Electronic Supplementary Information for

The Elusive Active Species in Nickel(II)-Mediated Oxidations of Hydrocarbons by Peracids: A Ni^{II}–Oxyl, an Aroyloxy Radical, or a Ni^{II}-Peracid complex?

Zhimin Wu,[a,b] Dongru Sun[a,b] Yong-Min Lee,[c] Yufen Zhao,[a,b] Wonwoo Nam*[c] and Yong Wang*[a,b]*

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

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

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

Email: yong@nbu.edu.cn, wwnam@ewha.ac.kr, sundongru@nbu.edu.cn

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Part I. The calculated data on the oxidants 1

Table S1. Benchmark of the performance of the employed B3LYP functional with other **5** functionals. Calculations were performedat the B2 level.

	B3LYP-D3BJ	*ΔE*	B3PW91-D3BJ	*ΔE*	PBE0-D3BJ	*ΔE*	M06	*ΔE*	TPSSh	*ΔE*	OPBE	*ΔE*
^{1}**1**	-2548.285836	**28.8**	-2547.643945[a]	**31.0**	-2546.056068	**34.8**	-2546.927026	**24.0**	-2548.109735	**27.6**	-2547.685073	**13.1**
^{3}**1**	-2548.331751	**0.0**	-2547.693351	**0.0**	-2546.111597	**0.0**	-2546.965281	**0.0**	-2548.153703	**0.0**	-2547.705977	**0.0**

a. Absolute energies are in au units and the relative ones are in kcal mol^{-1} units

Table S2. Various SCF and Gibbs free energies of **1** on the different spin states. Calculations were performed at the UB3LYP-D3(BJ)/B2//B1 level in solvent.

	OPT/B1	*ΔE*	OPT/B1+ZPE	*ΔE*	SPE	*ΔE*	SPE/B2+ZPE	*ΔE*	*G*	*ΔG*
^{1}**1**	-2547.859570[a]	**29.1**	-2547.287164	**29.5**	-2548.285836	**28.8**	-2547.713429	**29.3**	-2547.368211	**31.1**
^{3}**1**	-2547.905882	**0.0**	-2547.334194	**0.0**	-2548.331751	**0.0**	-2547.760063	**0.0**	-2547.417782	**0.0**
^{5}**1**	-2547.787534	**74.3**	-2547.218684	**72.5**	-2548.212592	**74.8**	-2547.643742	**73.0**	-2547.300313	**73.7**

a. Absolute energies are in au units and the relative ones are in kcal mol^{-1} units

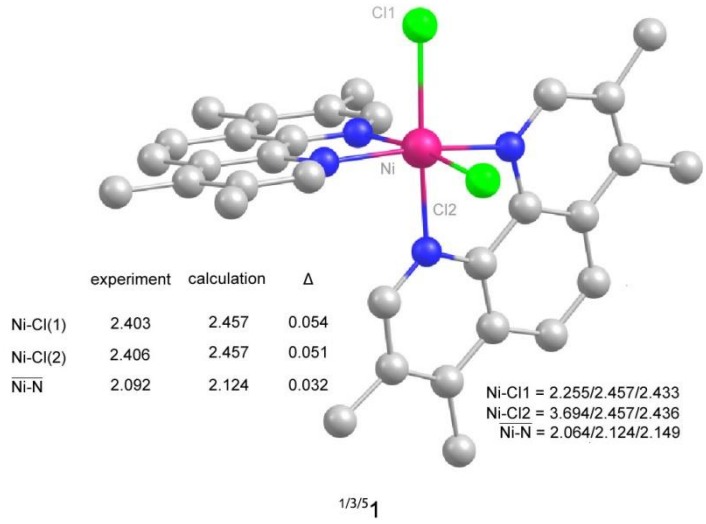

Fig. S1 Optimized structures of **1** on the different spin states. Calculations were done at the UB3LYP-D3(BJ)/B1 level in solvent. Lengths are in Å units. Hydrogen atoms of the supporting ligand are omitted for clarity.

Table S3. Mulliken spin densities and charges of **1** on the different spin states. Calculations were done at the UB3LYP-D3(BJ)/B1 level in solvent.

	charge				Spin density			
	Ni	Ligand	Cl1	Cl2	Ni	Ligand	Cl1	Cl2
^{1}**1**	0.36	0.96	-0.46	-0.87	0.00	0.00	0.00	0.00
^{3}**1**	0.33	0.85	-0.59	-0.59	1.59	0.26	0.08	0.08
^{5}**1**	0.26	0.89	-0.58	-0.58	1.60	2.23	0.09	0.09

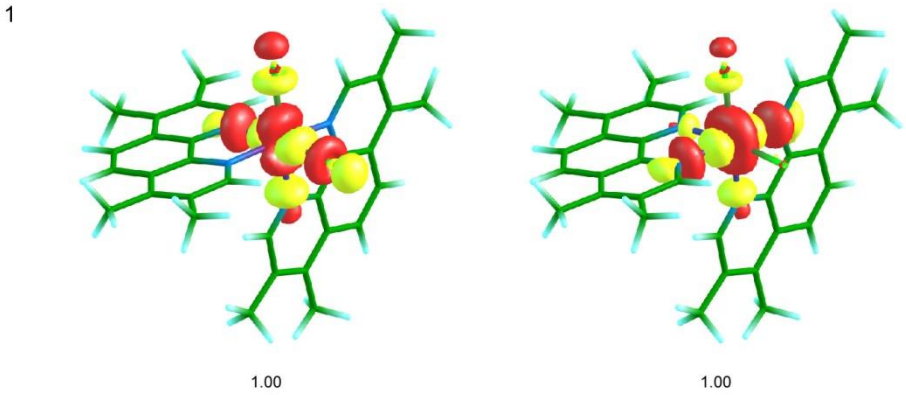

Fig. S2. Singly-occupied natural orbitals (SNOs) of **1** on the triplet spin states. Calculations were performed at the UB3LYP-D3(BJ)/B1 level in solvent. Positive values represent alpha-electron occupations.

Part II. The conversion of a Ni^{II}-*m*CPBA complex to a Ni^{III}-oxyl species and a *m*CBA$^{\bullet}$ radical.

Table S4. Various SCF and Gibbs free energies in the conversion of a Ni^{II}-*m*CPBA complex **2** to a Ni^{III}-oxyl species *via* a complex of a Ni^{III}-OH species and a *m*CBA$^{\bullet}$ radical on the singlet and triplet spin states. Calculations were performed at the UB3LYP-D3(BJ)/B2//B1 level in solvent.

	OPT/B1	*ΔE*	OPT/B1+ZPE	*ΔE*	SPE	*ΔE*	SPE/B2+ZPE	*ΔE*	*G*	*ΔG*
^{1}**2**	-3542.406577[a]	**13.0**	-3541.693215	**13.2**	-3542.997435	**14.0**	-3542.284073	**14.3**	-3541.794396	**13.1**
^{3}**2**	-3542.427219	**0.0**	-3541.714308	**0.0**	-3543.019764	**0.0**	-3542.306853	**0.0**	-3541.815234	**0.0**
^{5}**2**	-3542.327355	**62.7**	-3541.619517	**59.5**	-3542.920023	**62.6**	-3542.212185	**59.4**	-3541.720745	**59.3**
^{1}**TS$_{23}$**	-3542.335991	**57.2**	-3541.627030	**54.8**	-3542.937761	**51.5**	-3542.228800	**49.0**	-3541.570057	**53.1**
^{3}**TS$_{23}$**	-3542.386999	**25.2**	-3541.676860	**23.5**	-3542.985704	**21.4**	-3542.275786	**19.5**	-3541.780030	**22.1**
^{1}**3**	-3542.411580	**9.8**	-3541.698911	**9.7**	-3543.003592	**10.1**	-3542.290923	**10.0**	-3541.794731	**12.9**
^{3}**3**	-3542.403037	**15.2**	-3541.692636	**13.6**	-3543.002720	**10.7**	-3542.292319	**9.1**	-3541.796193	**11.9**
^{3}**TS$_{34}$**	-3542.380643	**29.2**	-3541.675791	**24.2**	-3542.979754	**25.1**	-3542.274902	**20.0**	-3541.778902	**22.8**
^{1}**4**	-3542.373301	**33.8**	-3541.661098	**33.4**	-3542.975648	**27.7**	-3542.263445	**27.2**	-3541.762049	**33.4**
^{3}**4**	-3542.401741	**16.0**	-3541.690004	**15.3**	-3543.002202	**11.0**	-3542.290465	**10.3**	-3541.790523	**15.5**

a. Absolute energies are in au units and the relative ones are in kcal mol^{-1} units

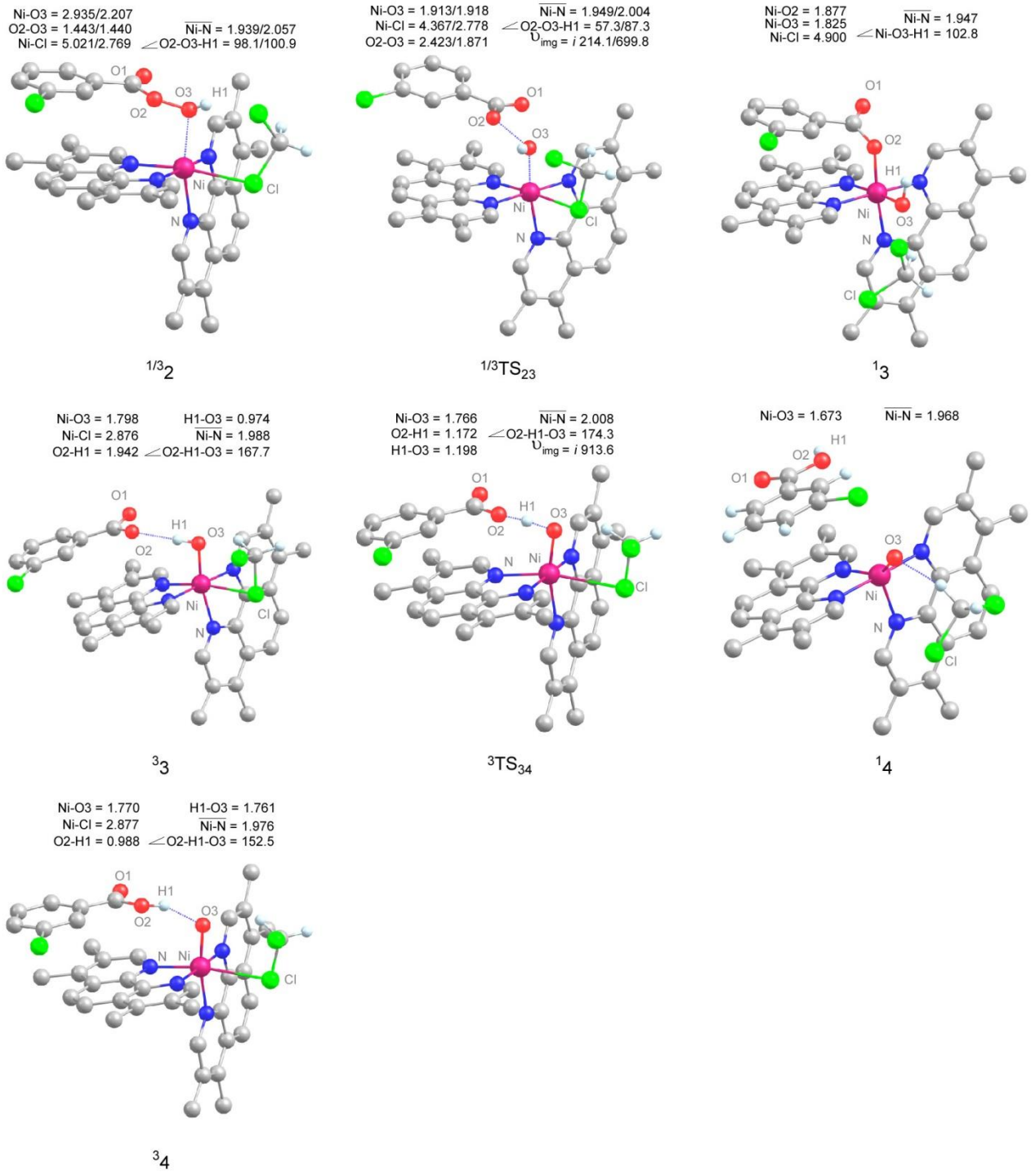

Fig. S3 The geometric information of the reaction intermediates in the conversion of a Ni^{II}-*m*CPBA complex **2** to a Ni^{III}-oxyl species *via* a complex of a Ni^{III}-OH species and a *m*CBA$^{\bullet}$ radical on the singlet and triplet spin states. Calculations were performed at the UB3LYP-D3(BJ)/B1 level in solvent. Lengths are in Å units, bond angles are in ° units and imaginary frequencies are in cm^{-1} units. Hydrogen atoms of the supporting ligand are omitted for clarity.

Table S5. Mulliken spin densities and charges of the reaction intermediates in the conversion of a Ni^{II}-*m*CPBA complex **2** to a Ni^{III}-oxyl species *via* a complex of a Ni^{III}-OH species and a *m*CBA$^{\bullet}$ radical on the singlet and triplet spin states. Calculations were performed at the UB3LYP-D3(BJ)/B1 level in solvent.

	charge						Spin density					
	Ni	Ligand	mCPBA-OH	O3	H	CH_2Cl_2	Ni	Ligand	mCPBA-OH	O3	H	CH_2Cl_2
^{1}**2**	0.67	1.20	-0.02	-0.28	0.37	0.05	0.00	0.00	0.00	0.00	0.00	0.00
^{3}**2**	0.59	1.07	0.06	-0.29	0.39	0.19	1.61	0.34	0.00	0.03	0.00	0.02
^{1}**TS$_{23}$**	0.78	1.64	-0.30	-0.47	0.34	0.00	0.00	0.00	0.00	0.00	0.00	0.00
^{3}**TS$_{23}$**	0.58	1.40	-0.12	-0.41	0.36	0.18	1.21	0.20	0.49	0.07	0.00	0.03
^{1}**3**	0.60	1.86	-0.30	-0.53	0.35	0.01	0.00	0.00	0.00	0.00	0.00	0.00
^{3}**3**	0.59	1.46	0.08	-0.60	0.02	0.44	0.84	0.18	1.00	-0.05	0.03	0.00
^{3}**TS$_{34}$**	0.57	1.74	-0.19	-0.66	0.01	0.54	0.93	0.66	0.46	-0.07	0.02	0.00
^{1}**4**	0.77	1.51	-0.16	-0.49	0.36	0.01	0.00	0.00	0.00	0.00	0.00	0.00
^{3}**4**	0.64	1.60	-0.36	-0.38	0.03	0.47	0.73	0.24	0.00	1.00	0.03	-0.01

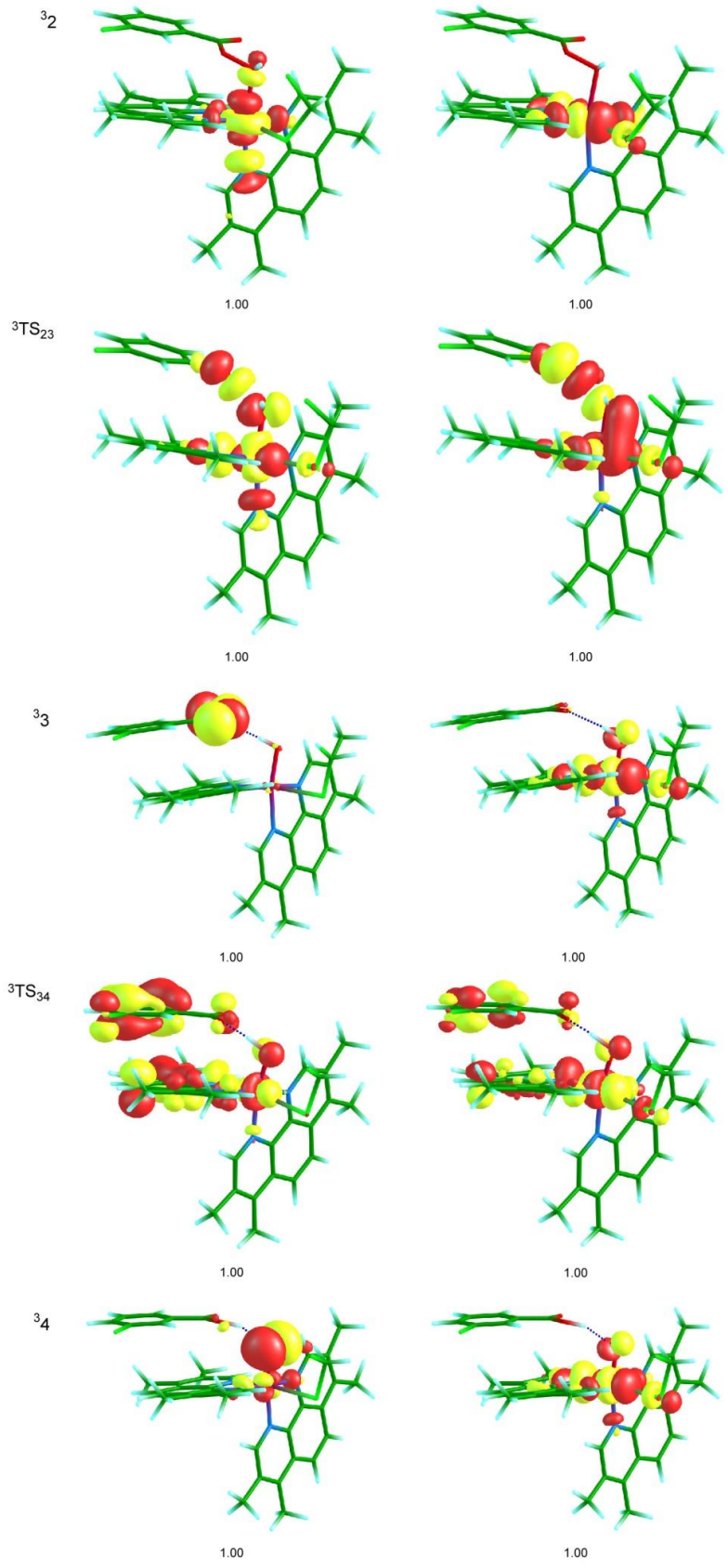

Fig. S4 Singly-occupied natural orbitals (SNOs) of the reaction intermediates in the conversion of a Ni^{II}-*m*CPBA complex **2** to a Ni^{III}-oxyl species *via* a complex of a Ni^{III}-OH species and a *m*CBA radical on the singlet and triplet spin states. Calculations were performed at the B1 level in solvent. Positive values represent alpha-electron occupations.

Part III. C-H bond activation by *m*CBA• and by the Ni^{III}-OH species

Table S6. Various SCF and Gibbs free energies of the reaction intermediates for the hydrogen atom abstraction of cyclohexane by a *m*CBA• radical on the doublet spin states. Calculations were performed at the UB3LYP-D3(BJ)/B2//B1 level in solvent.

	OPT/B1	*ΔE*	OPT/B1+ZPE	*ΔE*	SPE/B2	*ΔE*	SPE/B2+ZPE	*ΔE*	*G*	*ΔG*
^{2}**3'+CH**	-1115.717942[a]	**0.0**	-1115.454189	**0.0**	-1115.903701	**0.0**	-1115.639949	**0.0**	-1115.508276	**0.0**
^{2}TS$_{3'+CH}$	-1115.708400	**6.0**	-1115.448986	**3.3**	-1115.896119	**4.8**	-1115.636705	**2.0**	-1115.497997	**6.5**
^{2}IM$_{3'+CH}$	-1115.725600	**-4.8**	-1115.462253	**-5.1**	-1115.914730	**-6.9**	-1115.651383	**-7.2**	-1115.512825	**-2.9**

a. Absolute energies are in au units and the relative ones are in kcal mol^{-1} units

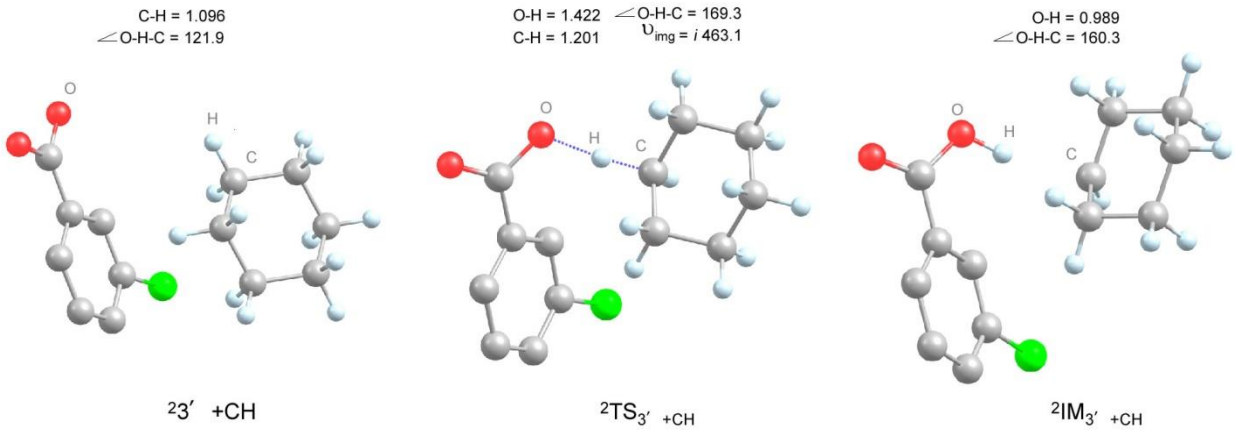

Fig. S5 The geometric information of the reaction intermediates for the hydrogen atom abstraction of cyclohexane by a mCBA• on the doublet spin states. Calculations were performed at the UB3LYP-D3(BJ)/B1 level in solvent. Lengths are in Å units, bond angles are in ° units and imaginary frequency is in cm-1 units. Hydrogen atoms of the mCPBA are omitted for clarity.

