Electronic Supporting Information

Oxidative properties of a nonheme $Ni^{II}(O_2)$ complex: Reactivity patterns for C–H activation, aromatic hydroxylation and heteroatom oxidation

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Computational Methods.

The studies presented in this work use density functional theory (DFT) methods as implemented in the *Jaguar* and *Gaussian*-03 program packages.[1] We use the unrestricted B3LYP density functional method[2] combined with a basis set (BS1) that contains LACVP on Ni and 6-31G on the rest of the atoms for geometry optimizations and frequency calculations.[3] Further improvement of the energetics was obtained through single point calculations using an LACV3P+ basis set on Ni and 6-311+G* on the rest of the atoms; BS2. The geometry optimizations and frequency calculations using PPh_3 as a substrate were performed using basis set BS2. All local minima were characterized with real frequencies only, whereas the transition states have a single imaginary frequency for the correct mode of action. Transition states were located by running a geometry scan between two local minima by stepwise changing the reaction coordinate in a full geometry optimization with one degree of freedom fixed. The maximum point of these geometry scans was used as a starting point for the transition state optimizations and established that the transition state is indeed connected to the minima on each side of the barrier. These methods have been shown to accurately reproduce structures and free energies of activation of reaction processes of metal-oxo reactivities.[4] All energies reported in this work were taken from the UB3LYP/BS2 calculations and were corrected for ZPE. Test calculations with alternative density functional methods (see below) gave the same spin state ordering and only minor differences in relative energies.

To test the effect of the environment on the barrier heights we did single point calculations in a dielectric constant of $\varepsilon = 37.5$, however, these studies only gave minor changes in relative energies and no changes in the spin state ordering and regioselectivities.

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Table S1. Absolute energies, zero–point energies, free energies of UB3LYP/BS1 optimized geometries for the reaction of $^{2,4}\mathbf{R}_1$ with ethylbenzene (EB), xanthene (XA) and 1,4-cyclohexadiene (CHD). UB3LYP/BS2 single points and also solvent single points obtained from UB3LYP/BS2//UB3LYP/BS1.

Substrate	E (BS1) (au)	ZPE (BS1) (kcal/mol)	G (BS1) (au)	E (BS2) (au)	E+Esolvent (BS2)
$^{4}\mathbf{R}_{1EB}$	-1401.822804	402.344	-1401.245609	-1402.427109	-1402.500699
$^{2}\mathbf{R}_{1EB}$	-1401.818900	402.419	-1401.240799	-1402.422860	-1402.497500
$^{4}\mathbf{R}_{2XA}$	-1667.517644	425.014	-1666.906231	-1668.257425	-1668.334683
$^{2}\mathbf{R}_{2XA}$	-1667.512925	425.082	-1666.900609	-1668.252171	-1668.330251
$^{4}\mathbf{TS}_{1Ar}$	-1401.778050	401.606	-1401.200869	-1402.375927	-1402.441117
$^{2}\mathbf{TS}_{1Ar}$	-1401.780768	401.712	-1401.203215	-1402.378595	-1402.443501
$^{4}\mathbf{I}_{1Ar}$	-1401.783784	402.436	-1401.205448	-1402.386483	-1402.452802
$^{2}\mathbf{I}_{1Ar}$	-1401.783369	402.504	-1401.203126	-1402.386113	-1402.452234
$^{4}\mathbf{TS}_{1HA,EB}$	-1401.785000	398.572	-1401.209660	-1402.382532	-1402.453020
$^{4}\mathbf{TS}_{1HA,XA}$	-1667.480590	421.496	-1666.871889	-1668.210874	-1668.284460
$^{4}\mathbf{TS}_{2HA,XA}$	-1667.489415	421.508	-1666.880590	-1668.222933	-1668.296490
$^{4}\mathbf{TS}_{1HA,CHD}$	-1324.349079	376.811	-1323.808732	-1324.916136	-1324.987709
$^{2}\mathbf{TS}_{1HA,EB}$	-1401.786772	398.661	-1401.210547	-1402.384058	-1402.450293
$^{2}\mathbf{TS}_{1HA,XA}$	-1667.481956	421.604	-1666.872509	-1668.211635	-1668.283127
$^{2}\mathbf{TS}_{2HA,XA}$	-1667.489410	421.516	-1666.880241	-1668.222790	-1668.296212
$^{2}\mathbf{TS}_{1HA,CHD}$	-1324.350202	376.842	-1323.809203	-1324.916977	-1324.985976
$^{4}\mathbf{I}_{1HA,EB}$	-1401.799447	400.718	-1401.224250	-1402.402400	-1402.471397
$^{4}\mathbf{I}_{1HA,XA}$	-1667.501301	423.979	-1666.891213	-1668.237026	-1668.310894
$^{4}\mathbf{I}_{1HA,CHD}$	-1324.373889	379.095	-1323.833146	-1324.945781	-1325.015740
$^{2}\mathbf{I}_{1HA,EB}$	-1401.799354	400.871	-1401.222084	-1402.401882	-1402.470247
$^{2}\mathbf{I}_{1HA,XA}$	-1667.501891	423.985	-1666.891665	-1668.237984	-1668.308946
$^{2}\mathbf{I}_{1HA,CHD}$	-1324.373942	379.064	-1323.832618	-1324.945665	-1325.015540

Table S2. Relative energies of UB3LYP/BS1 optimized geometries for the reaction of $^{2,4}\mathbf{R}_1$ with ethylbenzene, xanthene and 1,4-cyclohexadiene. UB3LYP/BS2 single points and also solvent single points obtained from UB3LYP/BS2//UB3LYP/BS1.

	ΔE (BS1)	ΔE (BS2)	ΔE+ZPE (BS1)	ΔE+ZPE (BS2)	ΔG (BS1)	ΔG (BS2)	$\Delta E_{Solvent}$ (BS2)	$\Delta(E_{Solvent}+ZPE)$ (BS2)	$\Delta G+E_{Solvent}$ (BS2)
$^4\mathbf{R}_{1EB}$	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
$^2\mathbf{R}_{1EB}$	2.45	2.67	2.52	2.74	3.02	3.23	2.01	2.52	2.58
$^4\mathbf{R}_{2XA}$	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
$^2\mathbf{R}_{2XA}$	2.96	3.30	3.03	3.36	3.53	3.86	2.78	3.03	3.35
$^4\mathbf{TS}_{1Ar}$	28.08	32.12	27.35	31.38	28.07	32.11	37.39	27.35	37.38
$^2\mathbf{TS}_{1Ar}$	26.38	30.44	25.75	29.81	26.60	30.67	35.89	25.75	36.12
$^4\mathbf{I}_{1Ar}$	24.49	25.49	24.58	25.58	25.20	26.21	30.06	24.58	30.77
$^2\mathbf{I}_{1Ar}$	24.75	25.73	24.91	25.89	26.66	27.64	30.41	24.91	32.32
$^4\mathbf{TS}_{1HA,EB}$	23.72	27.97	19.95	24.20	22.56	26.81	29.92	19.95	28.75
$^4\mathbf{TS}_{1HA,XA}$	16.99	21.22	13.47	17.69	14.42	18.65	24.62	13.47	22.05
$^4\mathbf{TS}_{2HA,XA}$	11.21	17.29	8.21	14.29	22.84	28.92	27.92	8.21	39.55
$^4\mathbf{TS}_{1HA,CHD}$	17.76	22.02	14.16	18.41	16.04	20.30	24.07	14.16	22.36
$^2\mathbf{TS}_{1HA,EB}$	22.61	27.01	18.93	23.33	22.00	26.41	31.63	18.93	31.02
$^2\mathbf{TS}_{1HA,XA}$	16.13	20.74	12.72	17.32	14.03	18.64	25.45	12.72	23.35
$^2\mathbf{TS}_{2HA,XA}$	11.22	17.38	8.22	14.39	23.06	29.22	28.10	8.22	39.94
$^2\mathbf{TS}_{1HA,CHD}$	17.05	21.49	13.48	17.92	15.74	20.18	25.16	13.48	23.85
$^4\mathbf{I}_{1HA,EB}$	14.66	15.50	13.03	13.88	13.40	14.25	18.39	13.03	17.13
$^4\mathbf{I}_{1HA,XA}$	3.99	4.80	2.96	3.77	2.29	3.11	8.03	2.96	6.33
$^4\mathbf{I}_{1HA,CHD}$	2.19	3.41	0.87	2.10	0.72	1.94	6.48	0.87	5.01
$^2\mathbf{I}_{1HA,EB}$	14.71	15.83	13.24	14.36	14.76	15.88	19.11	13.24	19.16
$^2\mathbf{I}_{1HA,XA}$	3.62	4.20	2.59	3.17	2.01	2.59	9.25	2.59	7.64
$^2\mathbf{I}_{1HA,CHD}$	2.16	3.49	0.81	2.14	1.05	2.38	6.61	0.81	5.51

Table S3. Group spin densities and charges of UB3LYP/BS1 optimized geometries for the reaction of $^{2,4}\mathbf{R}_1$ with ethylbenzene, xanthene and 1,4-cyclohexadiene.

(a) Group spin densities.

	ρ_{Ni}	ρ_{O1}	ρ_{O2}	ρ_{TMC}	ρ_{SubH}	ρ_{Total}
$^4\mathbf{R}_{1EB}$	1.49	0.59	0.68	0.25	0.00	3.00
$^2\mathbf{R}_{1EB}$	1.54	-0.22	-0.57	0.25	0.00	1.00
$^4\mathbf{R}_{2XA}$	1.47	0.60	0.71	0.22	0.00	3.00
$^2\mathbf{R}_{2XA}$	1.53	-0.18	-0.57	0.23	0.00	1.00
$^4\mathbf{TS}_{1Ar}$	1.57	0.21	0.34	0.25	0.62	3.00
$^2\mathbf{TS}_{1Ar}$	1.55	0.15	-0.32	0.23	-0.61	1.00
$^4\mathbf{I}_{1Ar}$	1.58	0.19	0.06	0.26	0.92	3.00
$^2\mathbf{I}_{1Ar}$	1.57	0.16	-0.09	0.24	-0.89	1.00
	ρ_{Ni}	ρ_{O1}	ρ_{OH}	ρ_{TMC}	$\rho_{Sub.}$	ρ_{Total}
$^4\mathbf{TS}_{1HA,EB}$	1.54	0.29	0.32	0.24	0.61	3.00
$^4\mathbf{TS}_{1HA,XA}$	1.53	0.33	0.32	0.24	0.59	3.00
$^4\mathbf{TS}_{2HA,XA}$	1.51	0.35	0.34	0.21	0.58	3.00
$^4\mathbf{TS}_{1HA,CHD}$	1.53	0.32	0.35	0.23	0.57	3.00
$^2\mathbf{TS}_{1HA,EB}$	1.55	0.10	-0.29	0.24	-0.60	1.00
$^2\mathbf{TS}_{1HA,XA}$	1.54	0.07	-0.29	0.24	-0.56	1.00
$^2\mathbf{TS}_{2HA,XA}$	1.53	0.09	-0.28	0.21	-0.56	1.00
$^2\mathbf{TS}_{1HA,CHD}$	1.54	0.07	-0.31	0.24	-0.54	1.00
$^4\mathbf{I}_{1HA,EB}$	1.57	0.19	0.02	0.25	0.98	3.00
$^4\mathbf{I}_{1HA,XA}$	1.57	0.18	0.01	0.25	0.99	3.00
$^4\mathbf{I}_{1HA,CHD}$	1.57	0.18	0.02	0.25	0.98	3.00
$^2\mathbf{I}_{1HA,EB}$	1.57	0.18	-0.04	0.25	-0.96	1.00
$^2\mathbf{I}_{1HA,XA}$	1.57	0.18	-0.02	0.25	-0.99	1.00
$^2\mathbf{I}_{1HA,CHD}$	1.57	0.18	-0.03	0.25	-0.98	1.00

(b) Charges

	Q_{Ni}	Q_{O1}	Q_{O2}	Q_{TMC}	Q_{SubH}	Q_{Total}
$^4\mathbf{R}_{1EB}$	0.52	-0.29	-0.18	0.93	0.02	1.00
$^2\mathbf{R}_{1EB}$	0.54	-0.31	-0.19	0.95	0.01	1.00
$^4\mathbf{R}_{2XA}$	0.53	-0.28	-0.18	0.90	0.03	1.00
$^2\mathbf{R}_{2XA}$	0.55	-0.31	-0.19	0.92	0.03	1.00
$^4\mathbf{TS}_{1Ar}$	0.54	-0.44	-0.29	0.88	0.31	1.00
$^2\mathbf{TS}_{1Ar}$	0.53	-0.43	-0.29	0.87	0.31	1.00
$^4\mathbf{I}_{1Ar}$	0.54	-0.43	-0.34	0.90	0.34	1.00
$^2\mathbf{I}_{1Ar}$	0.54	-0.44	-0.34	0.89	0.34	1.00
	Q_{Ni}	Q_{O1}	Q_{OH}	Q_{TMC}	$Q_{Sub.}$	Q_{Total}
$^4\mathbf{TS}_{1HA,EB}$	0.53	-0.40	-0.01	0.88	-0.01	1.00

$^{4}\mathbf{TS}_{\mathbf{1}HA,XA}$	0.53	-0.39	0.01	0.89	-0.03	1.00
$^{4}\mathbf{TS}_{\mathbf{1}HA,CHD}$	0.53	-0.39	-0.01	0.88	-0.01	1.00
$^{4}\mathbf{TS}_{\mathbf{2}HA,CHD}$	0.53	-0.38	0.02	0.87	-0.04	1.00
$^{2}\mathbf{TS}_{\mathbf{1}HA,EB}$	0.53	-0.41	-0.01	0.89	0.01	1.00
$^{2}\mathbf{TS}_{\mathbf{1}HA,XA}$	0.53	-0.40	0.00	0.89	-0.02	1.00
$^{2}\mathbf{TS}_{\mathbf{2}HA,XA}$	0.53	-0.39	0.01	0.88	-0.03	1.00
$^{2}\mathbf{TS}_{\mathbf{1}HA,CHD}$	0.53	-0.40	-0.01	0.89	-0.01	1.00
$^{4}\mathbf{I}_{\mathbf{1}HA,EB}$	0.54	-0.43	-0.05	0.89	0.06	1.00
$^{4}\mathbf{I}_{\mathbf{1}HA,XA}$	0.54	-0.43	-0.05	0.89	0.06	1.00
$^{4}\mathbf{I}_{\mathbf{1}HA,CHD}$	0.54	-0.44	-0.05	0.89	0.06	1.00
$^{2}\mathbf{I}_{\mathbf{1}HA,EB}$	0.54	-0.44	-0.05	0.89	0.06	1.00
$^{2}\mathbf{I}_{\mathbf{1}HA,XA}$	0.54	-0.44	-0.05	0.89	0.06	1.00
$^{2}\mathbf{I}_{\mathbf{1}HA,CHD}$	0.54	-0.44	-0.05	0.89	0.06	1.00

Table S4. Group spin densities and charges of UB3LYP/BS2 single points on UB3LYP/BS1 optimized geometries for the reaction of $^{2,4}\mathbf{R}_1$ with ethylbenzene, xanthene and 1,4-cyclohexadiene.

(a) Group spin densities.

	ρ_{Ni}	ρ_{O1}	ρ_{O2}	ρ_{TMC}	ρ_{SubH}	ρ_{Total}
$^4\mathbf{R}_{1EB}$	1.54	0.57	0.68	0.21	0.00	3.00
$^2\mathbf{R}_{1EB}$	1.59	-0.22	-0.58	0.21	0.00	1.00
$^4\mathbf{R}_{2XA}$	1.51	0.58	0.70	0.21	0.00	3.00
$^2\mathbf{R}_{2XA}$	1.58	-0.19	-0.58	0.19	0.00	1.00
$^4\mathbf{TS}_{1Ar}$	1.63	0.19	0.31	0.21	0.67	3.00
$^2\mathbf{TS}_{1Ar}$	1.61	0.15	-0.29	0.19	-0.66	1.00
$^4\mathbf{I}_{1Ar}$	1.63	0.17	0.04	0.22	0.95	3.00
$^2\mathbf{I}_{1Ar}$	1.61	0.16	-0.06	0.21	-0.92	1.00
	ρ_{Ni}	ρ_{O1}	ρ_{OH}	ρ_{TMC}	$\rho_{Sub.}$	ρ_{Total}
$^4\mathbf{TS}_{1HA,EB}$	1.59	0.26	0.31	0.21	0.63	3.00
$^4\mathbf{TS}_{1HA,XA}$	1.58	0.30	0.31	0.21	0.60	3.00
$^4\mathbf{TS}_{2HA,XA}$	1.57	0.32	0.32	0.19	0.60	3.00
$^4\mathbf{TS}_{1HA,CHD}$	1.58	0.30	0.33	0.21	0.58	3.00
$^2\mathbf{TS}_{1HA,EB}$	1.60	0.10	-0.29	0.20	-0.62	1.00
$^2\mathbf{TS}_{1HA,XA}$	1.59	0.07	-0.29	0.21	-0.57	1.00
$^2\mathbf{TS}_{2HA,XA}$	1.59	0.09	-0.28	0.18	-0.57	1.00
$^2\mathbf{TS}_{1HA,CHD}$	1.59	0.06	-0.31	0.21	-0.55	1.00
$^4\mathbf{I}_{1HA,EB}$	1.62	0.17	0.01	0.21	0.99	3.00
$^4\mathbf{I}_{1HA,XA}$	1.62	0.16	0.00	0.22	1.00	3.00
$^4\mathbf{I}_{1HA,CHD}$	1.62	0.16	0.01	0.22	0.99	3.00
$^2\mathbf{I}_{1HA,EB}$	1.62	0.17	-0.02	0.21	-0.98	1.00
$^2\mathbf{I}_{1HA,XA}$	1.62	0.17	-0.01	0.22	-0.99	1.00
$^2\mathbf{I}_{1HA,CHD}$	1.62	0.17	-0.02	0.21	-0.99	1.00

(b) Charges

	Q_{Ni}	Q_{O1}	Q_{O2}	Q_{TMC}	Q_{SubH}	Q_{Total}
$^4\mathbf{R}_{1EB}$	0.40	-0.12	-0.12	0.88	-0.04	1.00
$^2\mathbf{R}_{1EB}$	0.39	-0.14	-0.13	0.91	-0.03	1.00
$^4\mathbf{R}_{2XA}$	0.46	-0.09	-0.12	0.73	0.02	1.00
$^2\mathbf{R}_{2XA}$	0.46	-0.12	-0.12	0.77	0.02	1.00
$^4\mathbf{TS}_{1Ar}$	0.39	-0.28	0.00	0.83	0.06	1.00
$^2\mathbf{TS}_{1Ar}$	0.38	-0.28	0.00	0.84	0.06	1.00
$^4\mathbf{I}_{1Ar}$	0.45	-0.32	-0.02	0.84	0.05	1.00
$^2\mathbf{I}_{1Ar}$	0.48	-0.34	-0.04	0.82	0.07	1.00
	Q_{Ni}	Q_{O1}	Q_{OH}	Q_{TMC}	$Q_{Sub.}$	Q_{Total}
$^4\mathbf{TS}_{1HA,EB}$	0.45	-0.27	0.16	0.84	-0.18	1.00

$^{4}\mathbf{TS}_{\mathbf{1}HA,XA}$	0.49	-0.25	0.13	0.87	-0.24	1.00
$^{4}\mathbf{TS}_{\mathbf{2}HA,XA}$	0.45	-0.13	0.19	0.72	-0.24	1.00
$^{4}\mathbf{TS}_{\mathbf{1}HA,CHD}$	0.42	-0.22	0.06	0.90	-0.16	1.00
$^{2}\mathbf{TS}_{\mathbf{1}HA,EB}$	0.32	-0.21	0.12	0.97	-0.21	1.00
$^{2}\mathbf{TS}_{\mathbf{2}HA,EB}$	0.43	-0.12	0.19	0.73	-0.24	1.00
$^{2}\mathbf{TS}_{\mathbf{1}HA,XA}$	0.39	-0.18	0.13	0.88	-0.22	1.00
$^{2}\mathbf{TS}_{\mathbf{1}HA,CHD}$	0.41	-0.24	0.08	0.91	-0.16	1.00
$^{4}\mathbf{I}_{\mathbf{1}HA,EB}$	0.41	-0.32	0.10	0.91	-0.10	1.00
$^{4}\mathbf{I}_{\mathbf{1}HA,XA}$	0.45	-0.32	0.01	0.94	-0.08	1.00
$^{4}\mathbf{I}_{\mathbf{1}HA,CHD}$	0.45	-0.34	0.01	0.93	-0.05	1.00
$^{2}\mathbf{I}_{\mathbf{1}HA,EB}$	0.43	-0.34	0.04	0.99	-0.12	1.00
$^{2}\mathbf{I}_{\mathbf{1}HA,XA}$	0.41	-0.34	0.05	0.99	-0.11	1.00
$^{2}\mathbf{I}_{\mathbf{1}HA,CHD}$	0.44	-0.34	0.02	0.93	-0.05	1.00

Table S5. Group spin densities and charges of UB3LYP/BS2 solvent single points on UB3LYP/BS1 optimized geometries for the reaction of $^{2,4}\mathbf{R}_1$ with ethylbenzene, xanthene and 1,4-cyclohexadiene.

(a) Group spin densities.

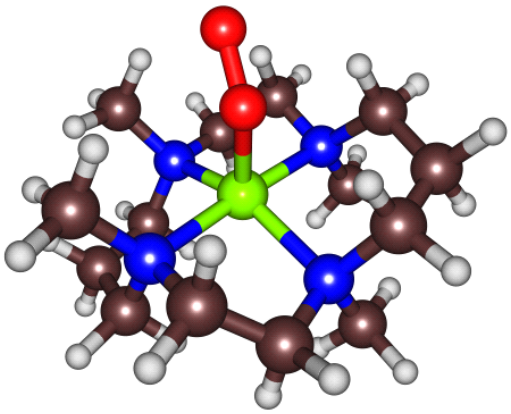
	ρ_{Ni}	ρ_{O1}	ρ_{O2}	ρ_{TMC}	ρ_{SubH}	ρ_{Total}
$^4\mathbf{R}_{1EB}$	1.57	0.56	0.63	0.24	0.00	3.00
$^2\mathbf{R}_{1EB}$	1.62	-0.28	-0.57	0.23	0.00	1.00
$^4\mathbf{R}_{2XA}$	1.56	0.56	0.64	0.24	0.00	3.00
$^2\mathbf{R}_{2XA}$	1.62	-0.25	-0.58	0.22	0.00	1.00
$^4\mathbf{TS}_{1Ar}$	1.64	0.17	0.33	0.22	0.63	3.00
$^2\mathbf{TS}_{1Ar}$	1.63	0.11	-0.32	0.20	-0.63	1.00
$^4\mathbf{I}_{1Ar}$	1.64	0.14	0.05	0.23	0.95	3.00
$^2\mathbf{I}_{1Ar}$	1.62	0.15	-0.07	0.22	-0.92	1.00
	ρ_{Ni}	ρ_{O1}	ρ_{OH}	ρ_{TMC}	$\rho_{Sub.}$	ρ_{Total}
$^4\mathbf{TS}_{1HA,EB}$	1.62	0.24	0.30	0.23	0.61	3.00
$^4\mathbf{TS}_{1HA,XA}$	1.61	0.29	0.30	0.24	0.56	3.00
$^4\mathbf{TS}_{2HA,XA}$	1.61	0.31	0.31	0.22	0.55	3.00
$^4\mathbf{TS}_{1HA,CHD}$	1.61	0.28	0.31	0.24	0.56	3.00
$^2\mathbf{TS}_{1HA,EB}$	1.62	0.05	-0.29	0.21	-0.59	1.00
$^2\mathbf{TS}_{1HA,XA}$	1.61	0.00	-0.30	0.22	-0.53	1.00
$^2\mathbf{TS}_{2HA,XA}$	1.62	0.01	-0.30	0.20	-0.53	1.00
$^2\mathbf{TS}_{1HA,CHD}$	1.61	0.01	-0.32	0.22	-0.52	1.00
$^4\mathbf{I}_{1HA,EB}$	1.64	0.14	0.01	0.22	0.99	3.00
$^4\mathbf{I}_{1HA,XA}$	1.63	0.14	0.00	0.23	1.00	3.00
$^4\mathbf{I}_{1HA,CHD}$	1.63	0.14	0.01	0.23	0.99	3.00
$^2\mathbf{I}_{1HA,EB}$	1.63	0.14	-0.02	0.22	-0.98	1.00
$^2\mathbf{I}_{1HA,XA}$	1.63	0.14	-0.01	0.23	-0.99	1.00
$^2\mathbf{I}_{1HA,CHD}$	1.64	0.14	-0.01	0.23	-0.99	1.00

(b) Charges

	Q_{Ni}	Q_{O1}	Q_{O2}	Q_{TMC}	Q_{SubH}	Q_{Total}
$^4\mathbf{R}_{1EB}$	0.41	-0.14	-0.20	0.96	-0.03	1.00
$^2\mathbf{R}_{1EB}$	0.41	-0.16	-0.21	0.98	-0.03	1.00
$^4\mathbf{R}_{2XA}$	0.49	-0.13	-0.21	0.83	0.01	1.00
$^2\mathbf{R}_{2XA}$	0.50	-0.15	-0.21	0.85	0.01	1.00
$^4\mathbf{TS}_{1Ar}$	0.41	-0.30	0.02	0.87	0.00	1.00
$^2\mathbf{TS}_{1Ar}$	0.40	-0.30	0.02	0.89	-0.01	1.00
$^4\mathbf{I}_{1Ar}$	0.47	-0.34	-0.02	0.88	0.01	1.00
$^2\mathbf{I}_{1Ar}$	0.50	-0.36	-0.03	0.85	0.04	1.00
	Q_{Ni}	Q_{O1}	Q_{OH}	Q_{TMC}	$Q_{Sub.}$	Q_{Total}
$^4\mathbf{TS}_{1HA,EB}$	0.47	-0.33	0.13	0.93	-0.19	1.00

$^{4}\mathbf{TS}_{\mathbf{1}HA,XA}$	0.51	-0.29	0.09	0.96	-0.26	1.00
$^{4}\mathbf{TS}_{\mathbf{2}HA,XA}$	0.47	-0.15	0.13	0.81	-0.27	1.00
$^{4}\mathbf{TS}_{\mathbf{1}HA,CHD}$	0.45	-0.27	0.01	0.98	-0.17	1.00
$^{2}\mathbf{TS}_{\mathbf{1}HA,EB}$	0.34	-0.20	0.10	1.01	-0.24	1.00
$^{2}\mathbf{TS}_{\mathbf{1}HA,XA}$	0.40	-0.17	0.09	0.95	-0.27	1.00
$^{2}\mathbf{TS}_{\mathbf{2}HA,XA}$	0.46	-0.13	0.14	0.81	-0.28	1.00
$^{2}\mathbf{TS}_{\mathbf{1}HA,CHD}$	0.43	-0.24	0.04	0.97	-0.19	1.00
$^{4}\mathbf{I}_{\mathbf{1}HA,EB}$	0.45	-0.39	0.07	0.96	-0.09	1.00
$^{4}\mathbf{I}_{\mathbf{1}HA,XA}$	0.48	-0.38	-0.03	1.00	-0.08	1.00
$^{4}\mathbf{I}_{\mathbf{1}HA,CHD}$	0.49	-0.38	-0.05	0.98	-0.04	1.00
$^{2}\mathbf{I}_{\mathbf{1}HA,EB}$	0.45	-0.34	-0.01	1.02	-0.11	1.00
$^{2}\mathbf{I}_{\mathbf{1}HA,XA}$	0.43	-0.36	0.01	1.02	-0.10	1.00
$^{2}\mathbf{I}_{\mathbf{1}HA,CHD}$	0.48	-0.38	-0.04	0.98	-0.05	1.00

(a)



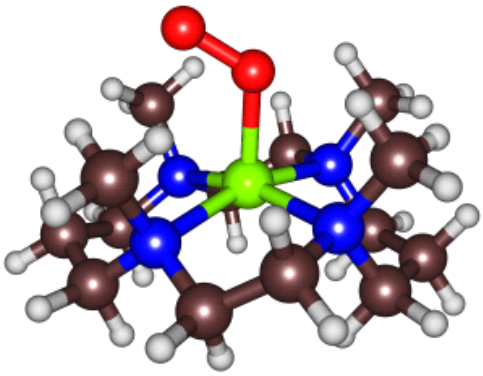
r_{Ni-O} = 2.005 (2.001)

r_{Ni-N1} = 2.146 (2.146)
r_{Ni-N2} = 2.141 (2.136)
r_{Ni-N3} = 2.177 (2.177)
r_{Ni-N4} = 2.165 (2.165)

r_{O-O} = 1.363 (1.373)

$^4R_1$ ($^2R_1$)

(b)



r_{Ni-O} = 1.992 (1.984)

r_{Ni-N1} = 2.200 (2.197)
r_{Ni-N2} = 2.200 (2.197)
r_{Ni-N3} = 2.207 (2.206)
r_{Ni-N4} = 2.205 (2.206)

r_{O-O} = 1.354 (1.367)

$^4R_2$ ($^2R_2$)

Figure S1. Optimized geometries of (a)-^{4,2}**R$_1$** and (b)-^{4,2}**R$_2$** as obtained at UB3LYP/BS1 in Jaguar. Bond lengths are in angstroms.

