

Supplementary Information for
Theoretical assessment of the mechanism and active sites in alkene
dimerization on Ni monomers grafted onto aluminosilicates: (Ni-OH)⁺
centers and C-C coupling mediated by Lewis acid-base pairs

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S1. Calculation of enthalpies and entropies using statistical mechanics formalisms

S2. Supporting calculations data

S3. DFT-optimized atomic coordinates

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S1. Calculation of enthalpies and entropies using statistical mechanics formalisms

Free energies were computed for a given state as the difference of enthalpy and entropy contributions:

$$G = H - TS \quad (S1)$$

The enthalpy of a given step reflects the sum of contributions from the DFT electronic energy (E_0), the zero-point vibrational enthalpy (E_{ZPV}), and vibrational, translational, and rotational enthalpy (H_{vib} , H_{trans} , and H_{rot}):

$$H = E_0 + E_{ZPV} + H_{vib} + H_{trans} + H_{rot} \quad (S2)$$

DFT-derived vibrational frequencies were used to compute E_{ZPV} and H_{vib} :

$$E_{ZPV} = \sum \frac{1}{2} h\nu_i \quad (S3)$$

$$H_{vib} = \sum \frac{h\nu_i e^{\frac{-h\nu_i}{k_B T}}}{1 - e^{\frac{-h\nu_i}{k_B T}}} \quad (S4)$$

Where h is Planck's constant, ν_i is a vibrational frequency mode, k_B is Boltzmann's constant, and T is temperature. Translational and rotational entropies were computed by:

$$H_{trans} = \frac{1}{2} k_B T \quad (S5)$$

$$H_{rot,linear} = k_B T \quad (S6)$$

Entropic contributions can likewise be decomposed into vibrational, translational, and rotational components:

$$S = S_{vib} + S_{trans} + S_{rot} \quad (S7)$$

Where the contributions are:

$$S_{vib} = R \sum_{i=1}^{3N-5} \left[\frac{h\nu_i}{k_B T \left(e^{\frac{h\nu_i}{k_B T}} - 1 \right)} - \ln \left(1 - e^{\frac{-h\nu_i}{k_B T}} \right) \right] \quad (S8)$$

$$S_{trans}^\circ = R \left(\ln \left[\left(\frac{2\pi M k_B T}{h^2} \right)^{\frac{3}{2}} \cdot \frac{V^\circ}{N_A} \right] + \frac{5}{2} \right) \quad (S9)$$

$$S_{rot} = k_B \left(\ln \left(\frac{\pi^{0.5}}{\sigma} \left(\frac{T^3}{\theta_x \theta_y \theta_z} \right)^{0.5} \right) + 1.5 \right) \quad (\text{S10})$$

where R is the ideal gas constant, M is the molecular mass of ethene, V is the molar volume, and N_A is Avogadro's number. The value σ reports the rotational symmetry numbers (4 and 1 for ethene and 1-butene, respectively) for the point group (D_{2h} and C_1 , respectively). Values of θ_i were computed using the moments of inertia, I_i , about each axis:

$$\theta_{x,y,z} = \frac{h^2}{8\pi^2 I_{x,y,z} k_B} \quad (\text{S11})$$

S2. Supporting calculations data

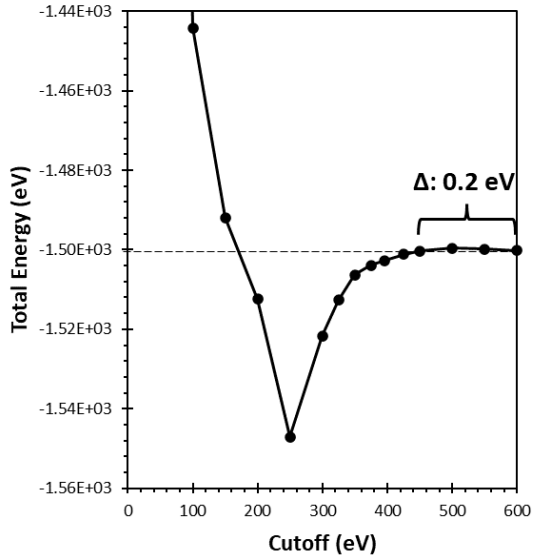


Figure S1. DFT electronic energy for the ethene adsorbed on a $(\text{Ni-OH})^+$ periodic slab as a function of electronic energy, justifying the use of 450 eV as the cutoff energy.