Table S7. Mulliken spin densities and charges of the reaction intermediates for the hydrogen atom abstraction of cyclohexane by a *m*CBA• on the doublet spin states. Calculations were performed at the UB3LYP-D3(BJ)/B1 level in solvent.

	Charge			Spin density		
	mCPBA-OH	Sub-H	H	mCPBA-OH	Sub-H	H
^{2}**3'+CH**	0.02	-0.10	0.09	1.00	0.00	0.00
^{2}TS$_{3'+CH}$	-0.34	0.07	0.24	0.58	0.42	0.00
^{2}IM$_{3'+CH}$	-0.39	0.06	0.34	0.04	0.92	0.04

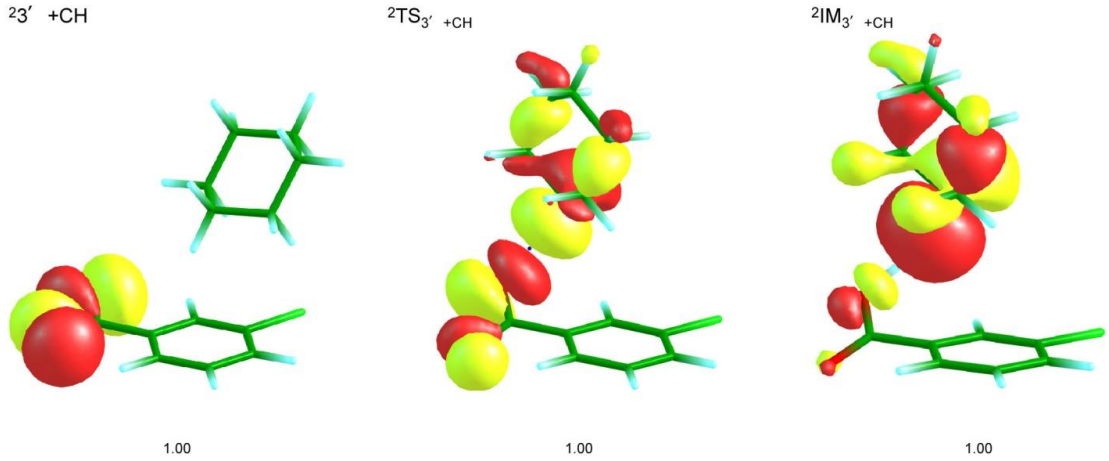

Fig. S6 Singly-occupied natural orbitals (SNOs) of the reaction intermediates for the hydrogen atom abstraction of cyclohexane by a *m*CBA• on the doublet spin states. Calculations were performed at the UB3LYP-D3(BJ)/B1 level in solvent. Positive values represent alpha-electron occupations.

Table S8. Various SCF and Gibbs free energies of the reaction intermediates for the hydrogen atom abstraction of cyclohexane by a Ni^{III}-OH species on the doublet spin states. Calculations were performed at the UB3LYP-D3(BJ)/B2//B1 level in solvent.

	OPT/B1	*ΔE*	OPT/B1+ZPE	*ΔE*	SPE/B2	*ΔE*	SPE/B2+ZPE	*ΔE*	*G*	*ΔG*
^{2}**3''+CH**	-2898.534439	**0.0**	-2897.746137	**0.0**	-2899.039090	**0.0**	-2898.250788	**0.0**	-2897.842742	**0.0**
$^2TS_{3''+CH}$	-2898.518863	**9.8**	-2897.736216	**6.2**	-2899.020969	**11.4**	-2898.238322	**7.8**	-2897.834281	**5.3**
$^2IM_{3''+CH}$	-2898.545108	**-6.7**	-2897.760107	**-8.8**	-2899.046853	**-4.9**	-2898.261852	**-6.9**	-2897.860183	**-10.9**

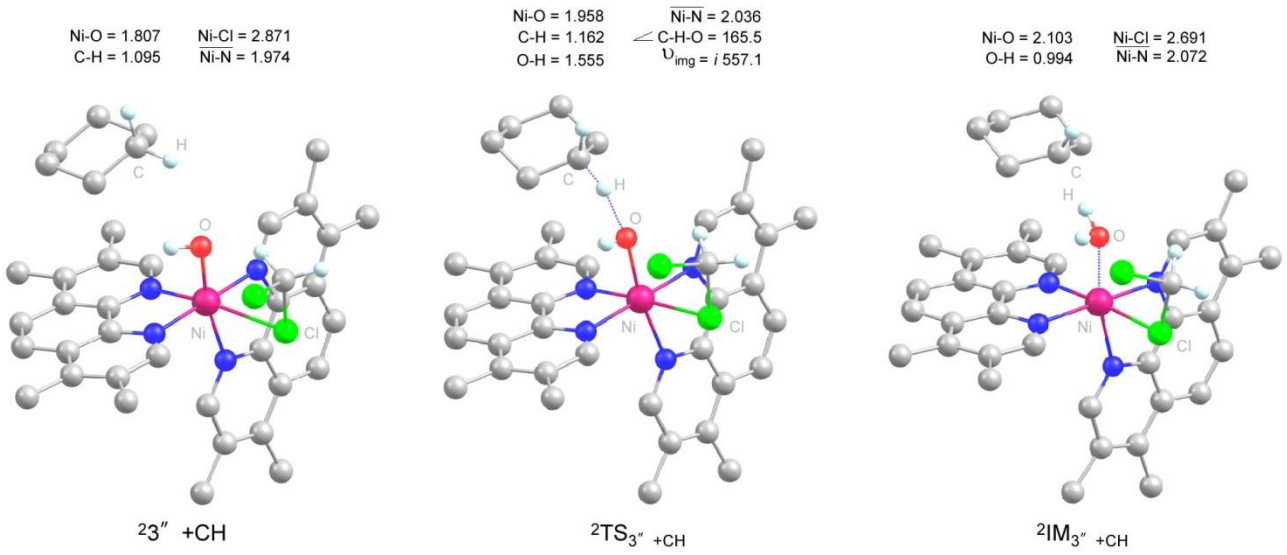

Fig. S7 The geometric information of the reaction intermediates in the hydrogen atom abstraction of cyclohexane by a Ni^{III}-OH species on the doublet spin states.Calculations were performed at the UB3LYP-D3(BJ)/B1 level in solvent. Lengths are in Å units, bond angles are in ° units and imaginary frequency is in cm^{-1} units. Hydrogen atoms of the supporting ligand and cyclohexane are omitted for clarity.

Table S9. Mulliken spin densities and charges of the reaction intermediates in the hydrogen atom abstraction of cyclohexane by a Ni^{III}-OH species on the doublet spin states. Calculations were performed at the UB3LYP-D3(BJ)/B1 level in solvent.

	charge						Spin density					
	Ni	Ligand	OH	H	Sub-H	CH_2Cl_2	Ni	Ligand	OH	H	Sub-H	CH_2Cl_2
^{2}**3''+CH**	0.62	1.52	-0.25	0.10	-0.11	0.12	0.84	0.18	-0.04	0.00	0.00	0.03
$^2TS_{3''+CH}$	0.58	1.20	-0.18	0.20	0.04	0.15	1.43	0.24	-0.39	0.00	-0.31	0.02
$^2IM_{3''+CH}$	0.55	1.06	-0.22	0.36	0.08	0.17	1.61	0.32	0.00	-0.05	-0.91	0.03

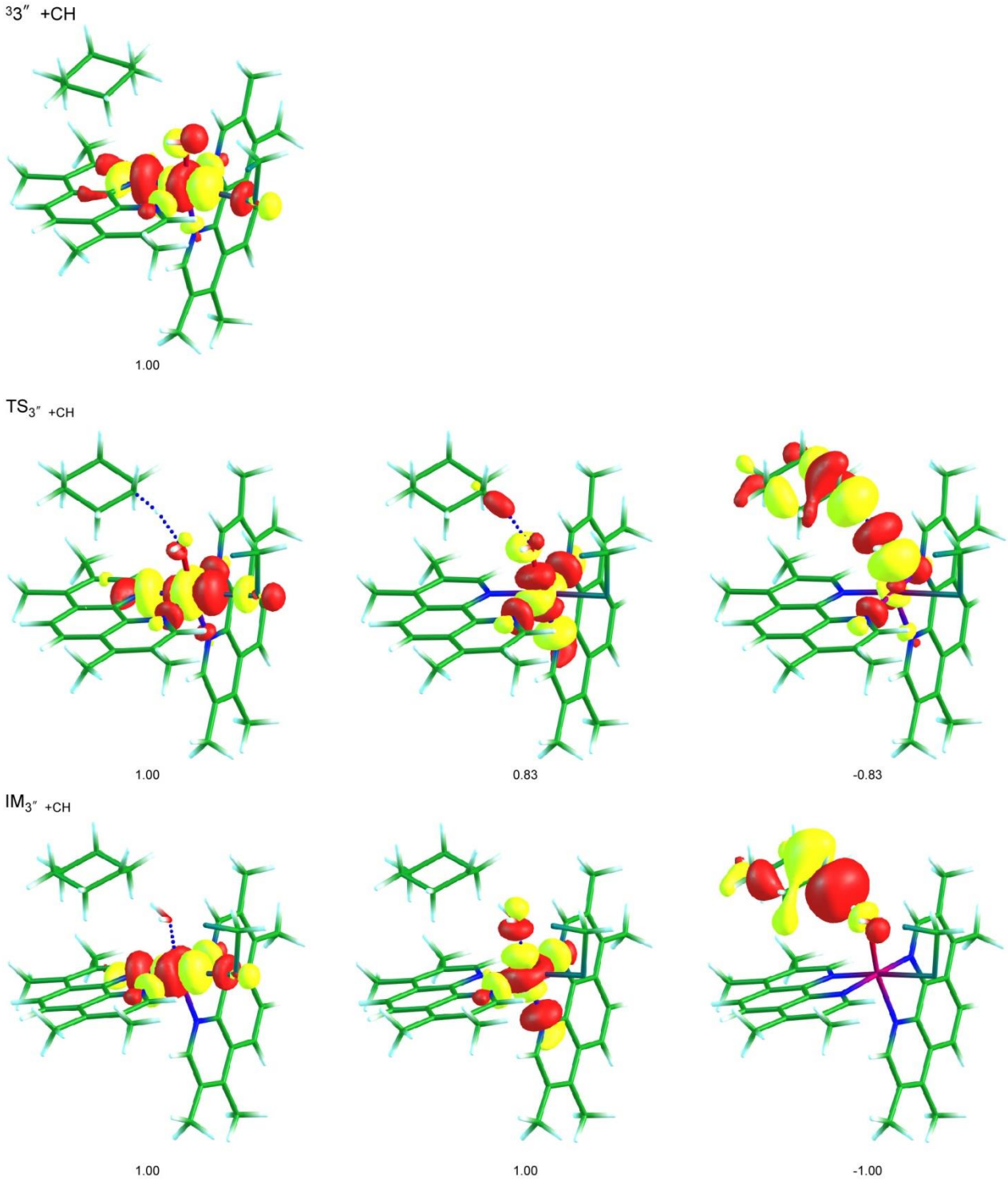

Fig. S8 Singly-occupied natural orbitals (SNOs) of the reaction intermediates in the hydrogen atom abstraction of cyclohexane by a Ni^{III}-OH species on the doublet spin states.Calculations were performed at the UB3LYP-D3(BJ)/B1 level in solvent. Positive values represent alpha-electron occupations.

Part IV. Reactions of R• with *m*CBA and dichlomethane

Table S10. Various SCF and Gibbs free energies of the reaction intermediates in reactions of carbon-centered R• species with *m*CPBA on the doublet spin states. Calculations were performed at the UB3LYP-D3(BJ)/B2//B1 level in solvent.

	OPT/B1	*ΔE*	OPT/B1+ZPE	*ΔE*	SPE/B2	*ΔE*	SPE/B2+ZPE	*ΔE*	*G*	*ΔG*
^{2}IM'	-1190.854607	**0.0**	-1190.588376	**0.0**	-1191.064282	**0.0**	-1190.798051	**0.0**	-1190.641442	**0.0**
^{2}TS$_{OH}$	-1190.838858	**9.9**	-1190.574995	**8.4**	-1191.046627	**11.1**	-1190.782764	**9.6**	-1190.625609	**9.9**
^{2}PC$_{OH}$	-1190.945309	**-56.9**	-1190.675829	**-54.9**	-1191.153879	**-56.2**	-1190.884399	**-54.2**	-1190.729622	**-55.3**

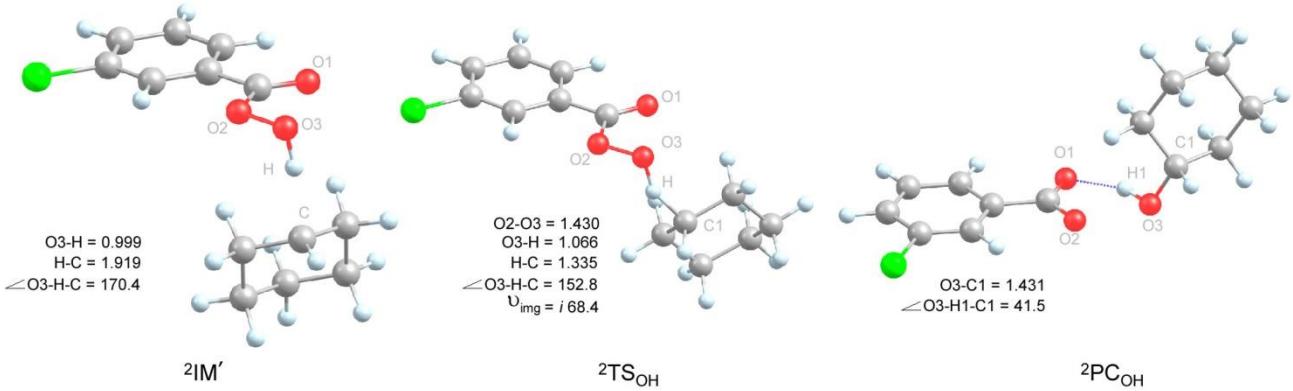

Fig. S9 The geometric information of the reaction intermediates in reactions of carbon-centered R• species with *m*CPBA on the doublet spin states.Calculations were done at the UB3LYP-D3(BJ)/B1 level in solvent. Lengths are in Å units, bond angles are in ° units and imaginary frequency is in cm^{-1} units.

Table S11. Mulliken spin densities and charges of the reaction intermediates in reactions of carbon-centered R• species with *m*CPBA on the doublet spin states. Calculations were performed at the UB3LYP-D3(BJ)/B1 level in solvent.

	charge				Spin density			
	mCPBA-OH	O	H	Sub-H	mCPBA-OH	O	H	Sub-H
^{2}IM'	-0.08	-0.33	0.36	0.05	0.00	0.05	0.04	0.91
^{2}TS$_{OH}$	-0.08	-0.31	0.36	0.04	0.02	0.24	0.01	0.72
^{2}PC$_{OH}$	-0.30	-0.44	0.37	0.38	0.58	0.38	0.00	0.05

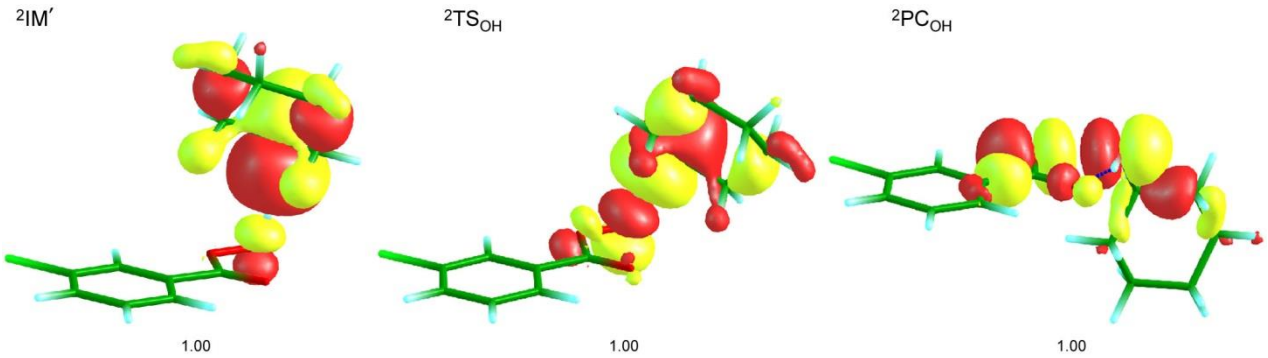

Fig. S10 Singly-occupied natural orbitals (SNOs) of the reaction intermediates in reactions of carbon-centered R• radical with *m*CPBA on the doublet spin states.Calculations were performed at the UB3LYP-D3(BJ)/B1 level in solvent. Positive values represent alpha-electron occupations.

Table S12. Various SCF and Gibbs free energies of the reaction intermediates in reactions of carbon-centered R• radical with dichloromethane on the doublet spin states. Calculations were performed at the UB3LYP-D3(BJ)/B2//B1 level in solvent.

	OPT/B1	*ΔE*	OPT/B1+ZPE	*ΔE*	SPE/B2	*ΔE*	SPE/B2+ZPE	*ΔE*	*G*	*ΔG*
^{2}IM''	-1194.967400	**0.0**	-1194.781541	**0.0**	-1195.085048	**0.0**	-1194.899189	**0.0**	-1194.830850	**0.0**
^{2}TS$_{Cl}$	-1194.951977	**9.7**	-1194.765715	**9.9**	-1195.068520	**10.4**	-1194.882258	**10.6**	-1194.807449	**14.7**
^{2}PC$_{Cl}$	-1194.977337	**-6.2**	-1194.792351	**-6.8**	-1195.095126	**-6.3**	-1194.910139	**-6.9**	-1194.840732	**-6.2**

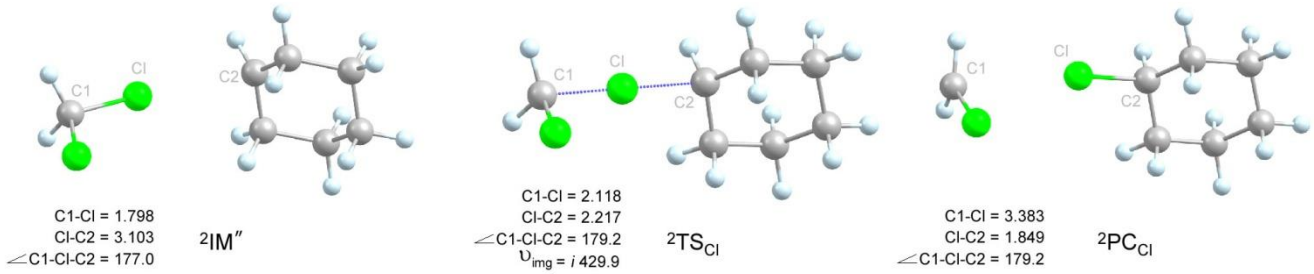

Fig. S11 The geometric information of the reaction intermediates inreactions of carbon-centered R• radical with dichloromethane on the doublet spin states. Calculations were performed at the UB3LYP-D3(BJ)/B1 level in solvent. Lengths are in Å units, bond angles are in ° units and imaginary frequency is in cm^{-1} units.

Table S13. Mulliken spin densities and charges of the reaction intermediates in reactions of carbon-centered R• radical with dichloromethane on the doublet spin states. Calculations were performed at the UB3LYP-D3(BJ)/B1 level in solvent.

	charge			Spin density		
	Sub-H	CH_2Cl	Cl	Sub-H	CH_2Cl	Cl
^{2}IM"	0.03	0.02	-0.04	0.97	0.02	0.01
$^2TS_{Cl}$	0.18	0.00	-0.18	0.57	0.53	-0.10
$^2PC_{Cl}$	0.14	0.01	-0.15	0.01	0.99	0.00

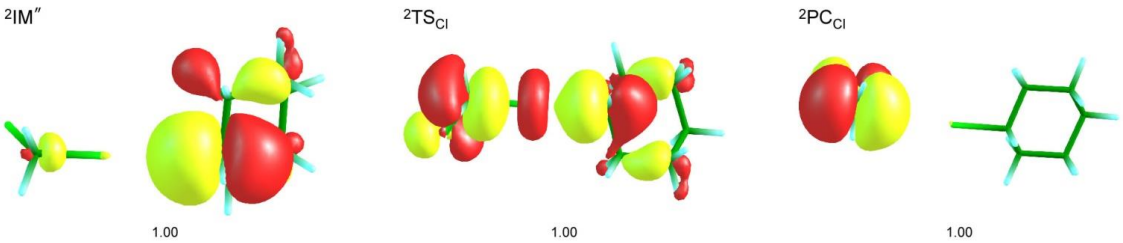

Fig. S12 Singly-occupied natural orbitals (SNOs) of the reaction intermediates in reactions of carbon-centered R• radical with dichloromethane on the doublet spin states. Calculations were performed at the UB3LYP-D3(BJ)/B1 level in solvent. Positive values represent alpha-electron occupations.