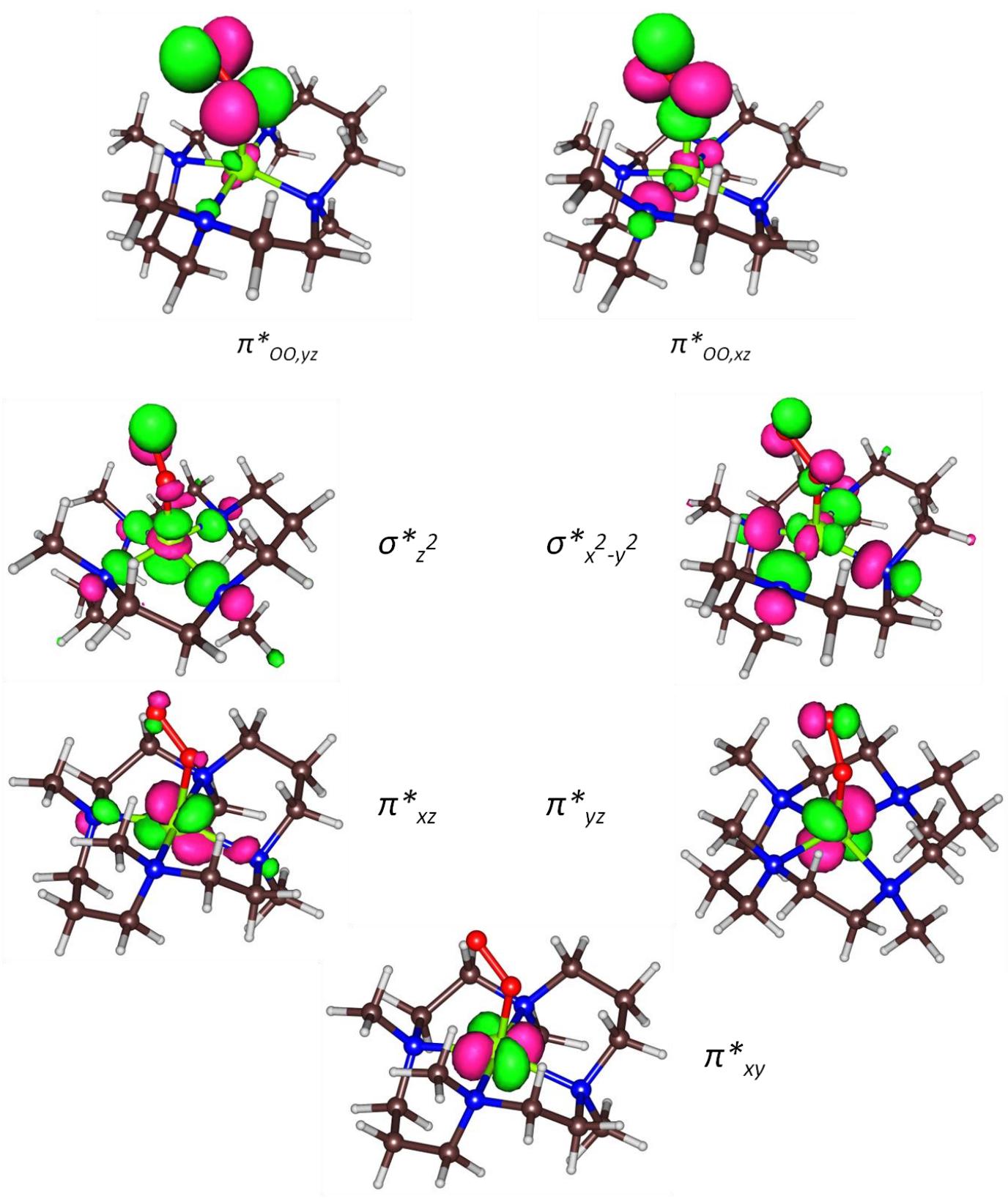


Figure S2. Molecular orbital of of ^{4,2}NiOO(TMC) as obtained at UB3LYP/BS1 in Jaguar.

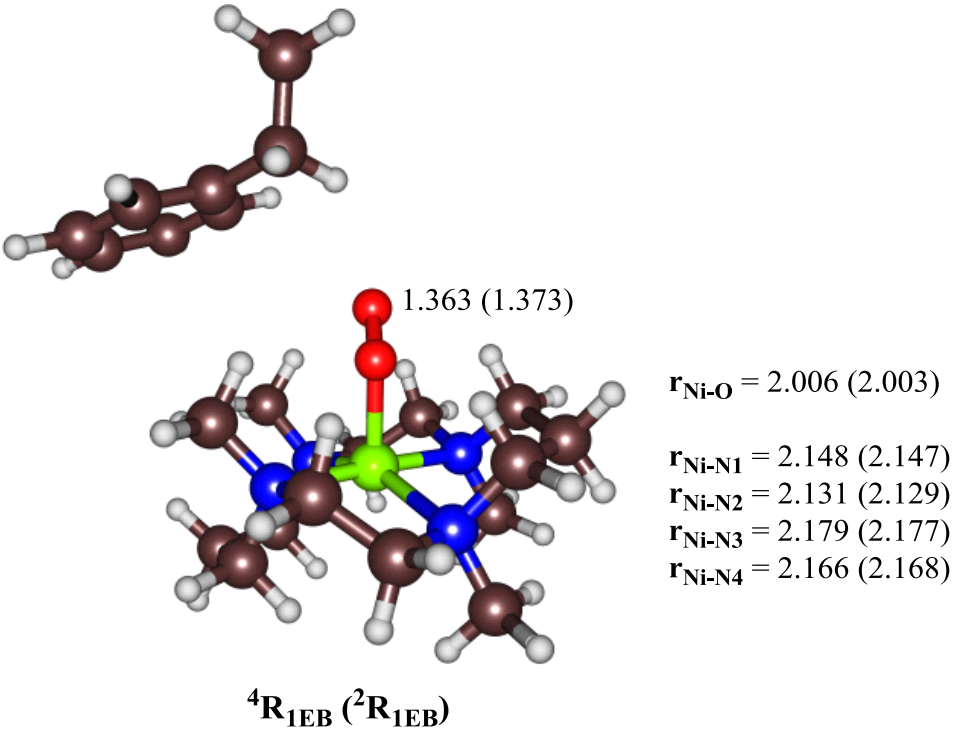


Figure S3. Optimized geometries of $^{4,2}\mathbf{R}_{1EB}$ and as obtained at UB3LYP/BS1 in Jaguar. Bond lengths are in angstroms.

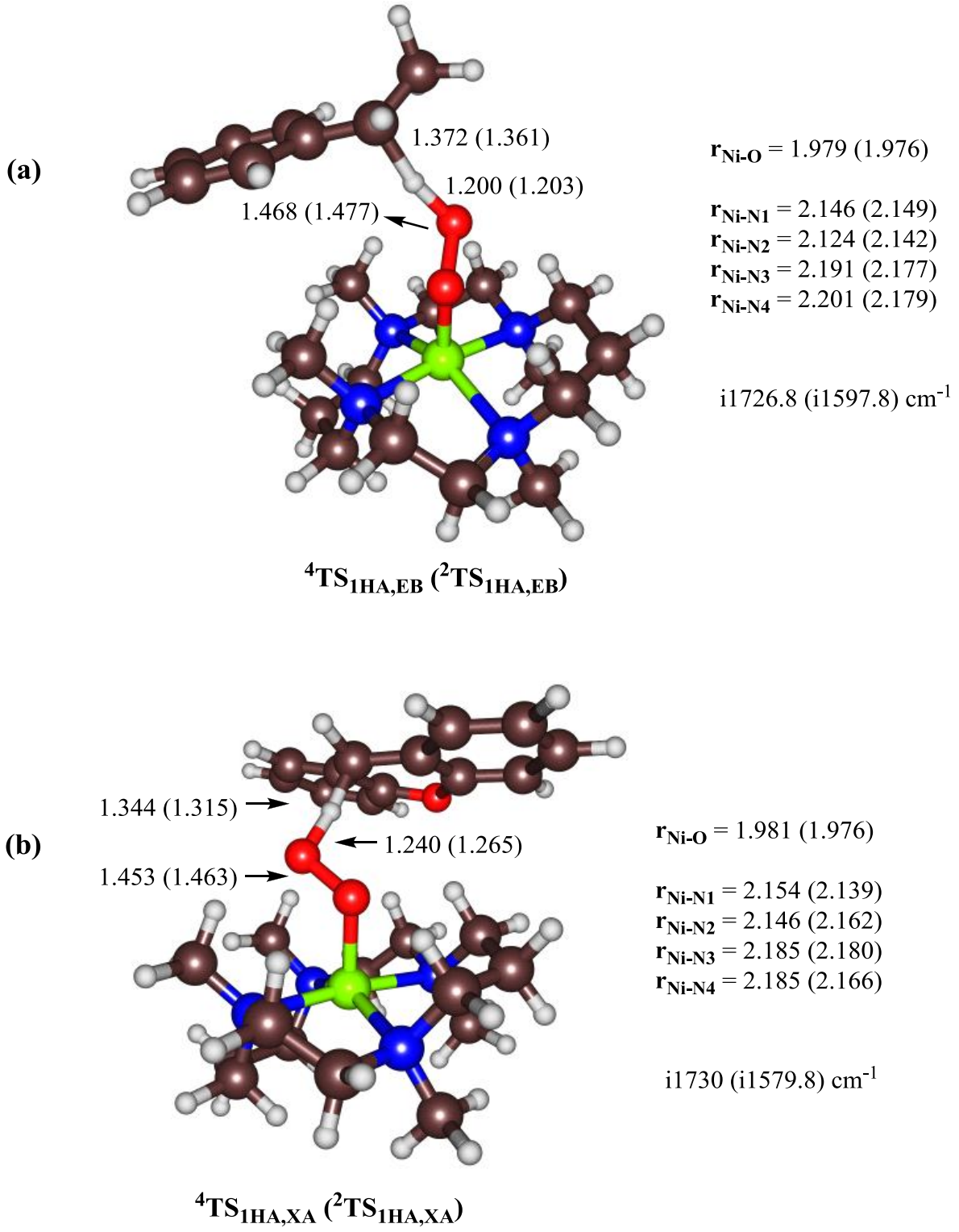


Figure S4. Optimized geometries of (a)-^{4,2}**TS**$_{1HA,EB}$ and (b)-^{4,2}**TS**$_{1HA,XA}$ as obtained at UB3LYP/BS1 in Jaguar. Bond lengths and imaginary frequencies are in angstroms and wave numbers respectively.

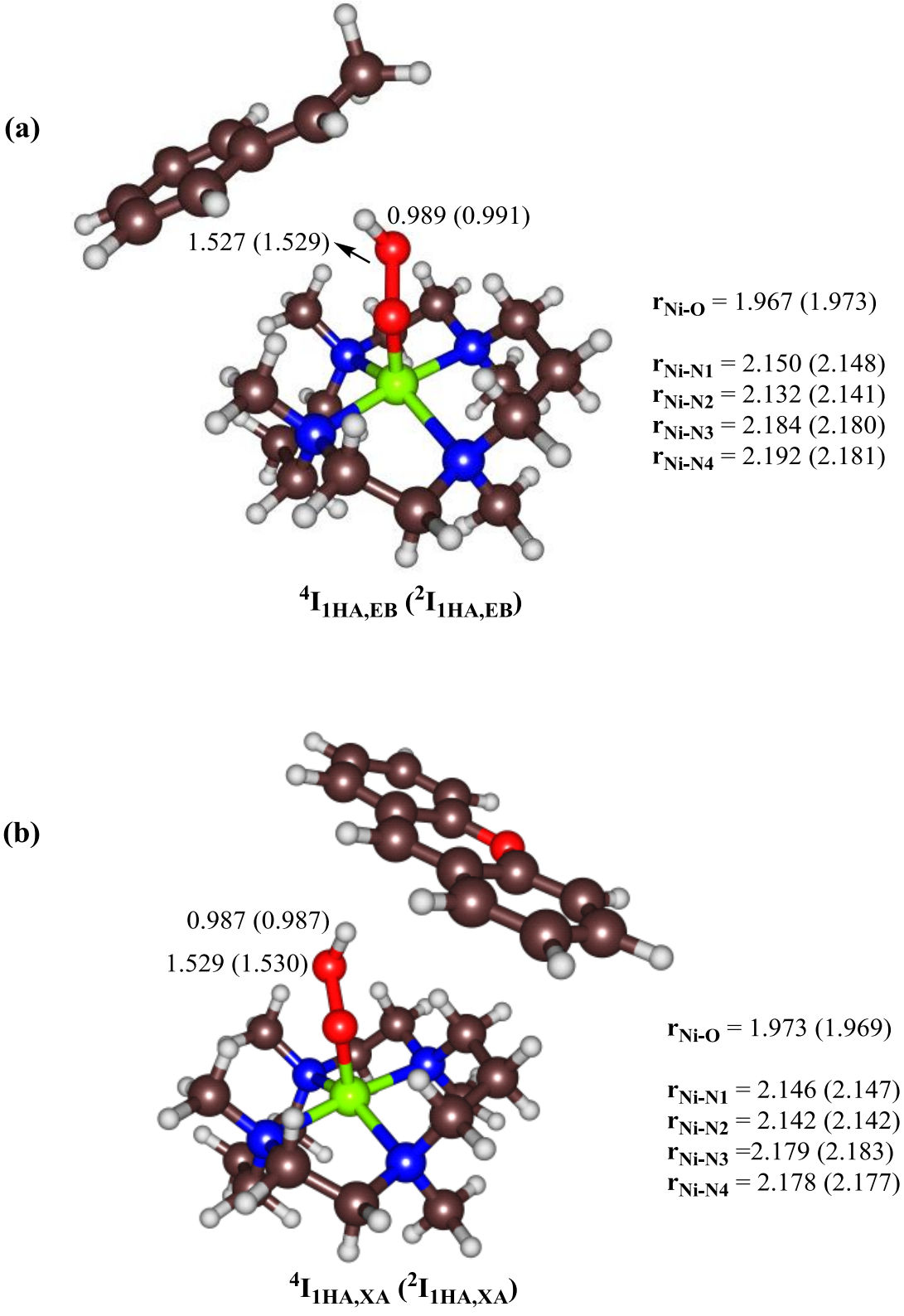


Figure S5. Optimized geometries of (a)-$^{4,2}\mathbf{I}_{1HA,EB}$ and (b)-$^{4,2}\mathbf{I}_{1HA,XA}$ as obtained at UB3LYP/BS1 in Jaguar with bond lengths given in angstroms.

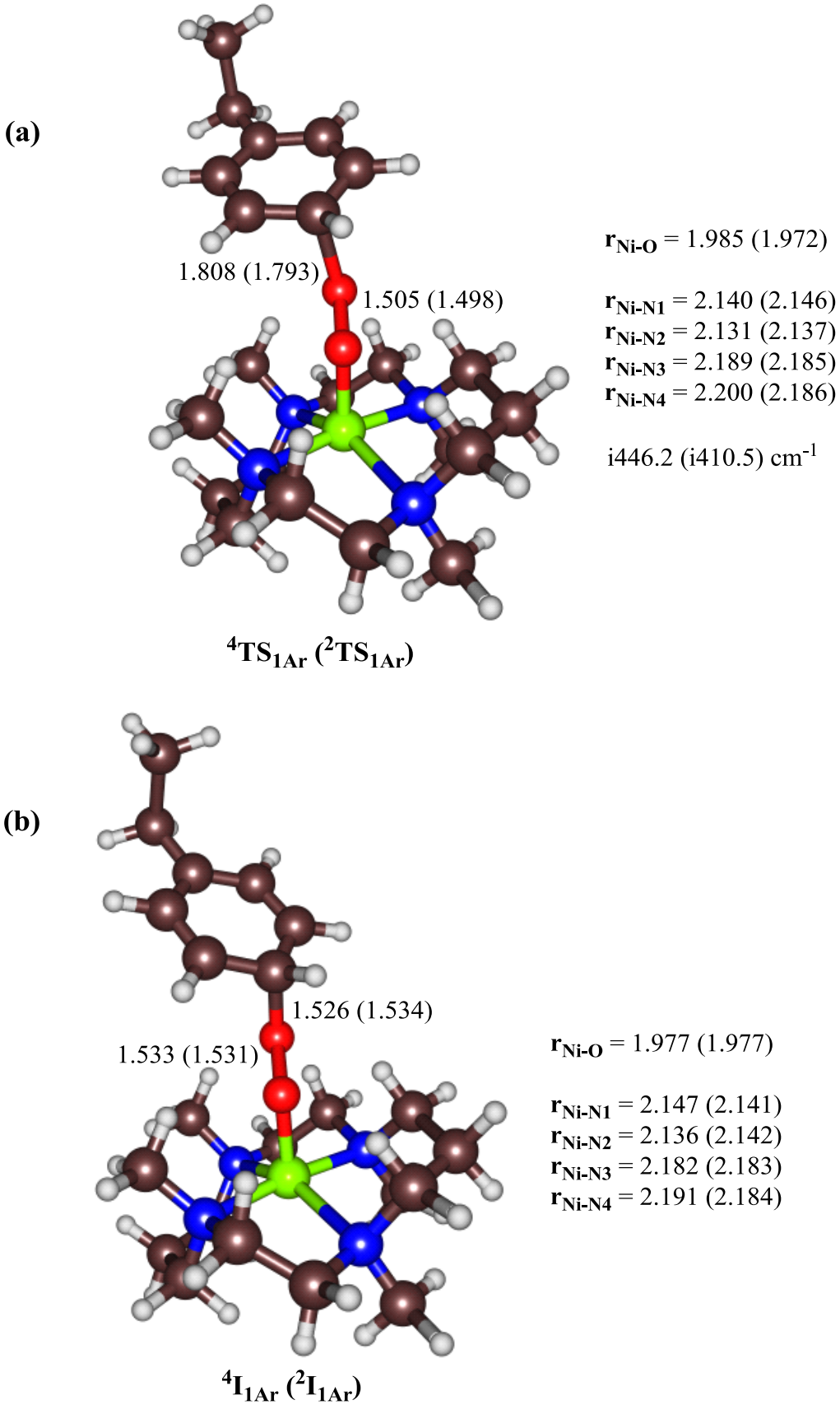


Figure S6. Optimized geometries of (a)- $^{4,2}TS_{1Ar}$ and (b)- $^{4,2}I_{1Ar}$ as obtained at UB3LYP/BS1 in Jaguar. Bond lengths and imaginary frequencies are in angstroms and wave numbers respectively.

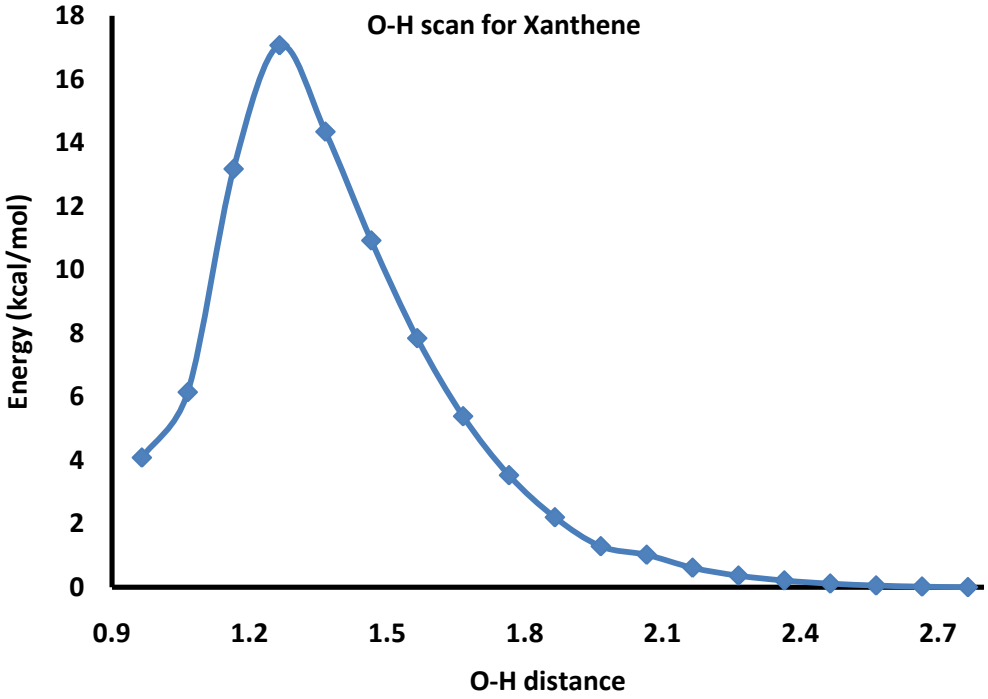


Figure S7. Hydrogen atom transfer scan starting from $^{4}\mathbf{R}_{1XA}$ in the direction of an Ni(II)-hydroperoxo complex. Energies are given in kcal mol^{-1}.

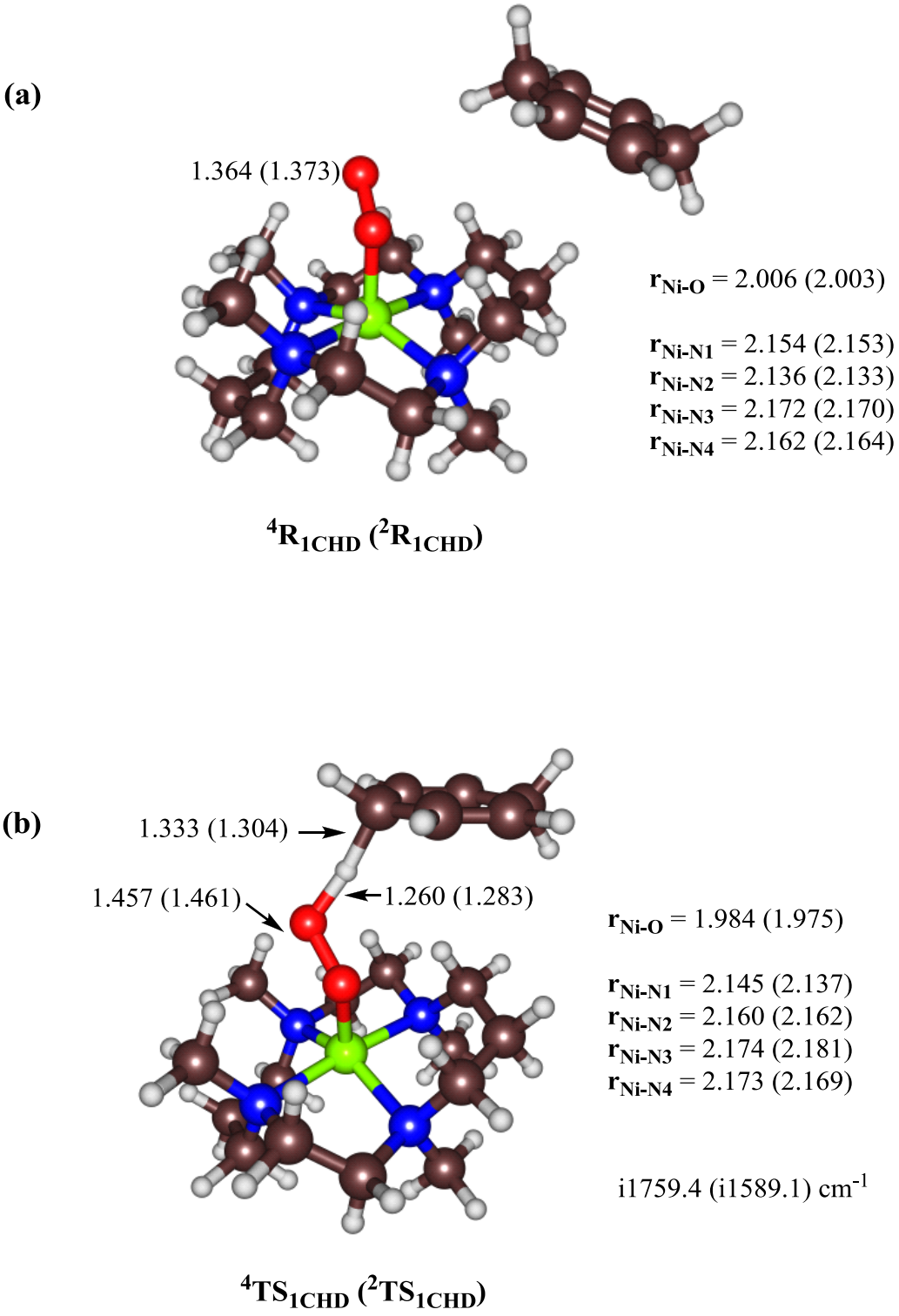


Figure S8. Optimized geometries of (a)- $^{4,2}\mathbf{R}_{1CHD}$ and (b)- $^{4,2}\mathbf{TS}_{1HA,CHD}$ as obtained at UB3LYP/BS1 in Jaguar. Bond lengths and imaginary frequencies are in angstroms and wave numbers respectively.

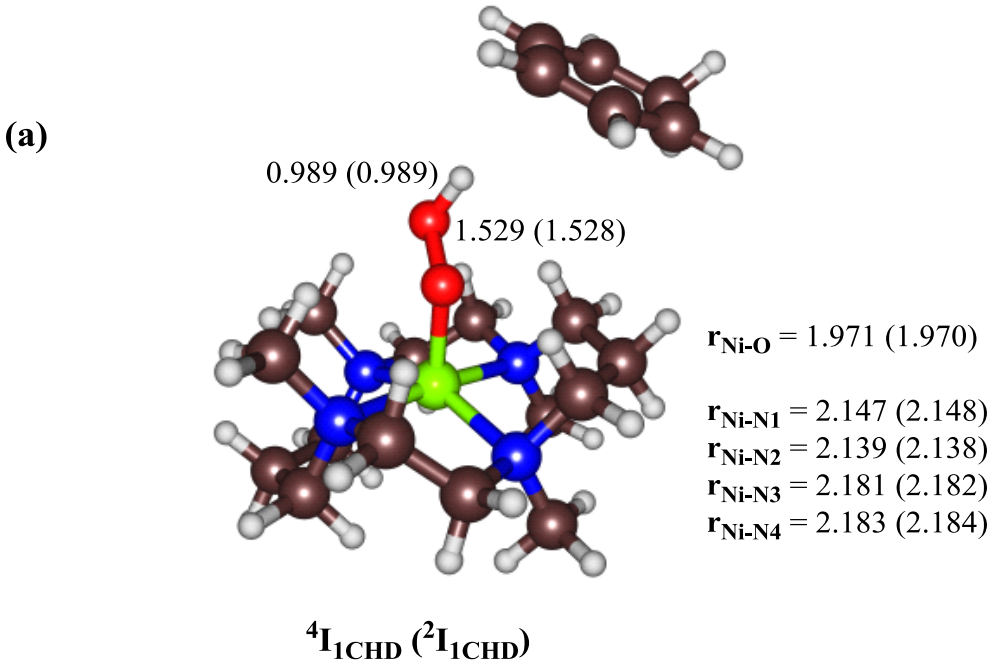


Figure S9. Optimized geometries of $^{4,2}I_{1HA,CHD}$ as obtained at UB3LYP/BS1 in Jaguar. Bond lengths are in angstroms.

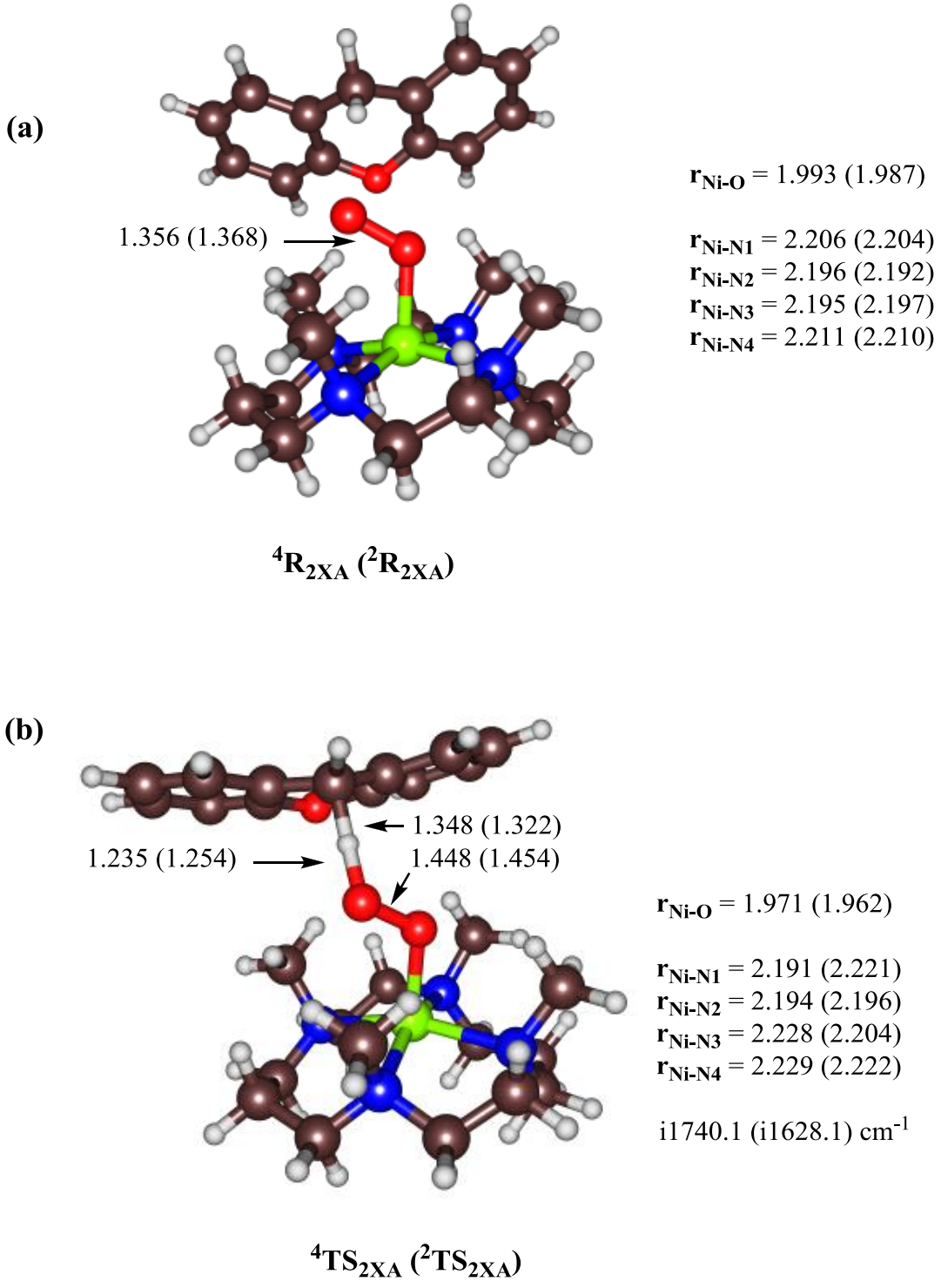
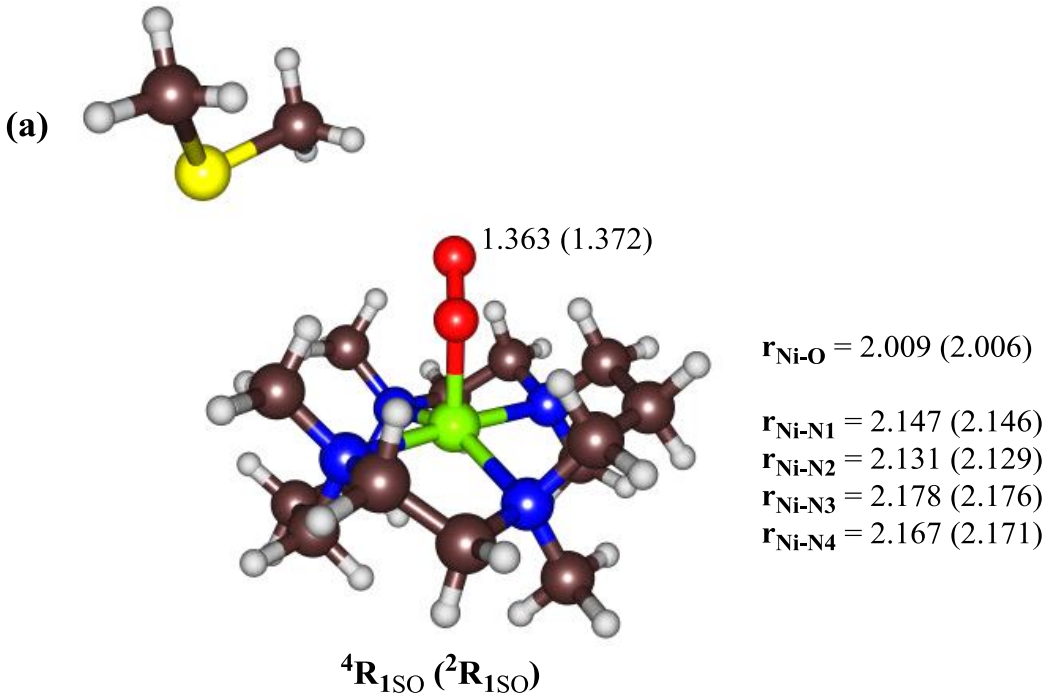


Figure S10. Optimized geometries of (a)-$^{4,2}\mathbf{R}_{2HA,XA}$ and (b)-$^{4,2}\mathbf{TS}_{2HA,XA}$ as obtained at UB3LYP/BS1 in Jaguar. Bond lengths and imaginary frequencies are in angstroms and wave numbers respectively.