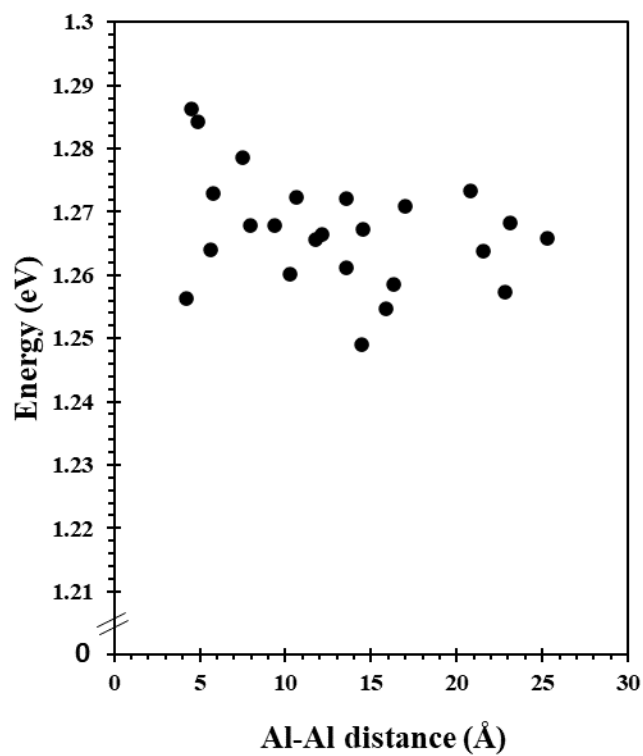


Figure S2. DFT-assessed electronic energy of $\text{Si}_{140}\text{Al}_2\text{O}_{335}\text{H}_{102}$ periodic slabs a function of Al-Al distance. Energies are referenced to the lowest energy single Si substitution by Al and distances are between the lowest energy single Al position and other Si substitution positions.

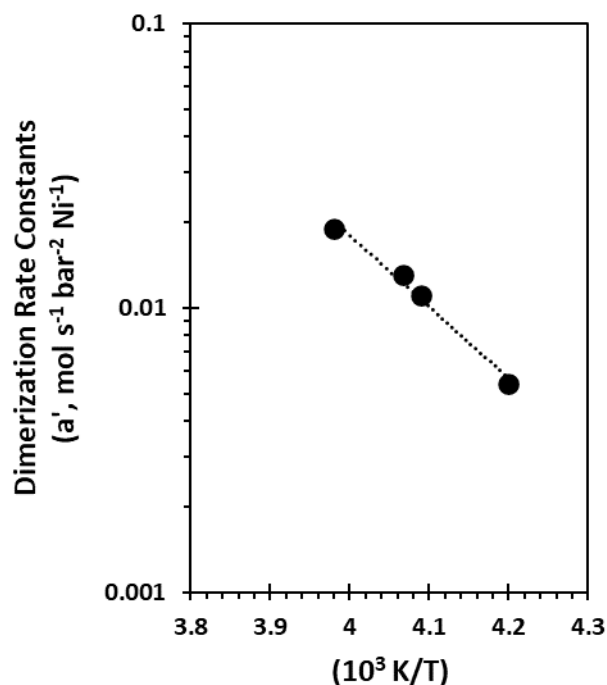


Figure S3. Second-order ethene dimerization constants (per $(\text{Ni-OH})^+$ site) as a function of reciprocal temperature (bottom abscissa) on small-pore Ni-Al-MCM-41 in the presence of intrapore liquids ($P/P_{\text{sat}} = 0.7\text{--}0.9$). Data were collected from *Journal of Catalysis* 389 (2020) 690–705 and rate constants are adapted to a reference state of 1 bar.