Part V. Robust oxidative ability of a Ni^{II}-*m*CPBA complex in hydroxyaltion

Table S14. Various SCF and Gibbs free energies of reaction intermediates of hydroxylation of cyclohexane by a Ni^{II}-*m*CPBA complex. on the singlet and triplet spin states. Calculations were performed at the UB3LYP-D3(BJ)/B2//B1 level in solvent.

	OPT/B1	*ΔE*	OPT/B1+ZPE	*ΔE*	SPE/B2	*ΔE*	SPE/B2+ZPE	*ΔE*	*G*	*ΔG*
^{1}**2+CH**	-3778.344156[a]	**8.9**	-3777.458579	**9.2**	-3778.984643	**10.7**	-3778.099066	**11.0**	-3777.570948	**9.3**
^{3}**2+CH**	-3778.358304	**0.0**	-3777.473263	**0.0**	-3779.001646	**0.0**	-3778.116605	**0.0**	-3777.585817	**0.0**
^{1}**TS**$_{2+CH}$	-3778.304227	**33.9**	-3777.425577	**29.9**	-3778.950650	**32.0**	-3778.072000	**28.0**	-3777.536868	**30.7**
^{3}**TS**$_{\2+CH}$	-3778.326773	**19.8**	-3777.447284	**16.3**	-3778.974803	**16.8**	-3778.095316	**13.4**	-3777.560438	**15.9**
^{1}**PC**$_{2+CH}$	-3778.458327	**-62.8**	-3777.570522	**-61.0**	-3779.103717	**-64.1**	-3778.215912	**-62.3**	-3777.681804	**-60.2**
^{3}**PC**$_{2+CH}$	-3778.479073	**-75.8**	-3777.591984	**-74.5**	-3779.126182	**-78.1**	-3778.239093	**-76.9**	-3777.703794	**-74.0**

a. Absolute energies are in au units and the relative ones are in kcal mol^{-1} units

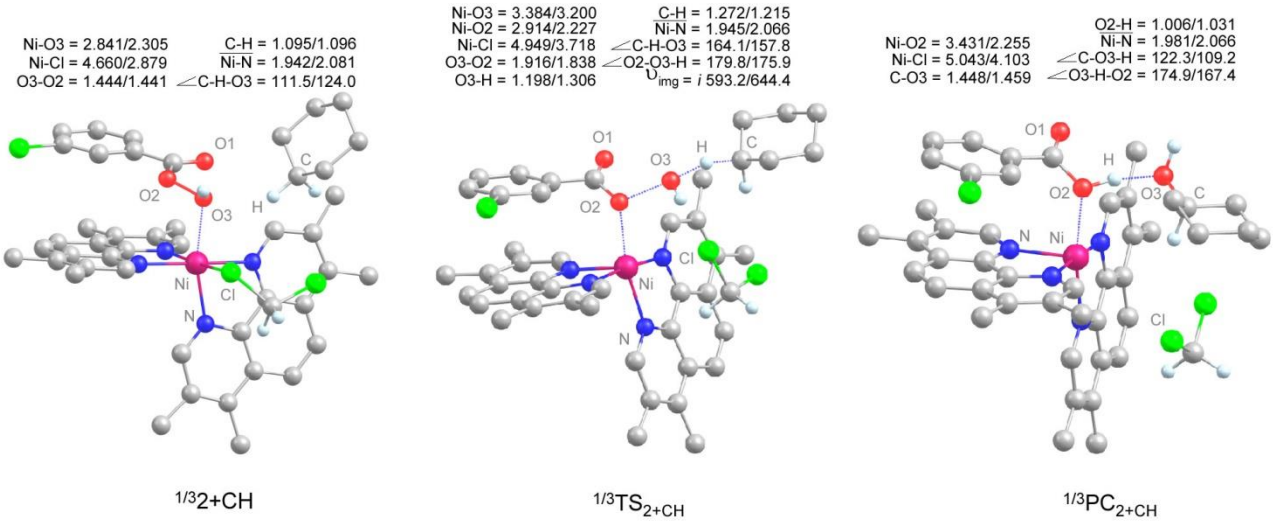

Fig. S13 The geometric information of reaction intermediates of hydroxylation of cyclohexane by a Ni^{II}-*m*CPBA complex on the singlet and triplet spin states.Calculations were performed at the UB3LYP-D3(BJ)/B1 level in solvent. Lengths are in Å units, bond angles are in ° units and imaginary frequency is in cm^{-1} units. Hydrogen atoms of the supporting ligand and cyclohexane are omitted for clarity.

Table S15. Mulliken spin densities and charges of reaction intermediates of hydroxylation of cyclohexane by a Ni^{II}-*m*CPBA complex on the singlet and triplet spin states. Calculations were performed at the UB3LYP-D3(BJ)/B1 level in solvent.

	charge							Spin density						
	Ni	Ligand	mCPBA-OH	OH	CH_2Cl_2	H	Sub-H	Ni	Ligand	mCPBA-OH	OH	CH_2Cl_2	H	Sub-H
^{1}**2+CH**	0.66	1.22	-0.01	0.10	0.05	0.07	-0.08	0.00	0.00	0.00	0.00	0.00	0.00	0.00
^{3}**2+CH**	0.63	1.07	0.06	0.12	0.12	0.07	-0.08	1.63	0.33	0.00	0.02	0.02	0.00	0.00
^{1}**TS**$_{2+CH}$	0.67	1.23	-0.02	0.10	0.05	0.09	-0.11	0.00	0.00	0.00	0.00	0.00	0.00	0.00
^{3}**TS**$_{2+CH}$	0.73	1.01	-0.20	0.00	0.06	0.27	0.15	1.64	0.32	0.05	0.00	0.00	0.00	-0.01
^{1}**PC**$_{2+CH}$	0.68	1.23	-0.39	-0.20	0.02	0.33	0.33	0.00	0.00	0.00	0.00	0.00	0.00	0.00
^{3}**PC**$_{2+CH}$	0.76	1.00	-0.33	-0.17	0.02	0.36	0.37	1.64	0.33	0.03	0.00	0.00	0.00	0.00

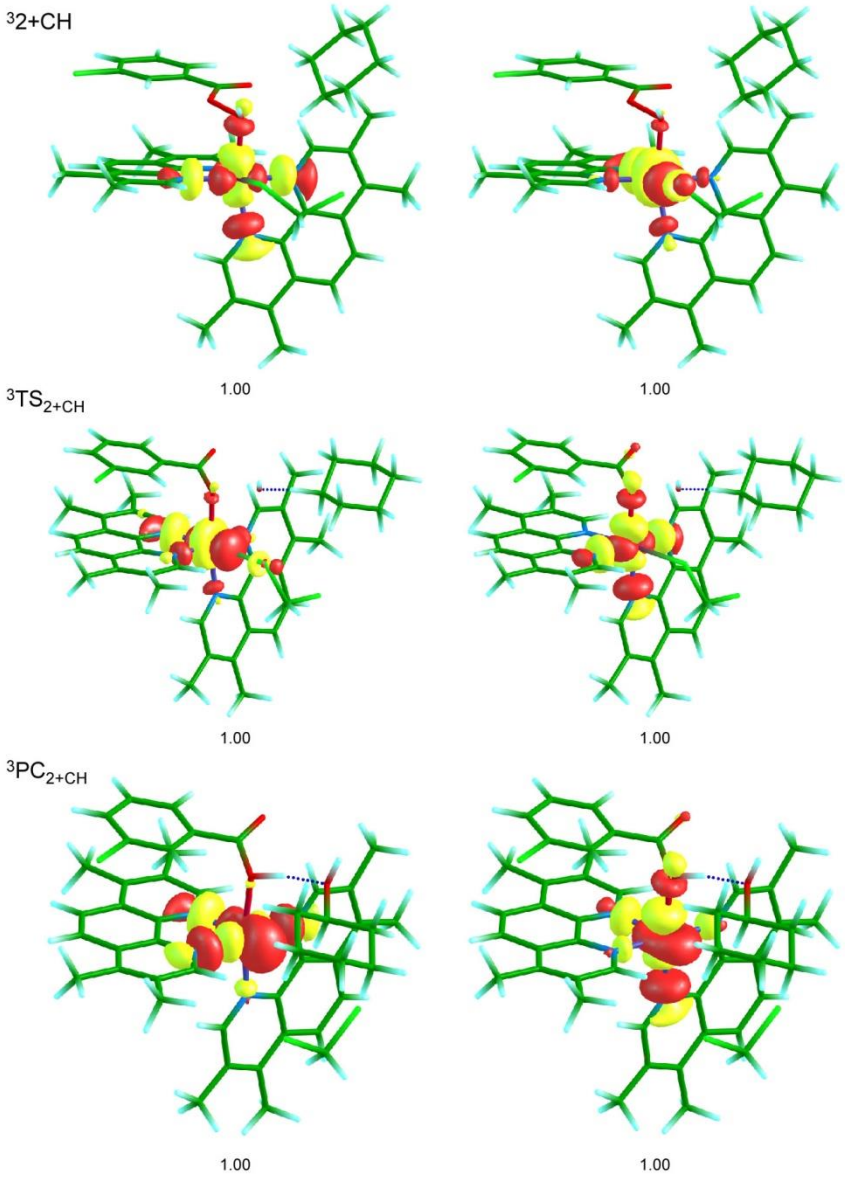

Fig. S14 Singly-occupied natural orbitals (SNOs) of reaction intermediates of hydroxylation of cyclohexane by a Ni^{II}-*m*CPBA complex on the singlet and triplet spin states.Calculations were performed at the UB3LYP-D3(BJ)/B1 level in solvent. Positive values represent alpha-electron occupations.

Part VI. C-H bond activation by the Ni^{III}-$O^{\bullet}$ species

Table S16. Various SCF and Gibbs free energies of the reaction intermediates in hydroxylation of CHA by a Ni^{III}-$O^{\bullet}$ specieson the triplet spin states. Calculations were performed at the UB3LYP-D3(BJ)/B2//B1 level in solvent.

	OPT/B1	*ΔE*	OPT/B1+ZPE	*ΔE*	SPE/B2	*ΔE*	SPE/B2+ZPE	*ΔE*	*G*	*ΔG*
^{3}**4+CH**	-2897.850075[a]	**0.0**	-2897.073966	**0.0**	-2898.352245	**0.0**	-2897.576136	**0.0**	-2897.174894	**0.0**
^{3}**TS**$_{4+CH}$	-2897.853310	**-2.0**	-2897.083565	**-6.0**	-2898.355513	**-2.1**	-2897.585768	**-6.0**	-2897.180406	**-3.5**
^{3}**PC**$_{4+CH}$	-2897.993519	**-90.0**	-2897.214681	**-88.3**	-2898.491934	**-87.7**	-2897.713097	**-85.9**	-2897.313210	**-86.8**

a. Absolute energies are in au units and the relative ones are in kcal mol^{-1} units

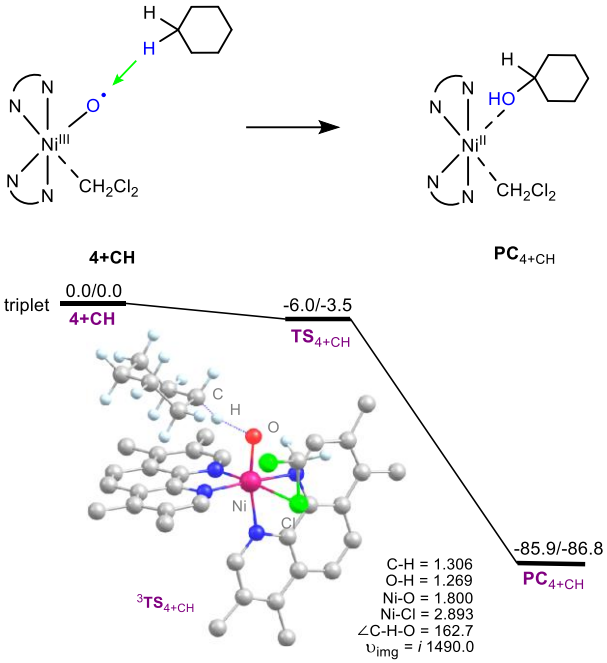

Fig. S15 Energy profiles (in kcal mol^{-1}) for hydroxylation of CHA by a Ni^{III}-$O^{\bullet}$ species on the triplet spin states . Calculations were performed at the UB3LYP-D3(BJ)/B2//B1 level in solvent. The geometric information of the transition states is presented. Hydrogen atoms of the supporting ligand are omitted for clarity. Lengths are in Å units, angles is in ° unit, and the imaginary frequency is in cm^{-1} units.

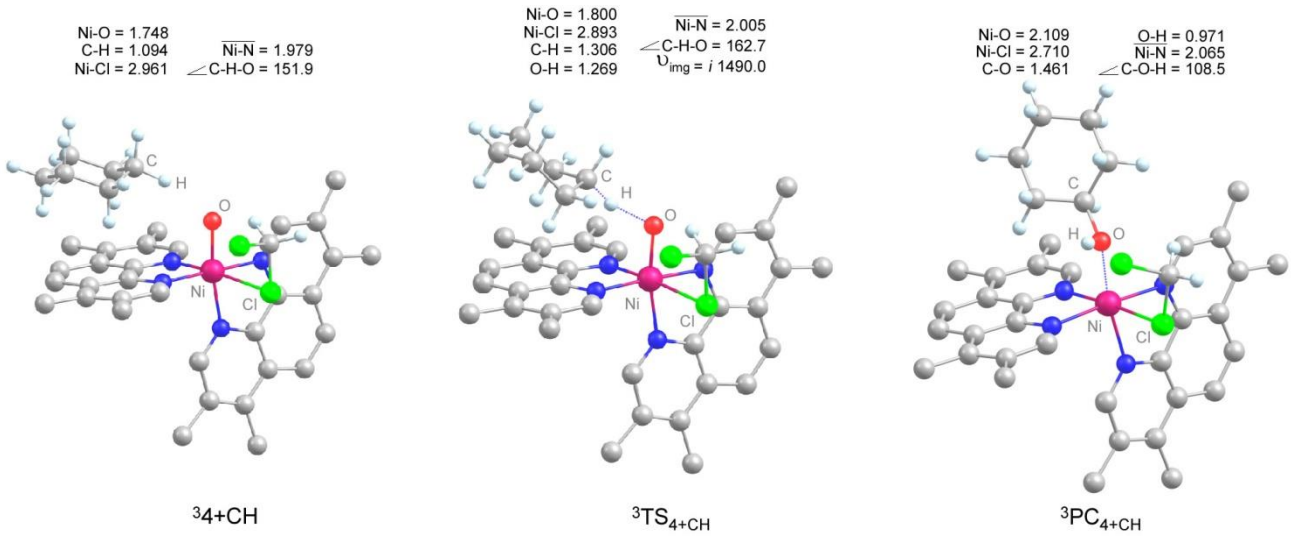

Fig. S16 The geometric information of the reaction intermediates of hydroxylation of CHA by a Ni^{III}-$O^{\bullet}$ species on the triplet spin states. Calculations were performedat the UB3LYP-D3(BJ)/B1 level in solvent. Lengths are in Å units, bond angles are in ° units and imaginary frequency is in cm^{-1} units. Hydrogen atoms of the supporting ligand are omitted for clarity.

Table S17. Mulliken spin densities and charges of the reaction intermediates for hydroxylation of CHA by a Ni^{III}-$O^{\bullet}$ species on the triplet spin states. Calculations were performedat the UB3LYP-D3(BJ)/B1 level in solvent.

	charge						Spin density					
	Ni	Ligand	O	CH_2Cl_2	H	Sub-H	Ni	Ligand	O	CH_2Cl_2	H	Sub-H
^{3}**4+CH**	0.67	1.57	-0.34	0.12	0.10	-0.11	0.72	0.24	1.02	0.02	0.00	0.00
^{3}**TS**$_{4+CH}$	0.66	1.50	-0.44	0.11	0.18	-0.01	0.76	0.21	0.79	0.02	-0.03	0.24
^{3}**PC**$_{4+CH}$	0.56	1.06	-0.55	0.17	0.36	0.41	1.61	0.32	0.04	0.03	0.00	0.00

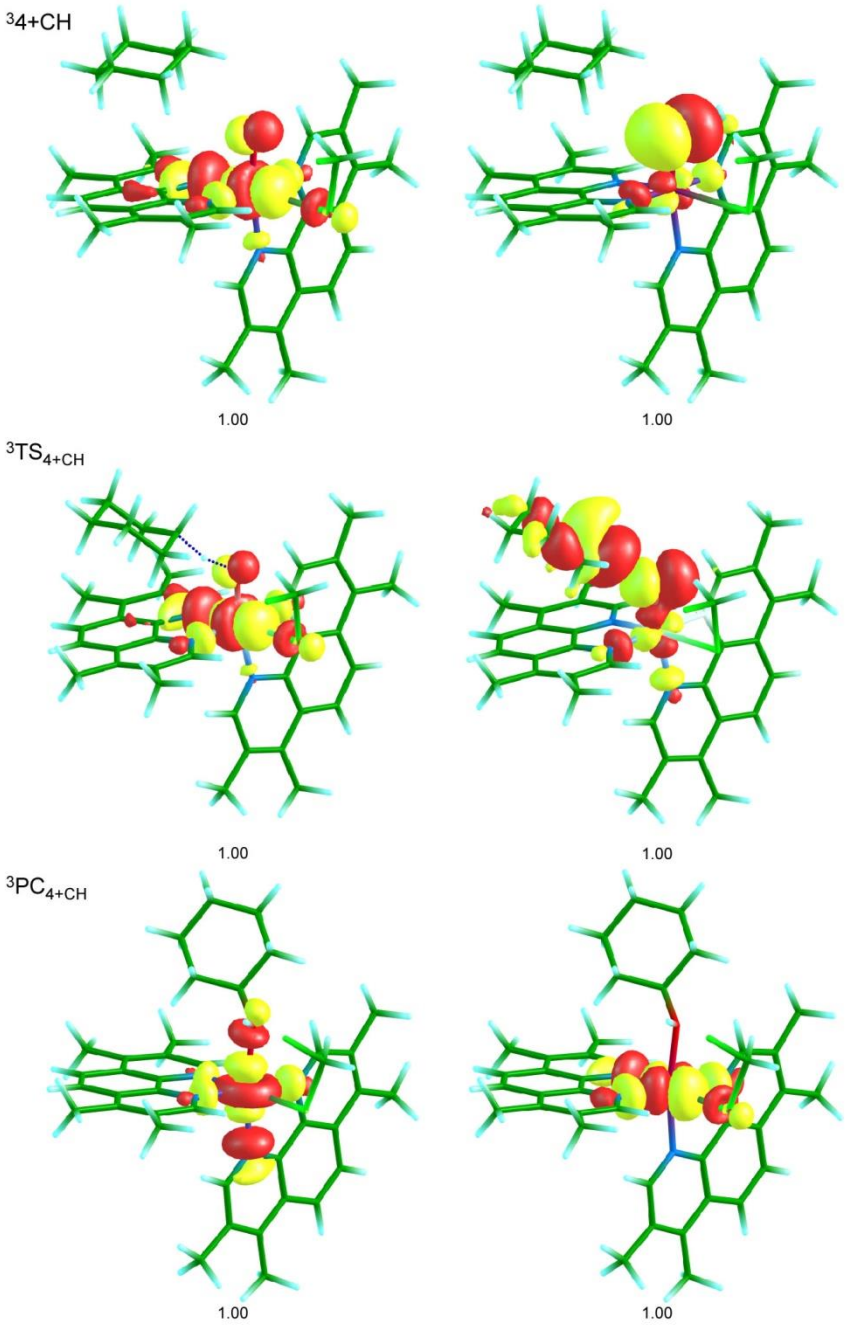

Fig. S17 Singly-occupied natural orbitals (SNOs) of the reaction intermediates for hydroxylation of CHA by a Ni^{III}-$O^{\bullet}$ species on the triplet spin states. Calculations were at the UB3LYP-D3(BJ)/B1 level in solvent. Positive values represent alpha-electron occupations.