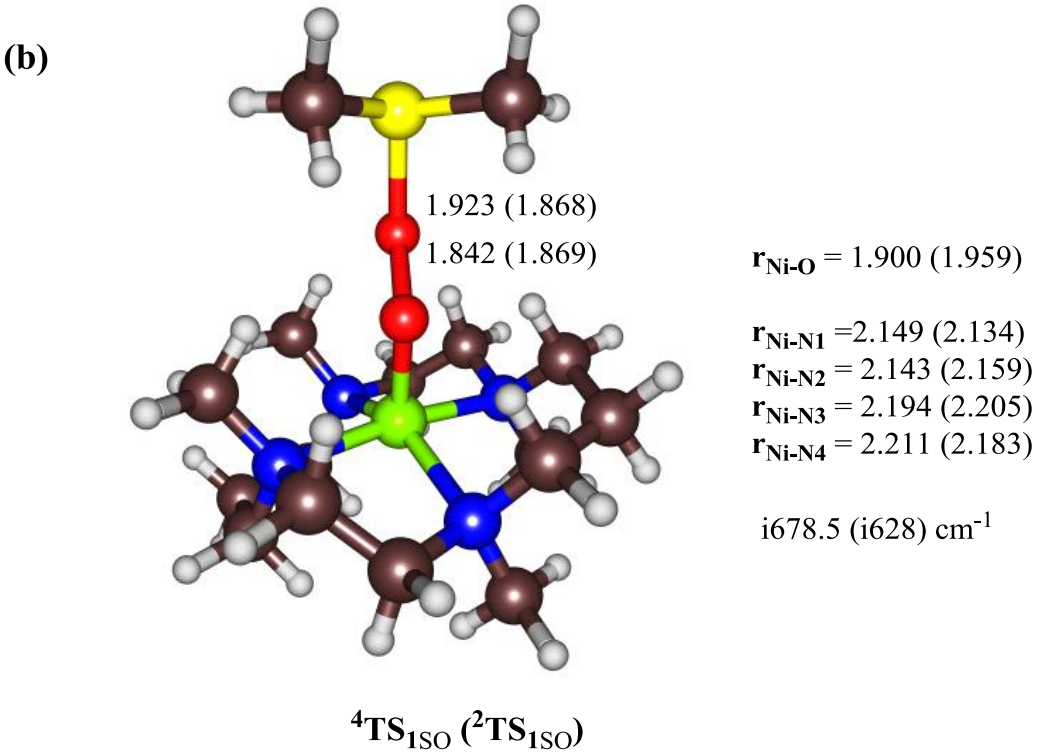


Figure S11. Optimized geometries of (a)- $^{4,2}\mathbf{R}_{1SO}$ and (b)- $^{4,2}\mathbf{TS}_{1SO}$ as obtained at UB3LYP/BS1 in Jaguar. Bond lengths and imaginary frequencies are in angstroms and wave numbers respectively.

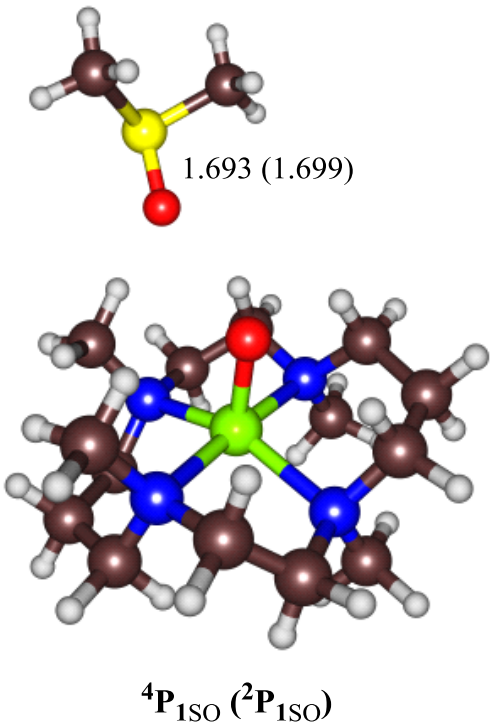


Figure S12. Optimized geometries of $^{4,2}P_{1SO}$ as obtained at UB3LYP/BS1 in Jaguar. Bond lengths are in angstroms.

Table S6. Relative energies for the sulfoxidation reaction of dimethylsulfide (DMS) by $^{2,4}[Ni^{II}OO(TMC)]^{+}$ as calculated with UB3LYP/BS1. Single point calculations done in solvent and with basis set BS2. ZPE calculated at UB3LYP/BS1.

	Basis set BS1					Basis set BS2			
	ΔE	ΔE+solv	ΔE+ZPE	ΔE+ZPE+Solv	ΔG	ΔE	ΔE+solv	ΔE+ZPE	ΔE+ZPE+Solv
$^{2}\mathbf{R_1}$ + DMS	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
$^{4}\mathbf{R_1}$ + DMS	-2.54	-1.82	-2.58	-1.86	-3.00	-2.79	-2.07	-2.83	-2.11
$^{2}\mathbf{R_1C}$	-3.43	1.52	-3.14	1.81	6.88	-2.40	2.55	-2.11	2.84
$^{4}\mathbf{R_1C}$	-5.83	-0.41	-5.70	-0.29	6.21	-5.11	0.30	-4.99	0.43
$^{2}\mathbf{TS_{1SO}}$	32.97	46.73	32.67	46.43	43.88	31.41	45.17	31.11	44.86
$^{4}\mathbf{TS_{1SO}}$	32.82	46.63	32.58	46.38	43.43	33.66	47.46	33.41	47.22
$^{2}\mathbf{P_{1SO}}$	22.10	31.52	22.05	31.46	33.53	6.49	15.90	6.44	15.85
$^{4}\mathbf{P_{1SO}}$	18.73	27.69	18.52	27.48	25.05	0.75	9.71	0.55	9.50

Table S7. Group spin densities and charges of UB3LYP/BS1 optimized geometries for the reaction of dimethylsulfide (DMS) with $^{2,4}[Ni^{II}OO(TMC)]^{+}$.

(a) BS1 Group Spin Densities and Group Charges

	Spin Densities					Group Charges				
	Ni	O1	O2	TMC	DMS	Ni	O1	O2	TMC	DMS
$^{2}\mathbf{R_1}$	1.53	-0.21	-0.57	0.25	-	0.55	-0.31	-0.19	0.94	-
$^{4}\mathbf{R_1}$	1.48	0.59	0.69	0.25	-	0.54	-0.29	-0.18	0.93	-
$^{2}\mathbf{R_1C}$	1.54	-0.23	-0.57	0.26	0.00	0.55	-0.31	-0.20	0.95	0.01
$^{4}\mathbf{R_1C}$	1.49	0.59	0.67	0.25	0.00	0.53	-0.28	-0.19	0.94	0.01
$^{2}\mathbf{TS_{1SO}}$	1.54	-0.39	-0.16	0.21	-0.20	0.49	-0.49	-0.46	0.81	0.65
$^{4}\mathbf{TS_{1SO}}$	1.58	0.75	0.16	0.25	0.26	0.50	-0.48	-0.43	0.81	0.61
$^{2}\mathbf{P_{1SO}}$	1.58	-0.82	-0.01	0.24	0.01	0.50	-0.46	-0.68	0.88	0.76
$^{4}\mathbf{P_{1SO}}$	1.53	1.19	0.00	0.28	0.00	0.48	-0.44	-0.69	0.89	0.77

(b) BS1-Solv. Group Spin Densities and Group Charges

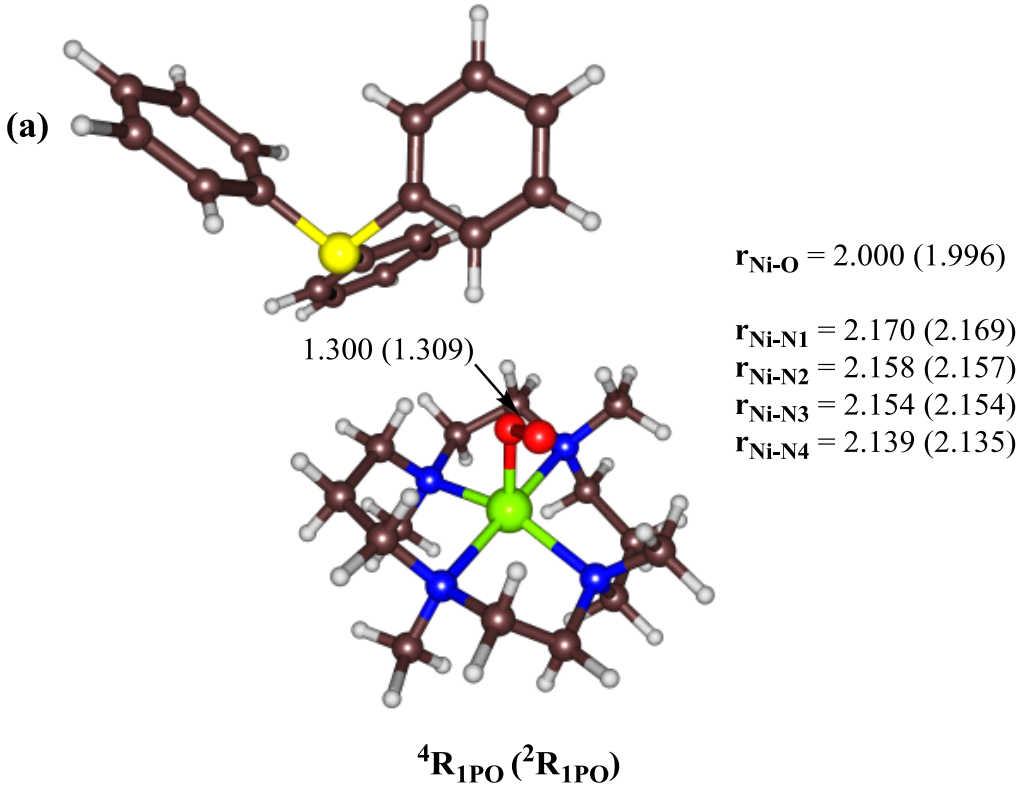
	Spin Densities					Group Charges				
	Ni	O1	O2	TMC	DMS	Ni	O1	O2	TMC	DMS
$^{2}\mathbf{R_1}$	1.57	-0.30	-0.56	0.28	-	0.55	-0.32	-0.27	1.03	-
$^{4}\mathbf{R_1}$	1.53	0.57	0.61	0.28	-	0.54	-0.30	-0.27	1.02	-
$^{2}\mathbf{R_1C}$	1.57	-0.29	-0.56	0.28	0.00	0.55	-0.32	-0.25	1.03	0.00
$^{4}\mathbf{R_1C}$	1.53	0.57	0.62	0.28	0.00	0.53	-0.30	-0.25	1.02	0.00
$^{2}\mathbf{TS_{1SO}}$	1.55	-0.41	-0.15	0.22	-0.21	0.48	-0.49	-0.47	0.84	0.64
$^{4}\mathbf{TS_{1SO}}$	1.59	0.74	0.16	0.25	0.26	0.49	-0.48	-0.43	0.84	0.59
$^{2}\mathbf{P_{1SO}}$	1.59	-0.83	-0.01	0.24	0.01	0.49	-0.48	-0.72	0.92	0.78
$^{4}\mathbf{P_{1SO}}$	1.56	1.14	0.00	0.30	0.00	0.48	-0.50	-0.71	0.94	0.78

(c) BS2 Group Spin Densities and Group Charges

	Spin Densities					Group Charges				
	Ni	O1	O2	TMC	DMS	Ni	O1	O2	TMC	DMS
$^{2}\mathbf{R_1}$	1.58	-0.21	-0.58	0.21	-	0.48	-0.18	-0.16	0.86	-
$^{4}\mathbf{R_1}$	1.53	0.57	0.68	0.22	-	0.48	-0.16	-0.15	0.83	-
$^{2}\mathbf{R_1C}$	1.59	-0.22	-0.58	0.21	0.00	0.41	-0.17	-0.16	0.93	-0.02
$^{4}\mathbf{R_1C}$	1.53	0.57	0.67	0.22	0.00	0.41	-0.15	-0.15	0.91	-0.02
$^{2}\mathbf{TS_{1SO}}$	1.59	-0.41	-0.13	0.17	-0.22	0.44	-0.44	-0.29	0.82	0.48
$^{4}\mathbf{TS_{1SO}}$	1.65	0.73	0.12	0.21	0.29	0.31	-0.37	-0.27	0.87	0.45
$^{2}\mathbf{P_{1SO}}$	1.64	-0.84	-0.01	0.20	0.00	0.40	-0.31	-0.63	0.91	0.62
$^{4}\mathbf{P_{1SO}}$	1.59	1.16	0.00	0.24	0.00	0.40	-0.30	-0.50	0.84	0.56

Table S8. Absolute energues of UB3LYP/BS1 optimized geometries for the reaction of dimethylsulfide (DMS) with $^{2,4}[Ni^{II}OO(TMC)]^{+}$ and single point solvent and UB3LYP/BS2 results.

	BS1 (Hartree)				BS2 (Hartree)	
	E	**E+ZPE**	**G**	**Solv (kcal/mol)**	**E**	**E+ZPE**
DMS	-477.968339	-477.891743	-477.919078	-4.008	-478.055895	-477.979299
$^{2}\mathbf{R_1}$	-1091.002381	-1090.520163	-1090.56902	-48.5147	-1091.472664	-1090.990446
$^{4}\mathbf{R_1}$	-1091.006427	-1090.524275	-1090.573798	-47.7938	-1091.477106	-1090.994954
$^{2}\mathbf{R_1C}$	-1568.976193	-1568.416912	-1568.477141	-47.5688	-1569.532392	-1568.973111
$^{4}\mathbf{R_1C}$	-1568.980009	-1568.420994	-1568.478202	-47.1068	-1569.536707	-1568.977692
$^{2}\mathbf{TS_{1SO}}$	-1568.918172	-1568.359841	-1568.418164	-38.7669	-1569.478504	-1568.920173
$^{4}\mathbf{TS_{1SO}}$	-1568.918417	-1568.359993	-1568.418881	-38.7151	-1569.474926	-1568.916502
$^{2}\mathbf{P_{1SO}}$	-1568.935501	-1568.376770	-1568.434658	-43.1070	-1569.518221	-1568.959490
$^{4}\mathbf{P_{1SO}}$	-1568.940866	-1568.382386	-1568.448173	-43.5645	-1569.527357	-1568.968876



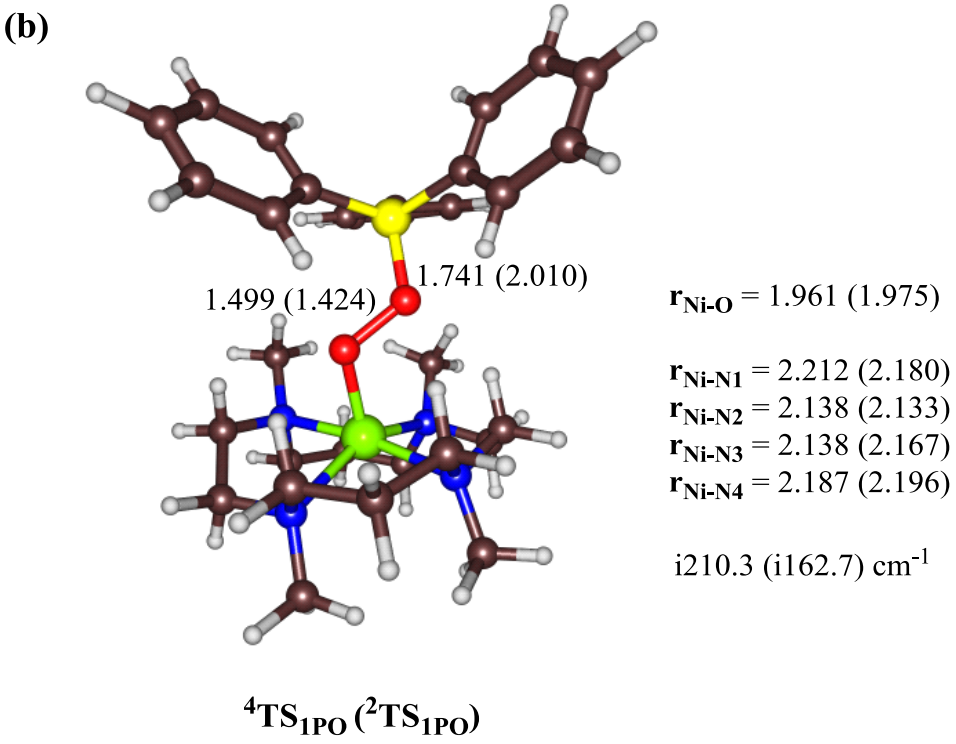
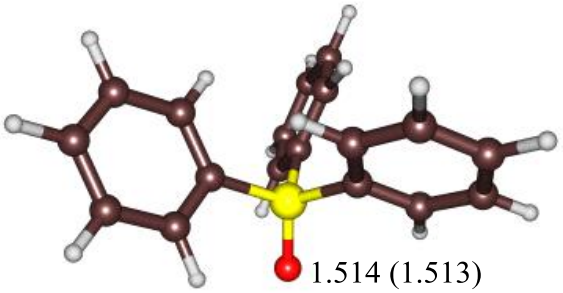
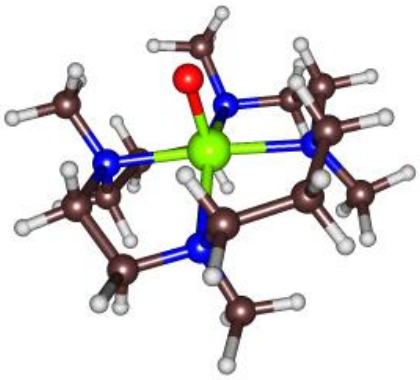


Figure S13. Optimized geometries of $^{4,2}\mathbf{R}_{1PO}$ and $^{4,2}\mathbf{TS}_{1PO}$ as obtained at UB3LYP/BS2 in Jaguar. Bond lengths and imaginary frequencies are in angstroms and wave numbers respectively.





r_{Ni-O} = 1.886 (1.924)

r_{Ni-N1} = 2.157 (2.180)
r_{Ni-N2} = 2.125 (2.154)
r_{Ni-N3} = 2.179 (2.126)
r_{Ni-N4} = 2.186 (2.177)

$^{4}\mathbf{P}_{1PO}$ ($^{2}\mathbf{P}_{1PO}$)

Figure S14. Optimized geometries of $^{4,2}\mathbf{P}_{1PO}$ as obtained at UB3LYP/BS2 in Jaguar. Bond lengths are in angstroms.

Table S9. Absolute energues of UB3LYP/BS2 optimized geometries for the oxidation reaction of triphenylphosphine (PPh_3) with $^{2,4}[Ni^{II}OO(TMC)]^{+}$ and single point solvent results.

	E	E+ZPE	G	E.Solvent (kcal/mol)
$^{4}\mathbf{R}_{1PO}$	-2127.961604	472.350	-2127.287557	-2128.036857
$^{2}\mathbf{R}_{1PO}$	-2127.957088	472.445	-2127.282262	-2128.033382
$^{4}\mathbf{TS}_{1PO}$	-2127.925914	471.583	-2127.246954	-2127.997616
$^{2}\mathbf{TS}_{1PO}$	-2127.931036	471.697	-2127.253553	-2127.996325
$^{4}\mathbf{P}_{1PO}$	-2128.036056	473.271	-2127.358468	-2128.103427
$^{2}\mathbf{P}_{1PO}$	-2128.032025	473.236	-2127.353697	-2128.100953

Table S10. Relative energies for the oxidation reaction of triphenylphosphine (PPh_3) with $^{2,4}[Ni^{II}OO(TMC)]^{+}$ as calculated with UB3LYP/BS2. Single point solvent calculations done in solvent with basis set BS2.

	ΔE	ΔE+ZPE	ΔG	ΔG+ZPE	ΔE(solv)	ΔE(solv)+ZPE	ΔG +ΔE(solv)
$^{4}\mathbf{R}_{1PO}$	0.00	0.00	0.00	0.00	0.00	0.00	0.00
$^{2}\mathbf{R}_{1PO}$	2.83	2.93	3.32	3.42	2.18	2.93	2.67
$^{4}\mathbf{TS}_{1PO}$	22.40	21.63	25.48	24.71	24.62	21.63	27.71
$^{2}\mathbf{TS}_{1PO}$	19.18	18.53	21.34	20.68	25.43	18.53	27.59
$^{4}\mathbf{P}_{1PO}$	-46.72	-45.80	-44.50	-43.58	-41.77	-45.80	-39.55
$^{2}\mathbf{P}_{1PO}$	-44.19	-43.30	-41.50	-40.62	-40.22	-43.30	-37.53

Table S11. Group spin densities and charges of UB3LYP/BS2 optimized geometries for the reaction of triphenylphosphine (PPh_3) with $^{2,4}[Ni^{II}OO(TMC)]^+$.

(a) B2 Group Spin Densities and Group Charges

	Spin Densities					Group Charges				
	Ni	O1	O2	TMC	PPh_3	Ni	O1	O2	TMC	PPh_3
$^4\mathbf{R}_{1PO}$	1.50	0.60	0.69	0.21	0.00	0.34	-0.04	-0.16	0.89	-0.03
$^2\mathbf{R}_{1PO}$	1.57	-0.22	-0.54	0.20	0.00	0.35	-0.07	-0.17	0.92	-0.04
$^4\mathbf{TS}_{1PO}$	1.63	0.20	0.09	0.21	0.87	0.37	-0.19	-0.30	0.80	0.31
$^2\mathbf{TS}_{1PO}$	1.49	0.17	-0.21	0.16	-0.62	0.46	-0.24	-0.24	0.68	0.34
$^4\mathbf{P}_{1PO}$	1.60	1.14	0.00	0.26	0.01	0.38	-0.28	-0.67	0.84	0.73
$^2\mathbf{P}_{1PO}$	1.64	-0.83	0.00	0.18	0.00	0.35	-0.26	-0.67	0.85	0.73

(b) B2-Solvent. Group Spin Densities and Group Charges

	Spin Densities					Group Charges				
	Ni	O1	O2	TMC	PPh_3	Ni	O1	O2	TMC	PPh_3
$^4\mathbf{R}_{1PO}$	1.55	0.59	0.63	0.23	0.00	0.37	-0.04	-0.26	0.98	-0.05
$^2\mathbf{R}_{1PO}$	1.60	-0.29	-0.54	0.22	0.00	0.38	-0.06	-0.27	1.01	-0.06
$^4\mathbf{TS}_{1PO}$	1.64	0.16	0.08	0.22	0.90	0.38	-0.19	-0.29	0.87	0.22
$^2\mathbf{TS}_{1PO}$	1.57	0.14	-0.26	0.19	-0.64	0.47	-0.23	-0.23	0.78	0.20
$^4\mathbf{P}_{1PO}$	1.61	1.12	0.00	0.27	0.01	0.41	-0.32	-0.65	0.87	0.70
$^2\mathbf{P}_{1PO}$	1.65	-0.84	0.00	0.19	0.00	0.39	-0.30	-0.68	0.88	0.71

Table S12. Energies and relative energies of optimized geometries of $^{2,4}[Ni^{II}OO(TMC)]^+$ using alternative density functional methods.

		ΔE
BP86/LACVP:	E (au)	(kcal/mol)
M2	-1091.113888	0.00
M4	-1091.120218	-3.97
BHandHLYP/LACV3P++**		
M2	-1081.113259	0.00
M4	-1081.115627	-1.49
BLYP/LACVP:		
M2	-1090.533733	0.00
M4	-1090.540212	-4.07
BP86-VWN5/LACVP:		
M2	-1091.178779	0.00
M4	-1091.185479	-4.20

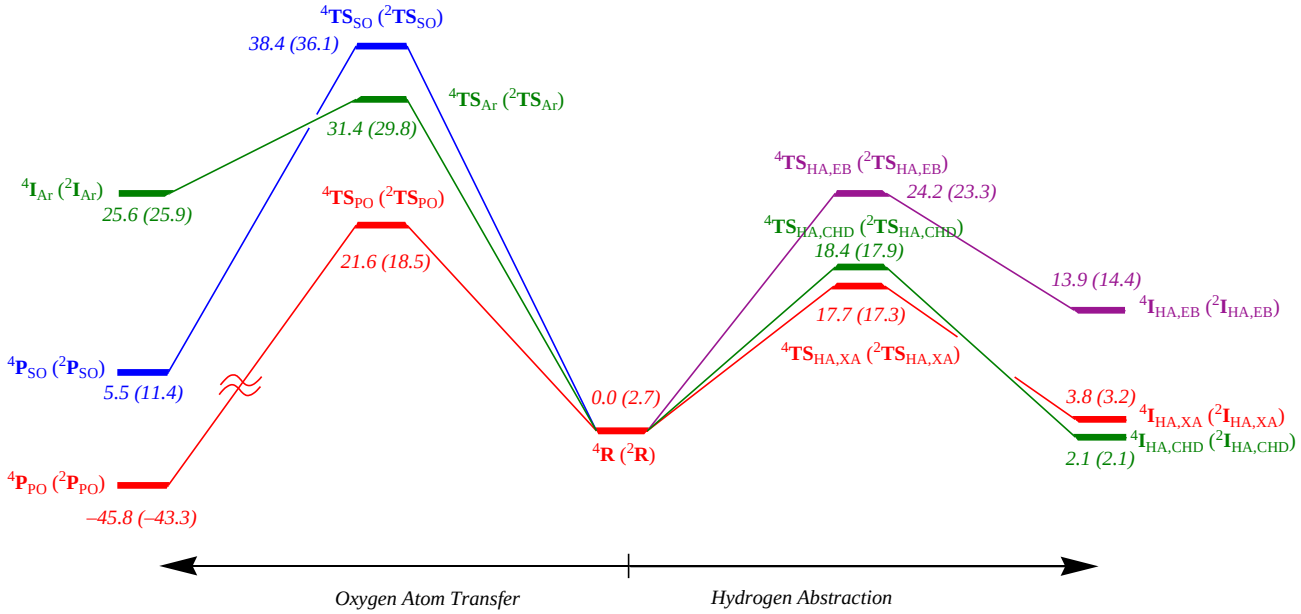


Figure S15. Potential energy profile of substrate oxidation (H-abstraction, heteroatom oxidation and aromatic hydroxylation) by $^{4,2}\mathbf{R_1}$. Relative energies are in kcal mol^{-1} and obtained at UB3LYP/BS2//UB3LYP/BS1 and corrected for ZPE at UB3LYP/BS1. Quartet spin data is in parenthesis

Cartesian Coordinates:

$^{4}R_{1}$:

O	-0.008663212	-0.001207327	0.003463877
N	0.000703795	0.000568085	2.844903752
C	2.527147452	-0.003309265	2.643804203
H	3.378708602	0.656719304	2.424921705
H	2.737159207	-0.474648373	3.607952391
C	1.256270670	0.825258086	2.735000630
H	1.334686408	1.513848516	3.591020405
H	1.128914708	1.429404196	1.832773831
C	-0.120382038	-0.802314000	4.110749578
H	-0.171493649	-0.124537237	4.978455075
H	0.794242018	-1.396711018	4.219612694
C	-1.346460499	-1.743604886	4.146020672
H	-2.274212753	-1.163911563	4.111931819
H	-1.344697293	-2.212701894	5.139245800
C	-1.408482278	-2.904183206	3.129405803
H	-0.507018426	-3.523556736	3.225635760
H	-2.267289919	-3.543242269	3.389541998
C	-1.132065063	0.973531273	2.695488735
H	-0.994868862	1.818242164	3.384934952
H	-2.085364428	0.508349158	2.924518036
H	-1.151819971	1.336266585	1.668414539
O	-1.106745217	-0.128439991	-0.793394702
N	-1.509715253	-2.503707297	1.675276285
C	-1.434385392	-3.699850555	0.752090212
H	-2.445413663	-4.049521380	0.508276201
H	-0.932201307	-4.517630818	1.275900185
C	-0.678930072	-3.322088158	-0.524350301
H	-0.722431040	-4.143886659	-1.254573248
H	-1.120145235	-2.429248112	-0.975344996
C	-2.784655996	-1.774837119	1.376011492
H	-3.646275274	-2.437817297	1.537534222
H	-2.760939692	-1.431757480	0.341781308
H	-2.892820331	-0.902165026	2.010763615
C	2.848718429	-1.705168997	-0.868731271
H	3.562251450	-2.508299428	-0.649567714
H	3.248707866	-1.217264360	-1.767990765
C	2.896178499	-0.635365301	0.244293925
H	3.934077735	-0.274242942	0.328205855
H	2.259697629	0.208949213	-0.030245400
C	1.481010141	-2.291380133	-1.279948525
H	1.638751749	-2.992512474	-2.114796626
H	0.827570967	-1.493983653	-1.632600009
N	0.748645466	-3.006557907	-0.167612943
N	2.445686479	-1.104829268	1.614845279
C	3.308897129	-2.225021499	2.113277965
H	4.333830647	-1.870335627	2.292676043
H	2.902838722	-2.608931709	3.052499346
H	3.349462541	-3.037665114	1.398440592
C	1.447597937	-4.287750663	0.186717079
H	2.524049106	-4.177982717	0.081850714
H	1.232290189	-4.588837686	1.213392027
H	1.131701974	-5.091993000	-0.491405651
Ni	0.332898134	-1.473394366	1.320717441

$^{2}R_{1}$:

O	-0.001169811	-0.000405459	0.000959016
N	0.000303663	0.000181056	2.837936169
C	2.527016036	-0.001455141	2.640498651
H	3.378786836	0.658151531	2.421548868
H	2.734785087	-0.470134753	3.606473473
C	1.255411976	0.826029244	2.724328218
H	1.330936316	1.520474646	3.575653586
H	1.127544718	1.422491925	1.817090735
C	-0.123964571	-0.796738183	4.106665917
H	-0.178292628	-0.115904299	4.971588582
H	0.790492321	-1.390608165	4.221134796
C	-1.350305604	-1.737662900	4.139668151
H	-2.277810216	-1.157852252	4.100751303
H	-1.352594212	-2.205237064	5.133581503
C	-1.408661188	-2.899795659	3.124753199
H	-0.509150253	-3.521290217	3.227316516

H	-2.270187398	-3.536604396	3.380669384
C	-1.132562443	0.972534843	2.678070019
H	-0.987148921	1.830668576	3.348726739
H	-2.084663205	0.514743010	2.926978137
H	-1.157814035	1.312623094	1.643366054
O	-1.077163738	-0.161608495	-0.836146473
N	-1.500763180	-2.503247979	1.668535376
C	-1.427072815	-3.703558622	0.749937809
H	-2.438834314	-4.050498116	0.505628243
H	-0.928594233	-4.520578935	1.278485124
C	-0.667659572	-3.330728421	-0.525221222
H	-0.708143919	-4.154903795	-1.252707164
H	-1.105122559	-2.437558934	-0.979774900
C	-2.768424813	-1.765633089	1.358284744
H	-3.635673069	-2.422214224	1.514552267
H	-2.733356994	-1.425067715	0.323302637
H	-2.874294223	-0.891081106	1.990644936
C	2.857851438	-1.711179869	-0.866911914
H	3.573282370	-2.511598577	-0.643808229
H	3.257974537	-1.224743136	-1.766898704
C	2.898439646	-0.637472199	0.242149796
H	3.934057994	-0.270693321	0.327438272
H	2.256215294	0.201357547	-0.035973213
C	1.492293415	-2.301123135	-1.278432947
H	1.651942427	-3.005741811	-2.109807058
H	0.837520577	-1.506132721	-1.633728120
N	0.759209623	-3.013566788	-0.164467289
N	2.448377927	-1.105581920	1.614006845
C	3.313520660	-2.223268841	2.115161842
H	4.337677914	-1.865990499	2.293262481
H	2.908718383	-2.605449853	3.055690019
H	3.355473972	-3.037554280	1.402255470
C	1.459352744	-4.292644920	0.196237218
H	2.535794652	-4.182066681	0.091878768
H	1.243112426	-4.590197548	1.223870676
H	1.144013490	-5.099866510	-0.478452776
Ni	0.335681960	-1.472554862	1.313538199

$^4R_2$:

Ni	0.012208649	0.241850181	-0.015959609
N	-0.068499634	-0.075255662	2.160060801
N	2.183816553	-0.022648108	0.262692680
N	0.159321206	-0.082599434	-2.193677317
N	-2.130320704	-0.136693888	-0.341101348
C	1.217209233	-0.798843108	2.446179390
H	1.402074443	-0.837271881	3.531086543
H	1.099196212	-1.831549049	2.101918391
C	2.391603688	-0.132093508	1.751544994
H	3.318201708	-0.686338020	1.962634495
H	2.533752799	0.879608544	2.136539609
C	2.581299402	-1.318232072	-0.400261739
H	3.646393838	-1.506662557	-0.187572335
H	2.011036563	-2.120995192	0.082434924
C	2.366556009	-1.386636529	-1.918459489
H	2.793381492	-2.344062602	-2.246769618
H	2.963150499	-0.624077857	-2.428907697
C	0.916188884	-1.367701336	-2.420075764
H	0.352789919	-2.169934339	-1.928488192
H	0.915082953	-1.588162565	-3.500162844
C	-1.260178972	-0.240112915	-2.675968921
H	-1.635262946	0.756430497	-2.917239121
H	-1.278014481	-0.821824854	-3.609581735
C	-2.149575797	-0.898720542	-1.636041135
H	-1.810060174	-1.918150675	-1.425313230
H	-3.178295586	-0.972427037	-2.022052230
C	-2.833560442	-0.962933780	0.705603927
H	-2.493302156	-1.998770410	0.590277697
H	-3.912315235	-0.951564280	0.484895828
C	-2.589387028	-0.520199927	2.148678562
H	-2.774334886	0.551572636	2.274931141
H	-3.336140402	-1.023309828	2.776607082

C	-1.209438515	-0.914440080	2.675999745
H	-1.006261805	-1.954489160	2.394849445
H	-1.198997858	-0.870026402	3.776226202
C	-0.086110121	1.255315519	2.857693003
H	0.007027240	1.113393908	3.944144081
H	0.724633644	1.886180638	2.499683337
H	-1.011211471	1.779477122	2.628751175
C	3.029489517	1.120368117	-0.218367935
H	4.066800810	1.000857552	0.125345553
H	2.611887611	2.052557820	0.161097501
H	3.031671903	1.172727038	-1.302539224
C	0.763938436	1.052896516	-2.967271239
H	1.828155969	1.134620578	-2.769879841
H	0.292352569	1.983933839	-2.653858630
H	0.622265669	0.899556156	-4.046529313
C	-2.850631616	1.172963876	-0.494852158
H	-2.362493603	1.792828594	-1.243799344
H	-2.811731590	1.727394471	0.440031788
H	-3.896661427	0.996810213	-0.784657569
O	0.181274491	2.217696023	-0.204257735
O	-0.673114641	3.015793171	0.478506847

$^{2}R_{2}$:

Ni	0.010873786	0.246978793	-0.015120881
N	-0.067661113	-0.075588960	2.156647821
N	2.182341336	-0.025029441	0.259065994
N	0.162169153	-0.085102868	-2.191256488
N	-2.127182103	-0.137025043	-0.341211441
C	1.219309529	-0.796961112	2.445008490
H	1.403353746	-0.831719949	3.529990440
H	1.103005154	-1.830979267	2.103809987
C	2.391603616	-0.129303222	1.748193060
H	3.319859901	-0.680336821	1.959828661
H	2.530999488	0.884040628	2.129625101
C	2.582468306	-1.321418377	-0.400884678
H	3.647816188	-1.507480619	-0.188030103
H	2.014050597	-2.124299919	0.084193828
C	2.367210664	-1.394013887	-1.918869686
H	2.790595882	-2.353940925	-2.244307365
H	2.966595564	-0.635256004	-2.431528404
C	0.917021257	-1.370928250	-2.421087435
H	0.351758776	-2.173711042	-1.932159232
H	0.915964587	-1.588597435	-3.501605945
C	-1.257295486	-0.237752491	-2.675511108
H	-1.629441067	0.760472791	-2.913958490
H	-1.275217292	-0.816671808	-3.610726184
C	-2.148439460	-0.897074134	-1.637833515
H	-1.811473665	-1.917874628	-1.429127533
H	-3.177456401	-0.967242252	-2.023170993
C	-2.831731974	-0.963974641	0.704534153
H	-2.492283359	-2.000082443	0.588652349
H	-3.910020768	-0.951227626	0.482450155
C	-2.588404253	-0.521873579	2.147763214
H	-2.774017901	0.549637756	2.274484429
H	-3.334595814	-1.026146733	2.775370140
C	-1.208008301	-0.915461178	2.674025700
H	-1.004483239	-1.955716106	2.393641611
H	-1.196072666	-0.869774659	3.774017229
C	-0.087028794	1.256785440	2.852286517
H	-0.001657169	1.114748741	3.939170848
H	0.727472026	1.884805103	2.498236390
H	-1.007837760	1.783837664	2.613877486
C	3.021294267	1.122519206	-0.225022154
H	4.052884661	1.023081115	0.140802500
H	2.580216359	2.053863241	0.129434713
H	3.045015087	1.155622079	-1.309649090
C	0.768516985	1.055518539	-2.957098901
H	1.837234178	1.118657755	-2.778291395
H	0.315651202	1.986601965	-2.617036576
H	0.605602853	0.921308137	-4.035675745
C	-2.845592750	1.174697003	-0.492780165
H	-2.360175126	1.791652187	-1.245740392
H	-2.796620892	1.731889730	0.439749318

H	-3.893461579	0.998991427	-0.775385284
O	0.183117622	2.213930560	-0.205560143
O	-0.686745393	3.005245018	0.491131805

$^{4}R_{EB}$:

O	-0.401695111	-0.262950824	0.080651286
N	-0.258215282	-0.122432480	2.889056532
C	2.237485179	0.196101038	2.571145480
H	2.983349305	0.951031627	2.283439989
H	2.546303604	-0.192814543	3.545520055
C	0.871065155	0.851751305	2.682206557
H	0.890907311	1.589239153	3.500158817
H	0.626566410	1.385447070	1.760033204
C	-0.222229253	-0.869588374	4.193218232
H	-0.321245235	-0.161255386	5.031974475
H	0.763000840	-1.342301298	4.284755221
C	-1.320873011	-1.949444276	4.325508774
H	-2.313202546	-1.488751218	4.300643455
H	-1.226770547	-2.362791601	5.338907890
C	-1.274584824	-3.160464185	3.369088249
H	-0.304742804	-3.666061236	3.466597319
H	-2.045666830	-3.879852856	3.688016704
C	-1.514026021	0.690868903	2.751996817
H	-1.450846180	1.584020969	3.389077064
H	-2.390032488	0.128802788	3.057912517
H	-1.636780085	0.990616248	1.712430984
O	-1.354976159	-0.629257047	-0.821523175
N	-1.459185380	-2.855132798	1.900170030
C	-1.265018566	-4.085291885	1.042448600
H	-2.231550493	-4.572647726	0.861662443
H	-0.644487537	-4.800626968	1.589111260
C	-0.608808500	-3.692570124	-0.282937278
H	-0.564377395	-4.557845115	-0.961098671
H	-1.176829170	-2.894459355	-0.767958946
C	-2.814611170	-2.291891541	1.598408423
H	-3.591807698	-3.035259377	1.825583621
H	-2.859974404	-2.015304803	0.545123212
H	-3.006501496	-1.395734204	2.176880424
C	2.648244644	-1.636248308	-0.866993817
H	3.475871275	-2.319297443	-0.641809363
H	2.939402579	-1.149394800	-1.807797452
C	2.590201367	-0.508861442	0.187695194
H	3.569816626	-0.003859434	0.202834455
H	1.830827629	0.223332877	-0.095946597
C	1.361985514	-2.429301515	-1.184025168
H	1.587922526	-3.152811829	-1.983558939
H	0.590091397	-1.755715234	-1.554770752
N	0.774356821	-3.167866731	-0.003816831
N	2.266903652	-0.959176008	1.599851542
C	3.298841769	-1.920756602	2.108360892
H	4.270005997	-1.417972443	2.220898028
H	2.990064148	-2.306191410	3.083244198
H	3.424338938	-2.756964827	1.431682638
C	1.653694381	-4.319844107	0.389387121
H	2.700742249	-4.072452436	0.233313203
H	1.516855879	-4.586401516	1.438868117
H	1.427492547	-5.197746620	-0.230871933
H	-5.924430344	-0.394415529	0.187481434
C	-5.378404532	0.524219071	0.383204301
C	-5.673555882	1.284629771	1.523219460
C	-4.396320420	0.955468268	-0.515799737
C	-4.980220724	2.479378118	1.753067866
H	-6.445101074	0.958465144	2.213959546
C	-3.692806864	2.155543344	-0.299338930
H	-4.171283205	0.362010985	-1.397211432
C	-4.000388301	2.908728932	0.847990460
H	-5.211775902	3.083231018	2.625517537
H	-3.476534010	3.844787532	1.025050711
C	-2.663048487	2.638177200	-1.304702161
H	-2.089219860	1.778436909	-1.671392191
H	-1.949881257	3.307507889	-0.804853993

C	-3.295619151	3.382010947	-2.502391063
H	-2.523688832	3.711787598	-3.207243388
H	-3.993182784	2.732218862	-3.043025016
H	-3.852651173	4.264742009	-2.168727972
Ni	0.211581268	-1.620922583	1.423463076

$^{4}R_{XA}$:

Ni	-0.224702807	-1.256795224	1.182897538
O	-0.440321782	0.494149895	0.226406630
N	0.114938981	-0.055537702	2.940719501
C	2.476479522	-0.571109756	2.176783270
H	3.411212463	-0.082346131	1.866258155
H	2.735583358	-1.249369208	2.994583063
C	1.494727969	0.480916674	2.665071868
H	1.902119906	0.963629019	3.567621965
H	1.357745601	1.256050896	1.906344533
C	0.029409925	-1.038953982	4.074607085
H	0.317322266	-0.546855160	5.018204653
H	0.763056580	-1.831747409	3.887534266
C	-1.370035377	-1.671785464	4.253510377
H	-2.106969570	-0.903151527	4.507004283
H	-1.308017932	-2.307318639	5.147333942
C	-1.913810278	-2.576692265	3.126463697
H	-1.203502357	-3.392388281	2.938068425
H	-2.848926946	-3.040072845	3.479694982
C	-0.738612543	1.152728054	3.190678963
H	-0.262881671	1.800109481	3.940800516
H	-1.718436817	0.874952058	3.565306581
H	-0.856671021	1.697592783	2.254705411
O	-1.607894549	0.718752496	-0.439962271
N	-2.164539079	-1.902589630	1.798142709
C	-2.570998996	-2.893134456	0.726939738
H	-3.664978125	-2.954601064	0.670434998
H	-2.209457529	-3.884832669	1.012404257
C	-1.992871356	-2.462279378	-0.621226736
H	-2.376934636	-3.092570165	-1.434188729
H	-2.266455071	-1.426091425	-0.835188982
C	-3.234945403	-0.858453286	1.883883116
H	-4.196091024	-1.321819610	2.147936995
H	-3.316272462	-0.355306197	0.920237409
H	-2.991454110	-0.110388701	2.630273986
C	1.704945986	-1.616843163	-1.517454614
H	2.225294707	-2.580525217	-1.572765955
H	2.039790421	-1.070625086	-2.409807402
C	2.221667329	-0.805755660	-0.309027096
H	3.313752191	-0.694795476	-0.410208792
H	1.773041350	0.190468133	-0.314877251
C	0.183730244	-1.810684273	-1.690781881
H	0.004739630	-2.366685223	-2.622768186
H	-0.305815984	-0.842213716	-1.785428851
N	-0.488147016	-2.534895371	-0.545263771
N	1.931906713	-1.414344544	1.050509384
C	2.561829683	-2.768195463	1.182186896
H	3.658069976	-2.685523080	1.169017991
H	2.257242941	-3.221959315	2.128666770
H	2.258624780	-3.422348248	0.374193964
C	-0.083500613	-3.981379570	-0.531516940
H	0.947532624	-4.093770339	-0.858060539
H	-0.176017853	-4.412429393	0.467143062
H	-0.712549417	-4.554530245	-1.225041188
H	-0.888462221	0.380878606	-5.823488852
C	-1.100046280	-0.658401331	-5.588328651
C	-0.290865566	-1.670731413	-6.116053578
C	-2.191289478	-0.958028789	-4.757880996
C	-0.571616702	-3.013552814	-5.824613739
H	0.543106687	-1.416433248	-6.761350358
C	-2.451017443	-2.309394857	-4.490873946
C	-1.661213323	-3.337610417	-5.011389816
H	0.040845397	-3.804431140	-6.244724471
C	-4.420158525	-0.418803166	-3.727209945
H	-1.927007976	-4.365857176	-4.793681560
C	-4.591020533	-1.789025013	-3.491615548
C	-5.533242067	0.415531384	-3.542895309

C	-5.808924041	-2.329531435	-3.075821980
H	-5.429370082	1.480374991	-3.730662133
C	-6.762863033	-0.101843608	-3.122823635
C	-6.899206975	-1.476849173	-2.885484945
H	-5.888188014	-3.400607436	-2.929242317
H	-7.611203782	0.560570893	-2.988977216
H	-7.853446618	-1.885084953	-2.569817052
C	-3.061082147	0.118370477	-4.135336157
H	-3.182223781	0.953741959	-4.835901691
H	-2.553596495	0.539462018	-3.250802372
O	-3.523877761	-2.700100500	-3.665388532

$^{4}R_{2XA}$:

Ni	0.011413484	-0.137740482	0.194454960
N	0.086051566	-0.263938636	2.395931814
N	2.215235860	-0.203075753	0.355082239
N	0.059617505	-0.651382362	-1.939611978
N	-2.098929604	-0.730028582	0.055162073
C	1.449325793	-0.836913791	2.662319055
H	1.699347153	-0.749682946	3.731374395
H	1.410994675	-1.905450156	2.426592311
C	2.512707450	-0.141570410	1.831054229
H	3.499133735	-0.584808121	2.034672198
H	2.576859168	0.913211220	2.105860800
C	2.676264727	-1.525855387	-0.204233076
H	3.763913698	-1.612983052	-0.046116764
H	2.201504455	-2.315995223	0.389931662
C	2.375541490	-1.761122760	-1.691192760
H	2.854799188	-2.713722037	-1.955189309
H	2.878041128	-1.012263661	-2.311294819
C	0.899646137	-1.894695532	-2.092588880
H	0.431596215	-2.683849034	-1.491716285
H	0.851253256	-2.220252347	-3.144681220
C	-1.369574472	-0.954020925	-2.319053557
H	-1.839077891	-0.013635601	-2.616862776
H	-1.389643308	-1.614531255	-3.198980616
C	-2.134283855	-1.594792895	-1.174299578
H	-1.699953344	-2.564754095	-0.909195813
H	-3.175698841	-1.778062062	-1.481223113
C	-2.659474018	-1.522668439	1.206915769
H	-2.230197443	-2.530480661	1.154695076
H	-3.745334419	-1.626307448	1.055779727
C	-2.377854807	-0.936339338	2.590555994
H	-2.661050334	0.120057774	2.641183172
H	-3.033103974	-1.451214100	3.305274472
C	-0.937577026	-1.153042092	3.055383842
H	-0.651944889	-2.191421922	2.849601431
H	-0.866417647	-1.009103134	4.144998406
C	-0.022620188	1.118413340	2.973049337
H	0.136046817	1.087486305	4.060961958
H	0.706785470	1.782689129	2.514748969
H	-1.003423447	1.533878008	2.752586349
C	2.941010675	0.944645463	-0.284731621
H	3.996910519	0.947369501	0.021389055
H	2.458711117	1.875553973	0.012141016
H	2.899274618	0.876256822	-1.367109351
C	0.530940415	0.443212278	-2.851517906
H	1.585586375	0.650163610	-2.699785542
H	-0.028543090	1.351773783	-2.635904235
H	0.377937887	0.156713342	-3.901357161
C	-2.939959738	0.498370896	-0.153050125
H	-2.571386357	1.078017689	-0.995341357
H	-2.881775610	1.139622641	0.723477152
H	-3.984824539	0.213527798	-0.340238002
O	0.036404162	1.824483004	-0.152639985
O	-0.864956477	2.618820433	0.476904389
H	-6.755762028	4.663362529	-0.521460309
C	-5.960845802	4.199481669	-1.095410698
C	-4.696016069	4.797023340	-1.144501519
C	-6.202740724	3.010798209	-1.797055497
C	-3.652943773	4.218640132	-1.881589465

H	-4.511781950	5.721929852	-0.605859978
C	-5.181994439	2.424633888	-2.553009321
H	-7.186090786	2.553159327	-1.773509676
C	-3.928471696	3.035587785	-2.580344886
C	-2.250734873	4.795076212	-1.938387267
H	-5.347404957	1.525865068	-3.136278131
O	-2.916113231	2.410512415	-3.352697526
C	-1.580747803	4.456421753	-3.256547801
H	-2.277658356	5.880441570	-1.791448369
C	-1.930116320	3.265518995	-3.907853775
C	-0.606943343	5.266208802	-3.858120878
C	-1.344553010	2.871781445	-5.111057719
H	-0.328105120	6.200304212	-3.379273433
C	0.003377553	4.887174066	-5.059443575
C	-0.364012159	3.688132359	-5.684792141
H	-1.677217364	1.957497211	-5.589442278
H	0.752686418	5.528606047	-5.510769852
H	0.094375131	3.399808384	-6.624880809
H	-1.654347454	4.379292625	-1.109185977

$^{4}R_{CHD}$:

Ni	0.145921992	-0.424299784	0.094680816
O	0.565735931	-1.195922888	1.898546087
N	2.257784821	-0.015110933	-0.017003379
C	1.313916741	2.209932632	0.746321045
H	1.382283342	2.944596621	1.561415523
H	1.493728867	2.756899632	-0.183573090
C	2.379363410	1.143872637	0.937133330
H	3.374769196	1.606907832	0.847099114
H	2.304930253	0.705325981	1.935761593
C	2.482680539	0.325237114	-1.463988589
H	3.516010034	0.681202675	-1.607817925
H	1.816427163	1.156967291	-1.721168505
C	2.226066062	-0.852234140	-2.432713942
H	2.926318545	-1.669770713	-2.234424983
H	2.493481814	-0.490000247	-3.434662832
C	0.788254860	-1.402148722	-2.552335507
H	0.108468183	-0.587737011	-2.835032239
H	0.768943183	-2.137019595	-3.372940817
C	3.243531909	-1.035967048	0.470634020
H	4.229113467	-0.569694198	0.609437948
H	3.357897864	-1.848093894	-0.240159715
H	2.889411754	-1.439325589	1.418683933
O	0.163784520	-2.469073380	2.175685043
N	0.212795630	-2.035047607	-1.306366863
C	-1.238710866	-2.419895893	-1.489276242
H	-1.311210810	-3.466291521	-1.811837315
H	-1.665646827	-1.809025226	-2.289222005
C	-1.997446462	-2.210214523	-0.177213216
H	-3.026125281	-2.590973268	-0.263271709
H	-1.496999251	-2.733997302	0.641580520
C	0.964666695	-3.262433040	-0.891146420
H	0.878939012	-4.039503586	-1.663850661
H	0.555566377	-3.626981916	0.051539429
H	2.014458250	-3.041295036	-0.733222536
C	-2.166232731	0.978323637	2.055169190
H	-2.844844850	1.671098403	1.543004748
H	-2.480467688	0.993033960	3.106469211
C	-0.727422268	1.536266701	2.043771004
H	-0.746129307	2.541122761	2.495637111
H	-0.083059515	0.902678220	2.656703051
C	-2.407438536	-0.469676279	1.581956548
H	-3.477402923	-0.701097187	1.702392636
H	-1.848832776	-1.161856894	2.210356080
N	-2.002453416	-0.741989630	0.150656228
N	-0.083535257	1.646034282	0.672655787
C	-0.868098659	2.561797056	-0.218444338
H	-0.827249777	3.593023982	0.160337362
H	-0.445933695	2.543107322	-1.226487194
H	-1.906744618	2.260495723	-0.273525054
C	-2.927061645	-0.041108815	-0.802524670
H	-3.258205936	0.906303151	-0.384900057
H	-2.440954458	0.156320069	-1.759706450

H	-3.822086009	-0.652620256	-0.979967788
C	-0.494172024	0.138262101	5.798076393
C	-1.198517445	1.260111782	6.012053581
C	-2.630269375	-1.137383267	5.438223816
C	-3.337074792	-0.016697260	5.652437329
C	-1.126131535	-1.214178948	5.563983354
H	-0.861604708	-1.892773738	6.393652045
H	-0.688091168	-1.689530674	4.671862560
H	-3.146564514	-2.062104540	5.186121493
H	-4.422542812	-0.035694273	5.572446837
H	-0.680842144	2.198579356	6.202795321
H	0.593845255	0.170102976	5.815449808
C	-2.709460730	1.301290100	6.047098251
H	-3.049866351	1.585563747	7.057809278
H	-3.083965529	2.111320422	5.398119636

$^{2}R_{EB}$:

O	-0.356929954	-0.274083895	0.044124583
N	-0.231734838	-0.108507719	2.854993443
C	2.264821751	0.203172572	2.539806393
H	3.012806713	0.952576408	2.243689742
H	2.569596975	-0.172309127	3.520723173
C	0.898879201	0.861819995	2.634979273
H	0.915960398	1.612953911	3.440264528
H	0.656619173	1.378297281	1.702450692
C	-0.199733491	-0.837404520	4.169319901
H	-0.301283743	-0.117947269	4.998034855
H	0.785238344	-1.308931984	4.270626317
C	-1.299077753	-1.915217350	4.311610879
H	-2.291245630	-1.454722599	4.279847229
H	-1.206948368	-2.318040895	5.329384554
C	-1.251342391	-3.135687690	3.367477490
H	-0.281839905	-3.641027009	3.471766094
H	-2.023045060	-3.851770274	3.691717985
C	-1.486714268	0.704428836	2.700932960
H	-1.415628913	1.616942730	3.308668683
H	-2.362071306	0.155863050	3.032550244
H	-1.614082937	0.970409594	1.652830487
O	-1.326163783	-0.659844831	-0.848072046
N	-1.433481015	-2.845337234	1.894788351
C	-1.243750607	-4.086348534	1.050753328
H	-2.212727611	-4.569468746	0.872760584
H	-0.629111767	-4.799390591	1.607046842
C	-0.582144811	-3.709452450	-0.276183283
H	-0.538619834	-4.581012247	-0.946100998
H	-1.143804686	-2.911558453	-0.769507195
C	-2.786404734	-2.279862873	1.584237622
H	-3.566706935	-3.015578785	1.825099027
H	-2.829699708	-2.022212815	0.526113775
H	-2.973200334	-1.372185826	2.145719958
C	2.684571609	-1.673576268	-0.872589194
H	3.508658472	-2.357051503	-0.635853099
H	2.981144616	-1.199333638	-1.818095969
C	2.624901716	-0.533185583	0.167420591
H	3.604830056	-0.029088101	0.180785192
H	1.866237927	0.195114567	-0.128233553
C	1.395629126	-2.463713933	-1.184144543
H	1.618740282	-3.197010177	-1.975370356
H	0.626951851	-1.789925387	-1.560982740
N	0.802678858	-3.187614837	0.002993866
N	2.295588160	-0.965461673	1.584320245
C	3.322495272	-1.923626799	2.109425750
H	4.294652446	-1.422320342	2.218946910
H	3.009136267	-2.295121025	3.088326289
H	3.447930666	-2.769023315	1.444179143
C	1.676163014	-4.338273338	0.412819392
H	2.724885062	-4.096499474	0.259226052
H	1.533082985	-4.593210961	1.464440776
H	1.449350343	-5.221832576	-0.198975230
H	-5.880387284	-0.419684829	0.195139022
C	-5.360037296	0.511629622	0.400891684

C	-5.715212658	1.279536502	1.518647751
C	-4.350649197	0.951032190	-0.463269824
C	-5.054690140	2.490099364	1.761059010
H	-6.507083850	0.946304624	2.182400664
C	-3.679864342	2.167835959	-0.233912989
H	-4.077241858	0.351808290	-1.326861015
C	-4.047965901	2.928291361	0.890425198
H	-5.331771591	3.099001814	2.616477746
H	-3.549853694	3.876506703	1.076673319
C	-2.618293120	2.655977522	-1.203134748
H	-1.996323493	1.806510892	-1.510877787
H	-1.957563086	3.369570452	-0.692581239
C	-3.215911970	3.333342588	-2.456770898
H	-2.421625161	3.668486493	-3.133649548
H	-3.860067402	2.638613158	-3.007704099
H	-3.821701400	4.204518682	-2.183263754
Ni	0.237024270	-1.619701885	1.403174165

$^{2}R_{XA}$:

Ni	-0.239132728	-1.256456593	1.136670001
O	-0.519277440	0.485486954	0.183526384
N	0.090464912	-0.059803554	2.895641919
C	2.455704511	-0.483215173	2.090028452
H	3.365631211	0.040286917	1.763234579
H	2.754682787	-1.152222055	2.901876459
C	1.443165911	0.530633852	2.595212977
H	1.846565980	1.029988827	3.490286517
H	1.260871188	1.297798908	1.837897775
C	0.064674878	-1.049441112	4.026936081
H	0.351150303	-0.550115990	4.966998792
H	0.825172636	-1.812351437	3.822780390
C	-1.305200757	-1.737590004	4.228922272
H	-2.066139542	-1.000306489	4.503553020
H	-1.200199097	-2.377263455	5.115752642
C	-1.836098419	-2.653995274	3.105154941
H	-1.098821950	-3.440331609	2.895314995
H	-2.745240415	-3.156439873	3.472102308
C	-0.805054982	1.114570866	3.162114268
H	-0.334678781	1.786675132	3.893448166
H	-1.760902961	0.799502273	3.568066468
H	-0.971197989	1.645195481	2.225128766
O	-1.730596434	0.672672843	-0.436082678
N	-2.139486280	-1.979337069	1.787846823
C	-2.532482039	-2.976515247	0.717204990
H	-3.624691902	-3.071359837	0.678379094
H	-2.136007411	-3.958293168	0.990537951
C	-1.990122505	-2.518627197	-0.636363745
H	-2.365998214	-3.157415471	-1.446212386
H	-2.300048037	-1.490048478	-0.838617566
C	-3.244870604	-0.974583959	1.902869054
H	-4.184230831	-1.475507491	2.176124452
H	-3.357889835	-0.463733726	0.946411348
H	-3.016400962	-0.227323184	2.654624907
C	1.662777490	-1.550285807	-1.590518593
H	2.214778945	-2.495653444	-1.655917305
H	1.962342965	-0.992927338	-2.488436683
C	2.168798500	-0.722144953	-0.390440754
H	3.254346776	-0.570620388	-0.506808558
H	1.681713995	0.255989518	-0.387377703
C	0.146796989	-1.793438768	-1.737523339
H	-0.030119846	-2.352431639	-2.666938613
H	-0.374473863	-0.840807227	-1.817867964
N	-0.482527408	-2.542754171	-0.583146550
N	1.922014242	-1.343856991	0.971805764
C	2.599211904	-2.676030491	1.089920722
H	3.691548991	-2.556497234	1.056210913
H	2.328201738	-3.140512714	2.041470602
H	2.303007360	-3.339269079	0.286755038
C	-0.031075983	-3.975404787	-0.582377143
H	0.997424949	-4.052864306	-0.926605371
H	-0.093591048	-4.414197813	0.415274409
H	-0.652446939	-4.564718776	-1.269128182
H	-0.670600123	0.253510333	-5.584585610

C	-0.952455845	-0.774404302	-5.374194694
C	-0.163053607	-1.825156540	-5.855194688
C	-2.113824768	-1.018724304	-4.624116355
C	-0.535280660	-3.153322000	-5.598743767
H	0.725020367	-1.611552722	-6.440276368
C	-2.465117469	-2.356088415	-4.391697503
C	-1.696403583	-3.422199544	-4.868374926
H	0.060519464	-3.973636055	-5.984873076
C	-4.360393578	-0.363216045	-3.697612432
H	-2.032965341	-4.435689386	-4.681215693
C	-4.621195903	-1.723945278	-3.493103195
C	-5.427625769	0.533419479	-3.534472309
C	-5.883369725	-2.196692622	-3.129444826
H	-5.253439539	1.593121442	-3.697361655
C	-6.699679526	0.084798618	-3.166021037
C	-6.926648598	-1.283276789	-2.960081174
H	-6.030671360	-3.263184035	-3.003888312
H	-7.510511682	0.795237419	-3.047247806
H	-7.913723209	-1.638301216	-2.683701015
C	-2.960739453	0.102936118	-4.051571584
H	-3.012646423	0.933344787	-4.766657107
H	-2.474556191	0.513558136	-3.150518554
O	-3.607295113	-2.697555700	-3.645372828

