-3.864812000
C	-12.188951000	0.278047000	-4.717864000	C	-4.890917000	1.244218000	-4.811014000
H	-12.521536000	-0.757530000	-4.852336000	H	-4.759625000	1.741104000	-5.769166000
H	-12.726966000	0.902706000	-5.436260000	C	-5.908137000	0.288959000	-4.671882000
H	-11.123365000	0.302106000	-4.975116000	C	-6.812470000	-0.045311000	-5.834945000
C	-13.255979000	1.863379000	-3.058187000	H	-6.767958000	-1.110553000	-6.087660000
H	-13.725675000	2.371048000	-3.897120000	H	-6.528679000	0.526848000	-6.722589000
C	-13.483132000	2.314055000	-1.755959000	H	-7.861153000	0.180197000	-5.606278000
H	-14.127052000	3.171330000	-1.579732000	F	-8.592647000	3.332649000	1.131345000
C	-12.877005000	1.659444000	-0.681202000				

VIII) Difluorination of PPh₃ by the cooperation of two 1F_s

¹ RC _{2,PF}				N	-0.618726000	1.342627000	-0.340246000
Ni	-1.313715000	0.773726000	1.380910000	C	-2.821403000	-0.023487000	3.842384000
N	-1.602763000	0.413734000	3.279546000	C	-3.280085000	-1.332805000	3.560589000
N	0.321731000	1.356544000	1.980831000	C	-2.461975000	-2.269633000	2.710799000

H	-1.426734000	-2.334133000	3.060530000	P	-6.855791000	-0.320378000	2.040877000
H	-2.892309000	-3.274915000	2.710612000	C	-8.562736000	-0.689034000	2.512207000
H	-2.441777000	-1.886747000	1.686825000	C	-6.612968000	1.446438000	1.790456000
C	-4.511205000	-1.741130000	4.075848000	C	-6.358557000	-1.314040000	0.622911000
H	-4.858419000	-2.752285000	3.880805000	C	-9.444197000	-1.368295000	1.650446000
C	-5.297157000	-0.875992000	4.853020000	C	-7.670985000	2.357181000	1.986067000
H	-6.238532000	-1.222768000	5.268439000	C	-5.781150000	-0.749588000	-0.530000000
C	-4.833228000	0.411348000	5.132490000	C	-9.002577000	-0.297544000	3.792053000
H	-5.435336000	1.083405000	5.738182000	C	-5.319251000	1.919107000	1.479342000
C	-3.606006000	0.858227000	4.636047000	C	-6.490919000	-2.716105000	0.721169000
C	-3.143073000	2.262888000	4.925503000	C	-10.749153000	-1.633339000	2.062698000
H	-2.828613000	2.771100000	4.007605000	C	-7.441580000	3.723476000	1.847100000
H	-2.279122000	2.255752000	5.597850000	C	-5.379435000	-1.574362000	-1.578603000
H	-3.941079000	2.848229000	5.389368000	C	-10.310665000	-0.562458000	4.190921000
C	-0.556757000	0.719071000	4.090342000	C	-5.113088000	3.290444000	1.335712000
O	-0.469334000	0.587903000	5.321755000	C	-6.090647000	-3.528825000	-0.334863000
C	0.594213000	1.269433000	3.288241000	C	-11.183779000	-1.232321000	3.328759000
C	1.832888000	1.681438000	3.770839000	C	-6.164246000	4.192624000	1.522686000
H	2.042933000	1.607696000	4.831388000	C	-5.533698000	-2.959995000	-1.485360000
C	2.767376000	2.182132000	2.857127000	H	-9.117899000	-1.676068000	0.663593000
H	3.741264000	2.510689000	3.205822000	H	-8.665093000	2.001367000	2.231107000
C	2.450536000	2.263334000	1.496446000	H	-5.658214000	0.322863000	-0.614310000
H	3.147930000	2.648601000	0.761906000	H	-8.325833000	0.210884000	4.471547000
C	1.192769000	1.833035000	1.083830000	H	-4.485003000	1.232122000	1.336493000
C	0.640199000	1.842560000	-0.319665000	H	-6.909469000	-3.166751000	1.615715000
O	1.324735000	2.271501000	-1.264498000	H	-11.427793000	-2.149421000	1.390975000
C	-1.336543000	1.329967000	-1.568947000	H	-8.260641000	4.421572000	1.988597000
C	-1.804324000	2.538199000	-2.133364000	H	-4.938479000	-1.130285000	-2.465169000
C	-1.545415000	3.867285000	-1.466208000	H	-10.644617000	-0.254871000	5.176636000
H	-1.873356000	3.860338000	-0.419815000	H	-4.121945000	3.654994000	1.083779000
H	-2.065746000	4.666878000	-1.998322000	H	-6.204785000	-4.605261000	-0.257431000
H	-0.474846000	4.098057000	-1.459717000	H	-12.200624000	-1.443937000	3.644540000
C	-2.523171000	2.496069000	-3.335976000	H	-5.989462000	5.259235000	1.419892000
H	-2.873420000	3.431958000	-3.763125000	H	-5.215856000	-3.597164000	-2.304811000
C	-2.781318000	1.282540000	-3.972643000	Ni	-3.363371000	7.427854000	-4.466471000
H	-3.336769000	1.262242000	-4.906692000	N	-5.228949000	7.204327000	-4.455719000
C	-2.321826000	0.093613000	-3.404620000	N	-3.775767000	9.165715000	-4.953391000
H	-2.513891000	-0.855084000	-3.900871000	N	-1.597770000	8.074505000	-4.418898000
C	-1.602336000	0.096749000	-2.202968000	C	-5.910044000	6.021549000	-4.050150000
C	-1.136615000	-1.199674000	-1.589857000	C	-6.529716000	5.973739000	-2.782547000
H	-0.068579000	-1.176854000	-1.349558000	C	-6.497131000	7.160130000	-1.850541000
H	-1.321272000	-2.041467000	-2.263498000	H	-7.118636000	7.978316000	-2.231263000
H	-1.676349000	-1.371379000	-0.653727000	H	-6.872322000	6.885969000	-0.861489000
F	-2.914016000	0.164219000	0.789235000	H	-5.482071000	7.554876000	-1.735902000

C	-7.176854000	4.792003000	-2.403898000	N	0.925053000	1.679529000	-1.922328000
H	-7.650288000	4.739354000	-1.427380000	N	-0.069057000	-0.274238000	-3.117653000
C	-7.212911000	3.688277000	-3.255290000	C	-0.608722000	0.815795000	1.550285000
H	-7.719485000	2.778739000	-2.945381000	C	-0.119513000	-0.316263000	2.240928000
C	-6.593833000	3.752219000	-4.503489000	C	1.139030000	-1.018602000	1.789755000
H	-6.622337000	2.892917000	-5.168065000	H	1.963798000	-0.312349000	1.651888000
C	-5.930624000	4.911096000	-4.920859000	H	1.446813000	-1.768832000	2.522811000
C	-5.252132000	4.966997000	-6.266144000	H	0.999994000	-1.530293000	0.830523000
H	-4.173903000	5.097678000	-6.134808000	C	-0.811405000	-0.767143000	3.371261000
H	-5.612765000	5.806703000	-6.869779000	H	-0.434858000	-1.632139000	3.910995000
H	-5.424984000	4.045012000	-6.827053000	C	-1.963344000	-0.117786000	3.815252000
C	-5.967213000	8.313865000	-4.824405000	H	-2.486580000	-0.477076000	4.696893000
O	-7.188307000	8.394095000	-4.908898000	C	-2.435757000	1.001036000	3.127922000
C	-5.059774000	9.476825000	-5.125770000	H	-3.330520000	1.512043000	3.473917000
C	-5.406192000	10.766622000	-5.514897000	C	-1.774915000	1.483876000	1.991269000
H	-6.448865000	11.025487000	-5.655683000	C	-2.293631000	2.699246000	1.265395000
C	-4.375369000	11.695267000	-5.706421000	H	-2.347279000	2.526974000	0.185655000
H	-4.615464000	12.708330000	-6.010759000	H	-1.629524000	3.556825000	1.417945000
C	-3.038607000	11.332465000	-5.499544000	H	-3.289934000	2.972130000	1.621032000
H	-2.223899000	12.035133000	-5.628078000	C	0.766893000	2.394603000	0.334270000
C	-2.769315000	10.024222000	-5.110473000	O	0.987303000	3.194839000	1.253836000
C	-1.438514000	9.398404000	-4.789645000	C	1.311727000	2.623961000	-1.056689000
O	-0.385959000	10.023839000	-4.860967000	C	2.124954000	3.661904000	-1.499966000
C	-0.463773000	7.345232000	-3.960944000	H	2.442798000	4.426311000	-0.801034000
C	0.072287000	6.323486000	-4.774548000	C	2.505746000	3.678782000	-2.847314000
C	-0.535570000	5.993491000	-6.114116000	H	3.139703000	4.478049000	-3.216830000
H	-1.535099000	5.573827000	-5.967955000	C	2.072956000	2.675338000	-3.722104000
H	0.076103000	5.262418000	-6.648796000	H	2.345793000	2.664299000	-4.770716000
H	-0.639924000	6.881514000	-6.746015000	C	1.262773000	1.663965000	-3.216528000
C	1.180483000	5.611882000	-4.303081000	C	0.662004000	0.496470000	-3.963663000
H	1.605666000	4.827841000	-4.923768000	O	0.857418000	0.344796000	-5.176476000
C	1.739142000	5.891844000	-3.056146000	C	-0.814739000	-1.383458000	-3.600131000
H	2.593594000	5.322312000	-2.702391000	C	-1.944629000	-1.178247000	-4.427865000
C	1.191781000	6.897880000	-2.260474000	C	-2.355662000	0.208431000	-4.855996000
H	1.621184000	7.112844000	-1.285642000	H	-2.416577000	0.886949000	-3.999041000
C	0.087353000	7.640066000	-2.693717000	H	-3.330819000	0.189846000	-5.349568000
C	-0.494451000	8.720575000	-1.815286000	H	-1.623670000	0.633798000	-5.550727000
H	-0.274426000	9.716348000	-2.215960000	C	-2.677501000	-2.293196000	-4.852620000
H	-0.077988000	8.664487000	-0.806581000	H	-3.535966000	-2.142303000	-5.502462000
H	-1.583860000	8.637336000	-1.742110000	C	-2.320470000	-3.583938000	-4.461947000
F	-2.966433000	5.738721000	-4.032269000	H	-2.901728000	-4.436993000	-4.800258000
¹ TM1 _{2,PF}				C	-1.210477000	-3.773528000	-3.640512000
Ni	-0.119538000	0.336054000	-1.304214000	H	-0.923093000	-4.778141000	-3.341054000
N	0.055333000	1.240342000	0.368120000	C	-0.444026000	-2.687881000	-3.199942000

C	0.764427000	-2.924353000	-2.325039000	C	-6.320469000	6.450915000	-4.228982000
H	1.617055000	-2.317883000	-2.643195000	C	-6.720808000	7.791149000	-3.666961000
H	1.058297000	-3.977190000	-2.349243000	H	-6.384578000	8.616751000	-4.303456000
H	0.562894000	-2.667780000	-1.277614000	H	-7.806606000	7.862468000	-3.555107000
F	-4.055650000	0.311825000	-1.859989000	H	-6.248197000	7.916887000	-2.688611000
P	-5.540829000	0.214909000	-1.277614000	C	-7.278873000	5.452530000	-4.439639000
C	-5.533920000	-1.191028000	-0.179453000	H	-8.321023000	5.667001000	-4.214643000
C	-5.816304000	1.760274000	-0.434968000	C	-6.917324000	4.197687000	-4.929888000
C	-6.583185000	-0.012980000	-2.708972000	H	-7.671641000	3.431581000	-5.085789000
C	-6.429154000	-2.256663000	-0.375726000	C	-5.578021000	3.930752000	-5.212309000
C	-6.373816000	1.780394000	0.855619000	H	-5.287795000	2.953387000	-5.590877000
C	-7.756729000	0.746250000	-2.852576000	C	-4.589134000	4.904609000	-5.018407000
C	-4.615741000	-1.215658000	0.889015000	C	-3.146333000	4.590891000	-5.329497000
C	-5.462697000	2.960801000	-1.082621000	H	-2.487678000	4.889652000	-4.506711000
C	-6.228798000	-0.974275000	-3.675343000	H	-2.811185000	5.139130000	-6.216727000
C	-6.401889000	-3.342967000	0.497230000	H	-3.008719000	3.521664000	-5.512963000
C	-6.570588000	3.004534000	1.492542000	C	-3.340684000	7.735971000	-5.336200000
C	-8.576833000	0.535060000	-3.960272000	O	-3.545596000	7.577012000	-6.552190000
C	-4.597093000	-2.310235000	1.748311000	C	-2.246260000	8.655580000	-4.854830000
C	-5.646836000	4.177747000	-0.430151000	C	-1.391556000	9.429227000	-5.634515000
C	-7.053471000	-1.166627000	-4.780320000	H	-1.494564000	9.412848000	-6.713187000
C	-5.488375000	-3.370413000	1.553317000	C	-0.421647000	10.203850000	-4.987813000
C	-6.201960000	4.191924000	0.855066000	H	0.257452000	10.817127000	-5.571608000
C	-8.225526000	-0.416317000	-4.920455000	C	-0.320984000	10.188458000	-3.591941000
H	-7.138508000	-2.238743000	-1.195303000	H	0.421179000	10.771404000	-3.059254000
H	-6.647763000	0.858134000	1.355520000	C	-1.207801000	9.390878000	-2.874301000
H	-8.027004000	1.490945000	-2.112147000	C	-1.261202000	9.200688000	-1.378689000
H	-3.923398000	-0.395777000	1.052758000	O	-0.438004000	9.768000000	-0.639684000
H	-5.036992000	2.948002000	-2.081451000	C	-2.398598000	7.944283000	0.312016000
H	-5.317084000	-1.554530000	-3.576300000	C	-1.429210000	7.085195000	0.880158000
H	-7.092927000	-4.166182000	0.350189000	C	-0.234545000	6.620275000	0.083674000
H	-7.002645000	3.027457000	2.487566000	H	-0.527346000	6.323342000	-0.929259000
H	-9.486115000	1.115957000	-4.072872000	H	0.253271000	5.768829000	0.565913000
H	-3.887621000	-2.330619000	2.568802000	H	0.497799000	7.428078000	-0.027165000
H	-5.344541000	5.106191000	-0.912090000	C	-1.593849000	6.660333000	2.205481000
H	-6.781843000	-1.900730000	-5.531559000	H	-0.847239000	6.001374000	2.642481000
H	-5.470915000	-4.220028000	2.228737000	C	-2.693435000	7.065253000	2.960840000
H	-6.342959000	5.140317000	1.364925000	H	-2.806758000	6.727571000	3.987497000
H	-8.865666000	-0.573783000	-5.782801000	C	-3.649651000	7.903472000	2.386918000
Ni	-3.317422000	7.681082000	-2.532365000	H	-4.510854000	8.222173000	2.969656000
N	-3.981681000	7.169536000	-4.286338000	C	-3.521963000	8.350081000	1.066242000
N	-2.125365000	8.662664000	-3.521735000	C	-4.578839000	9.232293000	0.451637000
N	-2.272632000	8.365347000	-1.040046000	H	-4.148784000	10.143636000	0.022262000
C	-4.967973000	6.175715000	-4.528374000	H	-5.329742000	9.521228000	1.192821000