PART VII. Cartesian coordinates

^{1}**1**

Ni	-0.111674000	9.972307000	8.010846000
N	0.172478000	9.019660000	9.641503000
N	-0.127923000	7.634416000	7.290886000
N	-0.269089000	10.979920000	6.360505000
N	1.809445000	10.058841000	7.642784000
C	0.349119000	9.713259000	10.762779000
H	0.351656000	10.797889000	10.653271000
C	0.555268000	9.109441000	12.015856000
C	0.757633000	10.006903000	13.210396000
H	0.743459000	11.054946000	12.904267000
H	1.716758000	9.811489000	13.700283000
H	-0.028843000	9.862520000	13.958252000
C	0.563905000	7.716803000	12.090019000
C	0.768318000	6.996432000	13.395144000
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H	0.889235000	7.688480000	14.226633000
H	1.657874000	6.359041000	13.353113000
C	0.378463000	6.970391000	10.890238000
C	0.382714000	5.535764000	10.864528000
H	0.521511000	4.995468000	11.792607000
C	0.217841000	4.840137000	9.703927000
H	0.227388000	3.757281000	9.729078000
C	0.036820000	5.509911000	8.449016000
C	-0.128457000	4.814072000	7.216361000
C	-0.127532000	3.308193000	7.201111000
H	-0.925093000	2.910777000	7.837676000
H	0.819166000	2.913642000	7.585341000
H	-0.272025000	2.911458000	6.197506000
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H	-0.391625000	7.576182000	5.261682000
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C	0.188432000	7.659849000	9.668266000
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H	2.569014000	12.600049000	3.127028000
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H	4.500693000	11.744027000	4.321756000
C	3.375685000	10.884923000	5.978225000
C	4.463580000	10.358870000	6.730462000
C	5.870310000	10.531907000	6.229480000
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H	6.116622000	11.594504000	6.131670000
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H	5.826083000	8.338022000	8.271242000
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H	2.597227000	9.059255000	9.257393000
C	2.072954000	10.707498000	6.479848000
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Cl	0.842142000	13.041908000	9.830881000

^{3}**1**

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C	0.888972000	6.644885000	13.505134000
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H	1.017884000	7.209634000	14.426876000
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C	0.487987000	5.563611000	10.772786000
H	0.674427000	4.883204000	11.594797000
C	0.307192000	5.060375000	9.517240000
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C	0.057336000	5.917158000	8.392873000
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C	-0.578685000	5.977894000	4.611162000
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^{5}**1**

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C	1.492653000	7.047525000	13.401141000
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H	1.307639000	7.458242000	14.392139000
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C	0.298177000	8.240530000	9.965026000
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C	-2.656784000	12.776574000	3.793959000
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C	-0.278790000	11.777051000	2.240314000
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H	-0.298060000	10.790521000	1.763393000
C	0.687667000	11.010642000	4.456047000
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H	1.933876000	10.464322000	2.769688000
C	2.778732000	9.737392000	4.596491000
H	3.595628000	9.255300000	4.073016000
C	2.718398000	9.658409000	6.002872000
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C	4.714625000	8.095496000	6.138779000
H	4.275132000	7.399055000	5.415274000
H	5.287770000	7.510456000	6.857283000
H	5.420148000	8.727811000	5.585162000
C	3.516479000	8.991883000	8.197945000
C	4.439596000	8.269804000	9.145079000
H	4.187837000	8.503386000	10.181933000
H	5.487177000	8.540218000	8.979574000
H	4.354663000	7.184942000	9.021774000
C	2.472306000	9.756837000	8.740939000
H	2.395541000	9.898283000	9.812060000
C	1.637414000	10.323625000	6.661927000
C	0.574888000	10.912821000	5.870458000
Cl	-3.029436000	10.544880000	8.608381000
Cl	-0.315366000	12.738393000	9.628198000

[1]**2**

Ni	0.678777000	9.208060000	7.239486000
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N	0.515287000	10.219718000	5.605657000
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H	1.554785000	10.063886000	10.076790000
C	0.536910000	8.781758000	11.480478000
C	1.081182000	9.544713000	12.660867000
H	1.692492000	10.385893000	12.329254000
H	1.701902000	8.905338000	13.296075000
H	0.272065000	9.941713000	13.281188000
C	-0.300147000	7.668992000	11.615646000
C	-0.705438000	7.132467000	12.957297000
H	-1.794555000	7.161983000	13.065047000
H	-0.265660000	7.698174000	13.776098000
H	-0.397281000	6.086842000	13.061005000
C	-0.792767000	7.052525000	10.429556000
C	-1.682143000	5.924057000	10.402070000
H	-1.990695000	5.476412000	11.338127000
C	-2.157168000	5.413439000	9.227070000
H	-2.827171000	4.563621000	9.250962000
C	-1.814870000	5.995670000	7.959416000
C	-2.309000000	5.546206000	6.701715000
C	-3.255990000	4.383567000	6.647582000
H	-4.153425000	4.600982000	7.235386000
H	-2.793648000	3.489287000	7.077987000
H	-3.564464000	4.150566000	5.630578000
C	-1.887911000	6.218927000	5.550532000
C	-2.335427000	5.823376000	4.167168000
H	-3.422390000	5.903221000	4.066667000
H	-2.057094000	4.790325000	3.938889000
H	-1.881641000	6.469083000	3.412878000
C	-1.026619000	7.326577000	5.680613000
H	-0.696942000	7.853850000	4.795360000
C	-0.949369000	7.102798000	7.974210000
C	-0.405269000	7.592514000	9.191092000
C	-0.562979000	10.400099000	4.845975000
H	-1.461535000	9.871724000	5.138625000
C	-0.582966000	11.266016000	3.734170000
C	-1.865305000	11.376903000	2.949522000
H	-2.207186000	12.414386000	2.891728000
H	-2.655517000	10.787666000	3.418754000
H	-1.737451000	11.013951000	1.924678000
C	0.573430000	11.980064000	3.403035000
C	0.635328000	12.891915000	2.211531000
H	0.785767000	13.929421000	2.529649000
H	-0.273734000	12.850104000	1.614844000
H	1.478750000	12.625631000	1.566777000
C	1.708603000	11.849754000	4.254210000
C	2.947497000	12.559522000	4.088704000

H	3.059054000	13.231146000	3.246486000
C	3.985039000	12.408193000	4.966034000
H	4.904562000	12.955309000	4.799211000
C	3.884235000	11.549284000	6.114301000
C	4.918567000	11.347334000	7.072999000
C	6.225306000	12.070892000	6.923720000
H	6.693254000	11.826947000	5.964347000
H	6.927442000	11.820412000	7.716278000
H	6.065935000	13.154227000	6.939855000
C	4.674701000	10.463161000	8.128452000
C	5.697337000	10.162436000	9.193039000
H	5.307154000	9.440347000	9.912955000
H	5.970059000	11.069130000	9.742284000
H	6.613432000	9.748045000	8.762162000
C	3.410329000	9.850997000	8.230923000
H	3.211965000	9.168792000	9.047005000
C	2.669263000	10.866980000	6.296757000
C	1.615319000	10.976922000	5.351046000
C	-3.289821000	9.336464000	7.628850000
C	-4.112364000	8.401903000	8.438983000
C	-4.011009000	8.338361000	9.834860000
C	-4.776796000	7.398235000	10.514936000
C	-5.639406000	6.532472000	9.844134000
C	-5.736655000	6.615788000	8.453161000
C	-4.975416000	7.542808000	7.747401000
O	-3.292532000	9.412866000	6.419379000
O	-2.492618000	10.084732000	8.440724000
Cl	-4.625061000	7.281309000	12.259934000
H	-3.342501000	8.992916000	10.377755000
H	-6.221344000	5.805810000	10.398698000
H	-6.410513000	5.950410000	7.924506000
H	-5.030346000	7.608410000	6.667522000
O	-1.652531000	10.945265000	7.642566000
H	-1.276250000	11.483076000	8.368181000
Cl	2.761950000	12.598017000	10.301507000
C	1.355820000	13.159442000	9.350866000
H	1.419642000	12.730445000	8.355455000
H	1.361864000	14.244992000	9.334012000
Cl	-0.205279000	12.632812000	10.082359000

^{3}**2**

Ni	-0.026053000	10.455341000	7.874398000
N	-0.108903000	9.588109000	9.746460000
N	-0.598937000	8.561125000	7.317539000
N	0.056913000	11.264670000	5.997924000
N	1.974923000	10.139850000	7.497052000
C	0.083836000	10.129949000	10.944016000
H	0.342738000	11.183022000	10.958777000
C	-0.035043000	9.419715000	12.154699000
C	0.195340000	10.157931000	13.448011000
H	0.442806000	11.204224000	13.257188000
H	1.018731000	9.716079000	14.017420000
H	-0.694578000	10.134284000	14.084534000
C	-0.361588000	8.062144000	12.102902000
C	-0.521976000	7.233533000	13.345776000
H	-1.528262000	6.803898000	13.388773000
H	-0.363021000	7.815952000	14.251129000
H	0.187521000	6.399558000	13.349813000
C	-0.557112000	7.461295000	10.825819000
C	-0.887858000	6.075990000	10.643303000
H	-0.977494000	5.437913000	11.512690000
C	-1.108008000	5.549985000	9.403922000
H	-1.366924000	4.502972000	9.310546000
C	-1.022637000	6.356712000	8.220611000
C	-1.299255000	5.871778000	6.910254000
C	-1.692122000	4.434647000	6.717400000
H	-2.603145000	4.209886000	7.280866000
H	-0.907532000	3.765773000	7.085537000
H	-1.875665000	4.196909000	5.671564000
C	-1.211259000	6.763467000	5.836926000
C	-1.508102000	6.364736000	4.414722000
H	-2.536073000	6.003031000	4.312033000
H	-0.841924000	5.566211000	4.074216000
H	-1.384219000	7.215613000	3.741690000
C	-0.849711000	8.098287000	6.099604000
H	-0.781459000	8.815498000	5.289566000
C	-0.677343000	7.715292000	8.374312000
C	-0.433290000	8.269171000	9.676306000
C	-0.924865000	11.789973000	5.271966000
H	-1.906905000	11.793801000	5.731811000
C	-0.740758000	12.298312000	3.971275000
C	-1.932969000	12.872370000	3.249911000
H	-1.779197000	13.927030000	3.000987000
H	-2.829100000	12.801474000	3.869804000
H	-2.128428000	12.339115000	2.314497000
C	0.536471000	12.245327000	3.406052000
C	0.815211000	12.768673000	2.024801000
H	1.589624000	13.542106000	2.053674000
H	-0.071760000	13.196815000	1.561964000
H	1.182820000	11.967206000	1.375323000
C	1.593134000	11.667602000	4.168754000
C	2.941570000	11.534595000	3.692542000
H	3.187976000	11.897699000	2.702632000

C	3.916366000	10.957255000	4.454072000
H	4.920007000	10.873159000	4.056475000
C	3.643466000	10.454520000	5.771236000
C	4.621660000	9.834674000	6.602307000
C	6.031874000	9.682865000	6.104521000
H	6.052682000	9.112528000	5.170220000
H	6.668482000	9.173010000	6.824906000
H	6.474427000	10.662590000	5.895412000
C	4.232622000	9.382919000	7.867032000
C	5.183127000	8.713549000	8.826034000
H	4.672134000	8.449010000	9.754150000
H	6.021908000	9.369094000	9.079401000
H	5.599854000	7.796078000	8.398878000
C	2.892577000	9.562786000	8.262138000
H	2.560418000	9.225469000	9.238556000
C	2.328681000	10.582331000	6.264077000
C	1.302826000	11.190139000	5.462910000
C	-3.461788000	9.451977000	7.643100000
C	-3.982430000	8.176960000	8.188304000
C	-3.914883000	7.870694000	9.555556000
C	-4.337261000	6.616358000	9.977057000
C	-4.819468000	5.666937000	9.074092000
C	-4.889430000	5.991111000	7.718002000
C	-4.473092000	7.241615000	7.269207000
O	-3.479435000	9.813026000	6.493150000
O	-2.859268000	10.170866000	8.662605000
Cl	-4.239879000	6.216210000	11.681358000
H	-3.530363000	8.583570000	10.272411000
H	-5.133852000	4.691965000	9.427702000
H	-5.265039000	5.258624000	7.012212000
H	-4.505369000	7.499848000	6.217809000
O	-2.078202000	11.238216000	8.092790000
H	-2.197155000	11.937498000	8.772313000
Cl	1.056767000	12.840595000	8.772500000
C	-0.161832000	14.166672000	8.782382000
H	-0.545146000	14.275596000	7.772130000
H	0.336387000	15.062780000	9.139495000
Cl	-1.532112000	13.811448000	9.882080000

^{1}**TS**$_{23}$

Ni	0.544821000	9.415129000	7.340656000
N	0.434609000	8.722368000	9.124475000
N	-0.661519000	7.872283000	6.909569000
N	0.502017000	10.289908000	5.646969000
N	2.390429000	10.094024000	7.417731000
C	0.889134000	9.302806000	10.239286000
H	1.454586000	10.217830000	10.121255000
C	0.650417000	8.786438000	11.523245000
C	1.217963000	9.530200000	12.703392000
H	1.748368000	10.426031000	12.376796000
H	1.919439000	8.904947000	13.263697000
H	0.424921000	9.840412000	13.390003000
C	-0.104370000	7.612399000	11.652601000
C	-0.388041000	6.993436000	12.986888000
H	-1.468085000	6.958804000	13.163324000
H	0.075609000	7.542529000	13.803256000
H	-0.021359000	5.961988000	13.014247000
C	-0.640412000	7.019018000	10.470094000
C	-1.472215000	5.854846000	10.449685000
H	-1.678041000	5.336687000	11.376795000
C	-2.035007000	5.394675000	9.286789000
H	-2.653241000	4.507743000	9.321504000
C	-1.821882000	6.052390000	8.032416000
C	-2.409707000	5.662823000	6.791417000
C	-3.345973000	4.497672000	6.699404000
H	-3.826626000	4.272253000	7.649548000
H	-2.794224000	3.605659000	6.376903000
H	-4.126415000	4.679732000	5.958724000
C	-2.062922000	6.383383000	5.639941000
C	-2.608071000	6.030265000	4.283701000
H	-3.695173000	6.161916000	4.256655000
H	-2.397240000	4.987301000	4.030037000
H	-2.173908000	6.665743000	3.510032000
C	-1.199891000	7.484423000	5.754371000
H	-0.941160000	8.055022000	4.873291000
C	-0.958818000	7.165367000	8.029891000
C	-0.362317000	7.626710000	9.231602000
C	-0.583720000	10.514579000	4.912077000
H	-1.524581000	10.116398000	5.285903000
C	-0.540479000	11.289759000	3.736559000
C	-1.822721000	11.462059000	2.963928000
H	-2.053615000	12.520142000	2.811523000
H	-2.656668000	11.006237000	3.500777000
H	-1.757412000	10.991622000	1.977420000
C	0.670087000	11.873830000	3.340816000
C	0.782530000	12.687100000	2.085241000
H	0.889232000	13.750623000	2.328632000
H	-0.091779000	12.574275000	1.447028000
H	1.666076000	12.394784000	1.511003000
C	1.802219000	11.723149000	4.194867000
C	3.083767000	12.339901000	3.993668000
H	3.243948000	12.942364000	3.108250000
C	4.102236000	12.191850000	4.895768000

H	5.055386000	12.667142000	4.700916000
C	3.940742000	11.425865000	6.100262000
C	4.947673000	11.238695000	7.091105000
C	6.286953000	11.892660000	6.927330000
H	6.801811000	11.489557000	6.048061000
H	6.927488000	11.741376000	7.793481000
H	6.171417000	12.969292000	6.769368000
C	4.648746000	10.423933000	8.191047000
C	5.651600000	10.118129000	9.273105000
H	5.228525000	9.438303000	10.014965000
H	5.959041000	11.031406000	9.792046000
H	6.550559000	9.651632000	8.860416000
C	3.357094000	9.880259000	8.310770000
H	3.121181000	9.253395000	9.158724000
C	2.691080000	10.818022000	6.305471000
C	1.656475000	10.935010000	5.347683000
C	-3.440568000	9.730660000	7.517813000
C	-4.143956000	8.625941000	8.279032000
C	-3.949713000	8.494027000	9.661044000
C	-4.521976000	7.410988000	10.314294000
C	-5.306141000	6.475443000	9.633087000
C	-5.520464000	6.639362000	8.260581000
C	-4.943800000	7.707547000	7.580892000
O	-3.220166000	9.592360000	6.307317000
O	-3.146868000	10.730448000	8.275073000
Cl	-4.244554000	7.205578000	12.035881000
H	-3.347212000	9.216191000	10.195954000
H	-5.745431000	5.641482000	10.167823000
H	-6.136480000	5.922450000	7.728827000
H	-5.085924000	7.840530000	6.515024000
O	-0.766559000	10.722517000	7.820313000
H	-1.137006000	10.477504000	8.685236000
Cl	2.146149000	12.899616000	9.430602000
C	0.371243000	13.184462000	9.384343000
H	-0.020275000	12.689058000	8.499804000
H	0.201748000	14.256616000	9.402169000
Cl	-0.466237000	12.459894000	10.799358000

^{3}**TS**$_{23}$

Ni	0.118333000	10.467479000	7.966769000
N	0.164494000	9.704860000	9.800561000
N	-0.412336000	8.541272000	7.458380000
N	0.093454000	11.221668000	6.147585000
N	2.051461000	10.155746000	7.568869000
C	0.470868000	10.313294000	10.943238000
H	0.805162000	11.340969000	10.872132000
C	0.372747000	9.686603000	12.198551000
C	0.741529000	10.480098000	13.425077000
H	1.060769000	11.487939000	13.153122000
H	1.558969000	10.004024000	13.974774000
H	-0.108832000	10.569565000	14.107797000
C	-0.072836000	8.361755000	12.254521000
C	-0.222589000	7.631010000	13.557816000
H	-1.256150000	7.295543000	13.692367000
H	0.045342000	8.252007000	14.410013000
H	0.412373000	6.739103000	13.573653000
C	-0.389844000	7.698615000	11.033717000
C	-0.845105000	6.338553000	10.956914000
H	-0.961897000	5.772168000	11.871958000
C	-1.136170000	5.745125000	9.762337000
H	-1.484957000	4.720584000	9.752015000
C	-1.004217000	6.451708000	8.520117000
C	-1.329204000	5.898760000	7.247336000
C	-1.837378000	4.488058000	7.159603000
H	-2.743497000	4.369553000	7.760514000
H	-1.092812000	3.785429000	7.548060000
H	-2.073566000	4.200627000	6.137225000
C	-1.180397000	6.702701000	6.113705000
C	-1.537730000	6.235649000	4.727301000
H	-2.601976000	5.987249000	4.664481000
H	-0.970499000	5.344629000	4.442805000
H	-1.332225000	7.016025000	3.991925000
C	-0.708106000	8.020741000	6.276994000
H	-0.592964000	8.670940000	5.417701000
C	-0.556571000	7.786160000	8.572581000
C	-0.254337000	8.410846000	9.824604000
C	-0.937039000	11.730135000	5.482096000
H	-1.888894000	11.721065000	5.997335000
C	-0.818282000	12.219324000	4.165056000
C	-2.053389000	12.770420000	3.500372000
H	-1.929075000	13.827328000	3.244947000
H	-2.917604000	12.682874000	4.161296000
H	-2.280692000	12.231463000	2.575692000
C	0.428235000	12.173178000	3.532087000
C	0.628427000	12.682190000	2.133468000
H	1.404811000	13.453724000	2.112781000
H	-0.282259000	13.107153000	1.716497000
H	0.959069000	11.872438000	1.474272000
C	1.532065000	11.616767000	4.243070000
C	2.861751000	11.485004000	3.714401000
H	3.063339000	11.831967000	2.708626000
C	3.873994000	10.929172000	4.445149000
H	4.861204000	10.848271000	4.007682000

C	3.662803000	10.446318000	5.781734000
C	4.670188000	9.851588000	6.595783000
C	6.064066000	9.698833000	6.058316000
H	6.058489000	9.102505000	5.140150000
H	6.729354000	9.216508000	6.771378000
H	6.486982000	10.677124000	5.806531000
C	4.321352000	9.424746000	7.882405000
C	5.306740000	8.783912000	8.825476000
H	4.827656000	8.532851000	9.773850000
H	6.145088000	9.453783000	9.038926000
H	5.718829000	7.862717000	8.402358000
C	2.993620000	9.598449000	8.320175000
H	2.697591000	9.275008000	9.311059000
C	2.367367000	10.573471000	6.315136000
C	1.313138000	11.153327000	5.552054000
C	-3.445476000	9.327707000	7.399590000
C	-4.156415000	8.016725000	7.588933000
C	-4.148601000	7.353124000	8.822170000
C	-4.758137000	6.105885000	8.912135000
C	-5.375718000	5.513506000	7.810037000
C	-5.376947000	6.190675000	6.588231000
C	-4.771838000	7.439387000	6.472075000
O	-3.206043000	9.796231000	6.298460000
O	-3.116358000	9.856991000	8.569352000
Cl	-4.723242000	5.248840000	10.445043000
H	-3.661598000	7.790383000	9.683338000
H	-5.840119000	4.538905000	7.904995000
H	-5.850733000	5.734214000	5.725918000
H	-4.755053000	7.970275000	5.527977000
O	-1.694389000	11.028447000	8.246000000
H	-1.798214000	11.336362000	9.166508000
Cl	1.011555000	12.994587000	8.695225000
C	-0.496908000	13.962065000	8.931704000
H	-1.134360000	13.788046000	8.069913000
H	-0.197445000	15.000748000	9.032300000
Cl	-1.375783000	13.467418000	10.405695000