$^{2}R_{2XA}$:

Ni	0.000000000	0.000000000	0.000000000
N	0.000000000	0.000000000	2.203576989
N	2.196784223	0.000000000	0.238954988
N	0.145187059	-0.640261337	-2.096780656
N	-2.082031282	-0.663527707	-0.179071841
C	1.367561236	-0.516668030	2.552497845
H	1.574965463	-0.357759909	3.622246355
H	1.366532919	-1.598225896	2.381476120
C	2.440794410	0.158557705	1.717563374
H	3.431122928	-0.242531083	1.980265696
H	2.466264749	1.229281428	1.929437403
C	2.717553939	-1.337672376	-0.224435938
H	3.800713396	-1.380307453	-0.023887391
H	2.245855242	-2.106575992	0.399598645
C	2.478366579	-1.669554748	-1.704180645
H	2.990639594	-2.622936888	-1.892385552
H	2.985425228	-0.945932721	-2.349905267
C	1.022253861	-1.866215639	-2.149962985
H	0.552638084	-2.633834682	-1.522665962
H	1.021247433	-2.250865578	-3.182904078
C	-1.261272411	-1.002255805	-2.508685054
H	-1.742977315	-0.093182192	-2.876049112
H	-1.231820097	-1.711137439	-3.349730314
C	-2.051155041	-1.598083526	-1.357018841
H	-1.603254960	-2.539611509	-1.021108227
H	-3.075940493	-1.825707523	-1.688446813
C	-2.662217406	-1.404455554	0.997622733
H	-2.202229393	-2.399792040	1.021389824
H	-3.737879535	-1.550436711	0.813323572
C	-2.450500085	-0.728627119	2.352565902
H	-2.763332374	0.320236343	2.328279257
H	-3.118468632	-1.218804803	3.072763618
C	-1.023803204	-0.875260066	2.881594406
H	-0.703475803	-1.915994721	2.752980614
H	-0.996758476	-0.660683793	3.961338610
C	-0.165685304	1.412417883	2.688922845
H	-0.048015888	1.451383054	3.781597165
H	0.563503064	2.066725933	2.216359643
H	-1.146151352	1.787108478	2.404434674
C	2.904474949	1.134193575	-0.444690016
H	3.943148822	1.203984974	-0.091912477
H	2.367986084	2.059267612	-0.234871263
H	2.917986789	0.991636412	-1.520429982
C	0.619141432	0.418456595	-3.050071562
H	1.670539462	0.639403474	-2.895693794
H	0.050434032	1.330641318	-2.877938514

H	0.481298212	0.085196837	-4.087820267
C	-2.947204645	0.527246132	-0.487569152
H	-2.569563005	1.061052026	-1.355611201
H	-2.927178713	1.225114326	0.346170042
H	-3.978614408	0.202425316	-0.682964494
O	-0.019570344	1.929434974	-0.474267538
O	-0.971265275	2.726960309	0.100640943
H	-6.858408302	4.530115148	-1.246995126
C	-6.032593901	4.055044702	-1.765643097
C	-4.782745486	4.683727597	-1.810219097
C	-6.219527422	2.820119759	-2.401526624
C	-3.700344806	4.092104286	-2.477057573
H	-4.641036263	5.644158575	-1.323211061
C	-5.158713707	2.218957314	-3.086863004
H	-7.190876847	2.337288738	-2.382193908
C	-3.921256970	2.862049550	-3.111020775
C	-2.313286434	4.705060569	-2.521834814
H	-5.280461869	1.282565821	-3.619483652
O	-2.868579339	2.218878164	-3.810887045
C	-1.582410061	4.298895676	-3.787492173
H	-2.376966959	5.796843596	-2.453139572
C	-1.879944931	3.062813367	-4.377424768
C	-0.600752082	5.092224093	-4.398717260
C	-1.237019784	2.610148443	-5.529762259
H	-0.361117976	6.059946862	-3.967760438
C	0.066654457	4.654760615	-5.548682531
C	-0.250322341	3.411815576	-6.113216367
H	-1.531097531	1.660977271	-5.963413160
H	0.820990856	5.284379451	-6.008276405
H	0.252153238	3.077252161	-7.014688391
H	-1.739809261	4.367106465	-1.642678632

$^{2}R_{CHD}$:

Ni	0.151220725	-0.423060204	0.095800023
O	0.576312065	-1.182820069	1.900256781
N	2.262394076	-0.019553751	-0.030208771
C	1.331523523	2.210872168	0.731876723
H	1.405638111	2.947721082	1.544407162
H	1.510627100	2.754020260	-0.200434932
C	2.391458828	1.139866573	0.923080168
H	3.389332288	1.596934433	0.831450264
H	2.314698758	0.701679579	1.921685651
C	2.486495129	0.316050746	-1.478273238
H	3.521276177	0.666041388	-1.625355280
H	1.824230255	1.150842850	-1.736407065
C	2.221146250	-0.863239431	-2.442545780
H	2.919483246	-1.682597401	-2.245120721
H	2.484602624	-0.505140244	-3.447013477
C	0.780849038	-1.408729510	-2.552876973
H	0.102137185	-0.593415990	-2.836311868
H	0.754746551	-2.147259207	-3.369782559
C	3.241715176	-1.045970954	0.459879043
H	4.226836812	-0.582374250	0.609331343
H	3.360696839	-1.853922435	-0.254960482
H	2.876342769	-1.452212332	1.402451473
O	0.166932428	-2.464590707	2.174245788
N	0.208693427	-2.034373272	-1.301222134
C	-1.244714172	-2.418189386	-1.476770539
H	-1.319292575	-3.465900359	-1.794160073
H	-1.673658019	-1.810407749	-2.278070802
C	-1.996075154	-2.201257924	-0.161906434
H	-3.026072276	-2.579755845	-0.240079202
H	-1.490743913	-2.719743073	0.657623619
C	0.959289094	-3.261109881	-0.880594495
H	0.864206997	-4.044017466	-1.646048625
H	0.555826249	-3.614881471	0.068658217
H	2.011002846	-3.042536543	-0.733097454
C	-2.147613312	0.996644233	2.057162676
H	-2.824748661	1.690270852	1.544046154
H	-2.458674542	1.017284039	3.109154092
C	-0.706403478	1.547072198	2.039683059
H	-0.716838602	2.552375570	2.490425717
H	-0.063022727	0.908506205	2.648528538

C	-2.394585542	-0.452294279	1.590787863
H	-3.464527124	-0.680930249	1.715085562
H	-1.834178126	-1.143595996	2.218279849
N	-1.995956079	-0.730723474	0.158396403
N	-0.068756055	1.652762081	0.664894736
C	-0.852938713	2.570794521	-0.224374148
H	-0.804853489	3.602308660	0.152515124
H	-0.435447930	2.548479151	-1.234363982
H	-1.893400937	2.274873877	-0.273799016
C	-2.923075142	-0.031107289	-0.793424993
H	-3.249208259	0.919082585	-0.378221182
H	-2.441514121	0.160387994	-1.754190376
H	-3.820618313	-0.640927840	-0.963343239
C	-0.509428804	0.160104916	5.816057950
C	-1.243703520	1.263101256	6.028461180
C	-2.608725344	-1.165399461	5.424292261
C	-3.345494915	-0.063734612	5.636096992
C	-1.104826819	-1.206357440	5.567998646
H	-0.833540367	-1.882270548	6.397701254
H	-0.644786893	-1.667130463	4.679365715
H	-3.098912614	-2.100924969	5.160238396
H	-4.429089958	-0.108717987	5.542383155
H	-0.751664646	2.213121006	6.229628444
H	0.577247550	0.218819087	5.845363160
C	-2.755559714	1.266516323	6.047339300
H	-3.113475959	1.533979588	7.056588574
H	-3.143890914	2.072596755	5.401458454

$^{4}TS_{Ar}$:

O	-0.241771634	0.040590142	0.388513628
N	0.342110291	-0.149360929	3.181682255
C	2.772540003	-0.060604559	2.468418564
H	3.549214018	0.638421180	2.124759448
H	3.179538393	-0.573014489	3.345155307
C	1.526527474	0.719407844	2.853205593
H	1.760170133	1.380160517	3.703276180
H	1.197015797	1.344443367	2.018846878
C	0.496592749	-1.013845988	4.398762369
H	0.612030417	-0.384055530	5.296329979
H	1.423728130	-1.588450847	4.286989621
C	-0.681909928	-1.988473516	4.627403836
H	-1.604849244	-1.431904227	4.819299008
H	-0.469671444	-2.514123915	5.568641526
C	-0.935842125	-3.090118826	3.575877938
H	-0.028002369	-3.696470465	3.457906383
H	-1.720831201	-3.759283376	3.963464896
C	-0.822834080	0.787936479	3.290148042
H	-0.560145304	1.647435547	3.922914065
H	-1.684709967	0.299072916	3.733435774
H	-1.067309206	1.112956691	2.278769618
O	-1.473961519	-0.292294481	-0.408551289
N	-1.324009708	-2.618533466	2.193827711
C	-1.415451566	-3.769918907	1.217461377
H	-2.449182188	-4.135106489	1.166963767
H	-0.803874070	-4.595043153	1.593428269
C	-0.938997243	-3.325587797	-0.167072965
H	-1.101981126	-4.129766240	-0.901173536
H	-1.480667729	-2.434372262	-0.494817250
C	-2.631687116	-1.885954412	2.174572754
H	-3.458339906	-2.580821099	2.379909884
H	-2.755069240	-1.415322288	1.197464322
H	-2.644405106	-1.102661792	2.924913238
C	2.402931914	-1.568967668	-1.123539861
H	3.160580677	-2.361895230	-1.100892598
H	2.601215082	-1.024720640	-2.057155121
C	2.654263616	-0.553686382	0.011875564
H	3.674760118	-0.151171899	-0.098686804
H	1.930887693	0.259625757	-0.078762876
C	0.987246634	-2.164848598	-1.276859138
H	0.974565416	-2.808304073	-2.171907117
H	0.257790002	-1.365291332	-1.409644595

N	0.520452980	-2.972316183	-0.087613930
N	2.513322905	-1.108252992	1.416406608
C	3.488550754	-2.217894823	1.664670175
H	4.519788832	-1.835539722	1.652844068
H	3.294043312	-2.665265509	2.643021475
H	3.404282932	-2.990835157	0.910713353
C	1.312121863	-4.238266559	0.049769747
H	2.346434610	-4.078544377	-0.243200130
H	1.300836008	-4.606969871	1.077404875
H	0.900746359	-5.016478831	-0.608121128
H	-2.737008513	2.115501636	0.845400991
C	-3.114905487	1.683023270	-0.075912336
C	-2.161588533	1.242712442	-1.072559438
C	-4.475499750	1.515901535	-0.266008331
C	-2.710008497	0.797764947	-2.340163981
H	-1.189317571	1.728291351	-1.082298745
C	-4.989182954	0.979763642	-1.472083213
H	-5.170539885	1.816598092	0.513531848
C	-4.069095781	0.638416052	-2.504179738
H	-2.023100930	0.543328551	-3.140060936
H	-4.458152858	0.262787392	-3.446719135
C	-6.477209524	0.837812854	-1.694165127
H	-6.986469366	0.739371090	-0.727079995
H	-6.680762837	-0.085001855	-2.254533471
C	-7.082670636	2.035636121	-2.466770354
H	-8.160075212	1.895784982	-2.603886687
H	-6.924636641	2.973601128	-1.922952954
H	-6.623666522	2.137914065	-3.456561825
Ni	0.348023432	-1.486714610	1.510857738

$^{2}TS_{Ar}$:

O	0.000000000	0.000000000	0.000000000
N	0.000000000	0.000000000	2.819539530
C	2.527852036	0.000000000	2.628592576
H	3.379164646	0.661976657	2.412121752
H	2.728273049	-0.458844632	3.601160092
C	1.252650607	0.823768371	2.694480894
H	1.325177204	1.536664988	3.531391027
H	1.122887055	1.397127206	1.772716753
C	-0.133911164	-0.783696628	4.092056667
H	-0.185891542	-0.098373340	4.954166771
H	0.774444250	-1.385805016	4.213625151
C	-1.369796388	-1.712933876	4.125324414
H	-2.290654661	-1.123087065	4.079840489
H	-1.381108862	-2.175924518	5.121531533
C	-1.439085772	-2.880537476	3.117077793
H	-0.554982705	-3.519635399	3.240397157
H	-2.317818616	-3.496571363	3.367396793
C	-1.132412403	0.962838166	2.617474548
H	-0.968345385	1.869793332	3.216209840
H	-2.079420996	0.530397884	2.925418733
H	-1.166881154	1.200478806	1.553861194
O	-0.992594997	-0.377185993	-1.056198729
N	-1.497860020	-2.501898542	1.656282226
C	-1.421158097	-3.718523647	0.762368883
H	-2.432872531	-4.066467393	0.516466190
H	-0.931438057	-4.526071710	1.314021631
C	-0.647302149	-3.384535455	-0.514303863
H	-0.675736675	-4.236938187	-1.210371840
H	-1.076486592	-2.510379595	-1.010248930
C	-2.737404301	-1.737830666	1.301640699
H	-3.619055470	-2.390361580	1.376103821
H	-2.631599359	-1.345093674	0.288933150
H	-2.872713239	-0.894317538	1.969647390
C	2.868337585	-1.743748911	-0.858187618
H	3.583269776	-2.543040129	-0.627442520
H	3.269636330	-1.267869860	-1.763764599
C	2.906878114	-0.655825341	0.236673271
H	3.938651542	-0.275048526	0.314609118
H	2.239167761	0.158505505	-0.053055914
C	1.499675409	-2.331447019	-1.263294294
H	1.655885410	-3.033722810	-2.098727068
H	0.831407631	-1.536296377	-1.595953883

N	0.773352720	-3.050056920	-0.149640479
N	2.463391063	-1.112378857	1.613214729
C	3.332536921	-2.218105577	2.128354255
H	4.354084639	-1.853229680	2.311053473
H	2.924252890	-2.596946144	3.069254979
H	3.385430005	-3.037505595	1.421832447
C	1.481006587	-4.317065426	0.227871320
H	2.558100847	-4.192807190	0.151486183
H	1.242050788	-4.618486892	1.249617552
H	1.194906714	-5.129168237	-0.454972897
H	-1.741178746	2.486439199	-0.722182066
C	-2.084936571	1.897458722	-1.565997957
C	-1.146231643	0.993811184	-2.201508255
C	-3.400252692	1.964020497	-1.983600172
C	-1.603713317	0.330606749	-3.408953724
H	-0.092803390	1.252175710	-2.145383835
C	-3.860182502	1.215735026	-3.098099199
H	-4.099693792	2.614208476	-1.465102530
C	-2.924078838	0.409115194	-3.800949249
H	-0.896318770	-0.267908706	-3.972700218
H	-3.258695166	-0.131621297	-4.682642331
C	-5.288981503	1.330829440	-3.576991087
H	-5.949102024	1.536039166	-2.724911667
H	-5.612510587	0.373220406	-4.006039642
C	-5.473959296	2.444309144	-4.637899870
H	-6.518999295	2.494874258	-4.961719560
H	-5.193323121	3.423078604	-4.233267058
H	-4.851965844	2.253726973	-5.519490555
Ni	0.331051412	-1.460707469	1.282991424

$^4I_{Ar}$:

O	-0.217706686	-0.083042704	0.050078334
N	-0.095046077	-0.030043795	2.879300930
C	2.405695160	0.224483400	2.556377988
H	3.171422464	0.962618341	2.276765333
H	2.701406989	-0.179166984	3.529019441
C	1.056669917	0.914649362	2.667496758
H	1.095439328	1.656365336	3.481207549
H	0.821668995	1.443127798	1.739550469
C	-0.077267698	-0.791298651	4.172199601
H	-0.156346496	-0.094082103	5.022466502
H	0.894922204	-1.291551755	4.255252831
C	-1.203356145	-1.844426042	4.289666878
H	-2.183340998	-1.356835830	4.284716116
H	-1.112346662	-2.283525235	5.292656810
C	-1.199310363	-3.034397477	3.305843186
H	-0.244037888	-3.569774518	3.386989435
H	-1.988516038	-3.737801116	3.616230573
C	-1.331252285	0.806223497	2.725085644
H	-1.228287052	1.740354742	3.294817643
H	-2.209352456	0.287550180	3.097760716
H	-1.451945864	1.013063143	1.661684316
O	-1.266572337	-0.604544935	-0.939608291
N	-1.383655514	-2.697970340	1.844423311
C	-1.231017965	-3.923052076	0.970435408
H	-2.214828162	-4.370347770	0.779758995
H	-0.642221893	-4.667842664	1.513095539
C	-0.553153736	-3.546573004	-0.347718676
H	-0.524386928	-4.416257914	-1.021946293
H	-1.091206162	-2.734422109	-0.841520324
C	-2.718826438	-2.081374737	1.554285836
H	-3.518871410	-2.816423541	1.721427270
H	-2.727793604	-1.731176629	0.521380469
H	-2.894480244	-1.223576427	2.194446664
C	2.767306350	-1.584184551	-0.894030780
H	3.565333626	-2.304112646	-0.675845236
H	3.080965634	-1.099311119	-1.828754728
C	2.745832551	-0.465794042	0.169412781
H	3.737900906	0.014341620	0.192024427
H	1.992276723	0.273121863	-0.111668730
C	1.445396540	-2.310891013	-1.219975543

H	1.629225270	-3.018121006	-2.045406851
H	0.692220239	-1.590184732	-1.538097993
N	0.841238830	-3.061670167	-0.056455203
N	2.406378511	-0.920983348	1.575711367
C	3.401140122	-1.920718162	2.080552861
H	4.387917000	-1.452439911	2.206463564
H	3.072900698	-2.307759496	3.048707834
H	3.504747465	-2.752668382	1.395149377
C	1.687201832	-4.240184767	0.324848444
H	2.741594485	-4.017259207	0.186845188
H	1.530359326	-4.523932710	1.367205277
H	1.447274405	-5.101317147	-0.314079272
H	-2.029346231	2.118313370	-0.491960410
C	-2.431885793	1.552437044	-1.324902196
C	-1.543422353	0.519376842	-1.933402726
C	-3.709391053	1.767802520	-1.773631048
C	-2.139779109	-0.157744176	-3.124267267
H	-0.539879477	0.917120712	-2.139715708
C	-4.254742946	1.053630096	-2.882449592
H	-4.332226422	2.513673364	-1.284850626
C	-3.422302875	0.096007191	-3.536249983
H	-1.520410844	-0.880851549	-3.645358901
H	-3.821232456	-0.433005904	-4.398439435
C	-5.644900547	1.348868449	-3.393246718
H	-6.281715655	1.680987505	-2.563190555
H	-6.096153732	0.429787965	-3.789976918
C	-5.659639490	2.432068125	-4.502314436
H	-6.683675991	2.614763116	-4.847657554
H	-5.249077996	3.378228681	-4.132212527
H	-5.058849878	2.119691549	-5.364290714
Ni	0.300592936	-1.481893073	1.348150523

$^{2}I_{Ar}$:

O	-0.208876144	-0.390553363	-0.942102747
N	1.292395287	2.033068091	-0.816088814
C	2.924472496	0.814698044	-2.324752976
H	3.064031025	0.492490420	-3.366816218
H	3.809932924	1.398091859	-2.056315661
C	1.678954347	1.680318985	-2.226741830
H	1.824542936	2.595502686	-2.822478375
H	0.813278301	1.147361155	-2.629101405
C	2.271612482	2.894605379	-0.074315873
H	2.359487961	3.876959584	-0.566688525
H	3.255552222	2.414957342	-0.135759004
C	1.907449064	3.117655756	1.411942735
H	0.968153792	3.672847067	1.495796512
H	2.671522291	3.793701277	1.819271667
C	1.882483082	1.892594128	2.351087600
H	2.859065973	1.391395055	2.322217184
H	1.738369418	2.254281693	3.381828746
C	-0.062140779	2.669389583	-0.921346397
H	-0.068019884	3.408744495	-1.734502916
H	-0.329281378	3.185638199	-0.004663234
H	-0.784092066	1.877325976	-1.118298207
O	-1.350905326	-0.789264162	-0.004123757
N	0.845249803	0.837846865	2.043991274
C	0.994367769	-0.367288904	2.947144254
H	0.323749796	-0.270928897	3.810356203
H	2.015542271	-0.387017971	3.338359817
C	0.683247544	-1.648970764	2.172042609
H	0.693447563	-2.515658939	2.850887725
H	-0.298715913	-1.582355970	1.696898498
C	-0.555600440	1.353817550	2.182522708
H	-0.767055750	1.591190025	3.234916090
H	-1.246375198	0.597781200	1.809165889
H	-0.698290710	2.249213642	1.588116269
C	2.177511190	-2.861097543	-1.212957294
H	3.183523357	-3.220829761	-0.964719224
H	1.757302885	-3.641272318	-1.862548445
C	2.260589498	-1.591182064	-2.085198662
H	2.848095850	-1.825172748	-2.988245452
H	1.249814612	-1.297711234	-2.378020514
C	1.280484239	-2.825423382	0.041916067

H	1.267551640	-3.830463147	0.494053629
H	0.264058967	-2.551564749	-0.241656772
N	1.709332423	-1.822014414	1.085520877
N	2.884675582	-0.384940069	-1.410640222
C	4.297223469	-0.663584123	-0.997206044
H	4.934316829	-0.818649650	-1.879886844
H	4.686985098	0.186323280	-0.430918439
H	4.356500771	-1.547785831	-0.374371197
C	3.013383268	-2.217623216	1.711792293
H	3.655811150	-2.707737768	0.984222628
H	3.544864173	-1.350491769	2.109036445
H	2.841241710	-2.930187102	2.530328906
H	-2.525252902	0.605786515	-2.242543289
C	-3.129357345	0.120208942	-1.484029779
C	-2.575315361	-1.120301209	-0.867422532
C	-4.329385973	0.654017992	-1.091113068
C	-3.516709614	-1.792188229	0.075888740
H	-2.171545511	-1.806647390	-1.623783490
C	-5.153788143	0.021253695	-0.111211096
H	-4.680192900	1.578617804	-1.544516916
C	-4.709810301	-1.218400734	0.438261147
H	-3.205679619	-2.743185773	0.497052546
H	-5.352873095	-1.728500217	1.151423891
C	-6.487184807	0.614158904	0.279001190
H	-6.412973428	1.710253883	0.295987837
H	-6.747726512	0.299004586	1.297789968
C	-7.633320788	0.206251194	-0.681535096
H	-8.580262100	0.658915123	-0.364354555
H	-7.423609245	0.534805708	-1.706089677
H	-7.762988993	-0.882363158	-0.696689563
Ni	1.392522232	0.103975993	0.107208251

$^{4}TS_{HA,EB}$:

O	-0.153252391	0.145497861	0.253103237
N	-0.088584726	-0.137753956	3.076241025
C	2.437058642	-0.062846495	2.858178562
H	3.270416206	0.636992209	2.697987518
H	2.662179922	-0.610244588	3.778088323
C	1.146427150	0.721510743	3.024019902
H	1.215631740	1.341726897	3.932090013
H	0.994206173	1.389361739	2.171882237
C	-0.179176921	-1.061114733	4.256887868
H	-0.227197856	-0.474702805	5.189493892
H	0.743397633	-1.652295402	4.294733710
C	-1.394754081	-2.015687804	4.209493968
H	-2.328881858	-1.445560966	4.229665423
H	-1.385160210	-2.575413956	5.154817344
C	-1.446889364	-3.078256898	3.090630722
H	-0.543942467	-3.700813898	3.138022399
H	-2.305170804	-3.741012418	3.286808930
C	-1.241811231	0.818880573	3.021186156
H	-1.096105384	1.627076619	3.752139137
H	-2.180518174	0.326571419	3.254537984
H	-1.294544676	1.223347463	2.011846254
O	-0.995798947	-0.109448114	-0.921975305
N	-1.538120675	-2.555954515	1.676515637
C	-1.443776840	-3.672883868	0.661119787
H	-2.450328643	-4.018898152	0.392475015
H	-0.927683456	-4.520195599	1.120872029
C	-0.695007216	-3.186350194	-0.581915278
H	-0.712588397	-3.960916389	-1.364068296
H	-1.150999805	-2.274586928	-0.976118933
C	-2.803574296	-1.800346374	1.417799393
H	-3.672118935	-2.467365145	1.513488290
H	-2.763654442	-1.382143031	0.412159486
H	-2.916901422	-0.975363609	2.111883254
C	2.785862418	-1.449092921	-0.784898714
H	3.524159016	-2.245570019	-0.630567191
H	3.170053434	-0.877549620	-1.641013114
C	2.797288996	-0.470308955	0.409168551
H	3.817790301	-0.066927591	0.517269465

H	2.106120354	0.350664960	0.203978271
C	1.434117382	-2.035050895	-1.245612483
H	1.612223105	-2.665904498	-2.131900947
H	0.756975563	-1.229358702	-1.530170334
N	0.720339913	-2.856580805	-0.196173076
N	2.381319159	-1.070562459	1.739232745
C	3.283080968	-2.200022562	2.133304028
H	4.299900425	-1.831204075	2.331805848
H	2.901203388	-2.673543461	3.041274823
H	3.339385268	-2.948977292	1.353603212
C	1.454429012	-4.137845716	0.070344093
H	2.526836505	-3.993196347	-0.033860239
H	1.255156296	-4.512272213	1.076545076
H	1.155197883	-4.905225933	-0.657061729
H	-6.803314465	0.068418890	0.537727437
C	-5.949178208	0.732675340	0.625642407
C	-5.837912495	1.583892355	1.735460683
C	-4.978083924	0.746871729	-0.377677164
C	-4.743771444	2.457416693	1.829848519
H	-6.601584584	1.579314613	2.506371475
C	-3.863290180	1.619219470	-0.300211905
H	-5.090584980	0.093296792	-1.235918092
C	-3.771294334	2.472687298	0.829760226
H	-4.663575532	3.137210428	2.672419486
H	-2.937778410	3.166806811	0.895308647
C	-2.807659626	1.648751250	-1.318948056
H	-1.852337740	0.730289382	-0.964695601
H	-2.169290389	2.536375941	-1.247820161
C	-3.088124446	1.225750348	-2.750830950
H	-2.160237028	1.198472949	-3.329351662
H	-3.547144871	0.232919621	-2.813647493
H	-3.769183168	1.935726574	-3.241787994
Ni	0.236713867	-1.425431803	1.391015661

$^{4}TS_{HA,XA}$:

Ni	-0.293278124	-1.431369739	0.893452765
O	-0.371264941	-0.225461201	-0.675990894
N	-0.086021935	0.235680255	2.241457261
C	2.333001146	-0.365802105	1.771948783
H	3.256758855	0.048187890	1.342846136
H	2.586243003	-0.713255719	2.777670928
C	1.280344391	0.728613672	1.846938070
H	1.621297272	1.506051351	2.549361979
H	1.141437331	1.190611631	0.866341355
C	-0.173684089	-0.385352611	3.606407935
H	0.045740906	0.370913257	4.378237808
H	0.604299861	-1.154060944	3.678973745
C	-1.547325483	-1.024414642	3.917451573
H	-2.331875804	-0.261337444	3.918791820
H	-1.494652900	-1.377842457	4.956314572
C	-1.996033487	-2.240738542	3.078026456
H	-1.232707426	-3.028032217	3.136730579
H	-2.914347269	-2.648823134	3.530509572
C	-0.992735396	1.425321085	2.115029221
H	-0.549112250	2.288431080	2.632210725
H	-1.960639337	1.229788368	2.567700071
H	-1.139637117	1.647337407	1.057962465
O	-1.605903548	0.537362619	-0.754090371
N	-2.241330509	-1.978441339	1.609897013
C	-2.566970032	-3.247763620	0.853688131
H	-3.652896526	-3.340985136	0.730564468
H	-2.239140755	-4.107317330	1.444228677
C	-1.879020770	-3.229239363	-0.512916119
H	-2.204995004	-4.084551442	-1.123534430
H	-2.134915212	-2.314128582	-1.050689790
C	-3.361147271	-1.010152386	1.388555034
H	-4.297393395	-1.416128494	1.799000410
H	-3.468797635	-0.825949841	0.320950602
H	-3.148950952	-0.055827333	1.856281667
C	1.866273637	-2.643040923	-1.371103798
H	2.390119701	-3.551726139	-1.050181272
H	2.269642071	-2.425210098	-2.369341211
C	2.270531102	-1.447190489	-0.484258651

H	3.364820286	-1.325195981	-0.543042117
H	1.794162247	-0.537974845	-0.860660746
C	0.362717526	-2.909756744	-1.578299760
H	0.239924907	-3.728506366	-2.303925719
H	-0.101349626	-2.010590058	-1.982582554
N	-0.390488013	-3.250412426	-0.313993553
N	1.885562272	-1.567446352	0.977141443
C	2.513169758	-2.772304399	1.606914069
H	3.608810420	-2.677143835	1.618941155
H	2.161378259	-2.872064615	2.637000332
H	2.254104053	-3.675814751	1.067840250
C	0.009853942	-4.601465596	0.198099166
H	1.064278396	-4.784413895	0.004902632
H	-0.160744476	-4.689309685	1.272775547
H	-0.559940825	-5.388488057	-0.315603939
H	-0.382787761	1.063969190	-4.232735006
C	-0.641118091	0.034081947	-4.457789674
C	0.197289160	-0.742312089	-5.256687048
C	-1.839010207	-0.495160724	-3.929649285
C	-0.142658004	-2.075092918	-5.551342964
H	1.107100410	-0.313546205	-5.662508025
C	-2.147240393	-1.836890710	-4.242879133
C	-1.322496746	-2.625893212	-5.045247301
H	0.501130179	-2.674354533	-6.186093430
C	-4.076578556	-0.301361990	-2.845450787
H	-1.624922375	-3.641248343	-5.273036676
C	-4.318550473	-1.651079778	-3.177636118
C	-5.146411803	0.427398561	-2.282277337
C	-5.553299705	-2.264546421	-2.964796239
H	-4.990665790	1.471971676	-2.029686559
C	-6.386867118	-0.170186876	-2.061277293
C	-6.590730033	-1.519565359	-2.399679346
H	-5.685742732	-3.298579793	-3.260446907
H	-7.198970812	0.410349365	-1.637420523
H	-7.558356760	-1.981726442	-2.237786741
C	-2.737475603	0.273237462	-3.054641263
H	-2.726125367	1.353990961	-3.225802807
H	-2.128479500	0.325524570	-1.857975475
O	-3.314365374	-2.444561857	-3.755940369