H	-5.064918000	8.684206000	-0.360573000	C	0.973678000	2.252228000	-3.599947000
F	-4.567434000	6.808943000	-1.555823000	H	1.786004000	1.728262000	-4.092269000
2(L)Ni ^{III} F+ P ^{III} Ph ₃				C	1.022458000	3.630546000	-3.450660000
Ni	-2.613895000	5.463938000	-0.527016000	H	1.872481000	4.188200000	-3.830171000
N	-3.350256000	6.465895000	0.929522000	C	-0.006150000	4.332068000	-2.806421000
N	-4.363331000	5.435399000	-1.099808000	C	0.019316000	5.833359000	-2.767638000
N	-2.325795000	4.297329000	-2.062648000	H	-0.767508000	6.245893000	-3.410045000
C	-2.621551000	6.909332000	2.064688000	H	0.981782000	6.208998000	-3.121786000
C	-1.751340000	8.014259000	1.932296000	H	-0.165104000	6.184465000	-1.751552000
C	-1.615381000	8.732296000	0.613477000	F	-0.919217000	5.506735000	0.076693000
H	-2.580925000	9.106230000	0.256063000	P	12.690699000	-0.782722000	-0.384745000
H	-0.931314000	9.580759000	0.699502000	C	13.623701000	0.612594000	0.273109000
H	-1.231546000	8.050572000	-0.151504000	C	11.607399000	-1.526863000	0.833487000
C	-1.027540000	8.436273000	3.052749000	C	13.795980000	-1.953590000	-1.165428000
H	-0.370598000	9.297926000	2.963598000	C	15.024732000	0.529834000	0.441169000
C	-1.149301000	7.777843000	4.277559000	C	11.524974000	-1.013312000	2.144806000
H	-0.578358000	8.116567000	5.137428000	C	13.740766000	-3.344403000	-0.921332000
C	-2.009087000	6.686301000	4.394262000	C	12.938779000	1.787831000	0.649021000
H	-2.106540000	6.172382000	5.347088000	C	10.806099000	-2.626149000	0.462656000
C	-2.757575000	6.236326000	3.299867000	C	14.744570000	-1.451397000	-2.090890000
C	-3.688932000	5.058437000	3.444354000	C	15.717251000	1.603360000	0.991590000
H	-3.507518000	4.304556000	2.670993000	C	10.685862000	-1.629918000	3.068511000
H	-4.733581000	5.373396000	3.346555000	C	14.643278000	-4.193656000	-1.552269000
H	-3.566748000	4.583657000	4.421214000	C	13.649898000	2.849187000	1.203589000
C	-4.690240000	6.706096000	0.865755000	C	9.977705000	-3.243779000	1.393562000
O	-5.393103000	7.330792000	1.668129000	C	15.651764000	-2.310621000	-2.699795000
C	-5.275601000	6.090483000	-0.376348000	C	15.034633000	2.763926000	1.370523000
C	-6.603682000	6.120479000	-0.792444000	C	9.917719000	-2.739916000	2.698890000
H	-7.335740000	6.654817000	-0.198530000	C	15.600917000	-3.682919000	-2.434897000
C	-6.945491000	5.451468000	-1.973259000	H	15.562743000	-0.371599000	0.175864000
H	-7.971736000	5.463709000	-2.324381000	H	12.124067000	-0.161216000	2.442430000
C	-5.970442000	4.756136000	-2.697513000	H	13.031743000	-3.754858000	-0.213134000
H	-6.202426000	4.216117000	-3.607628000	H	11.866898000	1.853135000	0.496334000
C	-4.665308000	4.765216000	-2.213732000	H	10.827671000	-2.997289000	-0.554579000
C	-3.485528000	4.054663000	-2.799425000	H	14.780850000	-0.391306000	-2.314526000
O	-3.568975000	3.403225000	-3.835710000	H	16.790402000	1.528879000	1.134878000
C	-1.187113000	3.593752000	-2.412193000	H	10.635351000	-1.244582000	4.081714000
C	-1.207499000	2.159454000	-2.509256000	H	14.600084000	-5.256653000	-1.344322000
C	-2.369832000	1.346037000	-1.993761000	H	13.117570000	3.746645000	1.500834000
H	-2.931103000	1.884596000	-1.227327000	H	9.385695000	-4.101036000	1.079371000
H	-2.040707000	0.398599000	-1.557159000	H	16.388256000	-1.912208000	-3.389491000
H	-3.068449000	1.119557000	-2.805092000	H	15.582525000	3.598259000	1.797429000
C	-0.120421000	1.524348000	-3.093087000	H	9.265889000	-3.209624000	3.429142000
H	-0.121353000	0.440970000	-3.169999000	H	16.303504000	-4.354214000	-2.918314000

Ni	-5.217415000	-4.685190000	0.377420000	H	-7.598751000	0.000157000	2.437373000
N	-3.653165000	-5.847602000	0.495831000	C	-7.299429000	-1.887522000	1.454611000
N	-6.089771000	-6.279278000	0.102070000	C	-6.872968000	-2.600422000	2.712760000
N	-7.012986000	-3.955520000	0.183197000	H	-7.507151000	-3.469340000	2.920774000
C	-2.306117000	-5.440702000	0.695694000	H	-6.915443000	-1.930989000	3.576814000
C	-1.921277000	-4.916243000	1.950175000	H	-5.849470000	-2.968185000	2.597503000
C	-2.929617000	-4.773703000	3.061680000	F	-4.363303000	-3.108520000	0.641083000
H	-3.416756000	-5.727600000	3.291692000	³ RC _{2,PF}			
H	-2.457563000	-4.399797000	3.974730000	Ni	-1.313993000	0.771412000	1.381574000
H	-3.713157000	-4.075829000	2.753411000	N	-1.603335000	0.411511000	3.280105000
C	-0.589951000	-4.532453000	2.146894000	N	0.321623000	1.353541000	1.981611000
H	-0.291625000	-4.139995000	3.116079000	N	-0.618514000	1.339582000	-0.339597000
C	0.355429000	-4.665233000	1.129128000	C	-2.822584000	-0.024341000	3.842810000
H	1.390384000	-4.384214000	1.304982000	C	-3.282392000	-1.333326000	3.561508000
C	-0.037215000	-5.166990000	-0.111552000	C	-2.464887000	-2.271391000	2.712486000
H	0.692537000	-5.269513000	-0.911562000	H	-1.429715000	-2.336315000	3.062327000
C	-1.362928000	-5.551997000	-0.350950000	H	-2.895904000	-3.276385000	2.713042000
C	-1.762359000	-6.085144000	-1.704670000	H	-2.444325000	-1.889314000	1.688215000
H	-2.683600000	-5.612525000	-2.062053000	C	-4.514154000	-1.740214000	4.076470000
H	-1.957583000	-7.161865000	-1.655435000	H	-4.862181000	-2.751175000	3.881838000
H	-0.974257000	-5.910081000	-2.442311000	C	-5.299506000	-0.874015000	4.853029000
C	-3.905612000	-7.170485000	0.340547000	H	-6.241486000	-1.219631000	5.268051000
O	-3.109616000	-8.125074000	0.376511000	C	-4.834438000	0.412953000	5.132070000
C	-5.373762000	-7.409569000	0.105478000	H	-5.436084000	1.085906000	5.737230000
C	-6.002283000	-8.635131000	-0.095118000	C	-3.606616000	0.858464000	4.635765000
H	-5.410051000	-9.542609000	-0.089495000	C	-3.142517000	2.262821000	4.924820000
C	-7.386717000	-8.646273000	-0.298048000	H	-2.825456000	2.769748000	4.007121000
H	-7.902640000	-9.587828000	-0.457316000	H	-2.279921000	2.255197000	5.598923000
C	-8.108211000	-7.447334000	-0.296130000	H	-3.940707000	2.849624000	5.386517000
H	-9.180541000	-7.415948000	-0.449129000	C	-0.557551000	0.716957000	4.091105000
C	-7.414201000	-6.258901000	-0.089055000	O	-0.470535000	0.586352000	5.322614000
C	-7.988261000	-4.866976000	-0.047796000	C	0.593776000	1.266778000	3.289118000
O	-9.207020000	-4.680538000	-0.209043000	C	1.832374000	1.678807000	3.771891000
C	-7.363938000	-2.579434000	0.224787000	H	2.042157000	1.605344000	4.832512000
C	-7.756957000	-1.906421000	-0.953892000	C	2.767108000	2.179212000	2.858269000
C	-7.819377000	-2.628950000	-2.277035000	H	3.740935000	2.507798000	3.207109000
H	-6.906211000	-3.206006000	-2.458640000	C	2.450573000	2.260137000	1.497502000
H	-7.953139000	-1.923823000	-3.102133000	H	3.148143000	2.645224000	0.763035000
H	-8.651973000	-3.340709000	-2.291528000	C	1.192861000	1.829838000	1.084703000
C	-8.095933000	-0.549327000	-0.876969000	C	0.640537000	1.839257000	-0.318888000
H	-8.405423000	-0.032778000	-1.782093000	O	1.325381000	2.267808000	-1.263674000
C	-8.042475000	0.140147000	0.333732000	C	-1.335902000	1.326911000	-1.568540000
H	-8.317302000	1.190139000	0.379115000	C	-1.803016000	2.535242000	-2.133270000
C	-7.640440000	-0.530555000	1.489143000	C	-1.544019000	3.864253000	-1.466019000

H	-1.870067000	3.856576000	-0.419067000	H	-4.117956000	3.657258000	1.083723000
H	-2.065694000	4.663721000	-1.996985000	H	-6.195675000	-4.598305000	-0.264692000
H	-0.473574000	4.095766000	-1.461230000	H	-12.198419000	-1.442632000	3.642008000
C	-2.521083000	2.493312000	-3.336362000	H	-5.983392000	5.262927000	1.423261000
H	-2.870901000	3.429299000	-3.763657000	H	-5.217696000	-3.585905000	-2.315161000
C	-2.779171000	1.279824000	-3.973134000	Ni	-3.364371000	7.426611000	-4.464977000
H	-3.333949000	1.259631000	-4.907588000	N	-5.229826000	7.201805000	-4.454248000
C	-2.320583000	0.090768000	-3.404638000	N	-3.777990000	9.164529000	-4.950575000
H	-2.512870000	-0.857919000	-3.900815000	N	-1.599217000	8.074455000	-4.416750000
C	-1.601902000	0.093722000	-2.202513000	C	-5.910015000	6.018202000	-4.049567000
C	-1.137350000	-1.202829000	-1.588783000	C	-6.529699000	5.968957000	-2.782028000
H	-0.069198000	-1.181031000	-1.348842000	C	-6.498045000	7.154640000	-1.849088000
H	-1.323094000	-2.044821000	-2.261877000	H	-7.118837000	7.973314000	-2.229913000
H	-1.676991000	-1.373367000	-0.652393000	H	-6.874612000	6.879682000	-0.860786000
F	-2.914452000	0.162510000	0.789711000	H	-5.483003000	7.548967000	-1.732810000
P	-6.854646000	-0.316540000	2.037082000	C	-7.175896000	4.786423000	-2.404258000
C	-8.561240000	-0.685666000	2.508852000	H	-7.649348000	4.732694000	-1.427804000
C	-6.610820000	1.450376000	1.789242000	C	-7.211017000	3.683275000	-3.256436000
C	-6.358003000	-1.308000000	0.617416000	H	-7.716890000	2.773118000	-2.947195000
C	-9.441872000	-1.367272000	1.648076000	C	-6.591959000	3.748636000	-4.504576000
C	-7.667743000	2.361949000	1.986826000	H	-6.619746000	2.889803000	-5.169784000
C	-5.786903000	-0.741007000	-0.537397000	C	-5.929693000	4.908358000	-4.921095000
C	-9.001569000	-0.292757000	3.788119000	C	-5.251227000	4.965772000	-6.266328000
C	-5.316780000	1.922038000	1.477797000	H	-4.173092000	5.097080000	-6.134862000
C	-6.485210000	-2.710514000	0.715606000	H	-5.612419000	5.805708000	-6.869307000
C	-10.746581000	-1.633027000	2.060614000	H	-5.423448000	4.044111000	-6.827955000
C	-7.436992000	3.728172000	1.849512000	C	-5.968861000	8.311130000	-4.822021000
C	-5.385993000	-1.563956000	-1.587723000	O	-7.190019000	8.390617000	-4.906276000
C	-10.309420000	-0.558389000	4.187236000	C	-5.062219000	9.474917000	-5.122596000
C	-5.109282000	3.293357000	1.335863000	C	-5.409535000	10.764814000	-5.510582000
C	-6.085716000	-3.521436000	-0.342111000	H	-6.452390000	11.023084000	-5.651106000
C	-11.181761000	-1.230461000	3.325996000	C	-4.379355000	11.694346000	-5.701307000
C	-6.159393000	4.196386000	1.524808000	H	-4.620156000	12.707505000	-6.004762000
C	-5.534887000	-2.950189000	-1.494330000	C	-3.042349000	11.332303000	-5.494704000
H	-9.115110000	-1.676294000	0.661770000	H	-2.228125000	12.035660000	-5.622531000
H	-8.662059000	2.006827000	2.232037000	C	-2.772147000	10.023897000	-5.106801000
H	-5.668567000	0.331987000	-0.621773000	C	-1.440919000	9.398796000	-4.786315000
H	-8.325361000	0.217282000	4.466936000	O	-0.388844000	10.025133000	-4.856845000
H	-4.483406000	1.234228000	1.333664000	C	-0.464741000	7.345784000	-3.958998000
H	-6.899022000	-3.162889000	1.611490000	C	0.072229000	6.324863000	-4.773045000
H	-11.424609000	-2.150887000	1.389644000	C	-0.535190000	5.995043000	-6.112855000
H	-8.255223000	4.426942000	1.992456000	H	-1.534612000	5.575012000	-5.967073000
H	-4.950225000	-1.118218000	-2.476013000	H	0.076856000	5.264298000	-6.647562000
H	-10.643797000	-0.249654000	5.172446000	H	-0.639623000	6.883197000	-6.744567000