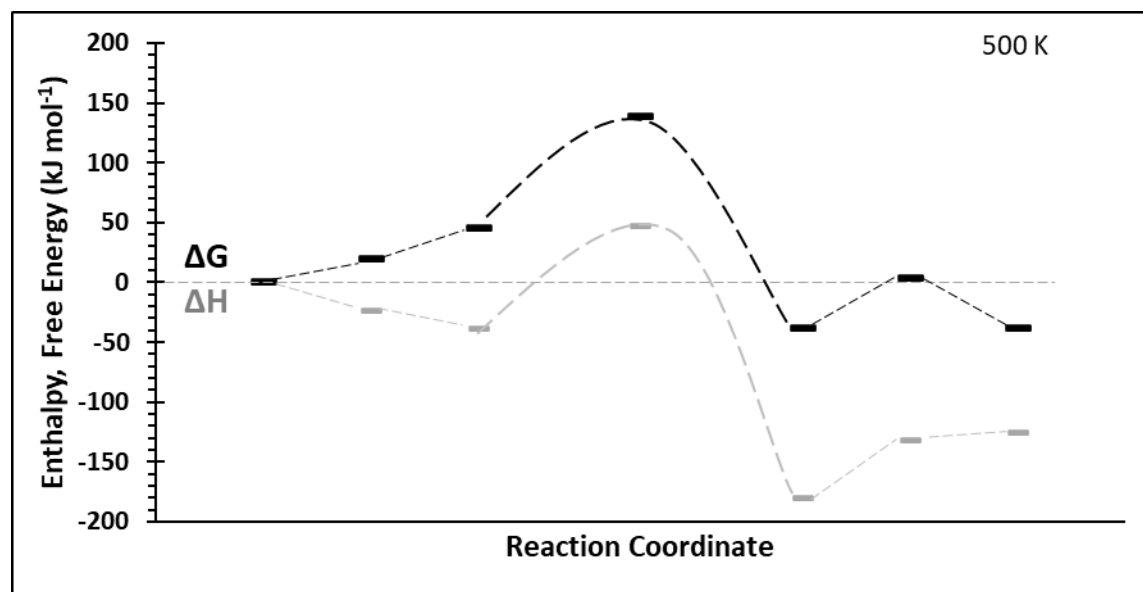


Figure S4. Reaction coordinate diagram of DFT-assessed ethene dimerization via a concerted acid-base mechanism over model $(\text{Ni-OH})^+$ sites. Enthalpies and free energies are reported with respect to a bare $(\text{Ni-OH})^+$ site and two gas phase ethene molecules at one bar, 500 K.

S3. DFT-optimized atomic coordinates

Ethene_(g) (I)

H	8.702470	9.305981	21.133051
H	8.770480	7.461161	21.332874
H	9.589746	9.089489	18.826004
H	9.657489	7.244525	19.024536
C	8.941650	8.333361	20.698685
C	9.418234	8.217138	19.458887

(Ni-OH)⁺ (*) (I)

Si	6.141571	3.904191	13.322562
Si	7.621518	12.256366	8.442000
Si	11.955669	10.554867	14.462399
Si	10.019951	6.824100	12.542282
Si	5.030561	12.629448	13.642000
Si	12.121967	5.142588	3.396400
Si	5.089982	6.236086	4.428400
Si	4.560124	6.121016	8.649600
Si	9.211920	5.814295	9.909600
Si	11.746457	10.779698	9.227201
Si	9.812782	12.048257	10.795200
Si	12.541766	0.089189	13.925600
Si	9.489394	5.305577	16.166904
Si	6.005562	3.693925	7.441600
Si	10.892969	2.767524	7.109600
Si	7.535115	7.937319	11.023600
Si	10.984008	9.467341	6.729600
Si	5.731494	10.501911	3.363200
Si	5.269097	6.215779	11.762400
Si	12.646716	5.129448	7.583200
Si	7.398423	11.266921	13.382401
Si	8.689230	2.733149	14.299601
Si	6.842045	3.766391	4.573600
Si	8.310841	11.745253	2.410400
Si	12.119840	5.856368	14.646000
Si	9.575190	9.643729	12.966000
Si	6.228600	11.080315	6.326000
Si	9.418234	2.664664	9.769600
Si	6.565253	10.646844	10.577200
Si	6.069852	7.946477	6.949200
Si	0.274987	8.055044	3.125600
Si	12.176368	9.218222	11.863199