$^{4}TS_{2HA,XA}$:

Ni	0.000000000	0.000000000	0.000000000
N	0.000000000	0.000000000	2.228560696
N	2.213569130	0.000000000	0.256776777
N	0.183540629	-0.710340307	-2.067937251
N	-2.057037043	-0.736896970	-0.163616647
C	1.375210296	-0.494262333	2.571629087
H	1.585529658	-0.327989092	3.640299930
H	1.391533847	-1.576482722	2.404853331
C	2.435698930	0.195344329	1.732185361
H	3.435329670	-0.170141295	2.013327619
H	2.424111888	1.270272563	1.921495206
C	2.756408301	-1.338324494	-0.169946054
H	3.840570922	-1.361183577	0.031291830
H	2.296362840	-2.099149541	0.472091950
C	2.522829746	-1.713097074	-1.640220792
H	3.040949379	-2.668369576	-1.802030988
H	3.026559313	-1.004120910	-2.304691710
C	1.068712982	-1.931079721	-2.082608428
H	0.602945196	-2.681709296	-1.432388923
H	1.072052643	-2.347536557	-3.103627571
C	-1.213715391	-1.090895131	-2.483579002
H	-1.697358082	-0.188291251	-2.862417105
H	-1.175007295	-1.807076944	-3.318600846
C	-2.013831516	-1.678959804	-1.333747465
H	-1.565263218	-2.616482545	-0.988476201
H	-3.034510158	-1.913976591	-1.674185945
C	-2.608027254	-1.480966213	1.024101908
H	-2.106070798	-2.455268917	1.064382705
H	-3.676512015	-1.675619389	0.839555698
C	-2.431122899	-0.776394341	2.370010085

H	-2.767663249	0.264327072	2.321372965
H	-3.097544393	-1.269963332	3.089514991
C	-1.008535739	-0.877584229	2.920787441
H	-0.666044093	-1.914931480	2.824519301
H	-1.000823362	-0.634898920	3.995255375
C	-0.175152135	1.416163237	2.696434965
H	0.016406840	1.481038613	3.778147572
H	0.489380161	2.081958207	2.151999565
H	-1.185406157	1.753216075	2.476764601
C	2.903921900	1.133222525	-0.444146332
H	3.926075673	1.257720546	-0.058894946
H	2.314270452	2.036914310	-0.286922573
H	2.964711054	0.948790679	-1.512589664
C	0.660299266	0.334391882	-3.033621704
H	1.717713805	0.535340715	-2.894719554
H	0.114066678	1.258025995	-2.847593073
H	0.502691685	-0.000314274	-4.068517311
C	-2.943182734	0.435521244	-0.470421374
H	-2.622245855	0.917466813	-1.390760739
H	-2.860681778	1.181171099	0.316727721
H	-3.985860980	0.104759876	-0.581404536
O	0.010237410	1.926574838	-0.415346684
O	-1.005953989	2.758473244	0.194617094
H	-6.465649825	4.564622377	0.207309975
C	-5.818612768	4.154938363	-0.560593757
C	-4.460393870	4.472398876	-0.567235287
C	-6.352895356	3.314499092	-1.552833357
C	-3.599065550	3.961143798	-1.561129866
H	-4.048712122	5.126812480	0.195305307
C	-5.526105674	2.799432580	-2.554719305
H	-7.410730386	3.075130362	-1.552918745
C	-4.170870603	3.127003671	-2.544860605
C	-2.151574414	4.226611684	-1.588903975
H	-5.911384724	2.168761887	-3.347289644
O	-3.380470463	2.583469108	-3.574921064
C	-1.477809918	3.954688916	-2.866962128
H	-1.846369461	5.155652754	-1.099018547
C	-2.110768445	3.131159617	-3.823483568
C	-0.200519338	4.460858439	-3.191524214
C	-1.524344272	2.825009239	-5.051552531
H	0.304992087	5.099393257	-2.473931067
C	0.403014914	4.159572443	-4.412023691
C	-0.258731179	3.340975038	-5.344655199
H	-2.071830334	2.213406200	-5.759330246
H	1.378671048	4.570393695	-4.648482340
H	0.201975949	3.122879608	-6.302097648
H	-1.567876852	3.396026591	-0.702110522

$^{4}TS_{HA,CHD}$:

Ni	0.084360026	-0.172796588	-0.116505814
O	0.163331416	-0.437744617	1.847951186
N	2.211268332	0.107084898	-0.080723027
C	1.360638624	2.484952730	0.108023492
H	1.383820145	3.362593123	0.769923574
H	1.701772323	2.825634712	-0.873715812
C	2.300781934	1.419675983	0.648835043
H	3.333918808	1.801326363	0.622523432
H	2.050199790	1.182257043	1.685948791
C	2.637057765	0.145790746	-1.519550180
H	3.708729961	0.395569531	-1.588859130
H	2.086048127	0.956211899	-2.010603154
C	2.388760145	-1.173394225	-2.287312834
H	3.002570072	-1.977947602	-1.870282609
H	2.780360165	-1.017212405	-3.301759546
C	0.932639975	-1.657232625	-2.464031564
H	0.339494260	-0.867509092	-2.944228128
H	0.939013754	-2.517893541	-3.152332326
C	3.026759852	-0.858498223	0.727141096
H	4.004987897	-0.416997394	0.965081558
H	3.204291356	-1.778488774	0.178650971
H	2.482047358	-1.085004507	1.643456956
O	0.103103854	-1.845699488	2.217040117
N	0.206404040	-2.040190286	-1.195548013

C	-1.241535552	-2.390816770	-1.451456711
H	-1.352488574	-3.478239333	-1.547037515
H	-1.548090334	-1.956328523	-2.406691898
C	-2.112159742	-1.866534169	-0.306697768
H	-3.146681145	-2.227282547	-0.412839657
H	-1.717747764	-2.209788629	0.653349412
C	0.845469531	-3.207021613	-0.506893812
H	0.759977994	-4.107807456	-1.131792125
H	0.356499841	-3.356042123	0.455102886
H	1.894627832	-3.016612449	-0.310932777
C	-2.345334471	1.747687229	1.120071364
H	-2.895046248	2.326836519	0.368245776
H	-2.801363097	2.029816323	2.078956328
C	-0.879660611	2.224698983	1.199097507
H	-0.878375301	3.305325923	1.418297468
H	-0.373171770	1.700099686	2.012515116
C	-2.613831670	0.237082798	0.959238503
H	-3.701330993	0.064853566	1.002489544
H	-2.143695476	-0.294238881	1.784614295
N	-2.072324608	-0.363836849	-0.314271351
N	-0.057627999	1.994321768	-0.053243149
C	-0.642085283	2.717994731	-1.227026105
H	-0.587625921	3.805955811	-1.076723582
H	-0.082001346	2.462364889	-2.130142365
H	-1.679866525	2.445574604	-1.378220574
C	-2.836073878	0.135121217	-1.504368284
H	-3.137574843	1.169349053	-1.357653276
H	-2.238269672	0.079840141	-2.415739212
H	-3.750487880	-0.458100948	-1.645124631
C	-1.896773518	-0.921344208	4.713505189
C	-3.148383267	-0.401427769	4.694610963
C	-2.730647340	-3.024673035	3.671838807
C	-3.989907690	-2.529403704	3.641736504
C	-1.582296216	-2.234935138	4.137962961
H	-0.812764877	-2.803934744	4.672581135
H	-0.786250731	-1.984307880	3.099026690
H	-2.544199009	-4.046085797	3.348671588
H	-4.813240875	-3.147710290	3.292362391
H	-3.341566567	0.573478986	5.136058905
H	-1.082549445	-0.359846490	5.163431440
C	-4.332825081	-1.147518460	4.135596628
H	-5.124473435	-1.214383617	4.903384930
H	-4.807469832	-0.560482787	3.326659315

$^{2}TS_{HA,EB}$:

O	-1.809919745	-0.578766967	1.002139547
N	-1.409590643	-1.399155582	3.658733369
C	0.393305093	0.377716034	3.756276000
H	0.534360930	1.464681282	3.846580312
H	0.979630258	-0.081117593	4.557747852
C	-1.078604486	0.042987515	3.930027503
H	-1.396759636	0.322718156	4.947107823
H	-1.684204828	0.610351486	3.218218371
C	-0.802044435	-2.389704710	4.608476419
H	-1.191886136	-2.224114937	5.626423111
H	0.278114118	-2.204455935	4.643258675
C	-1.053259283	-3.864949324	4.218201409
H	-2.123591840	-4.091135622	4.252563227
H	-0.610681701	-4.475102569	5.017372557
C	-0.444211548	-4.388810025	2.899442520
H	0.642609993	-4.233001442	2.912719957
H	-0.612116660	-5.476887959	2.853156821
C	-2.908609672	-1.468851503	3.644204773
H	-3.318352640	-0.942068479	4.517550705
H	-3.257345883	-2.496258932	3.684996338
H	-3.247359297	-1.003851837	2.718158290
O	-2.515544445	-1.215503412	-0.127886217
N	-0.957903674	-3.752852684	1.629104915
C	-0.206520893	-4.243852726	0.411922264
H	-0.737551032	-5.092424412	-0.038239375
H	0.772351267	-4.613203076	0.730383567

C	-0.058588302	-3.107698962	-0.602325790
H	0.389678581	-3.483997639	-1.534637904
H	-1.031884802	-2.663999731	-0.828971111
C	-2.416942145	-4.008801430	1.405790883
H	-2.589916807	-5.079811664	1.225495907
H	-2.753221891	-3.418554853	0.552187797
H	-3.000116399	-3.701450626	2.267084611
C	1.346398726	0.480945159	-0.038050746
H	2.435886112	0.360795147	0.006516842
H	1.182655031	1.341785703	-0.699599510
C	0.794882411	0.909429000	1.337926418
H	1.306848770	1.836406951	1.644568464
H	-0.274236242	1.109663273	1.243960693
C	0.689554544	-0.720566020	-0.748459969
H	1.152164946	-0.835427264	-1.742391262
H	-0.374654244	-0.531489913	-0.882054753
N	0.801285247	-2.029512193	-0.001886653
N	0.960352352	-0.111698634	2.447401425
C	2.405245711	-0.421580566	2.691435575
H	2.925896230	0.460350393	3.092048817
H	2.488722715	-1.235080876	3.417018203
H	2.901517384	-0.723266617	1.777122261
C	2.220990770	-2.510636809	0.033181997
H	2.907899707	-1.672701357	0.117958816
H	2.394187793	-3.182327700	0.876168129
H	2.463945281	-3.042758567	-0.896962705
H	-1.632848735	4.486366993	0.491454565
C	-1.602058563	3.776681928	-0.329601521
C	-0.647465912	3.927216022	-1.346088595
C	-2.527592126	2.731592700	-0.376600042
C	-0.624961712	3.017596177	-2.415364710
H	0.058476030	4.750419957	-1.314596951
C	-2.527379031	1.807789026	-1.451423626
H	-3.266930034	2.637242388	0.410429698
C	-1.546709566	1.971399935	-2.463714899
H	0.096977162	3.139947513	-3.216888752
H	-1.539275685	1.282170728	-3.304205014
C	-3.480939734	0.695192681	-1.534212128
H	-2.914735247	-0.307525547	-0.808943894
H	-3.502926040	0.222413064	-2.521246168
C	-4.846826962	0.796943685	-0.877781153
H	-5.398644962	-0.141016461	-0.990007055
H	-4.774334896	1.012327819	0.194155970
H	-5.444199825	1.595933820	-1.339625999
Ni	-0.384824007	-1.695778747	1.793241278

$^{2}TS_{HA,XA}$:

Ni	-0.508177905	-1.460025695	1.077102959
O	-0.836615461	-0.274066398	-0.469007428
N	0.271670890	0.234876488	2.122878983
C	2.362004082	-0.776050085	1.113538095
H	3.189393893	-0.548245535	0.426115076
H	2.817554090	-1.103132427	2.052771404
C	1.533565978	0.478405389	1.340586976
H	2.153492592	1.237957106	1.843119038
H	1.195043158	0.887242028	0.385199935
C	0.474519601	-0.218321056	3.539521902
H	0.975227445	0.573964907	4.120283276
H	1.151557600	-1.080303088	3.521909433
C	-0.829883675	-0.614072742	4.270285624
H	-1.481789658	0.257715508	4.385028653
H	-0.538300727	-0.884676721	5.294428185
C	-1.641195226	-1.811271309	3.727752066
H	-0.996761224	-2.699148998	3.676945341
H	-2.442620170	-2.037223475	4.449933707
C	-0.508485272	1.513443854	2.038933467
H	0.146806898	2.368308441	2.257408768
H	-1.318913056	1.526735056	2.761277240
H	-0.918987340	1.598238652	1.032772359
O	-2.243210367	0.121297423	-0.549815801
N	-2.244425272	-1.628158418	2.355023004
C	-2.924473422	-2.883437630	1.856421979
H	-4.000894195	-2.832801187	2.063376477

H	-2.535133052	-3.741308081	2.411518950
C	-2.678098615	-3.043666131	0.353882057
H	-3.278294756	-3.873582201	-0.049447650
H	-2.950392495	-2.123602742	-0.171264142
C	-3.251810810	-0.520497295	2.322231837
H	-4.112178560	-0.773768288	2.958672335
H	-3.567641163	-0.366592301	1.291029523
H	-2.820291388	0.410265184	2.672087453
C	0.704659804	-3.095000938	-1.567331244
H	1.158926085	-4.065124512	-1.331134612
H	0.827593375	-2.982096754	-2.652792425
C	1.523394186	-1.949453093	-0.935749458
H	2.563363193	-2.027651483	-1.293721185
H	1.111635462	-0.991328805	-1.260663608
C	-0.817286480	-3.121069573	-1.321237859
H	-1.262830821	-3.931926781	-1.917768917
H	-1.240596897	-2.173087208	-1.646778682
N	-1.212861103	-3.290656322	0.125769591
N	1.547362740	-1.929135147	0.580363406
C	2.148617469	-3.185426615	1.130636107
H	3.210010875	-3.259395635	0.854065327
H	2.072306442	-3.181217840	2.220846123
H	1.635776937	-4.061892683	0.753871299
C	-0.870940161	-4.665992921	0.614742719
H	0.052569075	-5.014666465	0.158991671
H	-0.745546312	-4.686158953	1.698862169
H	-1.662882088	-5.375789825	0.337888861
H	-0.854403599	1.967594708	-3.436500881
C	-0.681051562	1.006874288	-3.910394418
C	0.498844670	0.773569834	-4.614644152
C	-1.673050744	0.008999213	-3.800467052
C	0.718927716	-0.471556416	-5.230414652
H	1.243893603	1.557155787	-4.697260716
C	-1.419681622	-1.228775283	-4.429319961
C	-0.245177640	-1.478116776	-5.141366252
H	1.630256230	-0.648698035	-5.791161454
C	-3.969916260	-0.808738376	-3.264320146
H	-0.119178775	-2.437763938	-5.628536147
C	-3.647802527	-2.026644207	-3.898425380
C	-5.302607164	-0.636121368	-2.832699999
C	-4.589077788	-3.037926976	-4.097304544
H	-5.578786898	0.297798046	-2.352037711
C	-6.256112414	-1.636104865	-3.021814346
C	-5.898081903	-2.841361045	-3.652120528
H	-4.287324488	-3.945610230	-4.606666840
H	-7.277129805	-1.480685344	-2.690598027
H	-6.640726965	-3.616590345	-3.807537002
C	-2.917401304	0.198265315	-3.036313576
H	-3.275874204	1.231457003	-3.000789832
H	-2.559643879	0.104560497	-1.774190895
O	-2.351611439	-2.274301378	-4.376140052

$^{2}TS_{2HA,XA}$:

Ni	0.000000000	0.000000000	0.000000000
N	0.000000000	0.000000000	2.221455457
N	2.207759879	0.000000000	0.248324654
N	0.181500503	-0.723513942	-2.073656391
N	-2.061935110	-0.736555546	-0.167591209
C	1.374825765	-0.497525379	2.562930759
H	1.585135337	-0.335350874	3.632028756
H	1.390361165	-1.579111272	2.392005207
C	2.433212601	0.195466167	1.723620036
H	3.434202857	-0.167810503	2.002330259
H	2.419191621	1.270238190	1.913753329
C	2.757064068	-1.336029261	-0.178653198
H	3.841455286	-1.352231308	0.021165719
H	2.302454598	-2.098436601	0.465414324
C	2.523608959	-1.715219706	-1.647688000
H	3.046565801	-2.668076641	-1.807606348
H	3.022894668	-1.005294194	-2.314347076
C	1.070230876	-1.940847900	-2.088315532

H	0.608109510	-2.692679668	-1.436812332
H	1.074602408	-2.358981340	-3.108694518
C	-1.215857733	-1.107318156	-2.484476018
H	-1.700243857	-0.207350589	-2.867911120
H	-1.178418280	-1.828993375	-3.314767083
C	-2.015138224	-1.687300429	-1.330196894
H	-1.564597376	-2.620902691	-0.976984770
H	-3.034965710	-1.927509173	-1.669515240
C	-2.629471746	-1.467720060	1.020000553
H	-2.148948424	-2.452739868	1.061481195
H	-3.701905330	-1.639874768	0.836225605
C	-2.436224168	-0.766087008	2.364794459
H	-2.762509813	0.277946631	2.318591635
H	-3.103032713	-1.253376077	3.088201332
C	-1.010907836	-0.881882321	2.906514171
H	-0.673685316	-1.919551475	2.795761758
H	-0.996238834	-0.652407993	3.983723802
C	-0.174333737	1.412118875	2.702865911
H	0.019050517	1.465862685	3.784851107
H	0.488701953	2.084430300	2.164576574
H	-1.184954280	1.750483243	2.487927593
C	2.887164677	1.138632291	-0.455693723
H	3.902202061	1.284142635	-0.059730640
H	2.277493168	2.032136915	-0.316137343
H	2.964286830	0.943529910	-1.521308555
C	0.652054100	0.322491189	-3.040730440
H	1.708830881	0.528097984	-2.904412155
H	0.101854804	1.243011977	-2.851149665
H	0.493764036	-0.013479809	-4.075265601
C	-2.933681962	0.442895223	-0.489426095
H	-2.584956417	0.931241924	-1.396080267
H	-2.864763819	1.182888971	0.304212342
H	-3.975244128	0.118450031	-0.626725438
O	-0.029549748	1.901631713	-0.483276493
O	-0.986224805	2.736720022	0.224141069
H	-6.434096067	4.601641155	0.262128727
C	-5.775013311	4.215267354	-0.507527485
C	-4.417606607	4.535149927	-0.485764577
C	-6.292463938	3.401967800	-1.530550197
C	-3.541226985	4.053987490	-1.480686874
H	-4.018486429	5.167993495	0.301139469
C	-5.450180145	2.917062798	-2.534036719
H	-7.349485649	3.160320619	-1.552682870
C	-4.095738681	3.246988515	-2.495494708
C	-2.091318088	4.320704947	-1.476521984
H	-5.822180198	2.308053914	-3.349450806
O	-3.291128136	2.735478398	-3.529764429
C	-1.399123657	4.083718185	-2.753768647
H	-1.798696320	5.241588122	-0.964195817
C	-2.016411756	3.285865228	-3.740595646
C	-0.116883267	4.596605929	-3.043000320
C	-1.408722436	3.009342997	-4.965378037
H	0.376678235	5.215473288	-2.300390506
C	0.507530759	4.326009392	-4.260033605
C	-0.138245642	3.531007302	-5.223380589
H	-1.943833253	2.415784852	-5.697342829
H	1.487451960	4.741117153	-4.469166339
H	0.339199938	3.335741747	-6.177563308
H	-1.540923001	3.466802542	-0.631013700

$^{2}TS_{HA,CHD}$:

Ni	0.056345966	-0.183037213	-0.153862383
O	0.073159080	-0.504825127	1.794713481
N	2.177220158	0.061794200	-0.070068036
C	1.359584733	2.445150228	0.180257902
H	1.380878065	3.299883972	0.871342566
H	1.725247725	2.813178795	-0.782611799
C	2.272745435	1.348326308	0.704466803
H	3.312080755	1.713110717	0.711388736
H	1.995641411	1.079630445	1.726997684
C	2.634276198	0.140654456	-1.498031225
H	3.710894694	0.374670647	-1.536298733
H	2.106794096	0.976073272	-1.972995651

C	2.380940661	-1.147696904	-2.315182749
H	2.974272256	-1.975772421	-1.914880412
H	2.794164845	-0.962981231	-3.316171236
C	0.921114450	-1.602260788	-2.534387500
H	0.347883530	-0.787105199	-2.996067992
H	0.926663116	-2.438033468	-3.252681251
C	2.956311357	-0.945499150	0.723880444
H	3.927236484	-0.522258198	1.017210943
H	3.150066007	-1.840271372	0.140173325
H	2.375765261	-1.209001853	1.608007222
O	0.003673297	-1.932935492	2.093750796
N	0.168949288	-2.018239194	-1.291797478
C	-1.279843455	-2.340291158	-1.580101997
H	-1.403275984	-3.422440309	-1.712883007
H	-1.566109578	-1.870804528	-2.525105645
C	-2.159913854	-1.841634682	-0.430632873
H	-3.196565094	-2.188356627	-0.561608941
H	-1.779468224	-2.215428263	0.524469996
C	0.780058718	-3.217688271	-0.634894868
H	0.704897546	-4.090993457	-1.298947049
H	0.261412283	-3.403193922	0.304979520
H	1.824243501	-3.045102749	-0.400656576
C	-2.375509113	1.729570293	1.097972716
H	-2.904346029	2.335541174	0.352240876
H	-2.845421360	1.991900797	2.055685960
C	-0.906072996	2.186138699	1.216663078
H	-0.895776731	3.260549710	1.464074617
H	-0.421658038	1.633831167	2.025064140
C	-2.657224814	0.227084363	0.891314495
H	-3.747075893	0.064759692	0.916211019
H	-2.197790415	-0.332606800	1.704495001
N	-2.105654136	-0.339687383	-0.393522060
N	-0.061468875	1.979048992	-0.024800925
C	-0.612448830	2.741023286	-1.190443162
H	-0.550732548	3.823755635	-1.008781406
H	-0.034781087	2.504849547	-2.087847860
H	-1.649194925	2.483032380	-1.371698089
C	-2.848330496	0.203309842	-1.577506118
H	-3.138648378	1.236876580	-1.404747358
H	-2.240039450	0.166682941	-2.483011664
H	-3.768275793	-0.373751783	-1.746708194
C	-1.771229526	-0.901524530	4.694118282
C	-3.029712550	-0.400325638	4.697114108
C	-2.622882446	-3.089175929	3.854609318
C	-3.887951456	-2.610903843	3.847869092
C	-1.461718334	-2.251387701	4.198439383
H	-0.663283893	-2.769434393	4.741935901
H	-0.772032798	-2.068101593	3.106636283
H	-2.436481451	-4.129142866	3.597836692
H	-4.718198023	-3.262386688	3.585960414
H	-3.217647574	0.601813540	5.075915361
H	-0.945778120	-0.298548229	5.062384460
C	-4.227133815	-1.198887391	4.250299680
H	-4.983262455	-1.214800219	5.055446192
H	-4.743377726	-0.680312552	3.420533791

$^{4}I_{HA,EB}$:

O	-0.134665864	-0.111968133	0.095758880
N	-0.084597657	-0.118148825	2.916040120
C	2.432500780	0.062592025	2.674834138
H	3.229593996	0.784146451	2.445095651
H	2.683927291	-0.382906144	3.641766481
C	1.103743645	0.793476742	2.768834543
H	1.142196065	1.506722828	3.607793728
H	0.915219412	1.361218055	1.853519055
C	-0.130264596	-0.915572771	4.186481914
H	-0.212505630	-0.238405214	5.052643538
H	0.822170141	-1.450168635	4.284664801
C	-1.293239461	-1.933278475	4.241017144
H	-2.256161650	-1.413856145	4.210745502
H	-1.253039936	-2.395796060	5.236394976

C	-1.290408135	-3.102406525	3.232499930
H	-0.354763342	-3.668029705	3.334442794
H	-2.110492487	-3.788307406	3.499914646
C	-1.286130287	0.766314706	2.758210346
H	-1.179513929	1.661429607	3.387285195
H	-2.196306115	0.258259751	3.058708890
H	-1.359703325	1.044750027	1.707637443
O	-1.103520309	-0.576092565	-0.989518704
N	-1.413045280	-2.728585563	1.774273237
C	-1.263754446	-3.936297072	0.875977883
H	-2.251548704	-4.359961396	0.652386701
H	-0.701508933	-4.704980399	1.414684894
C	-0.546824980	-3.540909238	-0.416849745
H	-0.523276620	-4.393012183	-1.113352151
H	-1.054669235	-2.703540862	-0.899658326
C	-2.717079064	-2.065655299	1.452036160
H	-3.547521681	-2.771665082	1.596853697
H	-2.686950328	-1.719126199	0.418877200
H	-2.879436720	-1.199658720	2.083993026
C	2.832961282	-1.643581360	-0.824294420
H	3.608572802	-2.388713835	-0.609680733
H	3.180904670	-1.136482766	-1.734872778
C	2.811393886	-0.558809058	0.273999220
H	3.813759398	-0.103494142	0.335345193
H	2.081814108	0.206030748	-0.001308201
C	1.503147642	-2.327863377	-1.207729506
H	1.695254053	-3.018068469	-2.045499850
H	0.779241035	-1.579899086	-1.532851116
N	0.851450637	-3.098259356	-0.081173080
N	2.428110037	-1.049671961	1.657449014
C	3.387031011	-2.088787527	2.152104869
H	4.380871058	-1.648976604	2.318370298
H	3.025721468	-2.500683572	3.098738709
H	3.489496200	-2.898613996	1.440445717
C	1.660067490	-4.307845167	0.283652639
H	2.722466558	-4.106348664	0.175181048
H	1.473417785	-4.618246936	1.313599516
H	1.414806871	-5.143987917	-0.385757029
H	-6.507366493	0.429298234	0.183071981
C	-5.625392576	1.060327770	0.130412710
C	-5.333258065	1.941751538	1.185916758
C	-4.806933149	1.003205256	-0.993819971
C	-4.203864480	2.776248147	1.098171557
H	-5.986149768	1.994073422	2.050757929
C	-3.647662492	1.833001798	-1.103691719
H	-5.060658672	0.330528998	-1.805814987
C	-3.376002179	2.725185735	-0.017576913
H	-3.985874612	3.477352349	1.898195724
H	-2.513162694	3.382512150	-0.085689854
C	-2.776717365	1.800253970	-2.230814398
H	-1.601747448	0.258181937	-1.173336694
H	-1.959449829	2.520272973	-2.245147872
C	-2.990280636	0.989673970	-3.475336884
H	-2.051433509	0.853362470	-4.020447565
H	-3.405557453	-0.004189177	-3.271016317
H	-3.690093674	1.489609123	-4.165734486
Ni	0.314506585	-1.548906363	1.362173843

$^{4}I_{HA,XA}$:

Ni	0.154886614	-0.257868420	-0.264381164
O	0.393389547	-0.532445299	1.675208097
N	2.200872011	0.388934846	-0.311884598
C	0.960430164	2.583688007	-0.069158686
H	0.866067056	3.457032892	0.592412177
H	1.188814286	2.970381779	-1.066562938
C	2.094267147	1.698218880	0.420822629
H	3.044014729	2.252433698	0.352471715
H	1.936498831	1.423058029	1.467097472
C	2.564457136	0.490933746	-1.763705784
H	3.574931026	0.918646267	-1.871549643
H	1.866600740	1.192072779	-2.236756399
C	2.517883769	-0.858842671	-2.517429512
H	3.272508399	-1.543671071	-2.117938709

H	2.843279132	-0.649171169	-3.545541816
C	1.159814127	-1.584171921	-2.641996586
H	0.428336179	-0.913341298	-3.112427978
H	1.291180662	-2.442290026	-3.320720895
C	3.185322668	-0.428358723	0.471785059
H	4.073122417	0.175432705	0.707003098
H	3.516411107	-1.295117765	-0.092097544
H	2.688076153	-0.752232208	1.386541695
O	0.268264809	-2.006824702	2.060769045
N	0.542343749	-2.064334005	-1.349040927
C	-0.834238742	-2.654609464	-1.564792895
H	-0.759464040	-3.743647239	-1.677570232
H	-1.240055431	-2.264754594	-2.502523185
C	-1.742246979	-2.301540579	-0.384483662
H	-2.706212596	-2.825424517	-0.468259149
H	-1.266499745	-2.585582162	0.557872736
C	1.383805346	-3.097232348	-0.662700288
H	1.431958115	-4.010128748	-1.273787250
H	0.951585420	-3.311052555	0.314456729
H	2.391844567	-2.731913894	-0.502050554
C	-2.501191802	1.206548170	1.129212597
H	-3.184656897	1.687826185	0.418987080
H	-2.945053597	1.394105041	2.116397369
C	-1.138485913	1.930579790	1.139113689
H	-1.310027708	2.993482746	1.376782561
H	-0.506892912	1.490745268	1.914232058
C	-2.512808665	-0.325699204	0.952825402
H	-3.546380550	-0.687169451	1.061771362
H	-1.903766945	-0.779087822	1.731925273
N	-1.950402770	-0.811237177	-0.362743260
N	-0.358250638	1.856472750	-0.159689408
C	-1.122728529	2.478368465	-1.287480133
H	-1.243586948	3.558802737	-1.121963204
H	-0.580624559	2.327999956	-2.224753150
H	-2.106752807	2.035933737	-1.384521573
C	-2.853496181	-0.434941150	-1.498931972
H	-3.306967273	0.537157841	-1.322107937
H	-2.309815593	-0.392335052	-2.444642874
H	-3.668452714	-1.166051826	-1.593060006
H	-0.473060110	-0.351283954	6.403162549
C	-1.435189721	-0.066406469	5.989363252
C	-1.979122639	1.183238858	6.269586062
C	-2.125367084	-0.999396760	5.170856164
C	-3.233770325	1.546794878	5.745250510
H	-1.438514231	1.876466857	6.904688884
C	-3.388132090	-0.594323607	4.656254947
C	-3.942357229	0.651448812	4.934289275
H	-3.661903051	2.515491803	5.977744271
C	-2.425873785	-3.197994666	4.079913859
H	-4.920123478	0.894307446	4.534753843
C	-3.683290943	-2.756503716	3.581524865
C	-2.043875315	-4.530746529	3.770023629
C	-4.515453267	-3.575081252	2.824781425
H	-1.095387856	-4.900424534	4.147604535
C	-2.868776786	-5.355696218	3.011523238
C	-4.106452676	-4.882696862	2.535802006
H	-5.471469498	-3.189246314	2.490823325
H	-2.561638924	-6.373706783	2.797179369
H	-4.753581935	-5.533758701	1.958788150
C	-1.630876029	-2.300252338	4.854667221
H	-0.696341370	-2.641979316	5.288234113
H	-0.184072852	-1.934795670	2.934715175
O	-4.133292519	-1.452586949	3.833904754