C	1.180966000	5.613946000	-4.301820000	C	0.957962000	0.846023000	-2.772195000
H	1.606833000	4.830539000	-4.922839000	O	1.476347000	0.766967000	-3.881704000
C	1.739249000	5.893720000	-3.054667000	C	-0.916975000	-0.532696000	-3.323387000
H	2.594122000	5.324704000	-2.701105000	C	-1.536373000	0.084941000	-4.433532000
C	1.190986000	6.898921000	-2.258568000	C	-1.561260000	1.585491000	-4.587465000
H	1.620067000	7.113728000	-1.283559000	H	-1.775847000	2.084972000	-3.637488000
C	0.085999000	7.640423000	-2.691569000	H	-2.318301000	1.887381000	-5.315484000
C	-0.496690000	8.720095000	-1.812693000	H	-0.591307000	1.959920000	-4.933232000
H	-0.276475000	9.716240000	-2.212358000	C	-2.114256000	-0.731527000	-5.411621000
H	-0.081034000	8.663227000	-0.803698000	H	-2.586882000	-0.267132000	-6.272840000
H	-1.586140000	8.636655000	-1.740487000	C	-2.093133000	-2.120176000	-5.294514000
F	-2.966057000	5.737433000	-4.032162000	H	-2.541125000	-2.738222000	-6.066931000
³ TS _{2,PF}				C	-1.511041000	-2.713776000	-4.175060000
Ni	-0.725048000	0.610701000	-0.550149000	H	-1.504408000	-3.795969000	-4.076241000
N	-0.687477000	0.979111000	1.327251000	C	-0.920661000	-1.937527000	-3.172211000
N	0.911606000	1.534830000	-0.520566000	C	-0.305301000	-2.598018000	-1.963438000
N	-0.230254000	0.265144000	-2.363433000	H	0.712845000	-2.243113000	-1.775449000
C	-1.578714000	0.501280000	2.331800000	H	-0.273441000	-3.683164000	-2.088665000
C	-1.365070000	-0.786271000	2.872087000	H	-0.895213000	-2.378994000	-1.066107000
C	-0.229129000	-1.655695000	2.390060000	F	-2.426030000	-0.173725000	-0.655214000
H	0.741515000	-1.174359000	2.553731000	P	-4.626005000	-0.230261000	-1.117159000
H	-0.224226000	-2.611845000	2.919101000	C	-5.164074000	-1.575040000	-0.046502000
H	-0.302606000	-1.862227000	1.317038000	C	-5.114941000	1.385012000	-0.510490000
C	-2.217047000	-1.229790000	3.890138000	C	-5.205131000	-0.519089000	-2.788249000
H	-2.055136000	-2.213238000	4.323308000	C	-6.377883000	-2.247623000	-0.294148000
C	-3.256980000	-0.425036000	4.356959000	C	-5.999331000	1.496182000	0.578157000
H	-3.911430000	-0.785956000	5.145035000	C	-5.740964000	0.514130000	-3.586070000
C	-3.450169000	0.845509000	3.816165000	C	-4.369381000	-1.938602000	1.053518000
H	-4.252324000	1.477126000	4.188058000	C	-4.623468000	2.545949000	-1.140284000
C	-2.613450000	1.334798000	2.806167000	C	-5.109503000	-1.825836000	-3.314157000
C	-2.783122000	2.734866000	2.275302000	C	-6.787159000	-3.267573000	0.561818000
H	-2.794410000	2.755597000	1.182298000	C	-6.413722000	2.758762000	0.999071000
H	-1.954311000	3.373830000	2.600315000	C	-6.198940000	0.230648000	-4.869160000
H	-3.713949000	3.178003000	2.635121000	C	-4.790703000	-2.963142000	1.899777000
C	0.355252000	1.779505000	1.752680000	C	-5.044939000	3.804693000	-0.715671000
O	0.546638000	2.197522000	2.891256000	C	-5.583236000	-2.096316000	-4.593581000
C	1.300981000	2.084349000	0.626426000	C	-5.994951000	-3.627126000	1.656002000
C	2.494730000	2.797278000	0.680191000	C	-5.944179000	3.904986000	0.352406000
H	2.814832000	3.239403000	1.616160000	C	-6.127504000	-1.071619000	-5.373485000
C	3.249030000	2.906645000	-0.494576000	H	-6.997860000	-1.973860000	-1.140250000
H	4.184799000	3.455028000	-0.483830000	H	-6.372598000	0.608439000	1.076254000
C	2.810845000	2.303830000	-1.679719000	H	-5.828688000	1.522498000	-3.200075000
H	3.378368000	2.359022000	-2.600989000	H	-3.428189000	-1.432938000	1.230697000
C	1.606626000	1.607287000	-1.652383000	H	-3.914478000	2.468361000	-1.958965000

H	-4.675794000	-2.624680000	-2.722791000	C	-0.255128000	6.838519000	-1.176304000
H	-7.725093000	-3.780190000	0.373450000	C	0.457949000	6.907660000	-2.504406000
H	-7.107044000	2.844232000	1.829919000	H	-0.236074000	6.747401000	-3.336809000
H	-6.623587000	1.027772000	-5.470648000	H	1.249036000	6.154973000	-2.563209000
H	-4.173227000	-3.241637000	2.746935000	H	0.908285000	7.894881000	-2.655217000
H	-4.672780000	4.699935000	-1.210185000	C	0.267754000	6.055097000	-0.139587000
H	-5.520689000	-3.106157000	-4.985358000	H	1.191668000	5.507789000	-0.309238000
H	-6.316688000	-4.426278000	2.316726000	C	-0.377131000	5.965353000	1.093334000
H	-6.274795000	4.884289000	0.685463000	H	0.040869000	5.350473000	1.886055000
H	-6.493318000	-1.286676000	-6.372588000	C	-1.566936000	6.665395000	1.296696000
Ni	-3.582839000	7.813589000	-3.054657000	H	-2.076723000	6.600367000	2.255097000
N	-4.962315000	7.639842000	-4.416474000	C	-2.122790000	7.458248000	0.285460000
N	-3.125122000	9.296344000	-4.031833000	C	-3.424476000	8.184687000	0.510159000
N	-2.028126000	8.323983000	-2.003194000	H	-3.336166000	9.254788000	0.293459000
C	-5.849890000	6.538137000	-4.554188000	H	-3.766531000	8.069199000	1.542748000
C	-6.900023000	6.371378000	-3.624171000	H	-4.177952000	7.773792000	-0.167960000
C	-7.088225000	7.357493000	-2.499627000	F	-4.090299000	6.412767000	-2.028362000
H	-7.197011000	8.382337000	-2.871177000	³ IM1 _{2,PF}			
H	-7.973109000	7.111902000	-1.905262000	Ni	-0.383044000	0.277632000	-1.272315000
H	-6.203499000	7.333166000	-1.857160000	N	-0.180723000	1.192113000	0.450764000
C	-7.751239000	5.267635000	-3.752115000	N	0.823048000	1.675118000	-1.855337000
H	-8.562980000	5.142935000	-3.039312000	N	-0.186874000	-0.302623000	-3.138276000
C	-7.577031000	4.337261000	-4.777327000	C	-0.814853000	0.840113000	1.678791000
H	-8.251010000	3.489562000	-4.867644000	C	-0.366630000	-0.303828000	2.375145000
C	-6.531878000	4.504628000	-5.685084000	C	0.812820000	-1.104540000	1.877255000
H	-6.386384000	3.781978000	-6.484833000	H	1.680419000	-0.467052000	1.680100000
C	-5.656183000	5.594123000	-5.588671000	H	1.102716000	-1.862517000	2.609898000
C	-4.526013000	5.745584000	-6.576950000	H	0.584095000	-1.622541000	0.937754000
H	-3.577764000	5.949989000	-6.067775000	C	-1.030505000	-0.684625000	3.548096000
H	-4.709115000	6.588134000	-7.252716000	H	-0.682366000	-1.560107000	4.090419000
H	-4.408030000	4.840027000	-7.178522000	C	-2.118445000	0.044092000	4.028474000
C	-4.969885000	8.613608000	-5.358161000	H	-2.621809000	-0.262258000	4.941111000
O	-5.724369000	8.744929000	-6.337760000	C	-2.551823000	1.172657000	3.332686000
C	-3.873478000	9.615127000	-5.094711000	H	-3.398799000	1.745283000	3.702237000
C	-3.582502000	10.759082000	-5.832192000	C	-1.913450000	1.589667000	2.156998000
H	-4.192259000	11.006204000	-6.693326000	C	-2.395448000	2.817127000	1.425625000
C	-2.501623000	11.551738000	-5.429506000	H	-2.470738000	2.636713000	0.348601000
H	-2.252851000	12.449391000	-5.986675000	H	-1.698585000	3.651279000	1.559625000
C	-1.738254000	11.190417000	-4.313415000	H	-3.375921000	3.131185000	1.791410000
H	-0.892358000	11.778036000	-3.976390000	C	0.609250000	2.311381000	0.423524000
C	-2.085469000	10.033265000	-3.622219000	O	0.862330000	3.077184000	1.361369000
C	-1.394032000	9.447194000	-2.416513000	C	1.215472000	2.561001000	-0.947061000
O	-0.379539000	9.988490000	-1.943404000	C	2.112440000	3.560966000	-1.320285000
C	-1.456888000	7.550221000	-0.956693000	H	2.450802000	4.292654000	-0.596539000

C	2.556513000	3.575501000	-2.650155000	H	-6.908483000	-2.257491000	-1.267160000
H	3.254361000	4.342416000	-2.970653000	H	-6.606216000	0.858102000	1.328673000
C	2.120718000	2.612544000	-3.570975000	H	-7.927676000	1.403117000	-2.146466000
H	2.462185000	2.606864000	-4.599212000	H	-3.864914000	-0.314610000	1.131616000
C	1.226128000	1.643251000	-3.120072000	H	-4.958566000	2.996541000	-2.060947000
C	0.629802000	0.487652000	-3.904902000	H	-5.012539000	-1.451389000	-3.603911000
O	0.911594000	0.343930000	-5.099776000	H	-6.863713000	-4.191139000	0.270594000
C	-0.836310000	-1.406999000	-3.765392000	H	-7.076431000	3.015626000	2.440084000
C	-1.905005000	-1.189366000	-4.664394000	H	-9.316903000	0.985508000	-4.148652000
C	-2.345256000	0.208063000	-5.026026000	H	-3.827960000	-2.256085000	2.638657000
H	-2.508707000	0.817398000	-4.131025000	H	-5.374081000	5.144469000	-0.906128000
H	-3.274563000	0.186931000	-5.601423000	H	-6.410073000	-1.840633000	-5.598740000
H	-1.581731000	0.715519000	-5.625039000	H	-5.326462000	-4.198469000	2.219833000
C	-2.555155000	-2.299719000	-5.218504000	H	-6.455654000	5.148025000	1.332982000
H	-3.371659000	-2.136250000	-5.917709000	H	-8.560444000	-0.630486000	-5.875197000
C	-2.167344000	-3.599927000	-4.894707000	Ni	-3.323838000	7.659736000	-2.528152000
H	-2.682276000	-4.449469000	-5.334263000	N	-4.037574000	7.130334000	-4.259332000
C	-1.112072000	-3.801189000	-4.006828000	N	-2.101645000	8.555660000	-3.562684000
H	-0.800080000	-4.811824000	-3.755579000	N	-2.226356000	8.340389000	-1.070982000
C	-0.433734000	-2.718699000	-3.432275000	C	-5.074739000	6.180603000	-4.464206000
C	0.713004000	-2.963109000	-2.480423000	C	-6.407397000	6.527196000	-4.149747000
H	1.597027000	-2.378318000	-2.752601000	C	-6.733465000	7.895144000	-3.606929000
H	0.989334000	-4.020931000	-2.471829000	H	-6.362317000	8.691818000	-4.260605000
H	0.454348000	-2.682110000	-1.451815000	H	-7.812989000	8.023401000	-3.485622000
F	-3.898046000	0.388428000	-1.804508000	H	-6.244233000	8.012386000	-2.635706000
P	-5.399122000	0.248844000	-1.270089000	C	-7.416572000	5.573270000	-4.326725000
C	-5.389912000	-1.159260000	-0.175113000	H	-8.443283000	5.842855000	-4.090437000
C	-5.748933000	1.784807000	-0.437054000	C	-7.124629000	4.293505000	-4.798245000
C	-6.386112000	-0.003719000	-2.736447000	H	-7.918032000	3.562974000	-4.928918000
C	-6.236684000	-2.254987000	-0.416360000	C	-5.804761000	3.955757000	-5.095521000
C	-6.348409000	1.788207000	0.834801000	H	-5.568962000	2.958361000	-5.459218000
C	-7.597866000	0.690186000	-2.894025000	C	-4.766477000	4.883269000	-4.935346000
C	-4.519707000	-1.157456000	0.933277000	C	-3.346318000	4.493695000	-5.264686000
C	-5.415948000	2.995963000	-1.076168000	H	-2.658414000	4.779228000	-4.461361000
C	-5.954214000	-0.922777000	-3.712107000	H	-3.003125000	5.005375000	-6.170583000
C	-6.209834000	-3.344780000	0.452125000	H	-3.263326000	3.415182000	-5.425331000
C	-6.610242000	3.005969000	1.460372000	C	-3.386330000	7.637619000	-5.333106000
C	-8.378506000	0.455342000	-4.025105000	O	-3.616948000	7.456212000	-6.541380000
C	-4.500642000	-2.256184000	1.787599000	C	-2.242441000	8.516436000	-4.893224000
C	-5.662878000	4.206961000	-0.433416000	C	-1.363964000	9.225929000	-5.706886000
C	-6.740917000	-1.138911000	-4.840365000	H	-1.484214000	9.184408000	-6.783066000
C	-5.344017000	-3.345979000	1.548040000	C	-0.348480000	9.971051000	-5.096682000
C	-6.262439000	4.204217000	0.831782000	H	0.350185000	10.534050000	-5.707414000
C	-7.950740000	-0.454391000	-4.994591000	C	-0.227932000	9.990786000	-3.702526000