Si	10.824993	10.336671	3.770400
Si	9.054027	5.850395	4.332000
Si	9.031193	7.028039	7.155600
Si	6.994024	7.723504	2.854400
Si	4.362893	7.686247	14.121722
Si	0.835714	1.705082	8.539599
Si	1.466075	8.518111	14.830400
Si	3.888379	9.619175	11.809601
Si	0.805332	7.973685	7.592400
Si	1.759330	7.829018	10.581200
Si	1.840227	2.479251	11.191999
Si	0.911156	2.943912	14.214400
Si	2.459718	11.386902	13.536400
Si	2.016362	5.002964	9.659200
Si	1.452010	3.940390	5.250000
Si	2.550819	10.164133	3.446400
Si	0.383942	12.374090	4.288400
Si	3.235090	2.327151	6.777600
Si	1.197727	12.042020	7.403600
Si	3.876153	12.711868	7.652400
Si	2.418584	7.757083	5.170000
Si	4.199781	0.495187	10.704401
Si	7.831317	1.404997	2.890000
Si	10.379497	1.248518	12.132000
Si	7.089207	0.285220	15.146000
Si	11.886435	2.203720	4.395200
Si	6.783931	1.687563	9.423600
Al	7.328919	6.298514	14.464025
O	6.759162	11.154772	2.246000
O	10.662036	10.322471	8.084400
O	4.808184	2.980041	13.377386
O	9.344977	0.033977	11.782000
O	6.799699	2.314676	3.812400
O	5.597132	5.221026	7.776000
O	8.695064	6.300286	13.365526
O	5.090491	10.195853	10.945200
O	4.689340	2.785043	7.269200
O	4.895081	7.608168	8.053600
O	8.191955	13.104727	3.340000
O	8.886584	12.063254	9.446400
O	11.269333	6.043298	13.288025
O	5.428379	4.622051	4.457600
O	7.528183	3.043933	13.188847

O	12.478667	10.454661	12.866401	O	7.572567	7.657541	7.511200
O	8.152338	4.531535	3.923600	O	6.329909	4.892284	14.584025
O	7.701066	11.511662	6.972000	O	11.283936	4.368817	7.116000
O	7.028008	3.563591	6.182400	O	8.365394	7.133554	3.569600
O	12.430955	6.724504	7.685600	O	9.816282	10.696614	11.728000
O	6.210792	7.564768	11.869201	O	10.374769	10.180988	14.355600
O	10.928246	8.435102	12.674246	O	8.269135	6.423984	15.977899
O	12.123152	12.162531	14.865600	O	9.380091	1.932834	2.936000
O	8.150500	12.504423	14.143200	O	9.403315	4.917802	17.758797
O	7.080863	12.953290	16.639599	O	9.222651	3.988538	15.201822
O	10.048716	8.165867	6.658000	O	9.373579	10.650427	3.060400
O	10.287496	6.299891	11.015220	O	8.875794	12.074802	0.912400
O	11.700548	3.457016	3.255200	O	7.347367	8.026111	1.292000
O	8.077121	9.829805	13.651600	O	12.749405	9.401511	15.374399
O	5.990423	11.345361	4.736000	O	5.859732	7.497592	14.899578
O	5.921060	9.520032	6.624000	O	3.312936	0.709533	6.626000
O	4.723644	6.119025	10.254001	O	2.978678	1.350449	11.330400
O	5.736908	6.666637	2.982400	O	1.068614	0.149711	8.228399
O	11.297309	12.089932	10.074000	O	0.204751	1.514095	14.714001
O	8.855690	8.253445	11.973213	O	0.721963	1.945575	10.135201
O	6.404660	11.582667	9.290401	O	1.122239	2.843706	12.597199
O	5.882887	7.027509	5.610400	O	0.463370	11.055894	8.455600
O	6.387131	9.033073	3.624000	O	2.104801	9.990797	14.309601
O	7.798911	6.595498	10.155200	O	2.886552	9.287635	4.802400
O	6.732806	3.159585	8.763600	O	2.586701	3.790945	10.562000
O	10.657479	5.656886	3.996000	O	0.464383	12.203410	5.936400
O	12.586321	9.084703	6.780000	O	1.159651	4.920012	6.494400
O	9.089299	4.226274	9.981200	O	3.494215	6.622971	4.619600
O	9.669577	2.455892	8.148001	O	0.788414	8.241385	11.837601
O	6.093790	4.842000	11.966909	O	1.783353	11.622352	3.714400
O	11.554258	8.938177	3.251200	O	3.994570	13.081898	9.267200
O	10.626290	10.290086	5.385600	O	1.786450	6.227858	10.691200
O	5.227203	12.081703	7.077200	O	3.047836	5.504786	8.475200
O	9.695821	6.302978	8.446400	O	2.093647	2.575607	7.928400
O	11.853836	11.571386	3.535200	O	0.145068	4.350900	14.561200
O	10.604074	2.179299	10.792399	O	2.930433	3.255809	5.437200
O	11.853820	9.559185	10.317201	O	2.750156	11.560105	7.304000
O	8.898306	5.963077	5.940400	O	0.516184	2.624980	5.283200
O	11.024648	5.873256	15.882025	O	4.215781	6.452354	13.017757
O	5.862259	11.234272	13.865200	O	0.916564	7.557336	4.547600
O	7.391491	9.295200	10.160399	O	3.206430	8.467013	10.895200
O	7.332047	11.494408	11.745600	O	2.383492	3.021952	14.969601
O	12.504366	6.544400	2.473200	O	1.437888	12.619760	13.326401