$^4I_{HA,CHD}$:

Ni	0.024990861	-0.066668690	-0.110141569
O	-0.027703106	-0.287469960	1.847445937
N	2.163328304	-0.079108550	0.079642482
C	1.648548217	2.401712348	0.093342047
H	1.761334962	3.306077061	0.708809318
H	2.093050716	2.628701992	-0.879941583

C	2.389754082	1.248727837	0.749314798
H	3.466122109	1.481278613	0.781447120
H	2.043755878	1.109217131	1.777093424
C	2.696459775	-0.195749140	-1.317805279
H	3.794712357	-0.098177664	-1.312868896
H	2.301206529	0.645083194	-1.900481727
C	2.322220970	-1.521966955	-2.019624485
H	2.777697375	-2.369874627	-1.498735736
H	2.811283344	-1.499462497	-3.002905684
C	0.830559691	-1.810306594	-2.296209053
H	0.404978147	-0.991297631	-2.891396134
H	0.766578644	-2.721565391	-2.912392961
C	2.756551860	-1.099589137	1.006838231
H	3.757000660	-0.778617857	1.329725794
H	2.861149278	-2.063588792	0.518546392
H	2.085842717	-1.190751182	1.861941356
O	-0.805686099	-1.538174428	2.256615772
N	-0.055302510	-1.970317113	-1.082450113
C	-1.510114074	-2.122544392	-1.467259406
H	-1.767755304	-3.186861055	-1.540991604
H	-1.656695893	-1.689677326	-2.461019775
C	-2.398151983	-1.429815900	-0.431526550
H	-3.459910537	-1.629548291	-0.643795251
H	-2.161251025	-1.784708463	0.575071227
C	0.327623764	-3.150356729	-0.241137487
H	0.149671755	-4.082656559	-0.796226168
H	-0.257887033	-3.134299161	0.678411429
H	1.374929840	-3.104169494	0.035562883
C	-2.178415943	2.224878083	0.896829443
H	-2.598315241	2.851959830	0.100962111
H	-2.643545274	2.594562165	1.820710614
C	-0.666816430	2.495775141	1.054387953
H	-0.524038011	3.571876894	1.247188928
H	-0.293141638	1.924984611	1.907270952
C	-2.651772960	0.763309452	0.753414598
H	-3.753870847	0.753713408	0.725058440
H	-2.322919945	0.187402845	1.616491696
N	-2.123530608	0.049269799	-0.467304821
N	0.186609567	2.110649575	-0.138423228
C	-0.217290309	2.870522433	-1.364404998
H	0.000674956	3.941535834	-1.243324822
H	0.339969760	2.496878263	-2.227423023
H	-1.276079657	2.759184194	-1.563905683
C	-2.717798385	0.619171164	-1.720763468
H	-2.860405952	1.692154386	-1.624289512
H	-2.077875326	0.435032880	-2.585739103
H	-3.703415367	0.171780181	-1.910316172
C	-2.376728346	0.715549009	4.918739969
C	-3.650522165	1.118073426	4.606032686
C	-3.105259223	-1.631499189	5.090222027
C	-4.395400611	-1.282712241	4.780231031
C	-2.068653847	-0.655684474	5.162910312
H	-1.070618351	-0.941058807	5.481029002
H	-1.160533552	-1.256700140	3.135707643
H	-2.865737432	-2.670692731	5.297980882
H	-5.174343715	-2.039558602	4.739936819
H	-3.873446337	2.171339473	4.454627493
H	-1.584128764	1.453835401	5.004414635
C	-4.798454094	0.145295696	4.519946649
H	-5.594398960	0.444191644	5.230305810
H	-5.300933419	0.226355227	3.535901123

$^{2}I_{HA,EB}$:

O	-0.082606110	0.196672416	0.336630767
N	-0.445621801	-0.183406473	3.109615766
C	2.045293747	0.252660787	3.268889589
H	2.785789690	1.065228298	3.239105386
H	2.208887110	-0.284678596	4.207554978
C	0.645472370	0.843428881	3.243840635
H	0.490758155	1.448311318	4.151643146
H	0.524247242	1.498204392	2.376625188
C	-0.586721238	-1.131094540	4.264034453
H	-0.869902289	-0.578200659	5.174879156

H	0.395513999	-1.580604896	4.452782891
C	-1.623100956	-2.254086207	4.026157497
H	-2.625968815	-1.829723494	3.915990279
H	-1.664611943	-2.837762596	4.955925890
C	-1.353803161	-3.274126167	2.898442918
H	-0.380346818	-3.754117088	3.065856925
H	-2.117393472	-4.065928286	2.963478511
C	-1.700244459	0.599186085	2.853671141
H	-1.776429064	1.432361151	3.566423451
H	-2.584033227	-0.019725679	2.974726477
H	-1.648304957	0.970335566	1.829682167
O	-1.011644548	-0.172001936	-0.819998781
N	-1.329519222	-2.723980692	1.491416959
C	-0.935383338	-3.781170846	0.483973560
H	-1.834314719	-4.249199748	0.062764462
H	-0.379321438	-4.568010440	1.001419720
C	-0.090025633	-3.153069581	-0.625902983
H	0.109060548	-3.890575847	-1.418546622
H	-0.605403685	-2.292094802	-1.059441901
C	-2.651024274	-2.154521817	1.072309820
H	-3.403542273	-2.953753139	1.010092014
H	-2.534184967	-1.663119670	0.106185557
H	-2.992829443	-1.408619116	1.780994036
C	3.115069322	-0.964812611	-0.294413531
H	3.921216872	-1.666974940	-0.048596277
H	3.531135276	-0.321141732	-1.080424344
C	2.830589387	-0.032329814	0.901535495
H	3.765966000	0.485822002	1.170317378
H	2.084266147	0.706870310	0.602820783
C	1.926360870	-1.699300344	-0.947331535
H	2.295234691	-2.251722744	-1.826243059
H	1.188688065	-0.973127602	-1.283096810
N	1.199991304	-2.657056809	-0.031804127
N	2.297395615	-0.720332688	2.144333973
C	3.269009813	-1.736378428	2.661543993
H	4.182458534	-1.244858548	3.026597970
H	2.816322371	-2.289152007	3.488917425
H	3.547927757	-2.441465933	1.888168653
C	2.061656486	-3.838587122	0.300300630
H	3.103874269	-3.541471254	0.384111173
H	1.760148891	-4.301522761	1.241938143
H	1.997300991	-4.590498600	-0.498472329
H	4.329014957	2.547760266	-2.386778441
C	3.532432332	2.005752867	-2.887666197
C	3.850575031	1.007729431	-3.825682495
C	2.204269524	2.322289815	-2.610688892
C	2.814346577	0.331293766	-4.494997864
H	4.886959552	0.775606033	-4.047120515
C	1.133957314	1.651146609	-3.278573015
H	1.977382049	3.107250630	-1.897700373
C	1.485130798	0.644619119	-4.231626096
H	3.053228276	-0.427494682	-5.233563888
H	0.690131162	0.131974384	-4.765928322
C	-0.235820514	1.961298206	-3.033798930
H	-0.720022555	0.480455434	-1.506708589
H	-0.975908922	1.479546353	-3.671343196
C	-0.712972824	3.033467999	-2.096987182
H	-1.798180098	2.990709885	-1.969685937
H	-0.256741079	2.946377477	-1.101154074
H	-0.468521755	4.039659885	-2.473127737
Ni	0.319800859	-1.358936484	1.482337953

$^{2}\mathbf{I}_{\mathbf{HA,XA}}$:

Ni	0.096148504	-0.009255264	-0.137015116
O	0.069108871	-0.307587614	1.809433317
N	2.222341895	-0.280542337	-0.019050045
C	1.999582321	2.237992871	0.146802248
H	2.227555653	3.085283580	0.809671543
H	2.446851624	2.471299423	-0.823788938
C	2.616789209	0.971249020	0.716114830
H	3.713439885	1.075856463	0.730940871

H	2.276930511	0.812274074	1.743025147
C	2.702177433	-0.376853161	-1.436647884
H	3.803868500	-0.411625502	-1.462194529
H	2.397050347	0.538332397	-1.957933147
C	2.152315205	-1.604830963	-2.199610678
H	2.518518144	-2.530492699	-1.744555382
H	2.612284937	-1.579691214	-3.196910796
C	0.629146961	-1.700443259	-2.437968077
H	0.284306747	-0.800276931	-2.964350069
H	0.440672057	-2.555347954	-3.107209939
C	2.712450567	-1.414456298	0.832505023
H	3.749667714	-1.229598683	1.145566258
H	2.695097506	-2.353770775	0.288339360
H	2.054785534	-1.478581496	1.699833988
O	-0.758772052	-1.541887665	2.174263237
N	-0.231192232	-1.838482855	-1.203415450
C	-1.706152356	-1.804464575	-1.537963187
H	-2.086119956	-2.827371892	-1.654761444
H	-1.835607766	-1.304797218	-2.502131838
C	-2.473176241	-1.072665237	-0.434260078
H	-3.557561132	-1.143976861	-0.609583503
H	-2.241357695	-1.503850390	0.543411336
C	0.041191401	-3.106298162	-0.452007710
H	-0.253998623	-3.974504037	-1.058770360
H	-0.514113227	-3.087019593	0.485638486
H	1.093828512	-3.193444873	-0.207884387
C	-1.803083011	2.466253717	1.044849767
H	-2.165876390	3.166481118	0.282267956
H	-2.201498781	2.851199997	1.992729060
C	-0.268235139	2.556146561	1.171602564
H	0.002089144	3.600092497	1.401155365
H	0.056837605	1.914671530	1.993407278
C	-2.438927337	1.073611229	0.859825092
H	-3.535265838	1.179453106	0.881378694
H	-2.136514560	0.425127276	1.680059954
N	-2.036173129	0.366528777	-0.413283705
N	0.509322071	2.126919058	-0.058712964
C	0.167738903	2.980734212	-1.240744272
H	0.499477344	4.016345582	-1.077040692
H	0.667947311	2.591423393	-2.131368554
H	-0.900235586	2.989556584	-1.421763541
C	-2.605485235	1.059843199	-1.614586682
H	-2.620219248	2.136464294	-1.465161185
H	-2.022488243	0.846831770	-2.512702795
H	-3.642324851	0.736817343	-1.782690530
H	-0.284590517	1.401875664	5.734167371
C	-1.272100580	1.664010936	5.367932431
C	-1.638320041	2.999704083	5.225177950
C	-2.181654463	0.617076316	5.061316117
C	-2.926613119	3.341479411	4.770049234
H	-0.932694228	3.782252094	5.483397946
C	-3.472913789	1.001662303	4.602585259
C	-3.848714771	2.334159412	4.458188135
H	-3.216165159	4.382707950	4.680309063
C	-2.888651908	-1.749273198	4.951518720
H	-4.854572822	2.562829755	4.125846215
C	-4.164548947	-1.325023564	4.486091888
C	-2.704968803	-3.145326800	5.138536731
C	-5.197841739	-2.216689359	4.219917276
H	-1.745424441	-3.499645246	5.502327393
C	-3.732692114	-4.044765512	4.874600434
C	-4.981291571	-3.585503146	4.414285269
H	-6.151360118	-1.831724782	3.878391849
H	-3.573635513	-5.106092661	5.031425714
H	-5.781832712	-4.289602132	4.216647650
C	-1.880570413	-0.770304265	5.204710262
H	-0.918707536	-1.074854858	5.604171870
H	-1.036788628	-1.307810834	3.092479344
O	-4.430778377	0.035588590	4.273936425

$^{2}I_{HA,CHD}$:

Ni	0.029394718	-0.072401714	-0.093070720
O	0.048658428	-0.285291336	1.865150644

N	2.174274936	-0.066346252	0.022106322
C	1.639597220	2.410702243	0.031669703
H	1.766120615	3.321724801	0.634790945
H	2.048435135	2.632262628	-0.958511641
C	2.412590363	1.269558573	0.671614101
H	3.487466650	1.511199903	0.664056904
H	2.104043994	1.136780369	1.712186130
C	2.657652964	-0.190781314	-1.392870463
H	3.754356226	-0.082408001	-1.428896586
H	2.232942489	0.640701128	-1.968354004
C	2.271390026	-1.527229804	-2.068459341
H	2.751425279	-2.366276876	-1.554955122
H	2.726736577	-1.510851376	-3.068185429
C	0.773625148	-1.830499085	-2.290964185
H	0.321607386	-1.021851836	-2.880604206
H	0.696413906	-2.749324571	-2.894250209
C	2.810437216	-1.072783511	0.936104180
H	3.818062239	-0.738734098	1.220626468
H	2.908199680	-2.040003342	0.452365013
H	2.171126261	-1.163523162	1.814889133
O	-0.730436970	-1.520961074	2.314449842
N	-0.069580494	-1.983369568	-1.046511013
C	-1.534698185	-2.151611018	-1.381198399
H	-1.785136266	-3.218801735	-1.436709638
H	-1.717814355	-1.729456223	-2.373382288
C	-2.393598659	-1.456351342	-0.322909593
H	-3.459863982	-1.665750562	-0.498786030
H	-2.122138976	-1.800249788	0.678482562
C	0.350877236	-3.150222448	-0.205094551
H	0.164733334	-4.090324362	-0.744326033
H	-0.205577496	-3.129679874	0.732215905
H	1.405792572	-3.090546441	0.037944479
C	-2.156014962	2.210780783	0.968525187
H	-2.608208077	2.828443025	0.182998448
H	-2.591311521	2.584718608	1.905283576
C	-0.641985592	2.494291504	1.071563137
H	-0.501089066	3.573004230	1.251223169
H	-0.234865429	1.932586482	1.915156183
C	-2.622807447	0.744532416	0.852975584
H	-3.725011037	0.726600678	0.862703209
H	-2.260109987	0.176971633	1.708017993
N	-2.131736887	0.024610260	-0.379997469
N	0.173097290	2.105900398	-0.146809513
C	-0.278680766	2.851588109	-1.364860928
H	-0.063337739	3.925121864	-1.261579423
H	0.250051586	2.473019059	-2.243692152
H	-1.343092654	2.732062336	-1.525820916
C	-2.774181528	0.578654567	-1.616313361
H	-2.916472267	1.652493102	-1.526809741
H	-2.166558601	0.386332611	-2.502634529
H	-3.764667754	0.126262450	-1.763561518
C	-2.063194163	0.710268927	5.029609413
C	-3.333396511	1.172183754	4.791994898
C	-2.894808452	-1.594546536	5.287915087
C	-4.183231544	-1.185520905	5.054226588
C	-1.808633629	-0.671306391	5.276353033
H	-0.808066456	-1.002125217	5.538021239
H	-1.030895039	-1.236736408	3.213088280
H	-2.693957922	-2.640712861	5.499428787
H	-4.999822342	-1.901416916	5.077203564
H	-3.513793475	2.233967797	4.641431657
H	-1.231527404	1.408960761	5.054751973
C	-4.530784606	0.256351380	4.791532794
H	-5.267426690	0.605480954	5.541289527
H	-5.086134278	0.346904170	3.836521429

$^{4}R_{SO}$:

Ni	0.013097000	0.023163000	-0.027939000
O	0.039077000	0.089577000	1.979960000
O	1.248884000	0.068622000	2.607587000
N	-1.202415000	1.788817000	0.096565000

N	1.746272000	1.055842000	-0.714313000
N	1.181889000	-1.802382000	-0.243750000
N	-1.841211000	-1.068138000	-0.289349000
C	-2.938114000	-0.037388000	-0.176087000
C	-2.509380000	1.213557000	0.572470000
C	-1.216683000	2.320630000	-1.309686000
C	0.166865000	2.793107000	-1.812237000
C	1.280812000	1.738079000	-1.980415000
C	-0.852304000	2.862117000	1.087680000
C	2.741480000	-0.045297000	-1.004245000
C	2.540752000	-1.195573000	-0.015092000
C	2.384401000	2.011658000	0.247557000
C	-0.739155000	-3.113370000	0.847728000
C	-1.828680000	-2.019013000	0.892596000
C	1.213185000	-2.573734000	-1.531789000
C	0.744961000	-2.690600000	0.898047000
C	-2.077757000	-1.804839000	-1.573737000
H	-3.819121000	-0.475101000	0.315105000
H	-3.244175000	0.222092000	-1.193405000
H	-3.306957000	1.969572000	0.497767000
H	-2.359508000	0.993186000	1.632765000
H	-1.924540000	3.162383000	-1.382302000
H	-1.589927000	1.527085000	-1.968064000
H	0.528969000	3.628142000	-1.204718000
H	0.003144000	3.220232000	-2.810914000
H	0.934864000	0.945618000	-2.657246000
H	2.142629000	2.222779000	-2.466186000
H	-1.713148000	3.529724000	1.234333000
H	-0.018894000	3.466635000	0.747647000
H	-0.576332000	2.400859000	2.034133000
H	3.764428000	0.345892000	-0.934683000
H	2.599634000	-0.385485000	-2.033598000
H	3.328189000	-1.953428000	-0.141662000
H	2.572239000	-0.824037000	1.012484000
H	3.280544000	2.460274000	-0.204294000
H	2.654923000	1.471083000	1.154613000
H	1.699607000	2.801657000	0.534017000
H	-0.918916000	-3.788408000	0.002686000
H	-0.904135000	-3.734946000	1.738380000
H	-2.811008000	-2.516108000	0.945655000
H	-1.703437000	-1.410476000	1.791256000
H	1.365896000	-3.600609000	0.903154000
H	0.946115000	-2.146367000	1.820355000
H	-3.088861000	-2.236170000	-1.588404000
H	-1.980940000	-1.113288000	-2.414371000
H	-1.362764000	-2.607463000	-1.704577000
H	0.418217000	-3.314751000	-1.553816000
H	1.092632000	-1.915377000	-2.393820000
H	2.166246000	-3.111332000	-1.627766000
S	1.544352000	4.144562000	3.911841000
C	2.594379000	2.711301000	4.560856000
C	0.204486000	4.149066000	5.244670000
H	3.493973000	2.680521000	3.943850000
H	2.045199000	1.773243000	4.469104000
H	2.874710000	2.904184000	5.598131000
H	0.656015000	4.349661000	6.217971000
H	-0.488770000	4.952139000	4.990751000
H	-0.320416000	3.191746000	5.259087000

$^{2}R_{SO}$:

Ni	0.015463000	0.008504000	-0.029182000
O	0.030632000	0.047697000	1.976322000
O	1.254350000	0.050022000	2.597738000
N	-1.203456000	1.769250000	0.103840000
N	1.743769000	1.048831000	-0.709444000
N	1.183175000	-1.812218000	-0.263969000
N	-1.839293000	-1.084267000	-0.308230000
C	-2.937166000	-0.055359000	-0.187320000
C	-2.509571000	1.187267000	0.574921000
C	-1.218746000	2.317003000	-1.296077000
C	0.164525000	2.795532000	-1.793013000
C	1.278810000	1.742356000	-1.970076000
C	-0.853324000	2.829654000	1.109211000

C	2.741539000	-0.048665000	-1.008354000
C	2.541458000	-1.205746000	-0.027702000
C	2.380783000	1.995628000	0.262746000
C	-0.735657000	-3.135987000	0.815593000
C	-1.825374000	-2.042602000	0.868527000
C	1.217303000	-2.574001000	-1.557942000
C	0.747273000	-2.710630000	0.870906000
C	-2.074722000	-1.812385000	-1.597812000
H	-3.818636000	-0.498657000	0.297897000
H	-3.241230000	0.213918000	-1.202705000
H	-3.307558000	1.943561000	0.509955000
H	-2.356822000	0.954581000	1.632142000
H	-1.927119000	3.158942000	-1.358843000
H	-1.591802000	1.530668000	-1.963336000
H	0.525624000	3.624900000	-1.177240000
H	0.001242000	3.231903000	-2.787705000
H	0.933743000	0.955797000	-2.654513000
H	2.141147000	2.230999000	-2.450558000
H	-1.717095000	3.489780000	1.270422000
H	-0.025469000	3.444203000	0.773881000
H	-0.570726000	2.353139000	2.046187000
H	3.763252000	0.344457000	-0.934086000
H	2.601523000	-0.380107000	-2.040900000
H	3.329606000	-1.962067000	-0.157856000
H	2.567628000	-0.840933000	1.002673000
H	3.281014000	2.442974000	-0.181676000
H	2.643105000	1.447162000	1.167455000
H	1.698485000	2.786829000	0.550728000
H	-0.914165000	-3.805410000	-0.034205000
H	-0.900309000	-3.763774000	1.701888000
H	-2.807849000	-2.539414000	0.919197000
H	-1.697153000	-1.439502000	1.770436000
H	1.371047000	-3.618544000	0.867813000
H	0.945939000	-2.172042000	1.796775000
H	-3.085039000	-2.245229000	-1.615272000
H	-1.979404000	-1.114914000	-2.433800000
H	-1.358456000	-2.613061000	-1.734282000
H	0.418535000	-3.310519000	-1.590246000
H	1.105289000	-1.908432000	-2.415710000
H	2.168177000	-3.115560000	-1.652639000
S	1.493343000	4.196503000	3.849067000
C	2.594027000	2.772325000	4.432278000
C	0.299305000	4.258496000	5.312794000
H	3.465945000	2.764980000	3.775981000
H	2.057088000	1.826293000	4.350714000
H	2.917292000	2.956276000	5.458590000
H	0.850635000	4.487155000	6.226716000
H	-0.411870000	5.059115000	5.104801000
H	-0.226732000	3.307116000	5.414282000

$^{4}TS_{SO}$:

Ni	0.006315000	-0.012792000	0.007909000
O	-0.036557000	-0.027876000	1.977315000
O	1.716561000	0.027987000	2.539052000
N	-1.135204000	1.806622000	0.064707000
N	1.748287000	0.922480000	-0.819725000
N	1.055203000	-1.911633000	-0.318864000
N	-1.937701000	-1.021821000	-0.293210000
C	-2.966965000	0.067609000	-0.137994000
C	-2.440508000	1.288539000	0.599940000
C	-1.175942000	2.330223000	-1.338600000
C	0.211129000	2.706428000	-1.907855000
C	1.258888000	1.586543000	-2.084979000
C	-0.667531000	2.829909000	1.053321000
C	2.675821000	-0.233880000	-1.120821000
C	2.444781000	-1.372159000	-0.124931000
C	2.468953000	1.874284000	0.085800000
C	-0.908373000	-3.120922000	0.803858000
C	-1.949965000	-1.983608000	0.876368000
C	1.017130000	-2.695153000	-1.594639000
C	0.586609000	-2.739552000	0.851961000

C	-2.233342000	-1.724975000	-1.580618000
H	-3.853855000	-0.319487000	0.385588000
H	-3.298346000	0.349731000	-1.141726000
H	-3.205285000	2.081875000	0.577537000
H	-2.232240000	1.037820000	1.643493000
H	-1.831043000	3.215647000	-1.394403000
H	-1.625938000	1.557139000	-1.971949000
H	0.643150000	3.536813000	-1.340349000
H	0.032614000	3.113935000	-2.912241000
H	0.840497000	0.791929000	-2.716939000
H	2.120659000	2.007615000	-2.628162000
H	-1.494014000	3.501287000	1.326764000
H	0.129365000	3.441245000	0.639671000
H	-0.301641000	2.282951000	1.923251000
H	3.718849000	0.104655000	-1.078014000
H	2.493087000	-0.570448000	-2.145456000
H	3.191240000	-2.167660000	-0.280344000
H	2.522521000	-1.008788000	0.905270000
H	3.408186000	2.204291000	-0.382275000
H	2.661136000	1.370626000	1.035329000
H	1.857378000	2.746708000	0.290750000
H	-1.120887000	-3.783109000	-0.044372000
H	-1.088817000	-3.744637000	1.690719000
H	-2.955311000	-2.431820000	0.947410000
H	-1.749070000	-1.386662000	1.769392000
H	1.185605000	-3.663972000	0.904465000
H	0.771546000	-2.128693000	1.736374000
H	-3.262043000	-2.115209000	-1.582882000
H	-2.125384000	-1.024941000	-2.413409000
H	-1.553735000	-2.553582000	-1.739636000
H	0.173117000	-3.380248000	-1.601899000
H	0.934310000	-2.039293000	-2.463534000
H	1.930021000	-3.299383000	-1.696489000
S	2.213280000	0.059165000	4.396747000
C	1.332570000	-1.537723000	4.876326000
C	0.874981000	1.292175000	4.894463000
H	1.980046000	-2.356388000	4.564031000
H	0.393430000	-1.550474000	4.323433000
H	1.181569000	-1.556479000	5.955440000
H	0.615830000	1.136164000	5.942474000
H	1.291505000	2.287477000	4.741457000
H	0.038127000	1.103267000	4.218362000

$^{2}TS_{SO}$:

Ni	0.007334000	-0.005975000	0.018740000
O	0.030504000	-0.018846000	1.977585000
O	1.763615000	-0.042754000	2.678045000
N	-1.063264000	1.839055000	0.091300000
N	1.798750000	0.893863000	-0.783242000
N	1.031322000	-1.934888000	-0.284525000
N	-1.935025000	-0.959070000	-0.271184000
C	-2.940517000	0.155078000	-0.130932000
C	-2.390777000	1.362753000	0.611534000
C	-1.077195000	2.383450000	-1.305550000
C	0.324166000	2.733132000	-1.858447000
C	1.347719000	1.591384000	-2.042907000
C	-0.563464000	2.831403000	1.098499000
C	2.688592000	-0.289270000	-1.082934000
C	2.426134000	-1.415047000	-0.078985000
C	2.534649000	1.803324000	0.151916000
C	-0.967877000	-3.081451000	0.836859000
C	-1.972227000	-1.910790000	0.906660000
C	0.994225000	-2.733677000	-1.550404000
C	0.537048000	-2.741715000	0.889860000
C	-2.235720000	-1.661430000	-1.557830000
H	-3.842314000	-0.209815000	0.382086000
H	-3.250623000	0.443658000	-1.139392000
H	-3.130708000	2.178688000	0.578250000
H	-2.203847000	1.108990000	1.658068000
H	-1.708034000	3.286673000	-1.352192000
H	-1.542378000	1.631780000	-1.953979000
H	0.770393000	3.545525000	-1.276178000
H	0.163104000	3.158640000	-2.858572000

H	0.918255000	0.819380000	-2.694780000
H	2.226126000	2.002173000	-2.567357000
H	-1.371923000	3.516620000	1.390994000
H	0.246469000	3.430370000	0.692341000
H	-0.205883000	2.253491000	1.952407000
H	3.742560000	0.016215000	-1.046152000
H	2.490607000	-0.624724000	-2.104887000
H	3.161770000	-2.223771000	-0.216444000
H	2.499353000	-1.041970000	0.947918000
H	3.504426000	2.086662000	-0.282296000
H	2.673364000	1.290909000	1.106317000
H	1.963960000	2.705968000	0.339653000
H	-1.196740000	-3.735378000	-0.013438000
H	-1.170089000	-3.700138000	1.722660000
H	-2.991147000	-2.325051000	0.986891000
H	-1.745260000	-1.312578000	1.793062000
H	1.111362000	-3.681284000	0.952751000
H	0.732544000	-2.126810000	1.769166000
H	-3.272152000	-2.029801000	-1.565853000
H	-2.106244000	-0.967046000	-2.392177000
H	-1.572417000	-2.504592000	-1.708171000
H	0.124631000	-3.386135000	-1.569111000
H	0.952153000	-2.086576000	-2.428891000
H	1.886729000	-3.371258000	-1.625770000
S	2.082015000	-0.122809000	4.516964000
C	1.278520000	-1.790358000	4.876998000
C	0.632676000	0.994676000	4.981923000
H	1.979235000	-2.557789000	4.550826000
H	0.358855000	-1.824372000	4.293196000
H	1.089197000	-1.872794000	5.948043000
H	0.291586000	0.744533000	5.987072000
H	1.001214000	2.019027000	4.939610000
H	-0.117374000	0.807464000	4.207239000

$^4P_{SO}$:

Ni	0.005371000	-0.000822000	-0.006468000
O	0.014640000	-0.009774000	1.913454000
O	4.436569000	-0.006583000	1.962013000
N	-1.169335000	1.807019000	0.027809000
N	1.804909000	0.975756000	-0.572579000
N	1.122316000	-1.877027000	-0.145900000
N	-1.859108000	-1.036240000	-0.438620000
C	-2.915988000	0.036909000	-0.441216000
C	-2.527156000	1.260322000	0.369779000
C	-1.049175000	2.403724000	-1.343387000
C	0.393110000	2.803840000	-1.726978000
C	1.446025000	1.682937000	-1.854729000
C	-0.855063000	2.797673000	1.108290000
C	2.780349000	-0.160383000	-0.802264000
C	2.473984000	-1.298639000	0.170553000
C	2.419515000	1.905380000	0.431496000
C	-0.919994000	-3.073280000	0.842078000
C	-1.968909000	-1.943401000	0.770699000
C	1.234697000	-2.707814000	-1.386120000
C	0.562051000	-2.677375000	1.002737000
C	-2.019807000	-1.802951000	-1.713919000
H	-3.866717000	-0.366580000	-0.062112000
H	-3.088362000	0.316305000	-1.484427000
H	-3.294540000	2.040309000	0.242114000
H	-2.475533000	1.007610000	1.431263000
H	-1.697417000	3.291719000	-1.425457000
H	-1.421219000	1.665891000	-2.063651000
H	0.764227000	3.586237000	-1.057431000
H	0.329591000	3.280043000	-2.714513000
H	1.087440000	0.917748000	-2.556596000
H	2.358749000	2.118524000	-2.292637000
H	-1.710803000	3.468452000	1.269045000
H	0.001115000	3.411030000	0.844433000
H	-0.640055000	2.238343000	2.019698000
H	3.805257000	0.187917000	-0.637999000
H	2.694158000	-0.489288000	-1.841869000

H	3.251228000	-2.073658000	0.104360000
H	2.471143000	-0.921633000	1.193658000
H	3.229393000	2.479617000	-0.042157000
H	2.849565000	1.321822000	1.246752000
H	1.680844000	2.588413000	0.833546000
H	-1.051758000	-3.767156000	0.003739000
H	-1.176052000	-3.661732000	1.733583000
H	-2.972953000	-2.398581000	0.774572000
H	-1.870563000	-1.302649000	1.651839000
H	1.160786000	-3.592827000	1.137426000
H	0.676268000	-2.045543000	1.887909000
H	-3.038662000	-2.209241000	-1.795478000
H	-1.838630000	-1.138673000	-2.562757000
H	-1.317797000	-2.626427000	-1.766885000
H	0.393171000	-3.391368000	-1.473465000
H	1.262982000	-2.080763000	-2.280005000
H	2.151034000	-3.314602000	-1.355017000
S	5.794272000	-0.028496000	2.973640000
C	5.666535000	-1.668167000	3.924399000
C	5.341785000	1.130096000	4.409039000
H	5.836551000	-2.457516000	3.193699000
H	4.663420000	-1.740473000	4.348575000
H	6.438492000	-1.680274000	4.695768000
H	6.123372000	1.061880000	5.167921000
H	5.295587000	2.133501000	3.987997000
H	4.367405000	0.827941000	4.795206000