H	0.548687000	10.552619000	-3.197054000	C	5.437421000	-1.614751000	-3.583611000
C	-1.141026000	9.257842000	-2.949906000	O	6.558081000	-1.317559000	-3.149130000
C	-1.182535000	9.117052000	-1.448866000	C	4.990941000	-1.181123000	-4.961302000
O	-0.324739000	9.669438000	-0.738365000	C	5.710733000	-0.456038000	-5.905293000
C	-2.353491000	7.979653000	0.298471000	H	6.726204000	-0.151415000	-5.680957000
C	-1.419131000	7.096940000	0.888340000	C	5.086777000	-0.142339000	-7.118791000
C	-0.264968000	6.536009000	0.093918000	H	5.627335000	0.421948000	-7.871649000
H	-0.591790000	6.207264000	-0.898521000	C	3.769162000	-0.545554000	-7.367045000
H	0.189274000	5.684419000	0.607840000	H	3.257128000	-0.310885000	-8.292813000
H	0.505111000	7.299033000	-0.067227000	C	3.103497000	-1.268447000	-6.382632000
C	-1.580124000	6.740146000	2.233973000	C	1.683459000	-1.787624000	-6.407587000
H	-0.859467000	6.064235000	2.688297000	O	0.935507000	-1.569333000	-7.369745000
C	-2.643337000	7.234058000	2.988463000	C	0.127097000	-2.981820000	-4.982508000
H	-2.754204000	6.948400000	4.031043000	C	-0.916879000	-2.104515000	-4.607529000
C	-3.566680000	8.093639000	2.393021000	C	-0.698551000	-0.611695000	-4.578003000
H	-4.400352000	8.480544000	2.974436000	H	0.201446000	-0.350516000	-4.010587000
C	-3.440894000	8.474764000	1.051818000	H	-1.551848000	-0.099807000	-4.125652000
C	-4.463517000	9.381616000	0.415316000	H	-0.558172000	-0.218054000	-5.591102000
H	-3.997165000	10.253327000	-0.056340000	C	-2.160442000	-2.648304000	-4.266396000
H	-5.188497000	9.736078000	1.153843000	H	-2.976570000	-1.998000000	-3.966402000
H	-4.988189000	8.826284000	-0.367490000	C	-2.371657000	-4.026842000	-4.288915000
F	-4.595376000	6.872956000	-1.507790000	H	-3.344799000	-4.418699000	-4.008996000
'IM1' _{2,PF}				C	-1.336157000	-4.883117000	-4.662857000
Ni	2.835630000	-2.500598000	-3.983979000	H	-1.500678000	-5.957538000	-4.687700000
N	4.451461000	-2.322481000	-2.978356000	C	-0.077493000	-4.379751000	-5.012441000
N	3.736549000	-1.554885000	-5.238955000	C	1.031038000	-5.315687000	-5.433001000
N	1.422136000	-2.469254000	-5.265479000	H	1.428859000	-5.047895000	-6.417639000
C	4.581508000	-2.775084000	-1.637849000	H	0.670743000	-6.346888000	-5.478241000
C	4.713100000	-4.160424000	-1.391124000	H	1.876891000	-5.287381000	-4.736511000
C	4.798170000	-5.148849000	-2.530214000	F	-7.189439000	5.930609000	1.950349000
H	5.540234000	-4.841395000	-3.273583000	P	-7.923981000	4.783567000	1.122074000
H	5.070367000	-6.141243000	-2.160997000	C	-7.430932000	5.100797000	-0.572625000
H	3.842758000	-5.244773000	-3.059810000	C	-7.317522000	3.273226000	1.876141000
C	4.780456000	-4.604741000	-0.065405000	C	-9.671233000	5.032535000	1.383930000
H	4.888726000	-5.668475000	0.130321000	C	-7.826627000	4.244535000	-1.616474000
C	4.717720000	-3.704869000	0.998078000	C	-7.517675000	2.028682000	1.252629000
H	4.770461000	-4.065742000	2.021384000	C	-10.287648000	4.483260000	2.524070000
C	4.587714000	-2.339857000	0.743140000	C	-6.672176000	6.255949000	-0.836836000
H	4.537446000	-1.636407000	1.570407000	C	-6.690702000	3.358062000	3.133177000
C	4.514761000	-1.853379000	-0.567181000	C	-10.399751000	5.857069000	0.506313000
C	4.372169000	-0.374282000	-0.827349000	C	-7.461138000	4.566979000	-2.923047000
H	3.544864000	-0.167876000	-1.515003000	C	-7.092728000	0.874450000	1.910251000
H	5.278816000	0.028575000	-1.292000000	C	-11.622978000	4.775054000	2.787743000
H	4.191870000	0.170300000	0.103084000	C	-6.317308000	6.557104000	-2.150285000

C	-6.268382000	2.191317000	3.767940000	C	-9.889317000	-4.396322000	-1.841725000
C	-11.736163000	6.136182000	0.780417000	H	-10.838102000	-4.874958000	-1.629603000
C	-6.714956000	5.716980000	-3.191948000	C	-8.764885000	-5.116700000	-2.259363000
C	-6.473327000	0.950930000	3.160171000	H	-8.826562000	-6.193483000	-2.380597000
C	-12.343739000	5.600506000	1.919600000	C	-7.560853000	-4.453653000	-2.521203000
H	-8.385665000	3.329022000	-1.444776000	H	-6.670491000	-4.978825000	-2.845914000
H	-7.978677000	1.924471000	0.271754000	C	-7.517064000	-3.072554000	-2.354362000
H	-9.731132000	3.838727000	3.195984000	C	-6.333468000	-2.167523000	-2.571789000
H	-6.365576000	6.911835000	-0.030804000	O	-5.244036000	-2.636793000	-2.949806000
H	-6.531012000	4.318961000	3.608388000	C	-5.637245000	0.107574000	-2.401285000
H	-9.928521000	6.275632000	-0.376221000	C	-4.574718000	0.132865000	-1.468724000
H	-7.761323000	3.911282000	-3.733045000	C	-4.473656000	-0.897662000	-0.371636000
H	-7.249180000	-0.088877000	1.435849000	H	-5.435611000	-1.046518000	0.128374000
H	-12.101364000	4.356032000	3.666584000	H	-3.735749000	-0.600320000	0.378547000
H	-5.733267000	7.448174000	-2.355770000	H	-4.178678000	-1.869677000	-0.781735000
H	-5.781774000	2.254826000	4.735673000	C	-3.593577000	1.126354000	-1.586947000
H	-12.301936000	6.770398000	0.106229000	H	-2.777755000	1.148224000	-0.868263000
H	-6.440725000	5.956619000	-4.214647000	C	-3.649537000	2.078057000	-2.604265000
H	-6.147721000	0.043743000	3.659668000	H	-2.881051000	2.842268000	-2.682048000
H	-13.385194000	5.823467000	2.129489000	C	-4.703085000	2.044695000	-3.518181000
Ni	-8.512180000	-0.585756000	-1.762874000	H	-4.752067000	2.781856000	-4.315730000
N	-10.376113000	-0.785857000	-1.249601000	C	-5.705009000	1.071285000	-3.431659000
N	-8.608771000	-2.410451000	-1.953736000	C	-6.842450000	1.055699000	-4.421184000
N	-6.656190000	-0.879970000	-2.304543000	H	-6.949875000	0.077446000	-4.901730000
C	-11.245478000	0.259808000	-0.834393000	H	-6.693455000	1.806802000	-5.202326000
C	-11.705652000	1.194639000	-1.787582000	H	-7.780960000	1.264555000	-3.898859000
C	-11.277313000	1.095279000	-3.229870000	F	-8.440207000	1.229169000	-1.592070000
H	-11.490860000	0.106688000	-3.650226000	¹ TS _{2,PF}			
H	-11.784527000	1.846354000	-3.842232000	Ni	2.171299000	-2.652211000	-4.079977000
H	-10.196947000	1.250816000	-3.301765000	N	3.972993000	-3.093838000	-3.620774000
C	-12.562220000	2.220845000	-1.372124000	N	2.878785000	-1.049581000	-4.537353000
H	-12.922913000	2.936492000	-2.107196000	N	0.525377000	-1.854392000	-4.619805000
C	-12.960949000	2.330917000	-0.040321000	C	4.337756000	-4.316103000	-2.995013000
H	-13.626428000	3.132350000	0.267081000	C	4.331428000	-5.506583000	-3.757066000
C	-12.491788000	1.410493000	0.895687000	C	4.015283000	-5.485644000	-5.234083000
H	-12.791820000	1.495980000	1.937326000	H	4.564421000	-4.693655000	-5.751943000
C	-11.632669000	0.369938000	0.520167000	H	4.269619000	-6.442965000	-5.696893000
C	-11.137365000	-0.613289000	1.552151000	H	2.949116000	-5.305524000	-5.419185000
H	-10.049035000	-0.728230000	1.503682000	C	4.637275000	-6.715494000	-3.121009000
H	-11.570049000	-1.605321000	1.383605000	H	4.641780000	-7.632607000	-3.704514000
H	-11.404495000	-0.287814000	2.561403000	C	4.940439000	-6.755431000	-1.760590000
C	-10.849218000	-2.055383000	-1.263522000	H	5.175260000	-7.701812000	-1.281654000
O	-11.988245000	-2.465699000	-0.981641000	C	4.940784000	-5.575448000	-1.017192000
C	-9.773753000	-3.017032000	-1.697067000	H	5.173650000	-5.603898000	0.044277000

C	4.638804000	-4.345436000	-1.612771000	C	-10.531339000	4.734758000	-1.363751000
C	4.637241000	-3.080347000	-0.791094000	C	-7.405972000	3.593985000	-4.219438000
H	3.714643000	-2.508957000	-0.940320000	C	-7.417144000	2.208550000	3.201676000
H	5.466061000	-2.425583000	-1.081472000	C	-11.826574000	4.749067000	1.116983000
H	4.734395000	-3.306839000	0.273816000	C	-5.928852000	5.393004000	-3.564373000
C	4.878996000	-2.101747000	-3.810609000	C	-5.812102000	4.018151000	3.162556000
O	6.093760000	-2.104436000	-3.571368000	C	-11.887837000	5.043848000	-1.283866000
C	4.197374000	-0.881207000	-4.385977000	C	-6.453147000	4.559119000	-4.553047000
C	4.772068000	0.337844000	-4.730662000	C	-6.394718000	2.932689000	3.819468000
H	5.839567000	0.477134000	-4.607078000	C	-12.534764000	5.054978000	-0.046862000
C	3.938818000	1.348906000	-5.224453000	H	-8.546848000	2.686682000	-2.626832000
H	4.363402000	2.308669000	-5.500178000	H	-8.640569000	1.998243000	1.438156000
C	2.561840000	1.134401000	-5.360102000	H	-9.928117000	4.222253000	1.963321000
H	1.890810000	1.899930000	-5.731631000	H	-5.983183000	5.962606000	-1.498685000
C	2.048759000	-0.106950000	-4.998698000	H	-5.831886000	5.269581000	1.421150000
C	0.608339000	-0.566032000	-5.033369000	H	-10.036374000	4.751605000	-2.327152000
O	-0.299368000	0.193623000	-5.396295000	H	-7.813089000	2.941129000	-4.984814000
C	-0.725180000	-2.514379000	-4.473302000	H	-7.870751000	1.362141000	3.707484000
C	-1.573439000	-2.194869000	-3.388146000	H	-12.325840000	4.759379000	2.080385000
C	-1.214552000	-1.097458000	-2.416091000	H	-5.185352000	6.142347000	-3.816342000
H	-0.215551000	-1.250431000	-1.991866000	H	-5.014198000	4.581052000	3.636047000
H	-1.941959000	-1.053049000	-1.602553000	H	-12.435630000	5.281614000	-2.189714000
H	-1.198762000	-0.124033000	-2.918793000	H	-6.120259000	4.661137000	-5.581511000
C	-2.763815000	-2.915626000	-3.228207000	H	-6.051873000	2.650490000	4.810189000
H	-3.407685000	-2.678736000	-2.384901000	H	-13.589740000	5.304220000	0.010563000
C	-3.111275000	-3.929753000	-4.121320000	Ni	-7.898455000	0.003654000	-0.509521000
H	-4.036413000	-4.482964000	-3.983754000	N	-9.782218000	-0.511228000	-0.428478000
C	-2.269667000	-4.233643000	-5.191361000	N	-7.653105000	-1.768403000	-0.048642000
H	-2.543910000	-5.018429000	-5.891907000	N	-5.915365000	-0.045561000	-0.622951000
C	-1.069494000	-3.539450000	-5.383466000	C	-10.912412000	0.252164000	-0.837723000
C	-0.173655000	-3.874833000	-6.552591000	C	-11.125965000	0.471004000	-2.216860000
H	0.097086000	-2.979280000	-7.120865000	C	-10.166966000	-0.077327000	-3.245482000
H	-0.668649000	-4.575783000	-7.230075000	H	-10.077569000	-1.166764000	-3.169425000
H	0.766238000	-4.336848000	-6.227837000	H	-10.500302000	0.166894000	-4.257917000
F	-7.672980000	5.910304000	0.076222000	H	-9.158761000	0.327227000	-3.109816000
P	-8.020986000	4.359026000	-0.234981000	C	-12.268816000	1.169717000	-2.623873000
C	-7.329643000	4.309891000	-1.911216000	H	-12.438225000	1.332534000	-3.685511000
C	-7.297457000	3.674095000	1.280519000	C	-13.194092000	1.637304000	-1.691514000
C	-9.816089000	4.422556000	-0.194943000	H	-14.080072000	2.172405000	-2.021662000
C	-7.837502000	3.453621000	-2.901971000	C	-12.974069000	1.416195000	-0.333186000
C	-7.863744000	2.565746000	1.930089000	H	-13.691558000	1.780193000	0.397795000
C	-10.470439000	4.436540000	1.050218000	C	-11.839054000	0.728573000	0.114430000
C	-6.370175000	5.282532000	-2.246702000	C	-11.639257000	0.474209000	1.588187000
C	-6.265119000	4.400320000	1.900388000	H	-10.618179000	0.709974000	1.904749000