O	0.612614	7.058433	14.690400	O	13.219235	4.612362	9.024000
O	2.190965	7.677449	6.776400	O	12.814268	4.350900	14.561200
O	0.550035	4.612362	9.024000	O	13.281814	7.058433	14.690400
O	2.993660	7.797837	15.073599	O	-0.164834	6.544400	2.473200
O	1.279718	8.335619	9.109200	O	-1.114942	8.938177	3.251200
O	2.861917	10.867428	12.039599	O	13.457614	8.241385	11.837601
O	3.622376	12.232078	14.337999	O	-0.538016	2.007291	7.788400
O	0.991568	4.858828	3.969200	O	0.080205	9.401511	15.374399
O	4.117428	10.476163	2.896400	O	-0.238245	6.724504	7.685600
O	1.492396	9.134474	2.577600	O	-0.082879	9.084703	6.780000
O	4.396040	9.048841	13.239684	O	-0.815364	11.571386	3.535200
O	10.672203	2.253358	5.550000	O	-0.038661	13.952423	3.919200
O	12.131184	2.007291	7.788400	O	1.335296	13.421932	8.228399
O	5.595158	0.513635	14.460401	O	3.579617	13.981754	6.626000
O	4.901489	12.889318	12.021600	O	3.727889	-0.190324	9.267200
O	8.150242	1.779009	10.280000	O	4.634808	-0.382904	12.021600
O	5.493874	1.418800	10.349999	O	7.925273	-0.167495	3.340000
O	6.987936	0.560486	8.251600	O	7.883819	-0.767798	14.143200
O	9.912067	2.121830	13.419600	O	6.814182	-0.318932	16.639599
O	11.742654	0.508326	12.582001	O	13.185384	2.624980	5.283200
O	12.363857	0.680201	3.919200	H	7.514091	-0.208639	17.302401
O	8.024569	1.615362	15.300400				
O	7.290307	1.459944	1.323600	Ethene* (II)			
O	7.135919	8.018453	18.299410	Si	6.149042	3.915223	13.330256
H	7.780772	13.063582	17.302401	Si	7.621518	12.256366	8.442000
H	9.535483	2.888301	2.830400	Si	11.955669	10.554867	14.462399
H	10.174930	4.472808	18.141293	Si	10.027813	6.827527	12.551401
H	8.480283	12.870338	0.506400	Si	5.030561	12.629448	13.642000
H	7.238176	8.941231	0.982400	Si	12.121967	5.142588	3.396400
H	4.055346	3.249006	13.943416	Si	5.089982	6.236086	4.428400
H	2.704204	2.173459	15.322400	Si	4.560124	6.121016	8.649600
H	6.381372	1.760295	1.167600	Si	9.211920	5.814295	9.909600
H	7.940010	7.548923	18.598356	Si	11.746457	10.779698	9.227201
Ni	6.681458	7.698425	16.643480	Si	9.812782	12.048257	10.795200
O	7.254618	13.832707	8.251600	Si	12.541766	0.089189	13.925600
O	5.861839	13.785856	14.460401	Si	9.484527	5.297910	16.179426
O	13.660769	4.858828	3.969200	Si	6.005562	3.693925	7.441600
O	13.132569	11.055894	8.455600	Si	10.892969	2.767524	7.109600
O	9.611659	13.306198	11.782000	Si	7.535115	7.937319	11.023600
O	11.856470	-1.109691	14.865600	Si	10.984008	9.467341	6.729600
O	13.840406	-0.652462	13.326401	Si	5.731494	10.501911	3.363200
O	12.873951	1.514095	14.714001	Si	5.269097	6.215779	11.762400
O	13.828851	4.920012	6.494400	Si	12.646716	5.129448	7.583200