^{1}**3**

Ni	-0.516569000	10.159627000	7.525941000
N	-0.527482000	9.321787000	9.259335000
N	-0.660745000	8.299058000	6.857020000
N	-0.432843000	10.936686000	5.762428000
N	1.423428000	10.035001000	7.373407000
C	-0.472838000	9.935954000	10.431979000
H	-0.387113000	11.014458000	10.401149000
C	-0.523721000	9.220185000	11.644469000
C	-0.411457000	9.998705000	12.928380000
H	-0.287049000	11.062854000	12.723946000
H	0.451124000	9.664659000	13.512806000
H	-1.306219000	9.870249000	13.543141000
C	-0.681122000	7.828064000	11.608190000
C	-0.794101000	7.011219000	12.860800000
H	-1.773843000	6.523261000	12.903754000
H	-0.678690000	7.616493000	13.756949000
H	-0.035608000	6.222466000	12.877794000
C	-0.751867000	7.180845000	10.340294000
C	-0.919420000	5.768917000	10.134003000
H	-1.002182000	5.120058000	10.996709000
C	-0.982365000	5.225871000	8.881483000
H	-1.112692000	4.156274000	8.784359000
C	-0.889483000	6.031717000	7.692809000
C	-0.973544000	5.559006000	6.352327000
C	-1.155747000	4.107260000	6.024843000
H	-1.261767000	3.478829000	6.906132000
H	-0.300648000	3.741493000	5.446066000
H	-2.043407000	3.970195000	5.399000000
C	-0.885916000	6.492007000	5.307078000
C	-0.960787000	6.071477000	3.865526000
H	-1.922376000	5.595949000	3.645946000
H	-0.177757000	5.344356000	3.628081000
H	-0.845089000	6.927770000	3.198940000
C	-0.736068000	7.856121000	5.607082000
H	-0.687784000	8.592800000	4.816147000
C	-0.724536000	7.416654000	7.884615000
C	-0.659325000	7.975659000	9.187222000
C	-1.439550000	11.358102000	5.008786000
H	-2.434358000	11.195624000	5.401380000
C	-1.219041000	11.959579000	3.751891000
C	-2.424113000	12.389574000	2.956151000
H	-2.409430000	13.467786000	2.770717000
H	-3.345482000	12.151892000	3.490352000
H	-2.455749000	11.885565000	1.985589000
C	0.093009000	12.134047000	3.293309000
C	0.394286000	12.774444000	1.969864000
H	1.029046000	13.655802000	2.107574000
H	-0.507719000	13.083971000	1.446630000
H	0.941009000	12.078343000	1.325067000
C	1.166819000	11.683396000	4.115321000
C	2.563179000	11.782124000	3.788903000
H	2.850752000	12.235643000	2.848612000
C	3.533966000	11.316936000	4.632206000
H	4.573948000	11.410121000	4.345473000
C	3.213597000	10.700489000	5.890838000

C	4.164250000	10.185279000	6.818803000
C	5.629612000	10.284926000	6.511628000
H	5.861752000	9.761080000	5.578551000
H	6.245718000	9.860725000	7.301336000
H	5.920634000	11.331830000	6.377341000
C	3.692819000	9.599226000	7.999207000
C	4.607678000	9.027262000	9.050299000
H	4.033537000	8.608950000	9.878675000
H	5.267509000	9.799756000	9.456257000
H	5.235530000	8.232076000	8.638134000
C	2.304371000	9.547800000	8.236269000
H	1.922755000	9.109177000	9.146588000
C	1.851115000	10.603639000	6.218222000
C	0.847918000	11.089337000	5.346653000
C	-3.209981000	9.439791000	7.356821000
C	-3.687952000	8.682626000	8.548954000
C	-3.651017000	9.260863000	9.823758000
C	-4.045866000	8.496059000	10.915792000
C	-4.454660000	7.169780000	10.769795000
C	-4.492359000	6.608180000	9.491694000
C	-4.129021000	7.363366000	8.380518000
O	-3.565713000	9.168281000	6.219954000
O	-2.367068000	10.457003000	7.617913000
Cl	-4.010466000	9.209177000	12.520885000
H	-3.318540000	10.282856000	9.948005000
H	-4.738499000	6.589556000	11.640052000
H	-4.805482000	5.576955000	9.371038000
H	-4.152847000	6.938616000	7.383846000
O	-0.280042000	11.818089000	8.249203000
H	-1.184675000	12.175434000	8.269396000
Cl	2.687855000	11.518948000	10.974184000
C	1.882325000	12.931243000	10.207660000
H	1.451332000	12.604004000	9.264305000
H	2.621129000	13.719123000	10.096571000
Cl	0.534066000	13.562283000	11.210342000

^{3}**3**

Ni	-0.094096000	10.730685000	7.685042000
N	-0.276135000	9.845959000	9.405120000
N	-0.670507000	8.864993000	6.960517000
N	0.156053000	11.554753000	5.943459000
N	1.796761000	10.180730000	7.457849000
C	-0.146529000	10.396872000	10.607707000
H	0.028477000	11.464297000	10.638497000
C	-0.220489000	9.651271000	11.798490000
C	-0.065951000	10.381901000	13.106929000
H	0.046314000	11.454805000	12.940322000
H	0.814422000	10.031219000	13.654402000
H	-0.938028000	10.229157000	13.749317000
C	-0.426048000	8.268829000	11.718864000
C	-0.495488000	7.408191000	12.946724000
H	-1.499406000	6.984754000	13.061254000
H	-0.258907000	7.965822000	13.850478000
H	0.202985000	6.569590000	12.869852000
C	-0.588319000	7.679125000	10.431672000
C	-0.840811000	6.282194000	10.209377000
H	-0.897470000	5.618531000	11.062634000
C	-1.032068000	5.776327000	8.955487000
H	-1.235515000	4.720016000	8.836639000
C	-0.995564000	6.616474000	7.792402000
C	-1.241820000	6.163837000	6.463324000
C	-1.546587000	4.713470000	6.220853000
H	-2.444636000	4.415458000	6.771989000
H	-0.725457000	4.081880000	6.574783000
H	-1.709665000	4.498081000	5.166978000
C	-1.207343000	7.098457000	5.423675000
C	-1.476336000	6.732493000	3.987351000
H	-2.474649000	6.300418000	3.868919000
H	-0.752869000	5.997065000	3.622204000
H	-1.413998000	7.613270000	3.345311000
C	-0.906695000	8.443499000	5.729141000
H	-0.860956000	9.188045000	4.941638000
C	-0.723327000	7.984467000	7.985897000
C	-0.519007000	8.512661000	9.298666000
C	-0.731226000	12.247021000	5.244746000
H	-1.689714000	12.399542000	5.729426000
C	-0.448365000	12.750944000	3.958583000
C	-1.525191000	13.526230000	3.244302000
H	-1.197170000	14.545816000	3.020045000
H	-2.425935000	13.589830000	3.857500000
H	-1.794806000	13.049878000	2.296781000
C	0.812375000	12.512380000	3.396581000
C	1.182416000	13.016205000	2.031267000
H	2.071823000	13.652292000	2.084880000
H	0.381007000	13.592726000	1.574095000
H	1.422043000	12.179562000	1.366398000
C	1.764755000	11.766979000	4.151755000
C	3.094382000	11.440577000	3.714310000
H	3.422462000	11.772768000	2.737156000
C	3.953134000	10.723930000	4.500622000
H	4.946741000	10.502240000	4.131635000
C	3.575201000	10.257442000	5.807211000
C	4.418778000	9.514087000	6.682121000

C	5.813689000	9.165022000	6.250631000
H	5.792725000	8.560720000	5.337726000
H	6.353170000	8.607356000	7.013296000
H	6.383347000	10.072530000	6.025233000
C	3.910784000	9.132822000	7.929553000
C	4.716737000	8.349660000	8.933721000
H	4.132033000	8.158266000	9.835535000
H	5.619976000	8.892767000	9.227666000
H	5.029533000	7.384223000	8.524566000
C	2.591439000	9.491311000	8.269159000
H	2.182485000	9.205712000	9.230208000
C	2.275258000	10.564656000	6.244205000
C	1.385382000	11.310660000	5.424809000
C	-3.851965000	8.856390000	8.555241000
C	-4.108943000	7.496801000	9.024304000
C	-3.996022000	7.225818000	10.392746000
C	-4.196294000	5.920507000	10.825226000
C	-4.508846000	4.899093000	9.926435000
C	-4.624676000	5.190948000	8.564632000
C	-4.423201000	6.488663000	8.104595000
O	-3.944556000	9.230890000	7.342418000
O	-3.485173000	9.823955000	9.287012000
Cl	-4.025965000	5.546124000	12.528718000
H	-3.751712000	8.016992000	11.091374000
H	-4.657426000	3.888088000	10.287387000
H	-4.874138000	4.397911000	7.868630000
H	-4.497529000	6.722994000	7.048443000
O	-1.681165000	11.564185000	7.827750000
Cl	1.128533000	13.131718000	8.691911000
C	-0.391188000	14.066061000	8.993663000
H	-1.180755000	13.506660000	8.494070000
H	-0.236392000	15.070226000	8.611443000
Cl	-0.776328000	14.161015000	10.735590000
H	-2.266899000	11.066544000	8.425380000

^{3}**TS**$_{34}$

Ni	-0.057932000	10.658884000	7.807631000
N	-0.188639000	9.790282000	9.562213000
N	-0.637720000	8.740684000	7.162930000
N	0.117025000	11.477319000	6.048584000
N	1.853272000	10.104811000	7.476173000
C	-0.048229000	10.378899000	10.750187000
H	0.182109000	11.436265000	10.736572000
C	-0.185091000	9.696158000	11.970519000
C	-0.012700000	10.472350000	13.248759000
H	0.189529000	11.523747000	13.037416000
H	0.819555000	10.078846000	13.840204000
H	-0.913955000	10.418459000	13.866371000
C	-0.476277000	8.325299000	11.946103000
C	-0.640882000	7.526167000	13.204151000
H	-1.675484000	7.179055000	13.298772000
H	-0.397683000	8.107932000	14.090451000
H	0.001922000	6.641012000	13.191019000
C	-0.636809000	7.697797000	10.674292000
C	-0.948253000	6.317893000	10.498995000
H	-1.047373000	5.682277000	11.369578000
C	-1.132010000	5.753002000	9.243756000
H	-1.341859000	4.693962000	9.184309000
C	-1.051823000	6.531997000	8.060420000
C	-1.298264000	6.039112000	6.738267000
C	-1.574326000	4.592985000	6.467472000
H	-1.863471000	4.034724000	7.355185000
H	-0.671845000	4.125762000	6.054145000
H	-2.361361000	4.478720000	5.719350000
C	-1.230125000	6.949566000	5.668189000
C	-1.489238000	6.527457000	4.249930000
H	-2.509006000	6.145772000	4.133934000
H	-0.805854000	5.728456000	3.945871000
H	-1.362877000	7.366715000	3.564289000
C	-0.902426000	8.285800000	5.937149000
H	-0.841616000	9.010139000	5.133153000
C	-0.724257000	7.905596000	8.206210000
C	-0.500165000	8.480235000	9.508234000
C	-0.804712000	12.173051000	5.400391000
H	-1.727817000	12.327267000	5.950046000
C	-0.593998000	12.677059000	4.100761000
C	-1.707785000	13.453478000	3.446627000
H	-1.388086000	14.467848000	3.189316000
H	-2.567188000	13.530443000	4.115274000
H	-2.041296000	12.968522000	2.523948000
C	0.633705000	12.437198000	3.471480000
C	0.929296000	12.940204000	2.087055000
H	1.784933000	13.623669000	2.101767000
H	0.083335000	13.468066000	1.651605000
H	1.190135000	12.109485000	1.423340000
C	1.628109000	11.696678000	4.175961000
C	2.935062000	11.383384000	3.667033000
H	3.207200000	11.720952000	2.674698000
C	3.841603000	10.675016000	4.405574000
H	4.816649000	10.463274000	3.984921000
C	3.537750000	10.204291000	5.729514000
C	4.438102000	9.470447000	6.554601000
C	5.812134000	9.140412000	6.045112000

H	5.749690000	8.546058000	5.127630000
H	6.397024000	8.580263000	6.771840000
H	6.360792000	10.055941000	5.800543000
C	4.005783000	9.081778000	7.827209000
C	4.876654000	8.309022000	8.784223000
H	4.341346000	8.101538000	9.712975000
H	5.782799000	8.868161000	9.036785000
H	5.188512000	7.352083000	8.354728000
C	2.702127000	9.425509000	8.237934000
H	2.349939000	9.134974000	9.220855000
C	2.259502000	10.495604000	6.239376000
C	1.318394000	11.236600000	5.467466000
C	-3.569065000	9.190716000	7.981685000
C	-3.948677000	7.815809000	8.471252000
C	-3.921328000	7.506142000	9.824612000
C	-4.164654000	6.184186000	10.217617000
C	-4.437137000	5.166960000	9.271479000
C	-4.498580000	5.499215000	7.926951000
C	-4.259457000	6.818543000	7.520706000
O	-3.598457000	9.420607000	6.766223000
O	-3.166475000	9.994849000	8.911839000
Cl	-4.173575000	5.779686000	11.902895000
H	-3.694264000	8.273558000	10.552573000
H	-4.615660000	4.153498000	9.610289000
H	-4.730836000	4.736001000	7.193444000
H	-4.309620000	7.105695000	6.477442000
O	-1.568800000	11.532003000	8.082361000
Cl	1.330940000	13.099558000	8.765887000
C	-0.200991000	13.997811000	9.095394000
H	-0.991614000	13.384251000	8.658262000
H	-0.099693000	14.990617000	8.668065000
Cl	-0.512229000	14.157312000	10.851288000
H	-2.416418000	10.797902000	8.504824000

^{1}**4**

Ni	-0.410142000	10.027844000	6.970325000
N	-0.686924000	8.927055000	8.522304000
N	-0.274707000	8.236655000	6.021890000
N	-0.140770000	11.068306000	5.379456000
N	1.585353000	9.936954000	7.008545000
C	-0.959906000	9.355029000	9.747044000
H	-1.050070000	10.428058000	9.863248000
C	-1.139417000	8.470674000	10.828421000
C	-1.447589000	9.054794000	12.182526000
H	-1.499591000	10.143760000	12.130175000
H	-0.677762000	8.788798000	12.913324000
H	-2.405965000	8.688996000	12.563077000
C	-1.034053000	7.092042000	10.602691000
C	-1.224681000	6.090407000	11.704785000
H	-2.108504000	5.473422000	11.508264000
H	-1.353549000	6.565526000	12.675056000
H	-0.365452000	5.415629000	11.766353000
C	-0.759293000	6.637062000	9.280634000
C	-0.666703000	5.258156000	8.887695000
H	-0.790527000	4.488416000	9.639071000
C	-0.441598000	4.893369000	7.590257000
H	-0.397220000	3.840577000	7.343906000
C	-0.283662000	5.865808000	6.542236000
C	-0.092693000	5.568426000	5.163359000
C	-0.045961000	4.157476000	4.658608000
H	0.196852000	3.437443000	5.438367000
H	0.687825000	4.051095000	3.857117000
H	-1.027298000	3.899036000	4.242885000
C	-0.009613000	6.635435000	4.257798000
C	0.133096000	6.408400000	2.778105000
H	-0.669627000	5.762184000	2.409622000
H	1.081949000	5.915915000	2.541662000
H	0.097961000	7.352442000	2.231294000
C	-0.105044000	7.954211000	4.736782000
H	-0.056053000	8.792008000	4.051351000
C	-0.366004000	7.222265000	6.914440000
C	-0.595796000	7.598041000	8.268863000
C	-1.068866000	11.656382000	4.635337000
H	-2.094252000	11.545003000	4.966084000
C	-0.747220000	12.401472000	3.484313000
C	-1.873741000	13.015712000	2.694409000
H	-1.776339000	14.104369000	2.647138000
H	-2.837945000	12.783328000	3.150248000
H	-1.887500000	12.639470000	1.666926000
C	0.599450000	12.553442000	3.126515000
C	1.016664000	13.349597000	1.923903000
H	1.618665000	14.212078000	2.229633000
H	0.164390000	13.717017000	1.356177000
H	1.635769000	12.742497000	1.255982000
C	1.594423000	11.947033000	3.946040000
C	3.012870000	12.050450000	3.735720000
H	3.377538000	12.610990000	2.884055000
C	3.910489000	11.470722000	4.588397000
H	4.970496000	11.582917000	4.397701000
C	3.487127000	10.721987000	5.740437000
C	4.361483000	10.113870000	6.686307000
C	5.847249000	10.223725000	6.498655000
H	6.142955000	9.816533000	5.526440000

H	6.400382000	9.693635000	7.271103000
H	6.157316000	11.273953000	6.518367000
C	3.799680000	9.436459000	7.775589000
C	4.632254000	8.772244000	8.841461000
H	3.995886000	8.306794000	9.596540000
H	5.278885000	9.496398000	9.346019000
H	5.273724000	7.994759000	8.415799000
C	2.396512000	9.375412000	7.892971000
H	1.936835000	8.864830000	8.730467000
C	2.102425000	10.601460000	5.948562000
C	1.169434000	11.209088000	5.063063000
C	-3.198218000	6.611518000	4.073460000
C	-3.460294000	7.132837000	5.441814000
C	-3.572075000	8.506068000	5.685822000
C	-3.813339000	8.935831000	6.989050000
C	-3.935699000	8.034498000	8.050402000
C	-3.820844000	6.669601000	7.790183000
C	-3.583212000	6.216653000	6.493069000
O	-3.081256000	5.430715000	3.798937000
O	-3.088473000	7.589830000	3.153298000
Cl	-3.943228000	10.647940000	7.300217000
H	-3.475019000	9.218286000	4.877571000
H	-4.112703000	8.398426000	9.055567000
H	-3.910360000	5.960420000	8.605046000
H	-3.486470000	5.159034000	6.279860000
O	-1.418349000	11.206747000	7.596428000
H	-2.945459000	7.166369000	2.289860000
Cl	1.410599000	13.897828000	7.111171000
C	0.475468000	13.381104000	8.550551000
H	-0.388213000	12.810381000	8.202256000
H	0.194884000	14.269294000	9.109440000
Cl	1.426728000	12.316132000	9.638050000

^{3}**4**

Ni	0.014404000	10.709531000	7.761601000
N	-0.133736000	9.842526000	9.488037000
N	-0.546570000	8.841149000	7.050081000
N	0.163004000	11.525800000	6.023029000
N	1.885337000	10.187628000	7.475462000
C	-0.000024000	10.410938000	10.683489000
H	0.235994000	11.466739000	10.699168000
C	-0.148221000	9.692796000	11.882908000
C	0.017202000	10.436959000	13.182424000
H	0.227868000	11.492419000	13.000614000
H	0.841339000	10.024248000	13.771913000
H	-0.890041000	10.374143000	13.790441000
C	-0.439211000	8.324230000	11.820623000
C	-0.613321000	7.494300000	13.058227000
H	-1.624846000	7.075935000	13.093100000
H	-0.450554000	8.070590000	13.966365000
H	0.086355000	6.652440000	13.057816000
C	-0.587144000	7.716537000	10.540499000
C	-0.894506000	6.328113000	10.336794000
H	-1.006335000	5.685099000	11.200236000
C	-1.068329000	5.806285000	9.087232000
H	-1.316412000	4.758165000	8.981115000
C	-0.967961000	6.622498000	7.911321000
C	-1.204879000	6.157574000	6.584971000
C	-1.561379000	4.716729000	6.359919000
H	-2.486829000	4.469268000	6.890047000
H	-0.777266000	4.059607000	6.749308000
H	-1.703168000	4.488235000	5.305743000
C	-1.117445000	7.072947000	5.532147000
C	-1.384166000	6.696746000	4.098455000
H	-2.403804000	6.319100000	3.975054000
H	-0.697859000	5.916464000	3.755896000
H	-1.265914000	7.561284000	3.442393000
C	-0.777426000	8.411214000	5.821061000
H	-0.700042000	9.140696000	5.022830000
C	-0.644601000	7.981130000	8.089307000
C	-0.444049000	8.522127000	9.394634000
C	-0.766606000	12.194363000	5.348460000
H	-1.719089000	12.340824000	5.846680000
C	-0.542442000	12.693611000	4.051417000
C	-1.662260000	13.436477000	3.370154000
H	-1.364305000	14.459726000	3.122937000
H	-2.541992000	13.487922000	4.014127000
H	-1.954142000	12.941302000	2.439256000
C	0.703953000	12.479930000	3.446247000
C	1.011918000	12.981021000	2.065645000
H	1.879524000	13.648506000	2.085907000
H	0.176873000	13.523434000	1.627798000
H	1.261150000	12.145268000	1.403403000
C	1.699732000	11.762594000	4.171079000
C	3.018763000	11.461146000	3.685734000
H	3.302400000	11.796746000	2.696206000
C	3.919586000	10.763112000	4.440872000
H	4.902607000	10.557963000	4.036126000
C	3.598674000	10.291654000	5.761010000
C	4.483426000	9.559126000	6.604331000
C	5.866156000	9.230864000	6.121946000
H	5.819147000	8.616331000	5.216781000
H	6.445593000	8.691337000	6.867998000