H	-11.806071000	-0.583365000	1.820709000	H	4.599501000	-5.253228000	0.491445000
H	-12.332626000	1.071775000	2.186286000	C	4.488342000	-3.227783000	1.215107000
C	-10.020498000	-1.786245000	-0.033606000	H	4.515240000	-3.516248000	2.262117000
O	-11.110566000	-2.367784000	0.096258000	C	4.411048000	-1.880718000	0.862127000
C	-8.731948000	-2.513248000	0.221067000	H	4.376164000	-1.118709000	1.636636000
C	-8.591071000	-3.829040000	0.650416000	C	4.371338000	-1.486781000	-0.480348000
H	-9.478952000	-4.415083000	0.856158000	C	4.285213000	-0.026047000	-0.847204000
C	-7.300195000	-4.346658000	0.796291000	H	3.469980000	0.160467000	-1.554715000
H	-7.160068000	-5.369691000	1.130306000	H	5.208706000	0.309014000	-1.332028000
C	-6.190241000	-3.546698000	0.508365000	H	4.119947000	0.590343000	0.040210000
H	-5.173100000	-3.907861000	0.602423000	C	5.334530000	-1.498591000	-3.494797000
C	-6.408616000	-2.239318000	0.084110000	O	6.462347000	-1.215005000	-3.069879000
C	-5.361111000	-1.234141000	-0.292332000	C	4.914663000	-1.143401000	-4.903202000
O	-4.157839000	-1.561015000	-0.293381000	C	5.667394000	-0.511018000	-5.887317000
C	-5.009441000	0.954699000	-1.088219000	H	6.692527000	-0.230798000	-5.675513000
C	-4.174708000	1.641199000	-0.179612000	C	5.062919000	-0.254951000	-7.124037000
C	-4.185423000	1.300869000	1.288766000	H	5.629265000	0.237014000	-7.908024000
H	-5.202382000	1.241220000	1.683163000	C	3.732050000	-0.622792000	-7.355921000
H	-3.632443000	2.044187000	1.868487000	H	3.234541000	-0.430593000	-8.299235000
H	-3.720332000	0.321901000	1.451223000	C	3.033232000	-1.252446000	-6.331275000
C	-3.287958000	2.607087000	-0.672680000	C	1.593922000	-1.716360000	-6.333521000
H	-2.647866000	3.140096000	0.026449000	O	0.861899000	-1.536699000	-7.315639000
C	-3.204170000	2.877444000	-2.037696000	C	-0.016132000	-2.752143000	-4.844221000
H	-2.510085000	3.628372000	-2.405136000	C	-1.030221000	-1.814751000	-4.538977000
C	-4.009343000	2.170073000	-2.929784000	C	-0.759347000	-0.332060000	-4.611080000
H	-3.935880000	2.363027000	-3.996654000	H	0.147057000	-0.064020000	-4.057227000
C	-4.913659000	1.202965000	-2.474782000	H	-1.596046000	0.239085000	-4.200634000
C	-5.730401000	0.402414000	-3.459455000	H	-0.601006000	-0.014300000	-5.647882000
H	-5.467403000	-0.661183000	-3.419768000	C	-2.293694000	-2.289439000	-4.168854000
H	-5.562179000	0.753696000	-4.480988000	H	-3.086120000	-1.590439000	-3.918874000
H	-6.801024000	0.471073000	-3.246111000	C	-2.553950000	-3.657868000	-4.097597000
F	-8.237681000	1.825380000	-0.739652000	H	-3.541123000	-3.995641000	-3.797302000
¹ IM2 _{2,PF}				C	-1.548144000	-4.573798000	-4.404953000
Ni	2.702700000	-2.307087000	-3.857369000	H	-1.750994000	-5.640846000	-4.357075000
N	4.317368000	-2.124685000	-2.852444000	C	-0.270463000	-4.140773000	-4.778848000
N	3.648285000	-1.486517000	-5.166106000	C	0.806384000	-5.143209000	-5.121413000
N	1.298414000	-2.306552000	-5.149590000	H	1.240252000	-4.944408000	-6.106934000
C	4.417486000	-2.484452000	-1.481630000	H	0.402616000	-6.159199000	-5.123073000
C	4.496993000	-3.852279000	-1.135400000	H	1.634446000	-5.115350000	-4.403499000
C	4.562296000	-4.920736000	-2.200984000	F	-6.914540000	4.376381000	1.327512000
H	5.341265000	-4.703963000	-2.938825000	P	-7.695927000	3.176450000	0.474921000
H	4.770772000	-5.897619000	-1.756705000	C	-7.269783000	3.961549000	-1.123345000
H	3.619424000	-5.003176000	-2.754301000	C	-6.840516000	1.873478000	1.437050000
C	4.532047000	-4.203033000	0.219228000	C	-9.323847000	3.646116000	1.139882000

C	-8.141574000	3.878938000	-2.221405000	C	-13.117894000	1.925767000	0.455742000
C	-7.485545000	0.665035000	1.746605000	H	-13.623154000	2.061556000	1.408213000
C	-9.710201000	3.189997000	2.408821000	C	-12.117478000	0.951819000	0.352074000
C	-6.145061000	4.799430000	-1.200068000	C	-11.784560000	0.081783000	1.538546000
C	-5.593248000	2.153517000	2.019414000	H	-10.705494000	0.021225000	1.708829000
C	-10.081604000	4.637587000	0.500420000	H	-12.139641000	-0.941375000	1.374086000
C	-7.901221000	4.639827000	-3.365106000	H	-12.252592000	0.467137000	2.448131000
C	-6.899905000	-0.236940000	2.636004000	C	-10.965307000	-1.520569000	-1.141343000
C	-10.850019000	3.711744000	3.021385000	O	-12.130130000	-1.921725000	-0.997994000
C	-5.894065000	5.530531000	-2.360518000	C	-9.868793000	-2.476423000	-1.505505000
C	-5.002006000	1.235429000	2.886979000	C	-9.986315000	-3.853016000	-1.665066000
C	-11.220373000	5.153577000	1.119906000	H	-10.945005000	-4.324017000	-1.483469000
C	-6.776105000	5.462795000	-3.439871000	C	-8.857027000	-4.575739000	-2.061196000
C	-5.657089000	0.044553000	3.206091000	H	-8.919006000	-5.651100000	-2.192508000
C	-11.604772000	4.695703000	2.380928000	C	-7.649438000	-3.911249000	-2.294506000
H	-9.013040000	3.241186000	-2.172919000	H	-6.752846000	-4.430041000	-2.611666000
H	-8.450747000	0.438686000	1.314444000	C	-7.605659000	-2.532609000	-2.113036000
H	-9.122430000	2.443139000	2.930231000	C	-6.426664000	-1.635764000	-2.339732000
H	-5.475320000	4.896510000	-0.355939000	O	-5.367711000	-2.098354000	-2.797044000
H	-5.091081000	3.089628000	1.813729000	C	-5.684927000	0.598695000	-2.288457000
H	-9.785147000	5.019940000	-0.469554000	C	-4.544213000	0.672492000	-1.459107000
H	-8.595227000	4.584275000	-4.197949000	C	-4.351535000	-0.285526000	-0.311764000
H	-7.420138000	-1.157386000	2.881929000	H	-5.264121000	-0.409599000	0.274180000
H	-11.139938000	3.352804000	4.004124000	H	-3.554559000	0.054341000	0.353905000
H	-5.015138000	6.165624000	-2.411440000	H	-4.079455000	-1.275147000	-0.696383000
H	-4.034101000	1.460708000	3.323763000	C	-3.544163000	1.603544000	-1.769726000
H	-11.800929000	5.920052000	0.616058000	H	-2.668077000	1.668227000	-1.128939000
H	-6.589736000	6.050735000	-4.333626000	C	-3.647984000	2.425220000	-2.891077000
H	-5.202729000	-0.659357000	3.896705000	H	-2.863688000	3.142117000	-3.117960000
H	-12.486593000	5.105980000	2.863624000	C	-4.758264000	2.312313000	-3.727313000
Ni	-8.568465000	-0.063098000	-1.377111000	H	-4.832266000	2.931939000	-4.616775000
N	-10.489860000	-0.251614000	-1.054122000	C	-5.783456000	1.402860000	-3.445408000
N	-8.700092000	-1.866175000	-1.732025000	C	-6.937016000	1.239188000	-4.404731000
N	-6.716615000	-0.351465000	-2.015861000	H	-6.981817000	0.217465000	-4.798643000
C	-11.466121000	0.775870000	-0.888236000	H	-6.838865000	1.925552000	-5.249870000
C	-11.825759000	1.562802000	-2.005562000	H	-7.899578000	1.433891000	-3.923689000
C	-11.200544000	1.329802000	-3.360798000	F	-8.500160000	1.761284000	-0.564374000
H	-11.299520000	0.284575000	-3.672312000	³ IMI' _{2,PF}			
H	-11.676323000	1.958195000	-4.118488000	Ni	2.870745000	-2.530007000	-3.701318000
H	-10.128871000	1.555127000	-3.367746000	N	4.563153000	-2.371482000	-2.729711000
C	-12.822719000	2.534852000	-1.856577000	N	3.851312000	-1.548746000	-5.048854000
H	-13.104919000	3.137645000	-2.716199000	N	1.444684000	-2.420498000	-5.032850000
C	-13.469883000	2.717693000	-0.635647000	C	4.836134000	-2.834586000	-1.408257000
H	-14.247016000	3.470385000	-0.536586000	C	5.029967000	-4.215683000	-1.191164000

C	5.020390000	-5.190844000	-2.344235000	F	-7.083625000	5.997078000	1.708463000
H	5.724094000	-4.895670000	-3.129379000	P	-7.872224000	4.821626000	0.975555000
H	5.288293000	-6.194886000	-2.004338000	C	-7.582693000	5.138140000	-0.765416000
H	4.032009000	-5.251662000	-2.816278000	C	-7.140881000	3.335564000	1.664075000
C	5.238214000	-4.670306000	0.117031000	C	-9.586629000	5.019703000	1.428353000
H	5.392354000	-5.732865000	0.287781000	C	-8.065439000	4.258098000	-1.751123000
C	5.253580000	-3.783405000	1.192735000	C	-7.404306000	2.075841000	1.096585000
H	5.415103000	-4.151429000	2.202044000	C	-10.063656000	4.442274000	2.620177000
C	5.059167000	-2.421302000	0.965591000	C	-6.896820000	6.313775000	-1.121727000
H	5.067059000	-1.725724000	1.801202000	C	-6.344529000	3.454851000	2.817973000
C	4.848670000	-1.926053000	-0.327067000	C	-10.426597000	5.830451000	0.642093000
C	4.635269000	-0.449608000	-0.554868000	C	-7.862138000	4.578847000	-3.092965000
H	3.735437000	-0.263209000	-1.151544000	C	-6.872685000	0.941580000	1.709453000
H	5.476030000	-0.011788000	-1.104055000	C	-11.371554000	4.692461000	3.026171000
H	4.534815000	0.081761000	0.395212000	C	-6.703017000	6.612149000	-2.469041000
C	5.551714000	-1.695480000	-3.395976000	C	-5.817973000	2.307420000	3.408410000
O	6.696518000	-1.450565000	-2.998933000	C	-11.733459000	6.068968000	1.059132000
C	5.109669000	-1.227711000	-4.773288000	C	-7.189127000	5.749025000	-3.452821000
C	5.852222000	-0.528260000	-5.723452000	C	-6.086251000	1.052179000	2.858803000
H	6.880991000	-0.254027000	-5.522143000	C	-12.202397000	5.505160000	2.249150000
C	5.219936000	-0.199778000	-6.931217000	H	-8.570406000	3.326545000	-1.509704000
H	5.772077000	0.344199000	-7.690964000	H	-7.991517000	1.945454000	0.189009000
C	3.886781000	-0.559849000	-7.174951000	H	-9.421336000	3.808537000	3.222096000
H	3.386555000	-0.310072000	-8.103100000	H	-6.523069000	6.987613000	-0.360078000
C	3.211227000	-1.258031000	-6.175178000	H	-6.136187000	4.427386000	3.248396000
C	1.774147000	-1.755237000	-6.184145000	H	-10.063588000	6.269276000	-0.280821000
O	1.051960000	-1.539407000	-7.163825000	H	-8.230928000	3.905824000	-3.859097000
C	0.110780000	-2.906400000	-4.885364000	H	-7.076963000	-0.033368000	1.279711000
C	-0.937874000	-2.013720000	-4.572031000	H	-11.743021000	4.251340000	3.944995000
C	-0.683939000	-0.530094000	-4.459295000	H	-6.175302000	7.518927000	-2.745769000
H	0.172213000	-0.319298000	-3.808666000	H	-5.201420000	2.397566000	4.296703000
H	-1.558528000	-0.012945000	-4.055905000	H	-12.384616000	6.692780000	0.456068000
H	-0.450514000	-0.095917000	-5.438046000	H	-7.041288000	5.986691000	-4.501734000
C	-2.221314000	-2.531597000	-4.360230000	H	-5.679560000	0.159844000	3.324487000
H	-3.040320000	-1.863738000	-4.110412000	H	-13.221691000	5.695998000	2.570162000
C	-2.470002000	-3.900551000	-4.455310000	Ni	-8.683039000	-0.589526000	-1.872532000
H	-3.474553000	-4.272583000	-4.278208000	N	-10.508276000	-0.810920000	-1.242075000
C	-1.427429000	-4.771504000	-4.769323000	N	-8.803345000	-2.402275000	-2.148413000
H	-1.615866000	-5.839515000	-4.848964000	N	-6.865983000	-0.864935000	-2.539917000
C	-0.128735000	-4.293661000	-4.987183000	C	-11.333455000	0.211513000	-0.698810000
C	0.989305000	-5.250184000	-5.328702000	C	-11.860784000	1.202349000	-1.555670000
H	1.499795000	-4.962059000	-6.253729000	C	-11.549056000	1.185923000	-3.030859000
H	0.604834000	-6.266179000	-5.453311000	H	-11.811542000	0.227289000	-3.491164000
H	1.756230000	-5.277796000	-4.544603000	H	-12.090520000	1.978643000	-3.555061000