$^{2}P_{SO}$:

Ni	-0.014175000	-0.000537000	-0.017891000
O	0.000777000	-0.001187000	1.939842000
O	3.182247000	-0.023906000	2.555042000
N	-1.158465000	1.821671000	0.031326000
N	1.748983000	0.931892000	-0.760386000
N	1.051446000	-1.901164000	-0.275663000
N	-1.930077000	-1.006778000	-0.336298000
C	-2.974084000	0.076690000	-0.236099000
C	-2.487459000	1.307801000	0.510342000
C	-1.147094000	2.359849000	-1.369252000
C	0.262485000	2.735334000	-1.880350000
C	1.303055000	1.606067000	-2.036324000
C	-0.734783000	2.846318000	1.042085000
C	2.689981000	-0.221411000	-1.041714000
C	2.437050000	-1.357259000	-0.050557000
C	2.450064000	1.877895000	0.169965000
C	-0.935027000	-3.093843000	0.820487000
C	-1.972878000	-1.950510000	0.849181000
C	1.053474000	-2.705924000	-1.539604000
C	0.560172000	-2.718959000	0.891909000
C	-2.183675000	-1.734485000	-1.620963000
H	-3.879542000	-0.313390000	0.251233000
H	-3.260644000	0.346612000	-1.256462000
H	-3.250669000	2.099334000	0.440781000
H	-2.340369000	1.077264000	1.569070000
H	-1.797945000	3.247117000	-1.436811000
H	-1.576583000	1.594406000	-2.026770000
H	0.682383000	3.550349000	-1.282299000
H	0.123500000	3.161629000	-2.883115000
H	0.896188000	0.820565000	-2.687818000
H	2.185816000	2.021945000	-2.547727000
H	-1.571563000	3.521079000	1.270517000
H	0.086223000	3.450698000	0.669255000
H	-0.416642000	2.305911000	1.934324000
H	3.728595000	0.122096000	-0.965379000
H	2.534658000	-0.553100000	-2.072827000
H	3.184816000	-2.153172000	-0.192667000
H	2.522106000	-0.995484000	0.981869000
H	3.330524000	2.304971000	-0.332794000
H	2.762274000	1.335768000	1.068591000
H	1.789434000	2.685149000	0.467640000
H	-1.133526000	-3.766723000	-0.022447000
H	-1.138230000	-3.701279000	1.713145000
H	-2.980665000	-2.394725000	0.901288000
H	-1.808091000	-1.343600000	1.743561000

H	1.155582000	-3.643365000	0.964058000
H	0.728527000	-2.104186000	1.777167000
H	-3.214425000	-2.116169000	-1.651096000
H	-2.039679000	-1.051442000	-2.461950000
H	-1.506126000	-2.570766000	-1.738192000
H	0.202453000	-3.381228000	-1.571775000
H	1.015043000	-2.062117000	-2.420207000
H	1.962589000	-3.320338000	-1.594460000
S	3.150965000	0.069891000	4.251344000
C	2.947813000	-1.736827000	4.789809000
C	1.402511000	0.670279000	4.689845000
H	3.831955000	-2.257840000	4.425964000
H	2.043001000	-2.133961000	4.327722000
H	2.894073000	-1.770195000	5.878911000
H	1.147413000	0.282243000	5.677798000
H	1.439162000	1.759560000	4.704071000
H	0.734978000	0.315825000	3.895071000

$^{4}R_{PO}$:

Ni	0.434871062	0.388111971	-0.420534987
O	1.060037484	1.262516542	1.265558194
O	1.824348385	2.310182096	1.180264361
N	-1.552359746	0.789381218	0.307515460
N	0.392452749	1.918700628	-1.913547505
N	2.391377322	-0.123516990	-1.208818220
N	0.126734363	-1.623671113	0.296359222
C	-1.216426608	-1.630565070	0.954816715
C	-1.704843784	-0.252917507	1.362300918
C	-2.414336890	0.583037529	-0.885983577
C	-2.159882230	1.576858072	-2.036208077
C	-0.793622871	1.550763351	-2.745411276
C	-1.872645030	2.075026037	0.975437393
C	1.674922485	1.726418915	-2.661595175
C	2.765236775	1.224975632	-1.715713692
C	0.334572423	3.333381751	-1.474231344
C	2.664146061	-1.779365157	0.718396193
C	1.236059564	-1.785784919	1.294217721
C	2.581063586	-1.105854164	-2.306863932
C	3.188848831	-0.528683402	-0.010430181
C	0.122475745	-2.754565719	-0.662630326
H	-1.207542302	-2.277984565	1.838783673
H	-1.920926469	-2.078674221	0.252569456
H	-2.754796310	-0.331019725	1.675936796
H	-1.142508853	0.103659672	2.225465255
H	-3.474211105	0.645908439	-0.598525035
H	-2.251035687	-0.435052532	-1.250777202
H	-2.406834044	2.594234242	-1.727039067
H	-2.898364831	1.340544998	-2.809932161
H	-0.612152113	0.544035798	-3.136793201
H	-0.849267819	2.218033722	-3.617086280
H	-2.857735385	2.016624449	1.454604081
H	-1.898393033	2.897589431	0.269870848
H	-1.118453132	2.288551440	1.728806107
H	1.984077459	2.665082796	-3.132078506
H	1.509633096	1.015316757	-3.471767084
H	3.733192680	1.195703452	-2.232580665
H	2.856967965	1.896182545	-0.861508299
H	0.313031307	4.002382144	-2.343278647
H	1.204185691	3.556386636	-0.860355361
H	-0.544321468	3.522076816	-0.869530221
H	2.830484040	-2.674655942	0.113038703
H	3.319464952	-1.912413094	1.585491033
H	1.092754148	-2.737299205	1.823011828
H	1.135669714	-0.994559891	2.035140039
H	4.228677825	-0.716329848	-0.312771788
H	3.201314015	0.316939487	0.672523345
H	-0.125666903	-3.692737423	-0.151218866
H	-0.621231159	-2.581526491	-1.441878987
H	1.086277247	-2.877988664	-1.137954090
H	2.653311681	-2.114794998	-1.916065061
H	1.756502277	-1.080985318	-3.018696181

H	3.512572971	-0.900808424	-2.846738086
P	1.842265772	-1.021565256	5.154958640
C	2.652342240	-1.916172291	6.556934495
C	4.053853311	-1.954491043	6.554062963
C	1.964575796	-2.546277002	7.601992021
C	4.751713464	-2.589800824	7.578154886
H	4.603732202	-1.482503364	5.744863234
C	2.663377050	-3.192260083	8.620666855
H	0.880143241	-2.539123219	7.622979779
C	4.056957724	-3.212775025	8.613322887
H	5.836663211	-2.605719027	7.563093212
H	2.117005380	-3.677152906	9.423247550
H	4.598592232	-3.715386506	9.407779183
C	0.117595633	-1.706904904	5.182316296
C	-0.057184566	-3.057007269	4.833831869
C	-1.022619402	-0.935387016	5.438031427
C	-1.327842564	-3.621340386	4.763802439
H	0.811556179	-3.680437407	4.640070267
C	-2.298291639	-1.498282753	5.355908148
H	-0.917000127	0.106101027	5.720771717
C	-2.456676055	-2.841051739	5.021742636
H	-1.437890072	-4.673577748	4.519926753
H	-3.168021393	-0.887108071	5.576844845
H	-3.447269582	-3.281929011	4.977786421
C	1.622329462	0.694892936	5.812249098
C	1.581459430	1.738934692	4.877470684
C	1.522473253	1.004136461	7.175232827
C	1.421126812	3.059643388	5.295296788
H	1.683561553	1.527206919	3.817906633
C	1.370043661	2.324868857	7.591218022
H	1.574303456	0.215096008	7.917114882
C	1.314700292	3.354986669	6.652730942
H	1.398181130	3.855918923	4.558146809
H	1.299241748	2.550147594	8.650570222
H	1.201863517	4.383379202	6.980478282

$^{2}R_{PO}$:

Ni	0.429987686	0.408996472	-0.430798311
O	1.122416903	1.261362375	1.235502279
O	1.950783136	2.268208427	1.119993338
N	-1.521531149	0.922112893	0.321819887
N	0.442749353	1.921190635	-1.937429028
N	2.343398443	-0.213763070	-1.241755828
N	0.028301403	-1.574564335	0.315209089
C	-1.302845411	-1.504272864	0.993854239
C	-1.709857134	-0.098210314	1.392413357
C	-2.414285247	0.749417260	-0.854047268
C	-2.126021095	1.715235724	-2.019843406
C	-0.773970172	1.609605154	-2.748074315
C	-1.758133519	2.230674984	0.981111766
C	1.702120581	1.656290430	-2.703092726
C	2.778311768	1.109407475	-1.767259656
C	0.467178916	3.339819184	-1.506676396
C	2.559962329	-1.855714300	0.704219532
C	1.142968738	-1.778902646	1.300136338
C	2.470988960	-1.216469451	-2.329857243
C	3.136085420	-0.643141742	-0.048109693
C	-0.047787282	-2.716335915	-0.627907652
H	-1.313319125	-2.142553645	1.884371045
H	-2.040843298	-1.922088959	0.307457254
H	-2.756682839	-0.115689948	1.724800705
H	-1.112516227	0.239368477	2.239542806
H	-3.463878971	0.872710827	-0.549771984
H	-2.312871853	-0.280135509	-1.209180000
H	-2.314596130	2.747468291	-1.719453219
H	-2.887184559	1.509233580	-2.780063790
H	-0.652025264	0.591172380	-3.132432016
H	-0.806501221	2.270720853	-3.625324016
H	-2.730989410	2.227213417	1.487555806
H	-1.763534662	3.044636228	0.265316906
H	-0.972178854	2.413342522	1.709641672
H	2.051032925	2.573903724	-3.186819546
H	1.487640318	0.947414016	-3.503645322

H	3.736227765	1.025250494	-2.296283749
H	2.914202410	1.782053088	-0.919807890
H	0.472603877	4.002923133	-2.380266500
H	1.354281927	3.517750369	-0.903116439
H	-0.393470016	3.579939693	-0.894390551
H	2.670894483	-2.766432313	0.109259199
H	3.220490406	-2.010644685	1.563779711
H	0.956262041	-2.711750620	1.847422500
H	1.095643745	-0.969537520	2.026689186
H	4.160538828	-0.886092156	-0.362750065
H	3.198884124	0.209860220	0.622587902
H	-0.336160498	-3.633187173	-0.099649579
H	-0.793098408	-2.515834583	-1.399060712
H	0.901685019	-2.895401225	-1.114161597
H	2.488901667	-2.223772769	-1.928876533
H	1.645435416	-1.152421481	-3.038099659
H	3.409327556	-1.068931332	-2.876456611
P	1.880435275	-1.040501043	5.170097916
C	2.698994238	-1.866387324	6.609637754
C	4.098359151	-1.797085215	6.662149179
C	2.020477369	-2.542066361	7.632037388
C	4.801117793	-2.370834142	7.718731144
H	4.642569982	-1.288779960	5.871304010
C	2.725409908	-3.126933976	8.683037951
H	0.938773407	-2.617761290	7.610817697
C	4.115353543	-3.039652966	8.731219298
H	5.883819733	-2.302940792	7.746862378
H	2.186209814	-3.648187124	9.467560678
H	4.661675566	-3.494298826	9.550980474
C	0.197811501	-1.824878311	5.157780700
C	0.110535173	-3.183314960	4.808806308
C	-0.991959034	-1.120489800	5.380727219
C	-1.123058840	-3.820217622	4.706120050
H	1.018706615	-3.755452683	4.638698170
C	-2.230447721	-1.756442812	5.266100165
H	-0.954479090	-0.074386753	5.663605157
C	-2.301767787	-3.106335773	4.931062397
H	-1.165388392	-4.877174756	4.461664375
H	-3.139781266	-1.196852842	5.463242120
H	-3.263576579	-3.603986215	4.861904125
C	1.540635872	0.666923042	5.800211260
C	1.492403517	1.702318736	4.856194647
C	1.355607715	0.977507240	7.154069723
C	1.243412294	3.015109249	5.255834586
H	1.661317627	1.491239251	3.804979109
C	1.112756005	2.290248688	7.551657632
H	1.411901621	0.196053559	7.903781141
C	1.052120064	3.311237780	6.603532651
H	1.219698524	3.806098145	4.513033084
H	0.976579103	2.517010912	8.604230568
H	0.870118507	4.334021995	6.917337685

$^{4}TS_{PO}$:

Ni	0.274340699	-0.173588776	0.066232119
O	-0.019180669	-0.010059584	1.998661238
O	0.870177170	-0.858486305	2.856257020
N	0.365512512	1.960236862	-0.024921356
N	2.332288016	-0.490659738	-0.418135391
N	0.066242391	-2.341351842	-0.134856791
N	-1.817204954	0.080684266	-0.605922243
C	-2.053577015	1.554231541	-0.616057474
C	-1.054324705	2.338999195	0.214205001
C	0.866407380	2.278773942	-1.386801024
C	2.285446763	1.755697987	-1.678952855
C	2.508774508	0.233944571	-1.713005032
C	1.144787675	2.675065366	1.013147796
C	2.448914338	-1.973391007	-0.598066273
C	1.445034574	-2.692360331	0.300878078
C	3.347121827	-0.079374218	0.581493471
C	-2.368865286	-2.121563443	0.601944830
C	-2.566180086	-0.597088274	0.501382093

C	-0.213626591	-3.043812257	-1.412863241
C	-0.964964328	-2.684844476	0.889783403
C	-2.266363507	-0.422265115	-1.925555615
H	-3.067972365	1.782064841	-0.266434619
H	-2.011577794	1.886292886	-1.654267451
H	-1.202513497	3.411447974	0.025068231
H	-1.229244084	2.169121718	1.277047509
H	0.853786904	3.366887933	-1.545302627
H	0.172517604	1.849246690	-2.115087830
H	3.014976969	2.231263510	-1.021200611
H	2.541609477	2.115771676	-2.681177638
H	1.814894090	-0.214689660	-2.432478501
H	3.520657759	0.045275704	-2.097966201
H	0.943829144	3.752710246	0.962439359
H	2.210766449	2.527840589	0.889313647
H	0.854679181	2.287826088	1.985171431
H	3.467156612	-2.301111385	-0.368198624
H	2.275426668	-2.219665482	-1.646308354
H	1.605251877	-3.777706542	0.256111991
H	1.565630888	-2.371370666	1.335308065
H	4.357486977	-0.249753868	0.190954906
H	3.210994726	-0.657475785	1.490429490
H	3.247444881	0.964556412	0.850755715
H	-2.817113125	-2.617284901	-0.263466442
H	-2.993159825	-2.441322652	1.443503071
H	-3.640525548	-0.403848150	0.366403565
H	-2.247966097	-0.132220880	1.433555944
H	-1.043950131	-3.778322911	0.974261903
H	-0.603941493	-2.296657469	1.838466212
H	-3.308609234	-0.136096355	-2.115486840
H	-1.645818349	0.000013837	-2.717345921
H	-2.200381946	-1.500075216	-1.985590570
H	-1.281005394	-3.126877975	-1.585652659
H	0.223903817	-2.525616725	-2.265882140
H	0.187901049	-4.063276981	-1.384840578
P	1.596837918	-0.143390697	4.267910403
C	3.151457042	0.682920833	4.163475809
C	3.243280140	2.079161652	3.876114345
C	4.362881787	-0.071928514	4.080540531
C	4.461837138	2.671992595	3.588623051
H	2.353244330	2.696379403	3.899673516
C	5.569235898	0.540395555	3.792889090
H	4.344883753	-1.141635319	4.255755724
C	5.642349808	1.919186801	3.543512890
H	4.497312405	3.742084137	3.405861900
H	6.472602233	-0.061500870	3.765489481
H	6.592819400	2.392160790	3.325157265
C	1.767983015	-1.663052618	5.243624042
C	0.952213918	-2.783867516	5.012733254
C	2.646756322	-1.683513035	6.341775303
C	1.029962571	-3.896855041	5.845872913
H	0.261873429	-2.781306803	4.180062671
C	2.727595018	-2.803766676	7.160265178
H	3.261587181	-0.818834028	6.562183506
C	1.919817643	-3.915661687	6.917165903
H	0.392256475	-4.753950313	5.654728206
H	3.413575467	-2.802209927	8.000688107
H	1.979583668	-4.784914581	7.563114363
C	0.319849935	0.936522413	4.952254679
C	-1.037894006	0.644725217	4.731318305
C	0.653723439	1.957261686	5.860201324
C	-2.028229341	1.373293301	5.384592337
H	-1.309908862	-0.142284273	4.041901454
C	-0.342436771	2.690595016	6.493953347
H	1.692036698	2.165720597	6.088663534
C	-1.688270169	2.403073598	6.259211590
H	-3.072478927	1.132930909	5.211556228
H	-0.066644628	3.476226253	7.189301960
H	-2.463080325	2.968193899	6.766222257

$^{2}TS_{PO}$:

Ni	0.224843814	0.009454516	-0.133929499
O	0.289351599	0.104810577	1.837738439

O	1.599964104	-0.093719525	2.356763737
N	-0.145723508	2.109967649	-0.159831037
N	2.198190590	0.165890671	-1.015616322
N	0.497958580	-2.163357927	-0.303431724
N	-1.933055742	-0.222666125	-0.338347876
C	-2.481539317	1.162967016	-0.274516610
C	-1.536804229	2.168800838	0.361681071
C	-0.001538565	2.534898643	-1.574260325
C	1.404945947	2.324548793	-2.168679648
C	1.948170690	0.889473836	-2.295750674
C	0.659658484	2.955461629	0.751982406
C	2.584247012	-1.260269972	-1.242431788
C	1.976459443	-2.153329340	-0.160047404
C	3.277961327	0.803339923	-0.230547343
C	-1.717909390	-2.453563716	0.923624728
C	-2.270944290	-1.015782847	0.885615641
C	0.144433316	-2.985152050	-1.484966476
C	-0.194018461	-2.676884833	0.914691322
C	-2.511614629	-0.850877711	-1.547276890
H	-3.435096189	1.173950984	0.268698205
H	-2.714258947	1.470061109	-1.295145434
H	-1.955509604	3.177478108	0.232411275
H	-1.454488732	1.983152275	1.432734871
H	-0.266792490	3.597903399	-1.678472799
H	-0.724686420	1.972800222	-2.171446298
H	2.133536044	2.961219475	-1.663231875
H	1.362296452	2.717253658	-3.190475375
H	1.240001824	0.287829488	-2.874587266
H	2.877147348	0.929850169	-2.883696964
H	0.210627180	3.952760214	0.845113247
H	1.670599261	3.084099628	0.380864987
H	0.699733405	2.469024519	1.723958880
H	3.674660374	-1.362157898	-1.247462620
H	2.243510646	-1.566874109	-2.231939216
H	2.386163209	-3.170190734	-0.235786265
H	2.215379404	-1.758461406	0.828345649
H	4.219008207	0.796690484	-0.796819133
H	3.405590121	0.266657967	0.706733849
H	3.030016210	1.829401795	0.016733634
H	-2.205703426	-3.064529854	0.158967253
H	-2.072940936	-2.876962639	1.869676522
H	-3.366422463	-1.073015719	0.974897973
H	-1.886590274	-0.463307201	1.741488556
H	-0.003560217	-3.755356410	1.017787478
H	0.247362349	-2.166596785	1.766796074
H	-3.608497846	-0.821416115	-1.515530731
H	-2.179691809	-0.317876966	-2.439129305
H	-2.207064750	-1.884539819	-1.642526014
H	-0.902373778	-3.267431823	-1.464136482
H	0.326188348	-2.452788819	-2.418003078
H	0.728610497	-3.913695508	-1.496733109
P	1.751604969	-0.337667322	4.345711814
C	3.504507558	0.113957734	4.482586630
C	4.014963665	1.130644150	3.656190959
C	4.371730350	-0.521349113	5.385531552
C	5.355181068	1.495377815	3.732600381
H	3.354775346	1.632898778	2.961056495
C	5.713991773	-0.157697535	5.448083470
H	3.999411804	-1.292682972	6.047991798
C	6.211575112	0.849211977	4.623028855
H	5.733130065	2.288608693	3.095523295
H	6.369750482	-0.657062994	6.152851187
H	7.256943744	1.133454777	4.678486729
C	1.454677455	-1.756720692	5.456299875
C	2.063324126	-2.984881818	5.131927950
C	0.541166097	-1.719811345	6.524370088
C	1.793563063	-4.127985027	5.875276271
H	2.753311152	-3.042495592	4.294740956
C	0.263594655	-2.873638209	7.253730915
H	0.059458002	-0.788335299	6.796983527
C	0.888676365	-4.078952801	6.937962136

H	2.284317125	-5.062229948	5.622109382
H	-0.435610314	-2.825627667	8.082543840
H	0.672425876	-4.973455830	7.512734014
C	0.742896470	1.040356985	4.971179134
C	-0.641161678	1.020552491	4.739159947
C	1.304368583	2.126644570	5.656034115
C	-1.445868570	2.059910763	5.199213484
H	-1.084997034	0.191494105	4.200695839
C	0.494886055	3.166131129	6.108517169
H	2.370444877	2.156363096	5.848616707
C	-0.880083371	3.135283411	5.882673271
H	-2.517056586	2.029709913	5.027156150
H	0.939318062	3.995125120	6.648661370
H	-1.509036316	3.942083733	6.244078404

$^{4}P_{PO}$:

Ni	-0.435189979	0.048289795	-0.352134552
O	-0.723081750	0.501004898	1.455616822
O	2.672043588	-0.340712280	3.020403285
N	-0.963185913	2.061637626	-0.919991637
N	1.644915081	0.303548465	-0.702247028
N	0.036112654	-2.048624901	0.009291401
N	-2.441716010	-0.486555095	-1.036435181
C	-3.097521318	0.800883202	-1.405719055
C	-2.443794465	2.024982452	-0.788218949
C	-0.469481117	2.219809815	-2.312101140
C	1.059381045	2.092439460	-2.459853347
C	1.722291160	0.744265741	-2.125286051
C	-0.512886650	3.179957680	-0.053287290
C	2.228448879	-1.063550554	-0.514708815
C	1.419377529	-1.839968529	0.520705166
C	2.366413196	1.229683120	0.207727133
C	-2.400365793	-2.405535601	0.679449208
C	-3.026579969	-1.077640346	0.212149300
C	0.078160317	-3.093011764	-1.042812388
C	-0.917130968	-2.434870375	1.091449832
C	-2.632001468	-1.398907625	-2.188176338
H	-4.159201388	0.783769861	-1.129617101
H	-3.070782682	0.881492803	-2.493353698
H	-2.892575414	2.924644864	-1.232934188
H	-2.648313932	2.062194941	0.282970624
H	-0.780869205	3.195046623	-2.714664649
H	-0.951250284	1.458495104	-2.932658839
H	1.565889080	2.900331130	-1.928687589
H	1.278244496	2.278389116	-3.516965470
H	1.266503889	-0.043310386	-2.736170400
H	2.776872804	0.801937422	-2.430612671
H	-1.113746065	4.076482725	-0.248524864
H	0.523599349	3.434714728	-0.243090804
H	-0.611604550	2.877223379	0.986743652
H	3.269256222	-0.985912091	-0.188757827
H	2.235402617	-1.579705725	-1.476321725
H	1.904060090	-2.802149490	0.731109739
H	1.390888506	-1.284062411	1.457522674
H	3.398008627	1.364640935	-0.143120001
H	2.385056700	0.812830963	1.213506544
H	1.879706707	2.196177035	0.249962313
H	-2.623130834	-3.200145787	-0.038158285
H	-2.961843742	-2.690222195	1.575900382
H	-4.100201587	-1.248968137	0.045497287
H	-2.916849965	-0.335845853	1.002258983
H	-0.675457178	-3.446230930	1.447797807
H	-0.762158960	-1.737120489	1.910879957
H	-3.696994535	-1.498928836	-2.433217080
H	-2.113813221	-1.006153545	-3.064213119
H	-2.241666457	-2.386200595	-1.982140502
H	-0.908187343	-3.506006051	-1.225554875
H	0.456358738	-2.700070827	-1.986387767
H	0.723359166	-3.922922614	-0.731884076
P	2.719292863	-0.256289462	4.530956393
C	4.415049579	0.026019921	5.149555178
C	5.291252298	0.764468208	4.344569885
C	4.856410077	-0.452223404	6.388906516

C	6.586735566	1.029899110	4.779523406
H	4.958344496	1.118271529	3.374902305
C	6.154134802	-0.184113636	6.821002662
H	4.196276416	-1.044109755	7.014248734
C	7.018347467	0.558392580	6.018752885
H	7.261461622	1.601333211	4.150613508
H	6.491147130	-0.560840626	7.780889903
H	8.028913793	0.764001019	6.355836984
C	2.143598323	-1.798527657	5.330739945
C	2.729227122	-3.005405490	4.920189272
C	1.136712724	-1.820869381	6.301382494
C	2.317074087	-4.211211618	5.478270624
H	3.510232495	-2.999676108	4.166312026
C	0.724511883	-3.032193194	6.857464855
H	0.671604517	-0.896844938	6.626062808
C	1.313814735	-4.225741122	6.448816515
H	2.781403597	-5.139757524	5.162070143
H	-0.055092463	-3.040023336	7.612119681
H	0.996151188	-5.166338971	6.886713380
C	1.679890961	1.099661849	5.178925251
C	0.526548165	1.443465739	4.460645118
C	1.995588742	1.792182443	6.354432344
C	-0.304064905	2.459002897	4.929804554
H	0.276424044	0.939176750	3.532526344
C	1.161482339	2.808683636	6.814659425
H	2.896292611	1.550888872	6.908076686
C	0.008670797	3.140272822	6.104979973
H	-1.198287102	2.716966188	4.371658617
H	1.415134636	3.343707598	7.723655207
H	-0.640313039	3.931919832	6.465256061

$^{2}P_{PO}$:

Ni	-0.459741713	0.056760676	-0.371439690
O	-0.794364485	0.491662466	1.472683988
O	2.780713846	-0.341622554	3.004148245
N	-0.968381496	2.076729464	-0.918248502
N	1.625130757	0.317830380	-0.695485758
N	-0.000237460	-2.033156788	0.030330711
N	-2.465920085	-0.468196120	-1.042211674
C	-3.095634916	0.823047796	-1.442457990
C	-2.451710325	2.042874343	-0.809621733
C	-0.454103733	2.270667493	-2.297766649
C	1.075386851	2.138196062	-2.427761657
C	1.720993269	0.777727403	-2.111548576
C	-0.532667669	3.169988979	-0.014891848
C	2.191977401	-1.058225279	-0.520445275
C	1.388818536	-1.821901538	0.528704828
C	2.355479584	1.221518091	0.230679309
C	-2.436918495	-2.331659161	0.731298056
C	-3.046607271	-1.008500661	0.230698381
C	0.023209526	-3.115333306	-0.981647133
C	-0.951198275	-2.366060769	1.132435677
C	-2.690501401	-1.406713497	-2.166177229
H	-4.166334974	0.817172053	-1.201737551
H	-3.031075505	0.892180929	-2.529515699
H	-2.889603841	2.946246312	-1.257286762
H	-2.667837240	2.067907515	0.258267227
H	-0.755766680	3.257506881	-2.678581424
H	-0.931147724	1.528233089	-2.944555094
H	1.579452384	2.930657336	-1.871525020
H	1.310495934	2.345613234	-3.477273642
H	1.260809637	0.004997682	-2.738320294
H	2.778849152	0.826530111	-2.406507724
H	-1.107048086	4.082248074	-0.218229423
H	0.516036879	3.406607553	-0.152677501
H	-0.693208322	2.856996491	1.015397182
H	3.239679450	-0.995907274	-0.213192169
H	2.173504042	-1.571517870	-1.483514574
H	1.871876305	-2.782512792	0.747550903
H	1.362821325	-1.253068835	1.456892903
H	3.387826313	1.353246619	-0.118625612

H	2.376803374	0.786494298	1.228878096
H	1.880548326	2.193325011	0.289035729
H	-2.674232340	-3.143336402	0.038232772
H	-2.995222377	-2.583009095	1.639626447
H	-4.125954240	-1.162620364	0.086247811
H	-2.914370748	-0.238165725	0.992641286
H	-0.719960985	-3.364814799	1.528573592
H	-0.771833443	-1.638958717	1.924409228
H	-3.759486499	-1.480675016	-2.402768157
H	-2.165355867	-1.054551747	-3.055272684
H	-2.329781574	-2.399672959	-1.934001744
H	-0.976295578	-3.480410343	-1.191542133
H	0.459172646	-2.776074447	-1.921052021
H	0.609992717	-3.966751609	-0.616860154
P	2.779289294	-0.255401849	4.514909538
C	4.451768390	0.046812884	5.185067314
C	5.345327064	0.788289936	4.402397854
C	4.859917818	-0.422552863	6.438965437
C	6.625032060	1.066968317	4.874585495
H	5.038660084	1.133865950	3.421128089
C	6.141894707	-0.141892833	6.907965481
H	4.185904643	-1.016390637	7.047333706
C	7.023339860	0.604718482	6.128441041
H	7.313460931	1.641007479	4.263079011
H	6.453663465	-0.511800210	7.879006181
H	8.021685890	0.820443292	6.494490544
C	2.195017392	-1.804928046	5.293947102
C	2.743020957	-3.011473861	4.835034454
C	1.228338776	-1.831291305	6.304296512
C	2.333312239	-4.222178951	5.384668712
H	3.491597521	-3.000639583	4.049315164
C	0.818375735	-3.047199330	6.851670315
H	0.791485837	-0.906947926	6.665290198
C	1.370282861	-4.241234031	6.394782239
H	2.768297985	-5.151243811	5.030663439
H	0.069355131	-3.058835143	7.636518334
H	1.054337404	-5.185696903	6.825585254
C	1.702953350	1.084518618	5.135851378
C	0.517394875	1.349369872	4.435520477
C	2.018763591	1.838269681	6.272664950
C	-0.343115984	2.348813330	4.884458318
H	0.262389116	0.794454961	3.537545263
C	1.153993767	2.838674233	6.712841517
H	2.941772985	1.656480136	6.811989968
C	-0.029473396	3.091889701	6.021965887
H	-1.261978595	2.543440913	4.340804282
H	1.407453438	3.421140731	7.592386631
H	-0.702635733	3.869814392	6.367702535