Si	7.398423	11.266921	13.382401	O	9.344977	0.033977	11.782000
Si	8.689230	2.733149	14.299601	O	6.799699	2.314676	3.812400
Si	6.842045	3.766391	4.573600	O	5.597132	5.221026	7.776000
Si	8.310841	11.745253	2.410400	O	8.718659	6.332808	13.414823
Si	12.119840	5.856368	14.646000	O	5.090491	10.195853	10.945200
Si	9.575190	9.643729	12.966000	O	4.689340	2.785043	7.269200
Si	6.228600	11.080315	6.326000	O	4.895081	7.608168	8.053600
Si	9.418234	2.664664	9.769600	O	8.191955	13.104727	3.340000
Si	6.565253	10.646844	10.577200	O	8.886584	12.063254	9.446400
Si	6.069852	7.946477	6.949200	O	11.284094	6.040246	13.278049
Si	0.274987	8.055044	3.125600	O	5.428379	4.622051	4.457600
Si	12.176368	9.218222	11.863199	O	7.529797	3.046755	13.189105
Si	10.824993	10.336671	3.770400	O	12.478667	10.454661	12.866401
Si	9.054027	5.850395	4.332000	O	8.152338	4.531535	3.923600
Si	9.031193	7.028039	7.155600	O	7.701066	11.511662	6.972000
Si	6.994024	7.723504	2.854400	O	7.028008	3.563591	6.182400
Si	4.356820	7.679688	14.116768	O	12.430955	6.724504	7.685600
Si	0.835714	1.705082	8.539599	O	6.210792	7.564768	11.869201
Si	1.466075	8.518111	14.830400	O	10.929487	8.435717	12.676115
Si	3.888379	9.619175	11.809601	O	12.123152	12.162531	14.865600
Si	0.805332	7.973685	7.592400	O	8.150500	12.504423	14.143200
Si	1.759330	7.829018	10.581200	O	7.080863	12.953290	16.639599
Si	1.840227	2.479251	11.191999	O	10.048716	8.165867	6.658000
Si	0.911156	2.943912	14.214400	O	10.279926	6.295975	11.023416
Si	2.459718	11.386902	13.536400	O	11.700548	3.457016	3.255200
Si	2.016362	5.002964	9.659200	O	8.077121	9.829805	13.651600
Si	1.452010	3.940390	5.250000	O	5.990423	11.345361	4.736000
Si	2.550819	10.164133	3.446400	O	5.921060	9.520032	6.624000
Si	0.383942	12.374090	4.288400	O	4.723644	6.119025	10.254001
Si	3.235090	2.327151	6.777600	O	5.736908	6.666637	2.982400
Si	1.197727	12.042020	7.403600	O	11.297309	12.089932	10.074000
Si	3.876153	12.711868	7.652400	O	8.856386	8.252687	11.971226
Si	2.418584	7.757083	5.170000	O	6.404660	11.582667	9.290401
Si	4.199781	0.495187	10.704401	O	5.882887	7.027509	5.610400
Si	7.831317	1.404997	2.890000	O	6.387131	9.033073	3.624000
Si	10.379497	1.248518	12.132000	O	7.798911	6.595498	10.155200
Si	7.089207	0.285220	15.146000	O	6.732806	3.159585	8.763600
Si	11.886435	2.203720	4.395200	O	10.657479	5.656886	3.996000
Si	6.783931	1.687563	9.423600	O	12.586321	9.084703	6.780000
Al	7.344418	6.318580	14.501011	O	9.089299	4.226274	9.981200
O	6.759162	11.154772	2.246000	O	9.669577	2.455892	8.148001
O	10.662036	10.322471	8.084400	O	6.096825	4.844862	11.969844
O	4.815321	2.991812	13.395929	O	11.554258	8.938177	3.251200