H	-10.474970000	1.332547000	-3.177796000	N	4.472690000	-2.141152000	-2.843687000
C	-12.672677000	2.205425000	-1.013370000	N	3.623923000	-1.392282000	-5.141072000
H	-13.085462000	2.964230000	-1.673985000	N	1.241538000	-2.310821000	-4.983762000
C	-12.961305000	2.238923000	0.350675000	C	4.825179000	-2.567453000	-1.528381000
H	-13.593360000	3.023189000	0.756891000	C	5.041804000	-3.941348000	-1.287285000
C	-12.424910000	1.264332000	1.190801000	C	4.975637000	-4.947402000	-2.411773000
H	-12.638765000	1.289987000	2.256684000	H	5.616629000	-4.658934000	-3.251042000
C	-11.607845000	0.244290000	0.686957000	H	5.289271000	-5.935813000	-2.065182000
C	-11.038598000	-0.799520000	1.616161000	H	3.958796000	-5.043546000	-2.812271000
H	-9.960210000	-0.921276000	1.466610000	C	5.326831000	-4.360581000	0.018255000
H	-11.497587000	-1.776775000	1.430995000	H	5.498686000	-5.417380000	0.206944000
H	-11.213489000	-0.529403000	2.661288000	C	5.396279000	-3.446184000	1.068427000
C	-10.989699000	-2.076359000	-1.289851000	H	5.617111000	-3.787004000	2.076054000
O	-12.107957000	-2.497842000	-0.947711000	C	5.179619000	-2.091644000	0.817792000
C	-9.954336000	-3.016576000	-1.850069000	H	5.229737000	-1.374564000	1.633532000
C	-10.091255000	-4.384827000	-2.064381000	C	4.892945000	-1.631148000	-0.473061000
H	-11.028077000	-4.869886000	-1.816625000	C	4.657461000	-0.162020000	-0.724869000
C	-9.003486000	-5.085883000	-2.596384000	H	3.730214000	0.004111000	-1.284310000
H	-9.082730000	-6.153603000	-2.774334000	H	5.469256000	0.268045000	-1.321712000
C	-7.813348000	-4.415161000	-2.899126000	H	4.595956000	0.390704000	0.216306000
H	-6.950740000	-4.925279000	-3.311129000	C	5.411204000	-1.464264000	-3.577999000
C	-7.746217000	-3.046184000	-2.657314000	O	6.570260000	-1.188365000	-3.248581000
C	-6.569551000	-2.137040000	-2.896239000	C	4.888650000	-1.041574000	-4.940877000
O	-5.507922000	-2.588835000	-3.363067000	C	5.568464000	-0.356066000	-5.946512000
C	-5.843907000	0.119559000	-2.624780000	H	6.600878000	-0.058771000	-5.805823000
C	-4.748675000	0.091252000	-1.731357000	C	4.869511000	-0.072333000	-7.128466000
C	-4.608932000	-1.002926000	-0.702055000	H	5.371786000	0.459909000	-7.929987000
H	-5.557720000	-1.198537000	-0.193111000	C	3.532928000	-0.462859000	-7.293023000
H	-3.858967000	-0.741321000	0.049473000	H	2.980899000	-0.248492000	-8.200458000
H	-4.308844000	-1.943438000	-1.176918000	C	2.922839000	-1.144651000	-6.241249000
C	-3.772195000	1.092048000	-1.826308000	C	1.497209000	-1.666532000	-6.164220000
H	-2.932001000	1.074777000	-1.136142000	O	0.719986000	-1.484503000	-7.108262000
C	-3.865088000	2.102071000	-2.783140000	C	-0.075359000	-2.809634000	-4.751577000
H	-3.100713000	2.872082000	-2.841971000	C	-1.112902000	-1.923562000	-4.386769000
C	-4.948421000	2.118046000	-3.662199000	C	-0.867321000	-0.436102000	-4.313645000
H	-5.025102000	2.899870000	-4.413709000	H	0.017562000	-0.206024000	-3.709448000
C	-5.945723000	1.138379000	-3.597438000	H	-1.725455000	0.082748000	-3.878687000
C	-7.113998000	1.169580000	-4.549981000	H	-0.684835000	-0.019615000	-5.310812000
H	-7.225705000	0.220653000	-5.085409000	C	-2.374980000	-2.450970000	-4.087352000
H	-6.997235000	1.967847000	-5.288564000	H	-3.184186000	-1.790326000	-3.789673000
H	-8.038218000	1.334673000	-3.988167000	C	-2.611868000	-3.824042000	-4.149575000
F	-8.595458000	1.217587000	-1.635983000	H	-3.598096000	-4.207390000	-3.905067000
³ TS _{2,PF}				C	-1.581748000	-4.688797000	-4.517386000
Ni	2.733834000	-2.356692000	-3.716124000	H	-1.763129000	-5.759619000	-4.571370000

C	-0.304388000	-4.200346000	-4.820768000	C	-11.558387000	0.713346000	-0.900420000
C	0.802420000	-5.147856000	-5.218753000	C	-11.895871000	1.553436000	-1.985007000
H	1.235502000	-4.878709000	-6.188124000	C	-11.249802000	1.370216000	-3.336707000
H	0.429365000	-6.173523000	-5.285137000	H	-11.418490000	0.360866000	-3.728328000
H	1.627102000	-5.137509000	-4.495493000	H	-11.649094000	2.087104000	-4.059508000
F	-6.914104000	4.732129000	1.452431000	H	-10.164766000	1.505667000	-3.283460000
P	-7.671729000	3.574337000	0.609441000	C	-12.875117000	2.537122000	-1.802659000
C	-7.234083000	4.182153000	-1.042044000	H	-13.140861000	3.179065000	-2.639081000
C	-6.948228000	2.166786000	1.494104000	C	-13.521979000	2.687593000	-0.576722000
C	-9.373651000	3.910273000	1.076671000	H	-14.284883000	3.450795000	-0.451010000
C	-8.059354000	3.967769000	-2.157943000	C	-13.181170000	1.854661000	0.487325000
C	-7.683175000	0.996936000	1.742804000	H	-13.680465000	1.969326000	1.446073000
C	-9.834554000	3.471152000	2.330985000	C	-12.201056000	0.864026000	0.347404000
C	-6.117047000	5.031082000	-1.145782000	C	-11.873411000	-0.044918000	1.506302000
C	-5.691354000	2.349558000	2.097500000	H	-10.792724000	-0.151303000	1.644408000
C	-10.134153000	4.831038000	0.335764000	H	-12.269874000	-1.050547000	1.328201000
C	-7.781465000	4.624568000	-3.355045000	H	-12.304253000	0.335627000	2.436445000
C	-7.173311000	0.033654000	2.612496000	C	-11.098214000	-1.587533000	-1.205723000
C	-11.047530000	3.943407000	2.827777000	O	-12.268512000	-1.979878000	-1.064023000
C	-5.836975000	5.660118000	-2.357818000	C	-10.010382000	-2.553715000	-1.575720000
C	-5.183003000	1.367864000	2.947143000	C	-10.144950000	-3.927213000	-1.751875000
C	-11.346702000	5.294392000	0.842808000	H	-11.112054000	-4.387832000	-1.588926000
C	-6.673529000	5.468551000	-3.458416000	C	-9.019716000	-4.661565000	-2.138881000
C	-5.926937000	0.217368000	3.216048000	H	-9.094804000	-5.734573000	-2.283177000
C	-11.802007000	4.855626000	2.087392000	C	-7.798585000	-4.012193000	-2.344024000
H	-8.892389000	3.284621000	-2.076839000	H	-6.904197000	-4.541505000	-2.650070000
H	-8.637827000	0.853173000	1.257432000	C	-7.738906000	-2.635860000	-2.147123000
H	-9.248477000	2.780624000	2.925568000	C	-6.538829000	-1.755175000	-2.334236000
H	-5.481805000	5.221118000	-0.290033000	O	-5.471253000	-2.235601000	-2.757707000
H	-5.121657000	3.255456000	1.930583000	C	-5.767234000	0.469650000	-2.220353000
H	-9.781319000	5.196959000	-0.620790000	C	-4.666921000	0.519005000	-1.336677000
H	-8.431449000	4.469480000	-4.210175000	C	-4.551697000	-0.450349000	-0.188134000
H	-7.753232000	-0.860830000	2.816453000	H	-5.487317000	-0.529032000	0.370162000
H	-11.397503000	3.602213000	3.796609000	H	-3.760649000	-0.148565000	0.502932000
H	-4.971882000	6.311092000	-2.433127000	H	-4.317415000	-1.452886000	-0.563461000
H	-4.212066000	1.513055000	3.409635000	C	-3.648156000	1.450453000	-1.576722000
H	-11.930759000	6.003556000	0.265627000	H	-2.803496000	1.495020000	-0.893274000
H	-6.462662000	5.975974000	-4.394923000	C	-3.696677000	2.303038000	-2.679169000
H	-5.535604000	-0.535442000	3.893403000	H	-2.899017000	3.020460000	-2.851380000
H	-12.743177000	5.226297000	2.481370000	C	-4.771912000	2.222976000	-3.563782000
Ni	-8.685954000	-0.148367000	-1.424645000	H	-4.806924000	2.871918000	-4.434631000
N	-10.608018000	-0.327064000	-1.105663000	C	-5.813041000	1.311801000	-3.352721000
N	-8.829915000	-1.956197000	-1.777542000	C	-6.942632000	1.201606000	-4.346805000
N	-6.819669000	-0.470169000	-2.011949000	H	-7.002333000	0.193066000	-4.771286000

H	-6.808961000	1.909983000	-5.168772000	H	-3.165181000	-1.711694000	-3.849266000
H	-7.909814000	1.403596000	-3.876916000	C	-2.620039000	-3.776895000	-4.027033000
F	-8.580566000	1.621780000	-0.835425000	H	-3.614368000	-4.124437000	-3.763192000
³ IM2 _{2,PF}				C	-1.599029000	-4.683795000	-4.307941000
Ni	2.756189000	-2.375824000	-3.683336000	H	-1.795620000	-5.752696000	-4.272442000
N	4.497977000	-2.119689000	-2.826302000	C	-0.311777000	-4.240997000	-4.638067000
N	3.665633000	-1.546924000	-5.179494000	C	0.783911000	-5.236618000	-4.937542000
N	1.262723000	-2.394618000	-4.951910000	H	1.257372000	-5.039257000	-5.904955000
C	4.839421000	-2.436670000	-1.477670000	H	0.387193000	-6.255445000	-4.952955000
C	5.037357000	-3.787154000	-1.118068000	H	1.582200000	-5.201802000	-4.185618000
C	4.959400000	-4.885502000	-2.151684000	F	-6.980700000	4.323963000	1.420724000
H	5.605101000	-4.679007000	-3.011263000	P	-7.774251000	3.151516000	0.538822000
H	5.259253000	-5.844419000	-1.720405000	C	-7.331702000	3.967803000	-1.039338000
H	3.941712000	-5.001917000	-2.544562000	C	-6.931644000	1.818782000	1.471532000
C	5.313975000	-4.095557000	0.219788000	C	-9.397368000	3.627347000	1.211975000
H	5.471727000	-5.134178000	0.499700000	C	-8.200366000	3.919434000	-2.141983000
C	5.392815000	-3.094702000	1.187233000	C	-7.587985000	0.609506000	1.753957000
H	5.607078000	-3.349881000	2.221262000	C	-9.802559000	3.134475000	2.460996000
C	5.193576000	-1.764290000	0.819937000	C	-6.195251000	4.791373000	-1.095401000
H	5.250691000	-0.980113000	1.570907000	C	-5.679359000	2.071351000	2.055623000
C	4.916112000	-1.413589000	-0.506897000	C	-10.136416000	4.648559000	0.597972000
C	4.699811000	0.031052000	-0.885834000	C	-7.945344000	4.699970000	-3.269234000
H	3.775414000	0.159782000	-1.459627000	C	-7.008001000	-0.319860000	2.618549000
H	5.517591000	0.397984000	-1.515790000	C	-10.942660000	3.649718000	3.078809000
H	4.644375000	0.664087000	0.003701000	C	-5.929590000	5.541925000	-2.240033000
C	5.451210000	-1.527334000	-3.612591000	C	-5.093671000	1.125893000	2.897173000
O	6.616251000	-1.250992000	-3.305258000	C	-11.275666000	5.157621000	1.222177000
C	4.936823000	-1.205171000	-5.005656000	C	-6.808519000	5.508278000	-3.323590000
C	5.628685000	-0.610714000	-6.059805000	C	-5.759706000	-0.065710000	3.189547000
H	6.666485000	-0.322742000	-5.941043000	C	-11.679085000	4.663047000	2.463300000
C	4.934199000	-0.403041000	-7.259995000	H	-9.081090000	3.293176000	-2.109662000
H	5.445741000	0.057918000	-8.098942000	H	-8.557198000	0.402432000	1.321368000
C	3.589890000	-0.778016000	-7.394721000	H	-9.229388000	2.363516000	2.963303000
H	3.040646000	-0.620162000	-8.315319000	H	-5.527538000	4.861760000	-0.246975000
C	2.968023000	-1.367306000	-6.295033000	H	-5.168744000	3.007393000	1.871466000
C	1.531707000	-1.850769000	-6.179128000	H	-9.825417000	5.058243000	-0.356245000
O	0.758467000	-1.727191000	-7.135831000	H	-8.636975000	4.671105000	-4.105405000
C	-0.062764000	-2.852571000	-4.686599000	H	-7.536796000	-1.240603000	2.844328000
C	-1.090405000	-1.924494000	-4.408087000	H	-11.247279000	3.262277000	4.046171000
C	-0.824456000	-0.439443000	-4.455609000	H	-5.041676000	6.165488000	-2.275232000
H	0.065976000	-0.174024000	-3.874677000	H	-4.121641000	1.330326000	3.335090000
H	-1.673866000	0.123728000	-4.060247000	H	-11.841847000	5.947094000	0.737851000
H	-0.640967000	-0.106082000	-5.483310000	H	-6.610606000	6.111310000	-4.204719000
C	-2.362941000	-2.407108000	-4.078735000	H	-5.309714000	-0.791313000	3.860296000

H	-12.561345000	5.067638000	2.949990000	C	-4.805726000	2.347916000	-3.700171000
Ni	-8.692319000	-0.003460000	-1.456002000	H	-4.859592000	2.992404000	-4.573314000
N	-10.630312000	-0.166910000	-1.171919000	C	-5.850287000	1.450599000	-3.452404000
N	-8.856576000	-1.804160000	-1.862085000	C	-6.998451000	1.336439000	-4.425459000
N	-6.832272000	-0.320441000	-2.078140000	H	-7.067899000	0.323933000	-4.838865000
C	-11.588777000	0.873324000	-0.987099000	H	-6.873073000	2.035436000	-5.256595000
C	-11.919644000	1.699556000	-2.084770000	H	-7.960307000	1.549784000	-3.950431000
C	-11.290014000	1.486523000	-3.441403000	F	-8.591304000	1.778559000	-0.521645000
H	-11.430916000	0.457473000	-3.789160000	¹ TS _{3,PF}			
H	-11.730967000	2.159558000	-4.181636000	Ni	2.787847000	-2.424844000	-3.769044000
H	-10.209537000	1.664536000	-3.431844000	N	4.400028000	-2.288760000	-2.749018000
C	-12.893541000	2.691758000	-1.916381000	N	3.752940000	-1.578786000	-5.047228000
H	-13.153099000	3.325402000	-2.760835000	N	1.392740000	-2.371728000	-5.067994000
C	-13.546917000	2.856203000	-0.696093000	C	4.489749000	-2.696580000	-1.390921000
H	-14.305806000	3.625203000	-0.581975000	C	4.560092000	-4.076057000	-1.091938000
C	-13.224529000	2.025006000	0.375151000	C	4.627081000	-5.107382000	-2.193398000
H	-13.734656000	2.146538000	1.326950000	H	5.413569000	-4.870650000	-2.917015000
C	-12.247275000	1.030020000	0.252058000	H	4.825547000	-6.100447000	-1.781594000
C	-11.943141000	0.120177000	1.416121000	H	3.688347000	-5.164133000	-2.756860000
H	-10.866817000	0.033087000	1.592737000	C	4.584465000	-4.473847000	0.249881000
H	-12.317206000	-0.890546000	1.219918000	H	4.644646000	-5.533226000	0.485835000
H	-12.410858000	0.489427000	2.332507000	C	4.539226000	-3.533589000	1.278798000
C	-11.125653000	-1.424251000	-1.298964000	H	4.557619000	-3.858457000	2.315282000
O	-12.299458000	-1.808604000	-1.183154000	C	4.471378000	-2.174666000	0.972381000
C	-10.041364000	-2.393565000	-1.669798000	H	4.435585000	-1.439852000	1.772697000
C	-10.183577000	-3.763577000	-1.863636000	C	4.442562000	-1.734192000	-0.355857000
H	-11.154087000	-4.220031000	-1.709951000	C	4.367565000	-0.261174000	-0.672577000
C	-9.061260000	-4.499164000	-2.256667000	H	3.558806000	-0.045375000	-1.379142000
H	-9.142282000	-5.569780000	-2.414131000	H	5.296668000	0.084825000	-1.138694000
C	-7.836023000	-3.854996000	-2.453026000	H	4.199391000	0.325227000	0.234397000
H	-6.944826000	-4.385349000	-2.766189000	C	5.427759000	-1.655259000	-3.366148000
C	-7.768313000	-2.481880000	-2.238594000	O	6.555945000	-1.396822000	-2.926359000
C	-6.566482000	-1.603998000	-2.424858000	C	5.020745000	-1.255795000	-4.766292000
O	-5.511552000	-2.081636000	-2.875982000	C	5.787059000	-0.605109000	-5.727675000
C	-5.777844000	0.613342000	-2.317039000	H	6.813419000	-0.341466000	-5.501074000
C	-4.644581000	0.644527000	-1.474740000	C	5.194668000	-0.310259000	-6.961559000
C	-4.483583000	-0.342939000	-0.347665000	H	5.771902000	0.196503000	-7.727986000
H	-5.404892000	-0.460927000	0.226020000	C	3.862106000	-0.658596000	-7.212879000
H	-3.687367000	-0.034189000	0.333887000	H	3.373687000	-0.436742000	-8.154414000
H	-4.227593000	-1.329212000	-0.751188000	C	3.149400000	-1.307892000	-6.210246000
C	-3.624381000	1.564479000	-1.751198000	C	1.706010000	-1.756954000	-6.235402000
H	-2.754104000	1.596430000	-1.100101000	O	0.985068000	-1.546560000	-7.219587000
C	-3.701526000	2.417220000	-2.851313000	C	0.068556000	-2.806966000	-4.790001000
H	-2.901560000	3.124590000	-3.051860000	C	-0.942405000	-1.862416000	-4.495649000