H	6.409175000	10.145996000	5.864527000
C	4.025090000	9.165661000	7.867671000
C	4.877275000	8.389399000	8.837963000
H	4.324868000	8.176083000	9.754912000
H	5.777141000	8.949497000	9.109526000
H	5.197501000	7.435825000	8.407620000
C	2.713991000	9.503642000	8.257219000
H	2.340996000	9.208022000	9.229552000
C	2.312321000	10.579581000	6.245008000
C	1.379296000	11.305670000	5.459840000
C	-3.735010000	8.735721000	8.008153000
C	-4.134095000	7.460998000	8.664687000
C	-4.053656000	7.311157000	10.053778000
C	-4.351570000	6.072096000	10.610352000
C	-4.732698000	4.987516000	9.822437000
C	-4.820712000	5.155708000	8.437760000
C	-4.520368000	6.385041000	7.857404000
O	-3.699103000	8.892265000	6.798018000
O	-3.375211000	9.684923000	8.884450000
Cl	-4.205908000	5.862859000	12.350801000
H	-3.744237000	8.138681000	10.677967000
H	-4.954012000	4.030969000	10.281242000
H	-5.122602000	4.318606000	7.817327000
H	-4.567158000	6.526319000	6.784083000
O	-1.561105000	11.465569000	8.045849000
Cl	1.264910000	13.121534000	8.707570000
C	-0.205465000	14.127008000	9.023321000
H	-1.020431000	13.652213000	8.484025000
H	0.014830000	15.135082000	8.686000000
Cl	-0.623942000	14.167880000	10.756389000
H	-2.935279000	10.420365000	8.392620000

^{2}3'+CH

C	-2.745287000	8.905938000	7.031672000
C	-3.984927000	8.184501000	7.342220000
C	-4.388906000	8.076690000	8.677594000
C	-5.579532000	7.418102000	8.955691000
C	-6.360566000	6.867383000	7.938225000
C	-5.938448000	6.979533000	6.612256000
C	-4.751071000	7.638633000	6.306244000
O	-2.257577000	9.037016000	5.869440000
Cl	-6.125563000	7.299341000	10.619669000
H	-3.788415000	8.506873000	9.469960000
H	-7.287787000	6.362539000	8.181867000
H	-6.545574000	6.554197000	5.821253000
H	-4.418307000	7.738801000	5.279218000
O	-2.015352000	9.490691000	7.886498000
C	-6.844987000	12.190768000	9.812354000
C	-8.170528000	11.593382000	10.305129000
C	-9.007155000	11.049693000	9.138563000
C	-8.211477000	10.032419000	8.309635000
C	-6.884604000	10.626770000	7.819113000
C	-6.050704000	11.169903000	8.986844000
H	-6.247007000	12.541494000	10.661777000
H	-7.055853000	13.072486000	9.190614000
H	-7.954107000	10.772602000	11.003653000
H	-8.740939000	12.342393000	10.866966000
H	-9.932274000	10.595817000	9.513172000
H	-9.306685000	11.886493000	8.491645000
H	-8.003298000	9.151119000	8.930776000
H	-8.807995000	9.681238000	7.459262000
H	-6.316381000	9.877267000	7.259812000
H	-7.097214000	11.447381000	7.119167000
H	-5.761492000	10.335200000	9.638754000
H	-5.118958000	11.613437000	8.616150000

^{2}TS$_{3'+CH}$

C	-3.625222000	9.759149000	7.319548000
C	-4.286595000	8.425567000	7.411127000
C	-4.595988000	7.860297000	8.653440000
C	-5.205425000	6.611261000	8.687817000
C	-5.517642000	5.918193000	7.518592000
C	-5.193090000	6.489370000	6.286842000
C	-4.569329000	7.733152000	6.228775000
O	-2.828080000	10.041968000	6.427500000
Cl	-5.598362000	5.894355000	10.246290000
H	-4.357746000	8.381554000	9.571609000
H	-6.001510000	4.950107000	7.572468000
H	-5.431164000	5.956116000	5.372890000
H	-4.309386000	8.183102000	5.277587000
O	-3.878485000	10.665691000	8.243238000
C	-6.464678000	12.097744000	9.591313000
C	-7.922678000	12.350651000	10.043037000
C	-8.919855000	11.844316000	8.995633000
C	-8.692644000	10.362912000	8.676746000
C	-7.236793000	10.104586000	8.219169000
C	-6.278364000	10.627189000	9.271212000
H	-5.764138000	12.420984000	10.367375000
H	-6.261338000	12.694852000	8.693622000
H	-8.098022000	11.835021000	10.996009000
H	-8.060793000	13.421617000	10.228549000
H	-9.945825000	11.997794000	9.350178000

H	-8.810888000	12.434185000	8.075596000
H	-8.898383000	9.759401000	9.570211000
H	-9.379771000	10.021068000	7.894849000
H	-7.082616000	9.037388000	8.039717000
H	-7.062847000	10.627903000	7.270490000
H	-6.260973000	9.999669000	10.170498000
H	-5.160337000	10.532938000	8.843268000

^{2}IM$_{3'+CH}$

C	-3.624763000	9.854540000	7.202662000
C	-4.280019000	8.518560000	7.356405000
C	-4.470564000	7.945227000	8.619269000
C	-5.099027000	6.707500000	8.706973000
C	-5.544708000	6.032794000	7.571618000
C	-5.334775000	6.609539000	6.317515000
C	-4.694515000	7.840757000	6.205207000
O	-2.938531000	10.147202000	6.243915000
Cl	-5.343587000	5.985577000	10.292654000
H	-4.125751000	8.441760000	9.517679000
H	-6.040466000	5.074054000	7.667354000
H	-5.675235000	6.090001000	5.428448000
H	-4.523405000	8.295158000	5.236423000
O	-3.824526000	10.744764000	8.194188000
C	-6.502215000	11.911052000	9.770127000
C	-7.978083000	12.348494000	9.974335000
C	-8.854478000	11.879881000	8.806384000
C	-8.760405000	10.363112000	8.600821000
C	-7.287489000	9.918815000	8.394769000
C	-6.443385000	10.434862000	9.519754000
H	-5.894415000	12.198555000	10.633279000
H	-6.110300000	12.453216000	8.897028000
H	-8.352489000	11.914954000	10.910310000
H	-8.024498000	13.438010000	10.082526000
H	-9.896926000	12.170257000	8.980729000
H	-8.534085000	12.389760000	7.887346000
H	-9.167276000	9.848837000	9.480760000
H	-9.360394000	10.049658000	7.738980000
H	-7.222392000	8.831070000	8.308604000
H	-6.939399000	10.342436000	7.441151000
H	-6.259143000	9.775508000	10.366745000
H	-4.591722000	10.484192000	8.761235000

^{2}IM'

C	-4.414725000	0.039136000	2.254962000
C	-4.967720000	-0.436008000	0.956482000
C	-4.159261000	-0.645925000	-0.168972000
C	-4.758902000	-1.076653000	-1.347116000
C	-6.132604000	-1.302610000	-1.431178000
C	-6.923873000	-1.089053000	-0.301547000
C	-6.348626000	-0.656475000	0.889400000
O	-5.063888000	0.263537000	3.250519000
O	-3.061040000	0.219525000	2.156463000
Cl	-3.756127000	-1.341452000	-2.768329000
H	-3.091737000	-0.476307000	-0.126825000
H	-6.572600000	-1.638062000	-2.362951000
H	-7.993062000	-1.261431000	-0.357994000
H	-6.950555000	-0.483776000	1.773279000
O	-2.489182000	0.680967000	3.391711000
H	-2.621008000	1.667189000	3.298144000
C	-3.011985000	3.468311000	1.363667000
C	-3.692514000	4.749301000	0.810046000
C	-5.099572000	4.915832000	1.396498000
C	-5.073910000	4.942892000	2.929846000
C	-4.396934000	3.665078000	3.495399000
C	-3.050975000	3.485478000	2.862281000
H	-1.987283000	3.383795000	0.989888000
H	-3.570164000	2.603930000	0.978020000
H	-3.080723000	5.621842000	1.071851000
H	-3.730446000	4.698518000	-0.283973000
H	-5.558475000	5.834415000	1.013031000
H	-5.731663000	4.082151000	1.060440000
H	-4.517208000	5.825140000	3.270706000
H	-6.089165000	5.027164000	3.333720000
H	-4.321259000	3.722961000	4.585443000
H	-5.041087000	2.807887000	3.259148000
H	-2.181417000	3.880771000	3.387500000

^{2}TS$_{OH}$

C	-4.860340000	0.319791000	1.673171000
C	-5.135604000	-0.616968000	0.548109000
C	-4.136724000	-1.423253000	-0.014306000
C	-4.476990000	-2.269792000	-1.063262000
C	-5.777851000	-2.334189000	-1.562001000
C	-6.761674000	-1.525893000	-0.990685000
C	-6.446723000	-0.669334000	0.059886000
O	-5.689053000	1.014692000	2.216689000
O	-3.530158000	0.300676000	1.994973000
Cl	-3.231509000	-3.286933000	-1.778531000
H	-3.121527000	-1.390756000	0.357675000
H	-6.014333000	-3.003904000	-2.380482000
H	-7.776081000	-1.569400000	-1.371762000
H	-7.200380000	-0.036392000	0.512459000
O	-3.239404000	1.118679000	3.131836000

H	-3.001244000	2.069005000	2.712435000
C	-3.587527000	3.681464000	1.231654000
C	-3.902412000	5.193566000	1.097627000
C	-4.906372000	5.640980000	2.166882000
C	-4.413251000	5.306791000	3.580282000
C	-4.090389000	3.798915000	3.715297000
C	-3.118400000	3.396695000	2.637554000
H	-2.841630000	3.379568000	0.489837000
H	-4.508312000	3.120701000	1.031209000
H	-2.971779000	5.765391000	1.204165000
H	-4.289205000	5.394361000	0.092088000
H	-5.091818000	6.717676000	2.078815000
H	-5.867387000	5.138778000	1.991290000
H	-3.510099000	5.890785000	3.800118000
H	-5.163671000	5.586259000	4.328348000
H	-3.690464000	3.583330000	4.711254000
H	-5.012629000	3.219845000	3.593473000
H	-2.074753000	3.666934000	2.833462000

$^{2}PC_{OH}$

C	-4.556418000	0.757593000	0.046682000
C	-5.034564000	-0.663269000	-0.013446000
C	-4.213245000	-1.715199000	0.408471000
C	-4.702830000	-3.014114000	0.334096000
C	-5.982976000	-3.287443000	-0.147117000
C	-6.789050000	-2.226870000	-0.563563000
C	-6.321333000	-0.916610000	-0.499555000
O	-5.279543000	1.695175000	-0.344164000
O	-3.366042000	0.916719000	0.532380000
Cl	-3.679548000	-4.346701000	0.861099000
H	-3.217281000	-1.518484000	0.784238000
H	-6.340027000	-4.309523000	-0.194496000
H	-7.786046000	-2.430279000	-0.939334000
H	-6.935534000	-0.083991000	-0.819764000
O	-3.247199000	3.131884000	0.255918000
H	-4.171558000	2.865353000	-0.038340000
C	-3.561580000	5.293182000	1.255934000
C	-3.583365000	6.074949000	2.577981000
C	-4.607102000	5.490915000	3.558064000
C	-4.348635000	3.998389000	3.799825000
C	-4.325382000	3.210994000	2.482710000
C	-3.292041000	3.798441000	1.521285000
H	-2.798047000	5.684514000	0.577357000
H	-4.531837000	5.385753000	0.751746000
H	-2.584180000	6.044111000	3.032005000
H	-3.803624000	7.127562000	2.369744000
H	-4.577566000	6.038532000	4.506361000
H	-5.617071000	5.621512000	3.146670000
H	-3.384361000	3.875382000	4.311090000
H	-5.111144000	3.578642000	4.464276000
H	-4.090107000	2.157765000	2.659548000
H	-5.313816000	3.251693000	2.008137000
H	-2.286637000	3.691491000	1.943726000

$^{2}IM''$

C	-4.414725000	0.039136000	2.254962000
C	-4.967720000	-0.436008000	0.956482000
C	-4.159261000	-0.645925000	-0.168972000
C	-4.758902000	-1.076653000	-1.347116000
C	-6.132604000	-1.302610000	-1.431178000
C	-6.923873000	-1.089053000	-0.301547000
C	-6.348626000	-0.656475000	0.889400000
O	-5.063888000	0.263537000	3.250519000
O	-3.061040000	0.219525000	2.156463000
Cl	-3.756127000	-1.341452000	-2.768329000
H	-3.091737000	-0.476307000	-0.126825000
H	-6.572600000	-1.638062000	-2.362951000
H	-7.993062000	-1.261431000	-0.357994000
H	-6.950555000	-0.483776000	1.773279000
O	-2.489182000	0.680967000	3.391711000
H	-2.621008000	1.667189000	3.298144000
C	-3.011985000	3.468311000	1.363667000
C	-3.692514000	4.749301000	0.810046000
C	-5.099572000	4.915832000	1.396498000
C	-5.073910000	4.942892000	2.929846000
C	-4.396934000	3.665078000	3.495399000
C	-3.050975000	3.485478000	2.862281000
H	-1.987283000	3.383795000	0.989888000
H	-3.570164000	2.603930000	0.978020000
H	-3.080723000	5.621842000	1.071851000
H	-3.730446000	4.698518000	-0.283973000
H	-5.558475000	5.834415000	1.013031000
H	-5.731663000	4.082151000	1.060440000
H	-4.517208000	5.825140000	3.270706000
H	-6.089165000	5.027164000	3.333720000
H	-4.321259000	3.722961000	4.585443000
H	-5.041087000	2.807887000	3.259148000
H	-2.181417000	3.880771000	3.387500000

$^{2}TS_{Cl}$

C	-4.860340000	0.319791000	1.673171000
C	-5.135604000	-0.616968000	0.548109000

C	-4.136724000	-1.423253000	-0.014306000
C	-4.476990000	-2.269792000	-1.063262000
C	-5.777851000	-2.334189000	-1.562001000
C	-6.761674000	-1.525893000	-0.990685000
C	-6.446723000	-0.669334000	0.059886000
O	-5.689053000	1.014692000	2.216689000
O	-3.530158000	0.300676000	1.994973000
Cl	-3.231509000	-3.286933000	-1.778531000
H	-3.121527000	-1.390756000	0.357675000
H	-6.014333000	-3.003904000	-2.380482000
H	-7.776081000	-1.569400000	-1.371762000
H	-7.200380000	-0.036392000	0.512459000
O	-3.239404000	1.118679000	3.131836000
H	-3.001244000	2.069005000	2.712435000
C	-3.587527000	3.681464000	1.231654000
C	-3.902412000	5.193566000	1.097627000
C	-4.906372000	5.640980000	2.166882000
C	-4.413251000	5.306791000	3.580282000
C	-4.090389000	3.798915000	3.715297000
C	-3.118400000	3.396695000	2.637554000
H	-2.841630000	3.379568000	0.489837000
H	-4.508312000	3.120701000	1.031209000
H	-2.971779000	5.765391000	1.204165000
H	-4.289205000	5.394361000	0.092088000
H	-5.091818000	6.717676000	2.078815000
H	-5.867387000	5.138778000	1.991290000
H	-3.510099000	5.890785000	3.800118000
H	-5.163671000	5.586259000	4.328348000
H	-3.690464000	3.583330000	4.711254000
H	-5.012629000	3.219845000	3.593473000
H	-2.074753000	3.666934000	2.833462000

^{2}PC$_{Cl}$

C	-4.556418000	0.757593000	0.046682000
C	-5.034564000	-0.663269000	-0.013446000
C	-4.213245000	-1.715199000	0.408471000
C	-4.702830000	-3.014114000	0.334096000
C	-5.982976000	-3.287443000	-0.147117000
C	-6.789050000	-2.226870000	-0.563563000
C	-6.321333000	-0.916610000	-0.499555000
O	-5.279543000	1.695175000	-0.344164000
O	-3.366042000	0.916719000	0.532380000
Cl	-3.679548000	-4.346701000	0.861099000
H	-3.217281000	-1.518484000	0.784238000
H	-6.340027000	-4.309523000	-0.194496000
H	-7.786046000	-2.430279000	-0.939334000
H	-6.935534000	-0.083991000	-0.819764000
O	-3.247199000	3.131884000	0.255918000
H	-4.171558000	2.865353000	-0.038340000
C	-3.561580000	5.293182000	1.255934000
C	-3.583365000	6.074949000	2.577981000
C	-4.607102000	5.490915000	3.558064000
C	-4.348635000	3.998389000	3.799825000
C	-4.325382000	3.210994000	2.482710000
C	-3.292041000	3.798441000	1.521285000
H	-2.798047000	5.684514000	0.577357000
H	-4.531837000	5.385753000	0.751746000
H	-2.584180000	6.044111000	3.032005000
H	-3.803624000	7.127562000	2.369744000
H	-4.577566000	6.038532000	4.506361000
H	-5.617071000	5.621512000	3.146670000
H	-3.384361000	3.875382000	4.311090000
H	-5.111144000	3.578642000	4.464276000
H	-4.090107000	2.157765000	2.659548000
H	-5.313816000	3.251693000	2.008137000
H	-2.286637000	3.691491000	1.943726000

^{1}2+CH

Ni	0.051461000	8.897042000	7.164197000
N	0.099347000	8.356315000	9.023827000
N	-0.903771000	7.216103000	6.908625000
N	-0.422491000	9.794077000	5.512868000
N	1.534000000	10.151171000	7.188456000
C	0.469406000	9.060332000	10.091242000
H	0.894423000	10.037637000	9.909519000
C	0.319071000	8.603471000	11.415172000
C	0.781986000	9.501515000	12.533264000
H	1.199036000	10.429050000	12.137341000
H	1.553212000	9.015484000	13.138337000
H	-0.045795000	9.764184000	13.198799000
C	-0.242763000	7.342309000	11.638195000
C	-0.421130000	6.777832000	13.017348000
H	-1.479125000	6.568981000	13.207092000
H	-0.063157000	7.456211000	13.789061000
H	0.119781000	5.830935000	13.117636000
C	-0.678772000	6.593447000	10.507427000
C	-1.299001000	5.299681000	10.575500000
H	-1.427162000	4.829576000	11.541921000
C	-1.744015000	4.658536000	9.454163000
H	-2.210195000	3.686312000	9.549169000
C	-1.632382000	5.253143000	8.151662000
C	-2.109483000	4.659151000	6.948941000

C	-2.785371000	3.320140000	6.997482000
H	-3.654967000	3.359039000	7.660881000
H	-2.105283000	2.560146000	7.396248000
H	-3.121751000	2.992388000	6.016045000
C	-1.924167000	5.357796000	5.752043000
C	-2.373726000	4.821163000	4.417654000
H	-3.456083000	4.659993000	4.402988000
H	-1.893707000	3.864847000	4.190071000
H	-2.129359000	5.520052000	3.615337000
C	-1.310620000	6.625622000	5.787595000
H	-1.154884000	7.167120000	4.864473000
C	-1.026066000	6.519041000	8.072576000
C	-0.513851000	7.159976000	9.231581000
C	-1.524051000	9.668740000	4.776974000
H	-2.250936000	8.939315000	5.104851000
C	-1.790020000	10.459630000	3.641730000
C	-3.058612000	10.189778000	2.873907000
H	-3.669666000	11.092172000	2.781313000
H	-3.657869000	9.428051000	3.376194000
H	-2.840149000	9.834593000	1.861731000
C	-0.875239000	11.450572000	3.271828000
C	-1.080601000	12.313522000	2.061044000
H	-1.255900000	13.353456000	2.357272000
H	-1.930689000	11.986809000	1.465348000
H	-0.191824000	12.302581000	1.423170000
C	0.259744000	11.657339000	4.107037000
C	1.244537000	12.685549000	3.909746000
H	1.144524000	13.351146000	3.061503000
C	2.298286000	12.844433000	4.765324000
H	3.020797000	13.628646000	4.576870000
C	2.474896000	11.993976000	5.910362000
C	3.558427000	12.086468000	6.829705000
C	4.599602000	13.153358000	6.652382000
H	5.132325000	13.014995000	5.705256000
H	5.333295000	13.149542000	7.455876000
H	4.133477000	14.142989000	6.620389000
C	3.623892000	11.149168000	7.866902000
C	4.748142000	11.120152000	8.869989000
H	4.620307000	10.294258000	9.572467000
H	4.784936000	12.048522000	9.448357000
H	5.717243000	10.997741000	8.377802000
C	2.589711000	10.201940000	7.997771000
H	2.632061000	9.472194000	8.795262000
C	1.506185000	10.998389000	6.124672000
C	0.429780000	10.812220000	5.216882000
C	-3.695504000	8.490213000	7.891580000
C	-4.270756000	7.372635000	8.683177000
C	-4.073733000	7.261449000	10.066100000
C	-4.601053000	6.157280000	10.725254000
C	-5.316604000	5.171474000	10.046365000
C	-5.510636000	5.301383000	8.669310000
C	-4.989605000	6.395091000	7.984026000
O	-3.830805000	8.655981000	6.699645000
O	-2.941853000	9.292799000	8.695601000
Cl	-4.328650000	5.988975000	12.451001000
H	-3.513382000	8.007654000	10.613306000
H	-5.711985000	4.318098000	10.584590000
H	-6.070259000	4.541557000	8.134873000
H	-5.121572000	6.502181000	6.914243000
O	-2.296137000	10.314906000	7.905153000
H	-1.999064000	10.886198000	8.641718000
Cl	1.013268000	12.868554000	9.404150000
C	-0.470465000	13.306629000	10.301618000
H	-1.074615000	13.953823000	9.672803000
H	-0.183455000	13.782869000	11.234132000
Cl	-1.467564000	11.864952000	10.719809000
C	-1.795075000	13.440379000	6.670885000
C	-1.971898000	14.249026000	5.378367000
C	-3.241764000	13.827363000	4.627273000
C	-4.485200000	13.925061000	5.521255000
C	-4.301940000	13.125060000	6.818432000
C	-3.036324000	13.565413000	7.566368000
H	-0.891530000	13.766571000	7.198953000
H	-1.645510000	12.381992000	6.417701000
H	-2.040112000	15.315851000	5.631641000
H	-1.089049000	14.138489000	4.739247000
H	-3.371137000	14.434933000	3.724166000
H	-3.129100000	12.787750000	4.296205000
H	-4.667726000	14.979236000	5.771782000
H	-5.369787000	13.572671000	4.978330000
H	-5.181676000	13.236848000	7.462503000
H	-4.215181000	12.055918000	6.581600000
H	-3.146912000	14.611365000	7.885007000
H	-2.924692000	12.971818000	8.480146000