O	10.626290	10.290086	5.385600	O	1.786450	6.227858	10.691200
O	5.227203	12.081703	7.077200	O	3.047836	5.504786	8.475200
O	9.695821	6.302978	8.446400	O	2.093647	2.575607	7.928400
O	11.853836	11.571386	3.535200	O	0.145068	4.350900	14.561200
O	10.604074	2.179299	10.792399	O	2.930433	3.255809	5.437200
O	11.853820	9.559185	10.317201	O	2.750156	11.560105	7.304000
O	8.898306	5.963077	5.940400	O	0.516184	2.624980	5.283200
O	11.013484	5.883865	15.872259	O	4.207298	6.449163	13.010658
O	5.862259	11.234272	13.865200	O	0.916564	7.557336	4.547600
O	7.391491	9.295200	10.160399	O	3.206430	8.467013	10.895200
O	7.332047	11.494408	11.745600	O	2.383492	3.021952	14.969601
O	12.504366	6.544400	2.473200	O	1.437888	12.619760	13.326401
O	7.572567	7.657541	7.511200	O	0.612614	7.058433	14.690400
O	6.348514	4.903883	14.587864	O	2.190965	7.677449	6.776400
O	11.283936	4.368817	7.116000	O	0.550035	4.612362	9.024000
O	8.365394	7.133554	3.569600	O	2.991441	7.795546	15.073055
O	9.816282	10.696614	11.728000	O	1.279718	8.335619	9.109200
O	10.374769	10.180988	14.355600	O	2.861917	10.867428	12.039599
O	8.242590	6.400996	16.043062	O	3.622376	12.232078	14.337999
O	9.380091	1.932834	2.936000	O	0.991568	4.858828	3.969200
O	9.467533	4.867182	17.765322	O	4.117428	10.476163	2.896400
O	9.223634	3.986418	15.202292	O	1.492396	9.134474	2.577600
O	9.373579	10.650427	3.060400	O	4.395122	9.045118	13.239109
O	8.875794	12.074802	0.912400	O	10.672203	2.253358	5.550000
O	7.347367	8.026111	1.292000	O	12.131184	2.007291	7.788400
O	12.749405	9.401511	15.374399	O	5.595158	0.513635	14.460401
O	5.845716	7.481173	14.902578	O	4.901489	12.889318	12.021600
O	3.312936	0.709533	6.626000	O	8.150242	1.779009	10.280000
O	2.978678	1.350449	11.330400	O	5.493874	1.418800	10.349999
O	1.068614	0.149711	8.228399	O	6.987936	0.560486	8.251600
O	0.204751	1.514095	14.714001	O	9.912067	2.121830	13.419600
O	0.721963	1.945575	10.135201	O	11.742654	0.508326	12.582001
O	1.122239	2.843706	12.597199	O	12.363857	0.680201	3.919200
O	0.463370	11.055894	8.455600	O	8.024569	1.615362	15.300400
O	2.104801	9.990797	14.309601	O	7.290307	1.459944	1.323600
O	2.886552	9.287635	4.802400	O	6.533332	7.949018	18.415377
O	2.586701	3.790945	10.562000	H	7.780772	13.063582	17.302401
O	0.464383	12.203410	5.936400	H	9.535483	2.888301	2.830400
O	1.159651	4.920012	6.494400	H	10.262617	4.412146	18.084375
O	3.494215	6.622971	4.619600	H	8.480283	12.870338	0.506400
O	0.788414	8.241385	11.837601	H	7.238176	8.941231	0.982400
O	1.783353	11.622352	3.714400	H	4.059357	3.264658	13.955483
O	3.994570	13.081898	9.267200	H	2.704204	2.173459	15.322400