C	-0.655913000	-0.381573000	-4.541211000	H	-5.613113000	6.220289000	-2.618363000
H	0.235990000	-0.128589000	-3.957466000	H	-3.744790000	2.063336000	3.189604000
H	-1.499664000	0.191668000	-4.148201000	H	-11.675023000	6.257687000	1.772437000
H	-0.464955000	-0.052180000	-5.568688000	H	-7.380142000	5.944211000	-4.347048000
C	-2.219174000	-2.327539000	-4.161020000	H	-4.480227000	-0.266902000	3.658731000
H	-3.009795000	-1.621938000	-3.923950000	H	-12.509074000	4.847880000	3.645003000
C	-2.495469000	-3.693805000	-4.111977000	Ni	-8.615980000	-0.071749000	-1.751429000
H	-3.492731000	-4.025337000	-3.839217000	N	-10.500117000	-0.290543000	-1.357671000
C	-1.492347000	-4.616782000	-4.406178000	N	-8.643380000	-1.897037000	-1.816139000
H	-1.707550000	-5.682049000	-4.375836000	N	-6.762081000	-0.311922000	-2.317393000
C	-0.201978000	-4.193451000	-4.746294000	C	-11.453830000	0.752752000	-1.183997000
C	0.870358000	-5.205134000	-5.076087000	C	-11.831614000	1.532788000	-2.300826000
H	1.350809000	-4.982743000	-6.034319000	C	-11.293123000	1.238777000	-3.681118000
H	0.448198000	-6.212272000	-5.128811000	H	-11.352213000	0.171488000	-3.915435000
H	1.666003000	-5.218922000	-4.321749000	H	-11.856468000	1.789521000	-4.439267000
F	-7.073825000	4.604605000	1.406830000	H	-10.241359000	1.526207000	-3.783098000
P	-7.872264000	3.286873000	0.699542000	C	-12.756380000	2.569035000	-2.120176000
C	-7.653409000	4.056765000	-0.953017000	H	-13.051566000	3.168225000	-2.977816000
C	-6.738565000	2.117713000	1.555965000	C	-13.313955000	2.823763000	-0.868148000
C	-9.398486000	3.730507000	1.599280000	H	-14.031922000	3.629591000	-0.743897000
C	-8.636011000	3.885683000	-1.942641000	C	-12.954517000	2.030888000	0.220866000
C	-7.131065000	0.789203000	1.800390000	H	-13.390927000	2.222286000	1.197309000
C	-9.873338000	2.935509000	2.648962000	C	-12.025984000	0.992245000	0.086248000
C	-6.569449000	4.913083000	-1.206037000	C	-11.666656000	0.136732000	1.273900000
C	-5.509516000	2.564438000	2.071273000	H	-10.582126000	0.027502000	1.368016000
C	-10.048486000	4.934805000	1.294104000	H	-12.082950000	-0.870098000	1.162421000
C	-8.542222000	4.575608000	-3.152424000	H	-12.051097000	0.572323000	2.199023000
C	-6.327911000	-0.057443000	2.565967000	C	-10.928797000	-1.576462000	-1.284338000
C	-10.987395000	3.342345000	3.386349000	O	-12.073080000	-2.000095000	-1.069334000
C	-6.463476000	5.571787000	-2.430768000	C	-9.790728000	-2.525262000	-1.537950000
C	-4.695201000	1.703374000	2.807261000	C	-9.839200000	-3.915099000	-1.543631000
C	-11.172646000	5.327737000	2.021332000	H	-10.775966000	-4.411910000	-1.320737000
C	-7.454078000	5.413972000	-3.402163000	C	-8.669219000	-4.619913000	-1.845374000
C	-5.106852000	0.395147000	3.068484000	H	-8.678642000	-5.704870000	-1.855341000
C	-11.641383000	4.535014000	3.071890000	C	-7.489735000	-3.930445000	-2.145003000
H	-9.480555000	3.232840000	-1.761868000	H	-6.568322000	-4.440729000	-2.398636000
H	-8.063798000	0.418843000	1.397842000	C	-7.511758000	-2.539595000	-2.121574000
H	-9.372459000	2.008957000	2.907220000	C	-6.382480000	-1.607890000	-2.459705000
H	-5.817489000	5.075064000	-0.444818000	O	-5.291597000	-2.058310000	-2.841691000
H	-5.197005000	3.587121000	1.910861000	C	-5.813511000	0.692431000	-2.677319000
H	-9.681637000	5.567207000	0.491966000	C	-4.652845000	0.897297000	-1.894684000
H	-9.321081000	4.454498000	-3.899229000	C	-4.363147000	0.052400000	-0.681290000
H	-6.657386000	-1.073272000	2.762214000	H	-5.255607000	-0.096226000	-0.069857000
H	-11.341698000	2.724857000	4.206283000	H	-3.592651000	0.514321000	-0.059185000

H	-4.013693000	-0.940367000	-0.985609000	C	2.964669000	-1.302884000	-6.176324000
C	-3.736555000	1.879921000	-2.292108000	C	1.544094000	-1.819913000	-6.197263000
H	-2.846305000	2.041408000	-1.689316000	O	0.823199000	-1.676542000	-7.193566000
C	-3.944265000	2.639374000	-3.442253000	C	-0.052865000	-2.902436000	-4.729080000
H	-3.221508000	3.395068000	-3.736836000	C	-1.114732000	-2.001791000	-4.479104000
C	-5.083931000	2.419523000	-4.214133000	C	-0.904076000	-0.510941000	-4.578008000
H	-5.245086000	2.998077000	-5.119913000	H	-0.035965000	-0.190234000	-3.991560000
C	-6.028596000	1.453211000	-3.849768000	H	-1.782289000	0.033025000	-4.220871000
C	-7.237862000	1.223822000	-4.723288000	H	-0.712881000	-0.212009000	-5.614664000
H	-7.433268000	0.158368000	-4.874361000	C	-2.369380000	-2.520541000	-4.139631000
H	-7.103059000	1.694092000	-5.701168000	H	-3.198794000	-1.848666000	-3.939827000
H	-8.138949000	1.657248000	-4.275347000	C	-2.575825000	-3.896572000	-4.042825000
F	-8.681807000	1.931555000	-0.064389000	H	-3.558702000	-4.269740000	-3.771565000
¹ PC _{2,PF}				C	-1.522450000	-4.775776000	-4.291973000
Ni	2.637666000	-2.358673000	-3.702440000	H	-1.682452000	-5.849031000	-4.224488000
N	4.227836000	-2.107726000	-2.674615000	C	-0.251897000	-4.298586000	-4.635536000
N	3.570631000	-1.507767000	-5.001094000	C	0.874500000	-5.265308000	-4.916267000
N	1.249774000	-2.409484000	-5.012312000	H	1.369354000	-5.040463000	-5.866380000
C	4.320459000	-2.452307000	-1.299280000	H	0.500958000	-6.292044000	-4.957163000
C	4.438859000	-3.813817000	-0.939324000	H	1.649361000	-5.226846000	-4.141311000
C	4.550507000	-4.889948000	-1.993295000	F	-7.075734000	4.861946000	2.128942000
H	5.317110000	-4.646600000	-2.735570000	P	-7.512319000	3.272222000	1.712429000
H	4.803475000	-5.851399000	-1.538529000	C	-7.517571000	3.758487000	-0.063962000
H	3.610775000	-5.021825000	-2.542601000	C	-5.976561000	2.617169000	2.500829000
C	4.467996000	-4.151276000	0.418851000	C	-9.037353000	3.429395000	2.730824000
H	4.565782000	-5.196324000	0.701467000	C	-8.390535000	3.136110000	-0.970987000
C	4.380688000	-3.169299000	1.405146000	C	-5.818485000	1.239332000	2.736598000
H	4.403750000	-3.447502000	2.455017000	C	-9.607423000	2.301316000	3.342771000
C	4.264598000	-1.828623000	1.038768000	C	-6.656712000	4.764634000	-0.531253000
H	4.195378000	-1.061337000	1.805719000	C	-4.941926000	3.487073000	2.890083000
C	4.229482000	-1.447883000	-0.307616000	C	-9.642126000	4.683143000	2.915811000
C	4.101059000	0.006253000	-0.688006000	C	-8.409499000	3.520505000	-2.312644000
H	3.291065000	0.160289000	-1.409204000	C	-4.663478000	0.750074000	3.347716000
H	5.020432000	0.367630000	-1.161608000	C	-10.750973000	2.428633000	4.132451000
H	3.901991000	0.623760000	0.191658000	C	-6.656422000	5.124261000	-1.879827000
C	5.230857000	-1.447977000	-3.305748000	C	-3.781912000	2.991144000	3.486101000
O	6.340575000	-1.119899000	-2.865620000	C	-10.803278000	4.801206000	3.680745000
C	4.819515000	-1.116723000	-4.722162000	C	-7.536142000	4.508798000	-2.772649000
C	5.562830000	-0.462190000	-5.698895000	C	-3.639453000	1.622565000	3.720501000
H	6.573627000	-0.142959000	-5.473818000	C	-11.356621000	3.676578000	4.296419000
C	4.967569000	-0.235356000	-6.945745000	H	-9.061954000	2.359122000	-0.630874000
H	5.526772000	0.273020000	-7.724372000	H	-6.596000000	0.550332000	2.438403000
C	3.654797000	-0.653548000	-7.194629000	H	-9.159726000	1.326051000	3.201584000
H	3.164532000	-0.485285000	-8.146260000	H	-5.989984000	5.268306000	0.156882000

H	-5.045649000	4.551291000	2.731528000	C	-6.048839000	0.352201000	-3.361011000
H	-9.204671000	5.564003000	2.463401000	C	-5.168912000	0.791109000	-2.346262000
H	-9.110380000	3.045509000	-2.992719000	C	-5.246225000	0.214266000	-0.954075000
H	-4.564845000	-0.316345000	3.527562000	H	-6.225535000	0.393962000	-0.497109000
H	-11.171470000	1.550227000	4.612960000	H	-4.488222000	0.662320000	-0.306637000
H	-5.974230000	5.893721000	-2.228857000	H	-5.085759000	-0.868853000	-0.967660000
H	-2.991868000	3.679280000	3.771823000	C	-4.223099000	1.774784000	-2.659210000
H	-11.268849000	5.774733000	3.802333000	H	-3.541578000	2.117261000	-1.884827000
H	-7.542901000	4.799360000	-3.819033000	C	-4.150148000	2.320806000	-3.941310000
H	-2.738446000	1.239078000	4.190395000	H	-3.413565000	3.087059000	-4.165837000
H	-12.253400000	3.771858000	4.901647000	C	-5.027015000	1.881254000	-4.933168000
Ni	-8.878369000	-0.191018000	-2.707628000	H	-4.968172000	2.301283000	-5.933935000
N	-10.750409000	-0.173523000	-2.309545000	C	-5.983799000	0.895804000	-4.663012000
N	-9.042869000	-1.982102000	-2.467785000	C	-6.912967000	0.413115000	-5.751054000
N	-7.046210000	-0.617667000	-3.065097000	H	-6.840531000	-0.671155000	-5.887164000
C	-11.521040000	1.015432000	-2.202267000	H	-6.676627000	0.893685000	-6.704010000
C	-11.854667000	1.725154000	-3.378603000	H	-7.961151000	0.630181000	-5.516012000
C	-11.481510000	1.192542000	-4.742539000	F	-7.982793000	1.690807000	1.264832000
H	-11.770355000	0.142922000	-4.854814000	³ TS _{3,PF}			
H	-11.972081000	1.771217000	-5.529721000	Ni	2.795972000	-2.503794000	-3.588831000
H	-10.401072000	1.242731000	-4.922541000	N	4.480148000	-2.395852000	-2.593518000
C	-12.563945000	2.926648000	-3.261506000	N	3.816581000	-1.526468000	-4.909964000
H	-12.828888000	3.473508000	-4.162726000	N	1.382510000	-2.318903000	-4.927422000
C	-12.940744000	3.419750000	-2.012732000	C	4.725339000	-2.884702000	-1.275977000
H	-13.490479000	4.353769000	-1.938835000	C	4.867737000	-4.274645000	-1.075057000
C	-12.613023000	2.707372000	-0.859458000	C	4.833332000	-5.235033000	-2.240043000
H	-12.907488000	3.088549000	0.114989000	H	5.546090000	-4.950063000	-3.020650000
C	-11.902197000	1.503391000	-0.930175000	H	5.072623000	-6.250155000	-1.911844000
C	-11.558335000	0.745080000	0.328339000	H	3.844274000	-5.263492000	-2.713868000
H	-10.483974000	0.542078000	0.397821000	C	5.048044000	-4.753072000	0.228790000
H	-12.071360000	-0.222214000	0.350339000	H	5.162650000	-5.822576000	0.386839000
H	-11.850805000	1.311850000	1.215554000	C	5.085705000	-3.881193000	1.316111000
C	-11.297797000	-1.384441000	-2.036253000	H	5.224935000	-4.267683000	2.321832000
O	-12.466150000	-1.654440000	-1.728574000	C	4.942284000	-2.510236000	1.105052000
C	-10.249451000	-2.464999000	-2.151053000	H	4.967659000	-1.826104000	1.949706000
C	-10.409058000	-3.833111000	-1.957119000	C	4.761202000	-1.991188000	-0.182731000
H	-11.386894000	-4.222829000	-1.699722000	C	4.602916000	-0.505161000	-0.392256000
C	-9.288332000	-4.659428000	-2.100425000	H	3.718540000	-0.278965000	-0.998155000
H	-9.386320000	-5.730044000	-1.953845000	H	5.466152000	-0.090130000	-0.923990000
C	-8.041079000	-4.114875000	-2.428823000	H	4.508118000	0.016254000	0.563899000
H	-7.154565000	-4.727349000	-2.543395000	C	5.494211000	-1.740014000	-3.240788000
C	-7.948840000	-2.739042000	-2.610579000	O	6.641155000	-1.532523000	-2.828894000
C	-6.723549000	-1.928888000	-2.959579000	C	5.079441000	-1.241440000	-4.615645000
O	-5.618453000	-2.470569000	-3.108296000	C	5.849276000	-0.543735000	-5.545111000