^{3}2+CH

Ni	-0.700710000	9.912190000	8.223171000
N	-0.628794000	8.763456000	9.974231000
N	-0.930564000	8.009193000	7.406031000
N	-0.787108000	10.955716000	6.443536000
N	1.336625000	10.175780000	7.887812000
C	-0.515109000	9.156269000	11.238377000
H	-0.409830000	10.223042000	11.404202000

C	-0.525367000	8.276471000	12.337959000
C	-0.405198000	8.854101000	13.724470000
H	-0.306645000	9.940811000	13.683610000
H	0.469770000	8.456287000	14.247431000
H	-1.285743000	8.619755000	14.330697000
C	-0.648776000	6.906424000	12.093629000
C	-0.685746000	5.899473000	13.208140000
H	-1.610259000	5.314443000	13.162817000
H	-0.629711000	6.369557000	14.187964000
H	0.148313000	5.195138000	13.121763000
C	-0.748468000	6.465841000	10.742144000
C	-0.856938000	5.084054000	10.367955000
H	-0.851133000	4.328186000	11.142265000
C	-0.978424000	4.703142000	9.063961000
H	-1.066049000	3.651073000	8.824759000
C	-1.011107000	5.666535000	8.001507000
C	-1.186527000	5.322661000	6.630305000
C	-1.332178000	3.879475000	6.239114000
H	-2.190307000	3.429988000	6.747977000
H	-0.444333000	3.308822000	6.530663000
H	-1.474634000	3.757780000	5.167238000
C	-1.228881000	6.351471000	5.684574000
C	-1.436052000	6.103805000	4.213165000
H	-2.393797000	5.607508000	4.027211000
H	-0.648797000	5.466932000	3.798648000
H	-1.433791000	7.044981000	3.659662000
C	-1.088974000	7.679143000	6.130245000
H	-1.121233000	8.499922000	5.422780000
C	-0.889850000	7.029633000	8.343400000
C	-0.746630000	7.433234000	9.715223000
C	-1.861305000	11.299092000	5.742142000
H	-2.814933000	10.980907000	6.146678000
C	-1.798050000	12.014568000	4.530757000
C	-3.089661000	12.352380000	3.831762000
H	-3.242905000	13.435155000	3.779418000
H	-3.939322000	11.921058000	4.364449000
H	-3.103492000	11.967286000	2.807922000
C	-0.544663000	12.384215000	4.035488000
C	-0.394726000	13.167333000	2.761687000
H	0.168185000	14.089042000	2.939871000
H	-1.357151000	13.438156000	2.331935000
H	0.159287000	12.588407000	2.014979000
C	0.616099000	11.994918000	4.766269000
C	1.958388000	12.294485000	4.354388000
H	2.116290000	12.846855000	3.436590000
C	3.039157000	11.898985000	5.089028000
H	4.034852000	12.144973000	4.742060000
C	2.889012000	11.162114000	6.312029000
C	3.982450000	10.722311000	7.114370000
C	5.389384000	11.027837000	6.683150000
H	5.589470000	10.605492000	5.692979000
H	6.127266000	10.628020000	7.375792000
H	5.543608000	12.109593000	6.610376000
C	3.706987000	10.014547000	8.288444000
C	4.786016000	9.503072000	9.207562000
H	4.350486000	8.985259000	10.064666000
H	5.406203000	10.320381000	9.588036000
H	5.447672000	8.800570000	8.691485000
C	2.361368000	9.770711000	8.627101000
H	2.114151000	9.229426000	9.534445000
C	1.579544000	10.860181000	6.739934000
C	0.442590000	11.278753000	5.967074000
C	-3.954339000	8.370668000	7.740028000
C	-4.245554000	6.951199000	8.043456000
C	-4.145786000	6.434539000	9.343837000
C	-4.355238000	5.074847000	9.536483000
C	-4.656658000	4.225144000	8.470312000
C	-4.759418000	4.756529000	7.183327000
C	-4.554738000	6.115802000	6.963043000
O	-4.027085000	8.915259000	6.666009000
O	-3.501163000	8.998935000	8.886738000
Cl	-4.218837000	4.415084000	11.154685000
H	-3.900040000	7.070156000	10.183862000
H	-4.808175000	3.166652000	8.646398000
H	-4.994263000	4.101426000	6.351859000
H	-4.617969000	6.538490000	5.967792000
O	-2.952993000	10.285185000	8.538020000
H	-3.244895000	10.814458000	9.302613000
Cl	-0.640113000	12.394085000	9.681797000
C	0.439134000	13.537718000	8.776355000
H	1.290151000	12.962079000	8.425993000
H	0.725626000	14.306928000	9.487060000
Cl	-0.373582000	14.293755000	7.391290000
C	-5.190506000	12.562674000	7.384565000
C	-6.199957000	13.235921000	6.444135000
C	-6.530075000	14.662648000	6.905202000
C	-5.258310000	15.508502000	7.059354000
C	-4.253016000	14.837004000	8.005276000
C	-3.923369000	13.414242000	7.537800000
H	-4.942076000	11.558170000	7.023769000
H	-5.653989000	12.431319000	8.373064000
H	-5.774803000	13.276619000	5.431259000
H	-7.114296000	12.635191000	6.375751000
H	-7.221439000	15.139210000	6.200582000

H	-7.049384000	14.615758000	7.872804000
H	-4.790291000	15.636562000	6.072754000
H	-5.509533000	16.512423000	7.420693000
H	-3.335100000	15.431730000	8.075235000
H	-4.681402000	14.794522000	9.016626000
H	-3.404295000	13.472908000	6.572378000
H	-3.217439000	12.945031000	8.231999000

^{1}**TS**$_{2+CH}$

Ni	-0.332807000	8.797141000	7.261830000
N	-0.124847000	8.285144000	9.109183000
N	-1.131130000	7.013464000	7.071642000
N	-0.882167000	9.568096000	5.578138000
N	1.079751000	10.146551000	7.184741000
C	0.202383000	9.046323000	10.149597000
H	0.449646000	10.077485000	9.942138000
C	0.228286000	8.577344000	11.477087000
C	0.622178000	9.543950000	12.564251000
H	0.868513000	10.520248000	12.143358000
H	1.497327000	9.187122000	13.115278000
H	-0.189713000	9.682184000	13.284774000
C	-0.097741000	7.241203000	11.730618000
C	-0.065800000	6.659239000	13.113601000
H	-1.067822000	6.327837000	13.405272000
H	0.284648000	7.375675000	13.853772000
H	0.589683000	5.783209000	13.148795000
C	-0.505442000	6.431447000	10.632438000
C	-0.919753000	5.060388000	10.738263000
H	-0.883541000	4.573143000	11.703956000
C	-1.382525000	4.368522000	9.655544000
H	-1.695391000	3.339486000	9.779040000
C	-1.486125000	4.976228000	8.357951000
C	-2.011220000	4.328996000	7.205238000
C	-2.514966000	2.918964000	7.306606000
H	-3.281548000	2.845475000	8.083892000
H	-1.702720000	2.238815000	7.584523000
H	-2.945407000	2.567557000	6.371031000
C	-2.037847000	5.045076000	6.004725000
C	-2.565957000	4.460517000	4.720225000
H	-3.623827000	4.195993000	4.816561000
H	-2.022568000	3.553665000	4.439351000
H	-2.474143000	5.176124000	3.900809000
C	-1.577065000	6.375624000	5.991468000
H	-1.579106000	6.926930000	5.061458000
C	-1.056609000	6.308865000	8.234716000
C	-0.535378000	7.013013000	9.352700000
C	-2.014228000	9.375449000	4.908632000
H	-2.712575000	8.657524000	5.312956000
C	-2.360802000	10.097279000	3.748386000
C	-3.689891000	9.797696000	3.105144000
H	-4.276853000	10.710551000	2.968986000
H	-4.270312000	9.115047000	3.728361000
H	-3.563218000	9.336217000	2.120239000
C	-1.473097000	11.053433000	3.249550000
C	-1.759840000	11.823008000	1.992082000
H	-2.034943000	12.858078000	2.227228000
H	-2.577574000	11.381828000	1.424700000
H	-0.878147000	11.860532000	1.346788000
C	-0.294538000	11.326153000	4.003466000
C	0.658675000	12.353978000	3.687049000
H	0.520760000	12.939464000	2.786616000
C	1.724545000	12.619694000	4.501322000
H	2.418807000	13.404050000	4.227359000
C	1.942673000	11.890477000	5.720008000
C	3.018606000	12.128132000	6.622164000
C	4.008808000	13.218807000	6.333148000
H	4.547735000	13.011912000	5.402125000
H	4.741733000	13.330168000	7.129643000
H	3.496388000	14.177490000	6.204472000
C	3.118880000	11.311788000	7.752696000
C	4.234889000	11.443006000	8.757508000
H	4.131516000	10.699918000	9.550667000
H	4.232971000	12.433176000	9.223916000
H	5.212352000	11.301510000	8.287175000
C	2.129556000	10.334973000	7.980917000
H	2.208904000	9.695623000	8.849137000
C	1.016885000	10.880643000	6.039471000
C	-0.066128000	10.577934000	5.172019000
C	-3.800898000	8.655411000	7.846169000
C	-4.135771000	7.394778000	8.610787000
C	-3.838218000	7.273980000	9.973395000
C	-4.180794000	6.097872000	10.630886000
C	-4.792715000	5.036036000	9.964588000
C	-5.080693000	5.171061000	8.605079000
C	-4.759293000	6.345903000	7.928155000
O	-4.317161000	8.876832000	6.750767000
O	-2.919324000	9.387356000	8.466847000
Cl	-3.827561000	5.946438000	12.347473000
H	-3.358231000	8.088041000	10.500759000
H	-5.041935000	4.127205000	10.499705000
H	-5.561747000	4.353617000	8.078240000
H	-4.985911000	6.468635000	6.876062000
O	-2.797774000	11.090902000	7.599034000

H	-2.481931000	11.351000000	8.487256000
Cl	0.732971000	12.792286000	9.981969000
C	-0.810620000	13.133823000	10.831635000
H	-1.283689000	13.981995000	10.345747000
H	-0.587620000	13.326934000	11.876611000
Cl	-1.948809000	11.745435000	10.763040000
C	-1.153311000	13.718901000	6.740312000
C	-0.983335000	15.168093000	6.213303000
C	-1.704183000	15.352756000	4.874651000
C	-3.186323000	14.980984000	4.981247000
C	-3.366269000	13.528257000	5.501880000
C	-2.621736000	13.398813000	6.807513000
H	-0.667582000	13.607196000	7.711716000
H	-0.660473000	13.042876000	6.039689000
H	-1.384353000	15.871901000	6.952536000
H	0.087785000	15.374959000	6.116602000
H	-1.604766000	16.390473000	4.537767000
H	-1.221793000	14.726114000	4.113421000
H	-3.693801000	15.671770000	5.665116000
H	-3.685579000	15.062985000	4.010078000
H	-4.426486000	13.293489000	5.624845000
H	-2.948635000	12.833925000	4.765594000
H	-3.139391000	13.846126000	7.659982000
H	-2.723625000	12.154766000	7.054009000

^{3}**TS**$_{2+CH}$

Ni	-1.064358000	9.508647000	8.050073000
N	-0.810125000	8.433863000	9.805416000
N	-0.993359000	7.612051000	7.254586000
N	-1.114612000	10.594991000	6.276190000
N	0.957770000	9.983084000	7.872191000
C	-0.745129000	8.867177000	11.058876000
H	-0.867860000	9.935065000	11.203466000
C	-0.529144000	8.023454000	12.165556000
C	-0.481492000	8.637670000	13.540696000
H	-0.641379000	9.716631000	13.487170000
H	0.485940000	8.464976000	14.022574000
H	-1.253156000	8.215387000	14.191689000
C	-0.376689000	6.652700000	11.940114000
C	-0.150126000	5.684191000	13.065803000
H	-0.987871000	4.982365000	13.136108000
H	-0.050160000	6.187361000	14.025517000
H	0.755733000	5.094209000	12.895149000
C	-0.462628000	6.172333000	10.601806000
C	-0.380672000	4.783206000	10.249156000
H	-0.223621000	4.050689000	11.030530000
C	-0.522922000	4.363362000	8.958807000
H	-0.475255000	3.304615000	8.737568000
C	-0.740347000	5.291357000	7.885207000
C	-0.932836000	4.901620000	6.529017000
C	-0.934168000	3.442622000	6.169810000
H	-1.724965000	2.917722000	6.716250000
H	0.015848000	2.972897000	6.444293000
H	-1.095766000	3.281430000	5.105876000
C	-1.138589000	5.898122000	5.570293000
C	-1.368388000	5.596465000	4.112243000
H	-2.270892000	4.993340000	3.971289000
H	-0.530247000	5.041536000	3.680141000
H	-1.490103000	6.519341000	3.541470000
C	-1.149653000	7.241351000	5.990060000
H	-1.306907000	8.039414000	5.272316000
C	-0.793039000	6.663572000	8.202360000
C	-0.676242000	7.104149000	9.565387000
C	-2.150885000	10.865513000	5.487394000
H	-3.104658000	10.449733000	5.790013000
C	-2.056509000	11.643712000	4.316628000
C	-3.307675000	11.872586000	3.507357000
H	-3.583184000	12.932190000	3.486865000
H	-4.145271000	11.314608000	3.930780000
H	-3.179777000	11.547566000	2.470610000
C	-0.814431000	12.169960000	3.957092000
C	-0.638433000	13.031932000	2.738455000
H	-0.204109000	13.999538000	3.009607000
H	-1.581968000	13.217724000	2.228945000
H	0.044824000	12.559180000	2.024819000
C	0.309397000	11.864508000	4.777697000
C	1.640283000	12.325835000	4.499723000
H	1.811389000	12.938692000	3.623565000
C	2.693311000	12.007414000	5.306733000
H	3.682165000	12.372291000	5.059053000
C	2.519791000	11.197429000	6.478611000
C	3.585404000	10.835597000	7.352993000
C	4.981250000	11.310135000	7.060739000
H	5.318208000	10.941150000	6.086246000
H	5.693818000	10.975880000	7.812175000
H	5.016946000	12.403757000	7.022055000
C	3.294214000	10.041368000	8.465983000
C	4.342848000	9.595678000	9.452322000
H	3.896951000	8.986321000	10.241331000
H	4.834756000	10.450829000	9.926057000
H	5.119399000	8.997846000	8.965348000
C	1.959673000	9.646474000	8.676802000
H	1.701040000	9.040125000	9.537630000

C	1.218985000	10.740329000	6.777147000
C	0.109291000	11.070429000	5.925636000
C	-3.966755000	8.619974000	7.650311000
C	-4.013877000	7.232956000	8.206861000
C	-3.841802000	6.991519000	9.575762000
C	-3.884196000	5.677892000	10.031203000
C	-4.066344000	4.606376000	9.156817000
C	-4.237545000	4.864188000	7.794986000
C	-4.221330000	6.171436000	7.317555000
O	-4.488993000	8.927231000	6.593663000
O	-3.258181000	9.456826000	8.426786000
Cl	-3.695165000	5.361383000	11.748545000
H	-3.683613000	7.813107000	10.261879000
H	-4.078512000	3.591408000	9.535983000
H	-4.384428000	4.036861000	7.109130000
H	-4.355635000	6.383735000	6.263888000
O	-3.808531000	11.152570000	7.979936000
H	-3.274958000	11.481549000	8.734703000
Cl	-1.701216000	12.389782000	10.312458000
C	-0.209511000	12.964341000	9.473969000
H	0.410605000	12.094205000	9.283501000
H	0.270739000	13.681048000	10.133220000
Cl	-0.560140000	13.763760000	7.918089000
C	-5.463005000	13.506261000	6.270861000
C	-5.551480000	14.938056000	5.681703000
C	-5.618543000	15.988810000	6.795685000
C	-4.431696000	15.864504000	7.756834000
C	-4.335748000	14.435158000	8.349197000
C	-4.270314000	13.454826000	7.201538000
H	-5.372948000	12.769059000	5.469285000
H	-6.381771000	13.289745000	6.827526000
H	-4.671474000	15.121184000	5.052156000
H	-6.430674000	14.995911000	5.031220000
H	-5.641717000	16.993716000	6.359320000
H	-6.554626000	15.864148000	7.355527000
H	-3.498920000	16.092444000	7.225851000
H	-4.516264000	16.581894000	8.579843000
H	-3.456223000	14.355084000	8.992439000
H	-5.224069000	14.237711000	8.960158000
H	-3.315025000	13.487426000	6.670046000
H	-4.281650000	12.320368000	7.635815000

^{1}**PC**$_{2+CH}$

Ni	-0.241468000	8.700366000	7.142762000
N	-0.093699000	8.279568000	9.054403000
N	-1.089318000	6.891173000	7.070524000
N	-0.765420000	9.431575000	5.381817000
N	1.141760000	10.119624000	7.038228000
C	0.262348000	9.080444000	10.056139000
H	0.518609000	10.097860000	9.799184000
C	0.310038000	8.669415000	11.401711000
C	0.742920000	9.675256000	12.437279000
H	0.989536000	10.630533000	11.970029000
H	1.628313000	9.331588000	12.980089000
H	-0.048472000	9.851370000	13.172419000
C	-0.030765000	7.351594000	11.719376000
C	0.042782000	6.823497000	13.121968000
H	-0.941426000	6.474473000	13.449126000
H	0.388590000	7.576147000	13.827505000
H	0.724794000	5.968303000	13.173056000
C	-0.482081000	6.504350000	10.667189000
C	-0.929274000	5.152258000	10.849469000
H	-0.897841000	4.718273000	11.840550000
C	-1.413424000	4.413417000	9.808465000
H	-1.749148000	3.400153000	9.988913000
C	-1.500006000	4.948126000	8.477969000
C	-2.025043000	4.239863000	7.361168000
C	-2.554731000	2.847560000	7.542670000
H	-3.306148000	2.824628000	8.337444000
H	-1.749217000	2.166298000	7.837886000
H	-3.009704000	2.459009000	6.633775000
C	-2.019973000	4.876244000	6.116568000
C	-2.537968000	4.219995000	4.863215000
H	-3.603992000	3.988629000	4.954949000
H	-2.012697000	3.283493000	4.654770000
H	-2.412031000	4.876572000	4.000148000
C	-1.530039000	6.192728000	6.026396000
H	-1.499338000	6.679592000	5.061764000
C	-1.046122000	6.263781000	8.280088000
C	-0.519179000	7.023336000	9.361007000
C	-1.847408000	9.157091000	4.657616000
H	-2.503208000	8.380095000	5.019529000
C	-2.207400000	9.862906000	3.491350000
C	-3.477164000	9.457357000	2.787288000
H	-4.124025000	10.320081000	2.606749000
H	-4.035263000	8.740334000	3.391468000
H	-3.261526000	8.996143000	1.817961000
C	-1.381989000	10.899071000	3.043836000
C	-1.686555000	11.675301000	1.795807000
H	-1.984874000	12.699524000	2.047442000
H	-2.490353000	11.221366000	1.219409000
H	-0.802603000	11.741903000	1.155256000
C	-0.249203000	11.240888000	3.838233000