H	6.882214000	-0.298860000	-5.328014000	C	-11.635584000	4.595681000	3.029092000
C	5.238335000	-0.176802000	-6.752709000	H	-9.578789000	3.253728000	-1.833064000
H	5.812097000	0.366879000	-7.496483000	H	-8.051768000	0.517565000	1.349773000
C	3.898523000	-0.496423000	-7.015442000	H	-9.283894000	2.144522000	2.898378000
H	3.413595000	-0.214482000	-7.942487000	H	-5.917795000	5.180043000	-0.637155000
C	3.195193000	-1.195669000	-6.035764000	H	-5.199952000	3.720756000	1.705844000
C	1.743398000	-1.646738000	-6.065042000	H	-9.811377000	5.567361000	0.329147000
O	1.036704000	-1.390540000	-7.046418000	H	-9.500849000	4.453290000	-3.987898000
C	0.030507000	-2.755886000	-4.792957000	H	-6.595813000	-0.928667000	2.712596000
C	-0.986452000	-1.827493000	-4.477686000	H	-11.230773000	2.852710000	4.233861000
C	-0.679087000	-0.354917000	-4.353263000	H	-5.794089000	6.303435000	-2.828126000
H	0.164696000	-0.177656000	-3.676756000	H	-3.699287000	2.240496000	2.979881000
H	-1.545296000	0.194485000	-3.975000000	H	-11.777888000	6.251781000	1.652827000
H	-0.401088000	0.071635000	-5.323472000	H	-7.601589000	5.974123000	-4.504770000
C	-2.288619000	-2.298929000	-4.271713000	H	-4.401967000	-0.082527000	3.528090000
H	-3.082064000	-1.603435000	-4.014190000	H	-12.492395000	4.906112000	3.619626000
C	-2.585822000	-3.657465000	-4.377163000	Ni	-8.686395000	-0.078881000	-1.724007000
H	-3.601968000	-3.998020000	-4.202069000	N	-10.551169000	-0.325151000	-1.259336000
C	-1.575761000	-4.563787000	-4.696331000	N	-8.687994000	-1.905015000	-1.779119000
H	-1.803367000	-5.623429000	-4.784485000	N	-6.852131000	-0.293864000	-2.358173000
C	-0.259643000	-4.132535000	-4.906268000	C	-11.515258000	0.702679000	-1.054946000
C	0.823523000	-5.128313000	-5.247602000	C	-11.946685000	1.470426000	-2.160872000
H	1.365894000	-4.842129000	-6.154673000	C	-11.450004000	1.180487000	-3.557624000
H	0.398820000	-6.123877000	-5.402789000	H	-11.511085000	0.112970000	-3.790905000
H	1.570558000	-5.206624000	-4.447820000	H	-12.039705000	1.728615000	-4.297384000
F	-7.113777000	4.707659000	1.253495000	H	-10.403287000	1.472746000	-3.692210000
P	-7.907495000	3.369046000	0.582787000	C	-12.885860000	2.488137000	-1.952494000
C	-7.746664000	4.121263000	-1.084145000	H	-13.222348000	3.077583000	-2.801631000
C	-6.737481000	2.230034000	1.430036000	C	-13.405869000	2.736468000	-0.683026000
C	-9.420369000	3.798068000	1.511133000	H	-14.136065000	3.527554000	-0.537258000
C	-8.752279000	3.920207000	-2.044599000	C	-12.992129000	1.956750000	0.396005000
C	-7.111567000	0.904943000	1.717523000	H	-13.398114000	2.144046000	1.386220000
C	-9.827248000	3.039396000	2.615127000	C	-12.046820000	0.937271000	0.233582000
C	-6.686680000	4.995002000	-1.375854000	C	-11.629769000	0.096755000	1.413439000
C	-5.498728000	2.699664000	1.899504000	H	-10.541635000	-0.006739000	1.462983000
C	-10.124650000	4.962710000	1.174223000	H	-12.043477000	-0.914006000	1.330685000
C	-8.704690000	4.597877000	-3.263889000	H	-11.977047000	0.539656000	2.349847000
C	-6.280581000	0.084413000	2.481856000	C	-10.955761000	-1.617341000	-1.160845000
C	-10.928601000	3.442223000	3.373457000	O	-12.083828000	-2.057563000	-0.898782000
C	-6.626445000	5.641169000	-2.610304000	C	-9.813407000	-2.549589000	-1.452921000
C	-4.656850000	1.863652000	2.633352000	C	-9.839633000	-3.940019000	-1.448303000
C	-11.234092000	5.352317000	1.925558000	H	-10.758902000	-4.450105000	-1.186020000
C	-7.639782000	5.453520000	-3.552438000	C	-8.671114000	-4.628296000	-1.791210000
C	-5.050150000	0.559346000	2.938856000	H	-8.663535000	-5.713310000	-1.794340000

C	-7.515422000	-3.922181000	-2.140575000	H	4.312229000	0.235614000	0.395691000
H	-6.596196000	-4.418940000	-2.426964000	C	5.429743000	-1.525754000	-3.345883000
C	-7.558999000	-2.531768000	-2.124192000	O	6.561228000	-1.234572000	-2.933944000
C	-6.458497000	-1.584649000	-2.510494000	C	4.972638000	-1.084234000	-4.721401000
O	-5.376965000	-2.020359000	-2.933595000	C	5.692912000	-0.365528000	-5.671168000
C	-5.932954000	0.721082000	-2.762078000	H	6.711973000	-0.065735000	-5.457227000
C	-4.749859000	0.952701000	-2.021794000	C	5.061127000	-0.052844000	-6.881541000
C	-4.406359000	0.125143000	-0.810471000	H	5.600578000	0.506112000	-7.639350000
H	-5.274049000	-0.025476000	-0.164927000	C	3.739869000	-0.449483000	-7.124006000
H	-3.618466000	0.602251000	-0.222583000	H	3.227314000	-0.215085000	-8.049453000
H	-4.057551000	-0.867448000	-1.116000000	C	3.076477000	-1.165090000	-6.131438000
C	-3.863522000	1.945127000	-2.460571000	C	1.651480000	-1.680619000	-6.150433000
H	-2.956703000	2.128487000	-1.889533000	O	0.916152000	-1.465897000	-7.124063000
C	-4.121788000	2.687032000	-3.612066000	C	0.059144000	-2.847826000	-4.755147000
H	-3.421340000	3.450078000	-3.939707000	C	-0.997341000	-1.955718000	-4.457151000
C	-5.282006000	2.439048000	-4.343444000	C	-0.776176000	-0.463113000	-4.467315000
H	-5.481953000	3.003211000	-5.250569000	H	0.093231000	-0.184120000	-3.861410000
C	-6.198789000	1.462892000	-3.936010000	H	-1.650870000	0.065385000	-4.079497000
C	-7.432223000	1.203394000	-4.766299000	H	-0.580251000	-0.104808000	-5.483937000
H	-7.626021000	0.133380000	-4.882057000	C	-2.256460000	-2.482931000	-4.147064000
H	-7.328769000	1.647014000	-5.760383000	H	-3.079444000	-1.816094000	-3.906873000
H	-8.322257000	1.645335000	-4.304832000	C	-2.473062000	-3.860614000	-4.126927000
F	-8.710061000	1.985735000	-0.146526000	H	-3.457588000	-4.244041000	-3.875543000
³ PC _{2,PF}				C	-1.425444000	-4.731886000	-4.423151000
Ni	2.800484000	-2.403592000	-3.707534000	H	-1.592481000	-5.806226000	-4.414147000
N	4.454925000	-2.230264000	-2.717388000	C	-0.150798000	-4.245103000	-4.737444000
N	3.717166000	-1.446707000	-4.994473000	C	0.971531000	-5.203477000	-5.059977000
N	1.367955000	-2.350860000	-5.005317000	H	1.486363000	-4.924783000	-5.984717000
C	4.641769000	-2.692506000	-1.385767000	H	0.590221000	-6.222200000	-5.171228000
C	4.791077000	-4.078564000	-1.155844000	H	1.732035000	-5.222021000	-4.269418000
C	4.833567000	-5.056365000	-2.306304000	F	-7.012856000	4.817037000	1.984031000
H	5.553602000	-4.746762000	-3.070360000	P	-7.853647000	3.379424000	1.645330000
H	5.110976000	-6.054150000	-1.955829000	C	-7.835293000	3.807483000	-0.145898000
H	3.861316000	-5.141099000	-2.806738000	C	-6.483330000	2.380245000	2.376017000
C	4.915198000	-4.534274000	0.162059000	C	-9.239796000	3.934638000	2.723550000
H	5.036840000	-5.599221000	0.343307000	C	-8.878472000	3.389871000	-0.988729000
C	4.891406000	-3.644349000	1.235405000	C	-6.664048000	1.016900000	2.671943000
H	4.987997000	-4.013555000	2.252546000	C	-10.076053000	2.998846000	3.354935000
C	4.743615000	-2.278200000	0.997135000	C	-6.782098000	4.560221000	-0.689733000
H	4.723335000	-1.581610000	1.831566000	C	-5.234887000	2.966643000	2.651640000
C	4.614933000	-1.781191000	-0.305206000	C	-9.473018000	5.303866000	2.932645000
C	4.453767000	-0.300657000	-0.546292000	C	-8.870633000	3.726133000	-2.343988000
H	3.595642000	-0.092589000	-1.194756000	C	-5.629301000	0.267358000	3.232564000
H	5.336927000	0.110459000	-1.047457000	C	-11.113466000	3.424879000	4.185089000

C	-6.763356000	4.869478000	-2.050647000	C	-10.012083000	-2.482053000	-1.909256000
C	-4.197126000	2.208276000	3.194938000	C	-10.088838000	-3.858181000	-1.700202000
C	-10.529098000	5.725767000	3.741352000	H	-11.036062000	-4.321446000	-1.450986000
C	-7.808367000	4.458106000	-2.880246000	C	-8.908984000	-4.603936000	-1.828783000
C	-4.391000000	0.857888000	3.491028000	H	-8.936250000	-5.677399000	-1.671114000
C	-11.347615000	4.788561000	4.374768000	C	-7.695803000	-3.987528000	-2.165519000
H	-9.702162000	2.813189000	-0.588973000	H	-6.778197000	-4.552383000	-2.278553000
H	-7.611493000	0.541417000	2.460567000	C	-7.701771000	-2.607229000	-2.359933000
H	-9.917511000	1.940252000	3.197003000	C	-6.536823000	-1.718174000	-2.755761000
H	-5.979077000	4.906305000	-0.051737000	O	-5.414290000	-2.214992000	-2.917111000
H	-5.075840000	4.015914000	2.445912000	C	-5.889343000	0.530509000	-3.267342000
H	-8.829192000	6.037232000	2.464662000	C	-4.937416000	0.956717000	-2.314972000
H	-9.698847000	3.415942000	-2.974130000	C	-4.934500000	0.392035000	-0.916085000
H	-5.792513000	-0.781580000	3.461503000	H	-5.930210000	0.437177000	-0.462814000
H	-11.742357000	2.689138000	4.677571000	H	-4.241001000	0.940704000	-0.273583000
H	-5.933624000	5.438227000	-2.459351000	H	-4.635194000	-0.661761000	-0.921452000
H	-3.238318000	2.678450000	3.392269000	C	-3.990163000	1.916593000	-2.693782000
H	-10.705337000	6.788086000	3.881864000	H	-3.258109000	2.250571000	-1.962660000
H	-7.797338000	4.710000000	-3.936590000	C	-3.978171000	2.448860000	-3.983166000
H	-3.584325000	0.271045000	3.920581000	H	-3.238102000	3.194509000	-4.259656000
H	-12.162444000	5.118448000	5.012623000	C	-4.923820000	2.019940000	-4.913926000
Ni	-8.799808000	-0.025108000	-2.526931000	H	-4.916354000	2.427168000	-5.921859000
N	-10.721962000	-0.196162000	-2.136335000	C	-5.886774000	1.061030000	-4.575688000
N	-8.839614000	-1.938241000	-2.213924000	C	-6.892455000	0.597667000	-5.602286000
N	-6.900714000	-0.407752000	-2.902875000	H	-6.883594000	-0.491631000	-5.713168000
C	-11.690144000	0.851415000	-2.105956000	H	-6.682153000	1.042518000	-6.578590000
C	-12.066248000	1.469960000	-3.319255000	H	-7.915898000	0.875141000	-5.322741000
C	-11.514701000	0.994207000	-4.642944000	F	-8.717956000	1.952103000	1.278428000
H	-11.587437000	-0.092611000	-4.746202000				
H	-12.055189000	1.455837000	-5.473792000				
H	-10.454233000	1.252595000	-4.758580000				
C	-12.973812000	2.536605000	-3.282092000				
H	-13.269429000	3.009400000	-4.215331000				
C	-13.504108000	2.988456000	-2.074759000				
H	-14.207142000	3.816523000	-2.062011000				
C	-13.127871000	2.368661000	-0.883962000				
H	-13.538195000	2.716728000	0.060725000				
C	-12.223155000	1.299228000	-0.875082000				
C	-11.826524000	0.653292000	0.430513000				
H	-10.739727000	0.649149000	0.562097000				
H	-12.167079000	-0.386242000	0.472458000				
H	-12.264360000	1.192150000	1.275166000				
C	-11.142327000	-1.469932000	-1.856308000				
O	-12.290821000	-1.845241000	-1.593662000				