C	0.630301000	12.342247000	3.560075000
H	0.468484000	12.931135000	2.666157000
C	1.652845000	12.672989000	4.403796000
H	2.292386000	13.511663000	4.159235000
C	1.898334000	11.940202000	5.614537000
C	2.939097000	12.241630000	6.539310000
C	3.845003000	13.411898000	6.288817000
H	4.405700000	13.273211000	5.358167000
H	4.560372000	13.556738000	7.095732000
H	3.260462000	14.331274000	6.181756000
C	3.085697000	11.413395000	7.655635000
C	4.174765000	11.605790000	8.679699000
H	4.113050000	10.842723000	9.457992000
H	4.094800000	12.584476000	9.163157000
H	5.166502000	11.543522000	8.222314000
C	2.164506000	10.366469000	7.853129000
H	2.273779000	9.719573000	8.712756000
C	1.042559000	10.861571000	5.900309000
C	-0.001232000	10.495758000	5.006035000
C	-3.988430000	8.665542000	7.408738000
C	-4.177895000	7.565661000	8.394451000
C	-3.816217000	7.725981000	9.738557000
C	-4.045507000	6.676204000	10.620345000
C	-4.612905000	5.473314000	10.197458000
C	-4.964636000	5.327232000	8.854809000
C	-4.749515000	6.367075000	7.953814000
O	-4.324677000	8.568466000	6.233669000
O	-3.413442000	9.751297000	7.920658000
Cl	-3.617352000	6.873944000	12.313073000
H	-3.377147000	8.653512000	10.081910000
H	-4.777637000	4.670791000	10.906665000
H	-5.411227000	4.398054000	8.517820000
H	-5.022731000	6.270313000	6.909977000
O	-3.342666000	11.719887000	6.196926000
H	-3.358298000	10.474415000	7.223921000
Cl	0.673917000	12.809643000	9.918458000
C	-0.966492000	12.893022000	10.655765000
H	-1.384220000	13.867369000	10.420190000
H	-0.859760000	12.741048000	11.725832000
Cl	-2.064721000	11.636240000	10.009786000
C	-1.395640000	13.130320000	6.706025000
C	-0.943831000	14.535345000	7.123853000
C	-1.483271000	15.592053000	6.151664000
C	-3.011241000	15.505424000	6.034574000
C	-3.465178000	14.093894000	5.631119000
C	-2.914989000	13.044465000	6.594631000
H	-1.032954000	12.371158000	7.404130000
H	-0.969409000	12.910207000	5.721962000
H	-1.310434000	14.754907000	8.135630000
H	0.149503000	14.571335000	7.171955000
H	-1.184954000	16.595035000	6.475578000
H	-1.033534000	15.430344000	5.162302000
H	-3.462952000	15.764950000	7.001415000
H	-3.383853000	16.235331000	5.308377000
H	-4.557197000	14.025303000	5.596153000
H	-3.092571000	13.866849000	4.621049000
H	-3.361720000	13.180016000	7.585230000
H	-3.041017000	11.547143000	5.293929000

^{3}**PC**$_{2+CH}$

Ni	-1.389105000	9.753079000	7.464125000
N	-1.323589000	9.036196000	9.391252000
N	-1.080750000	7.761326000	7.042187000
N	-1.322221000	10.507793000	5.531039000
N	0.602636000	10.313084000	7.392017000
C	-1.490265000	9.689350000	10.534569000
H	-1.713187000	10.747458000	10.452801000
C	-1.388500000	9.082083000	11.800691000
C	-1.605617000	9.931485000	13.025961000
H	-1.843178000	10.959818000	12.745639000
H	-0.713809000	9.954042000	13.660048000
H	-2.431709000	9.549126000	13.633159000
C	-1.096596000	7.716182000	11.862839000
C	-0.970324000	6.991028000	13.172185000
H	-1.751973000	6.229007000	13.260659000
H	-1.056407000	7.663305000	14.023542000
H	-0.006158000	6.477614000	13.240261000
C	-0.940591000	6.998623000	10.641534000
C	-0.707108000	5.583575000	10.571953000
H	-0.614970000	5.020835000	11.492029000
C	-0.629460000	4.928857000	9.377163000
H	-0.474393000	3.857371000	9.369460000
C	-0.753688000	5.624987000	8.127209000
C	-0.720100000	4.984669000	6.855443000
C	-0.568844000	3.491733000	6.780353000
H	-1.388781000	2.999460000	7.314025000
H	0.365076000	3.170641000	7.253010000
H	-0.569787000	3.130389000	5.753988000
C	-0.852124000	5.771589000	5.707121000
C	-0.846206000	5.196195000	4.314794000
H	-1.678679000	4.499795000	4.171949000
H	0.079396000	4.650104000	4.109653000
H	-0.941371000	5.988497000	3.569343000

C	-1.022051000	7.160051000	5.860574000
H	-1.132899000	7.798190000	4.990066000
C	-0.947681000	7.019964000	8.169281000
C	-1.061563000	7.705050000	9.427894000
C	-2.293503000	10.605355000	4.627733000
H	-3.267615000	10.232157000	4.919215000
C	-2.110978000	11.140113000	3.337846000
C	-3.299777000	11.197100000	2.412956000
H	-3.524739000	12.226226000	2.116087000
H	-4.186622000	10.787263000	2.900634000
H	-3.122927000	10.622286000	1.498619000
C	-0.841531000	11.593383000	2.974026000
C	-0.565087000	12.180674000	1.618620000
H	-0.206787000	13.211379000	1.711121000
H	-1.451248000	12.187669000	0.987042000
H	0.214985000	11.612012000	1.101983000
C	0.210848000	11.490292000	3.929285000
C	1.554835000	11.927714000	3.675953000
H	1.794743000	12.353881000	2.709877000
C	2.533649000	11.822850000	4.620548000
H	3.533980000	12.166998000	4.389782000
C	2.266247000	11.268551000	5.917315000
C	3.248262000	11.148183000	6.944278000
C	4.656330000	11.605865000	6.684968000
H	5.088304000	11.061230000	5.839074000
H	5.301682000	11.455051000	7.548077000
H	4.676007000	12.670159000	6.428652000
C	2.862939000	10.605719000	8.174538000
C	3.812552000	10.441484000	9.332865000
H	3.299986000	10.002583000	10.191430000
H	4.228444000	11.404019000	9.646227000
H	4.651530000	9.788962000	9.072503000
C	1.523819000	10.202436000	8.340209000
H	1.195076000	9.785974000	9.285556000
C	0.952372000	10.831714000	6.189495000
C	-0.078520000	10.940683000	5.194769000
C	-4.177007000	8.460882000	6.807915000
C	-4.161374000	7.184385000	7.559464000
C	-4.136528000	7.181409000	8.960561000
C	-4.157215000	5.960081000	9.625051000
C	-4.162161000	4.750895000	8.928662000
C	-4.182348000	4.770509000	7.532565000
C	-4.200650000	5.980899000	6.845235000
O	-4.623780000	8.595945000	5.685481000
O	-3.629657000	9.504300000	7.494861000
Cl	-4.179482000	5.941248000	11.380507000
H	-4.115252000	8.113158000	9.510161000
H	-4.158368000	3.812266000	9.470173000
H	-4.189702000	3.834157000	6.985557000
H	-4.228862000	6.007287000	5.762392000
O	-4.290625000	11.866258000	6.883392000
H	-3.970689000	10.412049000	7.145538000
Cl	-0.094437000	12.996078000	9.618351000
C	0.656087000	13.796724000	8.198334000
H	1.506608000	13.196330000	7.888868000
H	0.951258000	14.797746000	8.498302000
Cl	-0.467037000	13.937004000	6.810906000
C	-4.121522000	14.145882000	7.766187000
C	-3.637593000	14.995636000	8.951293000
C	-4.249266000	14.514845000	10.274073000
C	-3.965307000	13.025232000	10.507809000
C	-4.448253000	12.172933000	9.324466000
C	-3.838168000	12.669040000	8.014322000
H	-3.636261000	14.458464000	6.836067000
H	-5.204508000	14.281756000	7.634791000
H	-2.544044000	14.932442000	9.012746000
H	-3.883520000	16.047610000	8.773866000
H	-3.858175000	15.108226000	11.107588000
H	-5.335543000	14.675571000	10.251942000
H	-2.884481000	12.884288000	10.638836000
H	-4.442351000	12.679124000	11.430494000
H	-4.195165000	11.118477000	9.475809000
H	-5.542659000	12.236256000	9.250038000
H	-2.755709000	12.512993000	8.027509000
H	-5.242837000	12.006847000	6.764500000

^{3}4+CH

Ni	-0.036487000	10.703312000	7.661109000
N	-0.246375000	9.834105000	9.378751000
N	-0.627591000	8.856614000	6.924871000
N	0.164892000	11.560404000	5.945465000
N	1.846600000	10.182338000	7.413779000
C	-0.093142000	10.386873000	10.578453000
H	0.219398000	11.422507000	10.602181000
C	-0.318381000	9.680042000	11.772784000
C	-0.112649000	10.405123000	13.077322000
H	0.180701000	11.441692000	12.901508000
H	0.670369000	9.929052000	13.675272000
H	-1.029110000	10.411381000	13.674641000
C	-0.724452000	8.342211000	11.698878000
C	-0.989880000	7.527471000	12.931287000
H	-2.028324000	7.180377000	12.943533000
H	-0.811219000	8.092549000	13.843485000

H	-0.350494000	6.639024000	12.950082000
C	-0.895588000	7.751787000	10.413475000
C	-1.317922000	6.395459000	10.197728000
H	-1.512417000	5.764804000	11.055875000
C	-1.482825000	5.884832000	8.941904000
H	-1.808788000	4.858939000	8.825831000
C	-1.254037000	6.681266000	7.768864000
C	-1.463722000	6.227790000	6.434010000
C	-1.939017000	4.823758000	6.193389000
H	-2.943602000	4.687633000	6.609764000
H	-1.282159000	4.099931000	6.684820000
H	-1.978937000	4.580555000	5.133696000
C	-1.252253000	7.126147000	5.382769000
C	-1.479846000	6.762084000	3.939197000
H	-2.517891000	6.460448000	3.769151000
H	-0.838626000	5.930529000	3.631584000
H	-1.265952000	7.611240000	3.287297000
C	-0.826099000	8.436217000	5.685525000
H	-0.653891000	9.154046000	4.891039000
C	-0.836447000	8.012128000	7.959346000
C	-0.649029000	8.540581000	9.273748000
C	-0.747581000	12.236918000	5.256618000
H	-1.721866000	12.347073000	5.721710000
C	-0.480218000	12.784242000	3.987437000
C	-1.583578000	13.534560000	3.287563000
H	-1.294318000	14.571551000	3.092267000
H	-2.489923000	13.546917000	3.895631000
H	-1.827992000	13.071854000	2.326738000
C	0.792485000	12.609783000	3.426427000
C	1.146991000	13.163916000	2.077308000
H	2.017297000	13.823925000	2.150278000
H	0.328880000	13.729107000	1.636176000
H	1.411395000	12.353640000	1.389474000
C	1.768337000	11.877978000	4.163963000
C	3.107504000	11.605858000	3.717876000
H	3.424814000	11.979438000	2.752459000
C	3.986049000	10.886900000	4.479600000
H	4.985085000	10.704528000	4.104079000
C	3.620438000	10.363049000	5.767816000
C	4.479546000	9.603033000	6.613287000
C	5.882185000	9.304497000	6.169880000
H	5.875788000	8.745368000	5.228449000
H	6.431868000	8.721799000	6.905965000
H	6.432584000	10.233978000	5.990667000
C	3.978373000	9.156059000	7.841917000
C	4.800881000	8.345511000	8.809879000
H	4.218977000	8.094782000	9.698755000
H	5.688709000	8.897296000	9.133142000
H	5.139925000	7.410385000	8.354058000
C	2.651534000	9.471896000	8.195954000
H	2.244260000	9.135955000	9.141604000
C	2.315131000	10.624073000	6.216082000
C	1.404451000	11.372626000	5.423025000
O	-1.603297000	11.448446000	7.890278000
Cl	1.227751000	13.155429000	8.672902000
C	-0.275920000	14.085942000	9.047642000
H	-1.091089000	13.556229000	8.560795000
H	-0.131655000	15.098282000	8.683209000
Cl	-0.605489000	14.141280000	10.801377000
C	-4.552586000	9.359120000	6.200263000
C	-5.306308000	8.033167000	6.374701000
C	-4.875222000	7.305060000	7.655298000
C	-5.002102000	8.201397000	8.895180000
C	-4.259384000	9.532179000	8.709159000
C	-4.708101000	10.257830000	7.434334000
H	-4.904248000	9.879884000	5.301690000
H	-3.485727000	9.149860000	6.042772000
H	-6.384669000	8.239185000	6.422625000
H	-5.148166000	7.387354000	5.502498000
H	-5.462067000	6.388529000	7.787964000
H	-3.830160000	6.993950000	7.549882000
H	-6.064883000	8.407903000	9.083083000
H	-4.621658000	7.675902000	9.779381000
H	-4.404794000	10.174382000	9.586031000
H	-3.181832000	9.340158000	8.640044000
H	-5.762871000	10.549872000	7.535797000
H	-4.128654000	11.178093000	7.307984000

^{3}**TS**$_{4+CH}$

Ni	-0.184833000	10.487298000	7.221958000
N	-0.484132000	9.512322000	8.919907000
N	-0.556205000	8.624782000	6.400307000
N	0.197299000	11.462263000	5.559913000
N	1.797217000	10.176802000	7.222185000
C	-0.421240000	9.991473000	10.157429000
H	-0.155117000	11.035460000	10.259476000
C	-0.698276000	9.214385000	11.297564000
C	-0.611924000	9.874049000	12.649229000
H	-0.312919000	10.919326000	12.550749000
H	0.118095000	9.372147000	13.291305000
H	-1.577857000	9.847807000	13.162745000
C	-1.069319000	7.876643000	11.124793000
C	-1.420712000	6.995327000	12.288762000

H	-2.453111000	6.640644000	12.199691000
H	-1.322731000	7.514484000	13.239846000
H	-0.774961000	6.111788000	12.315215000
C	-1.128159000	7.353909000	9.800191000
C	-1.502954000	6.003307000	9.485968000
H	-1.754762000	5.327785000	10.293597000
C	-1.550167000	5.552934000	8.197423000
H	-1.840770000	4.527630000	8.005772000
C	-1.225721000	6.405523000	7.088176000
C	-1.267572000	5.996045000	5.723686000
C	-1.658415000	4.585424000	5.383284000
H	-2.663762000	4.363961000	5.756311000
H	-0.973700000	3.871368000	5.852486000
H	-1.650142000	4.405258000	4.310225000
C	-0.945681000	6.933043000	4.736651000
C	-0.959505000	6.608539000	3.265347000
H	-1.954547000	6.292700000	2.937027000
H	-0.262545000	5.798278000	3.030372000
H	-0.671893000	7.480383000	2.674239000
C	-0.599225000	8.241252000	5.134058000
H	-0.356409000	8.993742000	4.391217000
C	-0.858446000	7.735544000	7.373022000
C	-0.816789000	8.210483000	8.724780000
C	-0.660654000	12.089777000	4.766394000
H	-1.694962000	12.072065000	5.091904000
C	-0.263113000	12.740320000	3.581476000
C	-1.320586000	13.422418000	2.752108000
H	-1.121864000	14.494489000	2.658200000
H	-2.305346000	13.302010000	3.207553000
H	-1.363331000	13.005072000	1.741471000
C	1.090064000	12.728649000	3.223735000
C	1.587446000	13.401121000	1.976141000
H	2.339799000	14.157784000	2.221433000
H	0.786006000	13.887707000	1.424131000
H	2.065018000	12.673158000	1.311854000
C	2.012985000	12.054540000	4.075478000
C	3.426184000	11.956643000	3.833877000
H	3.841217000	12.422092000	2.948622000
C	4.256461000	11.291121000	4.691134000
H	5.315475000	11.241071000	4.470676000
C	3.761369000	10.652635000	5.879616000
C	4.571388000	9.942273000	6.811953000
C	6.050668000	9.829977000	6.577032000
H	6.250922000	9.320199000	5.628751000
H	6.552218000	9.278475000	7.369600000
H	6.506479000	10.823454000	6.513169000
C	3.951910000	9.365024000	7.925698000
C	4.711642000	8.589796000	8.971179000
H	4.036896000	8.218761000	9.745282000
H	5.468620000	9.213956000	9.455778000
H	5.225307000	7.729223000	8.532024000
C	2.559334000	9.512462000	8.082217000
H	2.058757000	9.074452000	8.937335000
C	2.379919000	10.739566000	6.131215000
C	1.515807000	11.434815000	5.236038000
O	-1.871981000	11.109610000	7.140881000
Cl	0.551508000	12.981542000	8.488213000
C	-1.129801000	13.619733000	8.687069000
H	-1.754048000	12.983558000	8.060240000
H	-1.116115000	14.666475000	8.399853000
Cl	-1.697224000	13.490761000	10.376502000
C	-4.216289000	8.783856000	7.658692000
C	-5.561408000	8.256667000	8.228790000
C	-5.553202000	8.289986000	9.760892000
C	-5.262830000	9.698863000	10.289350000
C	-3.917857000	10.233067000	9.725128000
C	-3.970994000	10.159144000	8.222694000
H	-4.237915000	8.796407000	6.565537000
H	-3.425574000	8.097008000	7.973771000
H	-6.382883000	8.875030000	7.847279000
H	-5.723008000	7.239058000	7.857469000
H	-6.516471000	7.937632000	10.146561000
H	-4.787725000	7.596155000	10.134626000
H	-6.072328000	10.379386000	9.999098000
H	-5.209372000	9.707029000	11.383260000
H	-3.731434000	11.253288000	10.069835000
H	-3.115985000	9.595958000	10.107527000
H	-4.581146000	10.940462000	7.760845000
H	-2.796373000	10.533290000	7.791299000

^{3}PC$_{4+CH}$

Ni	-0.209302000	10.339630000	7.855576000
N	-0.201715000	9.168202000	9.569938000
N	-0.660632000	8.525571000	6.995786000
N	-0.071214000	11.441765000	6.106997000
N	1.823030000	10.149503000	7.499459000
C	0.032937000	9.505169000	10.833402000
H	0.246521000	10.551879000	11.019023000
C	0.015095000	8.593287000	11.906193000
C	0.294760000	9.109147000	13.294174000
H	0.487812000	10.183682000	13.274894000
H	1.168573000	8.618365000	13.733858000
H	-0.553088000	8.932320000	13.963182000

C	-0.266138000	7.251940000	11.635090000
C	-0.313374000	6.215952000	12.722908000
H	-1.300485000	5.743660000	12.763104000
H	-0.103671000	6.641575000	13.702149000
H	0.417673000	5.422755000	12.534857000
C	-0.515653000	6.872336000	10.284329000
C	-0.819101000	5.527281000	9.883391000
H	-0.860726000	4.750662000	10.636723000
C	-1.060996000	5.205626000	8.579686000
H	-1.291081000	4.179871000	8.320245000
C	-1.019692000	6.196131000	7.541614000
C	-1.282930000	5.912369000	6.169974000
C	-1.624450000	4.509458000	5.752187000
H	-2.520995000	4.159215000	6.274158000
H	-0.811572000	3.821673000	6.007435000
H	-1.806262000	4.433499000	4.681971000
C	-1.217902000	6.961134000	5.248659000
C	-1.481014000	6.777699000	3.776456000
H	-2.495191000	6.407642000	3.596861000
H	-0.785126000	6.059316000	3.332430000
H	-1.370779000	7.724599000	3.243717000
C	-0.896960000	8.248586000	5.720632000
H	-0.837833000	9.081928000	5.028383000
C	-0.713481000	7.523944000	7.908450000
C	-0.468564000	7.866508000	9.283828000
C	-1.019036000	12.101366000	5.451682000
H	-1.997406000	12.120364000	5.916280000
C	-0.815081000	12.755945000	4.222055000
C	-1.980986000	13.461653000	3.578958000
H	-1.778623000	14.529094000	3.448261000
H	-2.879076000	13.363762000	4.192535000
H	-2.203368000	13.045569000	2.591482000
C	0.460193000	12.718161000	3.652138000
C	0.763108000	13.384391000	2.339218000
H	1.535830000	14.150262000	2.464204000
H	-0.115607000	13.860416000	1.908474000
H	1.143288000	12.656421000	1.615194000
C	1.493228000	12.028085000	4.349896000
C	2.843944000	11.927625000	3.872750000
H	3.105689000	12.394780000	2.931568000
C	3.804057000	11.260411000	4.576591000
H	4.811125000	11.208967000	4.181791000
C	3.513047000	10.627268000	5.832031000
C	4.481538000	9.925490000	6.607035000
C	5.897157000	9.819495000	6.112430000
H	5.928354000	9.338972000	5.129241000
H	6.525457000	9.243462000	6.788982000
H	6.342319000	10.813868000	6.001064000
C	4.077611000	9.354090000	7.816750000
C	5.014231000	8.590695000	8.717403000
H	4.490783000	8.240865000	9.609747000
H	5.852772000	9.213947000	9.042939000
H	5.432119000	7.716131000	8.209164000
C	2.733354000	9.498245000	8.211642000
H	2.392518000	9.064714000	9.145569000
C	2.192507000	10.710266000	6.321189000
C	1.179120000	11.407167000	5.577480000
O	-2.221408000	10.878138000	8.187349000
Cl	0.475314000	12.630867000	9.130037000
C	-1.073268000	13.496950000	9.469831000
H	-1.682146000	13.433648000	8.573650000
H	-0.816987000	14.516317000	9.741361000
Cl	-1.977525000	12.750884000	10.819057000
C	-3.902976000	9.075169000	8.159694000
C	-5.101363000	8.510800000	7.381142000
C	-6.202113000	9.565559000	7.212674000
C	-5.655547000	10.840535000	6.556643000
C	-4.451341000	11.397118000	7.333449000
C	-3.372151000	10.328533000	7.473753000
H	-3.112217000	8.327549000	8.244875000
H	-4.217109000	9.337612000	9.179799000
H	-4.758012000	8.176000000	6.393000000
H	-5.488597000	7.625827000	7.895882000
H	-7.026314000	9.159632000	6.616676000
H	-6.616045000	9.815171000	8.198778000
H	-5.344686000	10.615735000	5.527483000
H	-6.435483000	11.605544000	6.489767000
H	-4.041544000	12.282615000	6.835559000
H	-4.767723000	11.711138000	8.336868000
H	-2.976932000	10.067195000	6.488395000
H	-2.444783000	10.938820000	9.130207000