H	6.381372	1.760295	1.167600	Si	11.955669	10.554867	14.462399
H	7.367439	7.946788	18.938950	Si	10.011200	6.821604	12.549781
H	8.712812	9.280583	21.041180	Si	5.030561	12.629448	13.642000
H	8.762288	7.435349	21.246181	Si	12.121967	5.142588	3.396400
H	9.684555	9.051394	18.765177	Si	5.089982	6.236086	4.428400
H	9.725910	7.203089	18.969006	Si	4.560124	6.121016	8.649600
Ni	6.442107	7.525270	16.739767	Si	9.211920	5.814295	9.909600
C	8.962113	8.305484	20.617437	Si	11.746457	10.779698	9.227201
C	9.484815	8.180289	19.392874	Si	9.812782	12.048257	10.795200
O	7.254618	13.832707	8.251600	Si	12.541766	0.089189	13.925600
O	5.861839	13.785856	14.460401	Si	9.489118	5.306440	16.165745
O	13.660769	4.858828	3.969200	Si	6.005562	3.693925	7.441600
O	13.132569	11.055894	8.455600	Si	10.892969	2.767524	7.109600
O	9.611659	13.306198	11.782000	Si	7.535115	7.937319	11.023600
O	11.856470	-1.109691	14.865600	Si	10.984008	9.467341	6.729600
O	13.840406	-0.652462	13.326401	Si	5.731494	10.501911	3.363200
O	12.873951	1.514095	14.714001	Si	5.269097	6.215779	11.762400
O	13.828851	4.920012	6.494400	Si	12.646716	5.129448	7.583200
O	13.219235	4.612362	9.024000	Si	7.398423	11.266921	13.382401
O	12.814268	4.350900	14.561200	Si	8.689230	2.733149	14.299601
O	13.281814	7.058433	14.690400	Si	6.842045	3.766391	4.573600
O	-0.164834	6.544400	2.473200	Si	8.310841	11.745253	2.410400
O	-1.114942	8.938177	3.251200	Si	12.119840	5.856368	14.646000
O	13.457614	8.241385	11.837601	Si	9.575190	9.643729	12.966000
O	-0.538016	2.007291	7.788400	Si	6.228600	11.080315	6.326000
O	0.080205	9.401511	15.374399	Si	9.418234	2.664664	9.769600
O	-0.238245	6.724504	7.685600	Si	6.565253	10.646844	10.577200
O	-0.082879	9.084703	6.780000	Si	6.069852	7.946477	6.949200
O	-0.815364	11.571386	3.535200	Si	0.274987	8.055044	3.125600
O	-0.038661	13.952423	3.919200	Si	12.176368	9.218222	11.863199
O	1.335296	13.421932	8.228399	Si	10.824993	10.336671	3.770400
O	3.579617	13.981754	6.626000	Si	9.054027	5.850395	4.332000
O	3.727889	-0.190324	9.267200	Si	9.031193	7.028039	7.155600
O	4.634808	-0.382904	12.021600	Si	6.994024	7.723504	2.854400
O	7.925273	-0.167495	3.340000	Si	4.363807	7.682684	14.112592
O	7.883819	-0.767798	14.143200	Si	0.835714	1.705082	8.539599
O	6.814182	-0.318932	16.639599	Si	1.466075	8.518111	14.830400
O	13.185384	2.624980	5.283200	Si	3.888379	9.619175	11.809601
H	7.514091	-0.208639	17.302401	Si	0.805332	7.973685	7.592400
2Ethene* (III)				Si	1.759330	7.829018	10.581200
Si	6.143501	3.897510	13.319681	Si	1.840227	2.479251	11.191999
Si	7.621518	12.256366	8.442000	Si	0.911156	2.943912	14.214400
				Si	2.459718	11.386902	13.536400

Si	2.016362	5.002964	9.659200	O	8.077121	9.829805	13.651600
Si	1.452010	3.940390	5.250000	O	5.990423	11.345361	4.736000
Si	2.550819	10.164133	3.446400	O	5.921060	9.520032	6.624000
Si	0.383942	12.374090	4.288400	O	4.723644	6.119025	10.254001
Si	3.235090	2.327151	6.777600	O	5.736908	6.666637	2.982400
Si	1.197727	12.042020	7.403600	O	11.297309	12.089932	10.074000
Si	3.876153	12.711868	7.652400	O	8.854159	8.251783	11.976074
Si	2.418584	7.757083	5.170000	O	6.404660	11.582667	9.290401
Si	4.199781	0.495187	10.704401	O	5.882887	7.027509	5.610400
Si	7.831317	1.404997	2.890000	O	6.387131	9.033073	3.624000
Si	10.379497	1.248518	12.132000	O	7.798911	6.595498	10.155200
Si	7.089207	0.285220	15.146000	O	6.732806	3.159585	8.763600
Si	11.886435	2.203720	4.395200	O	10.657479	5.656886	3.996000
Si	6.783931	1.687563	9.423600	O	12.586321	9.084703	6.780000
Al	7.327168	6.274551	14.494328	O	9.089299	4.226274	9.981200
O	6.759162	11.154772	2.246000	O	9.669577	2.455892	8.148001
O	10.662036	10.322471	8.084400	O	6.099792	4.846679	11.972140
O	4.808115	2.973835	13.356284	O	11.554258	8.938177	3.251200
O	9.344977	0.033977	11.782000	O	10.626290	10.290086	5.385600
O	6.799699	2.314676	3.812400	O	5.227203	12.081703	7.077200
O	5.597132	5.221026	7.776000	O	9.695821	6.302978	8.446400
O	8.689021	6.302835	13.380956	O	11.853836	11.571386	3.535200
O	5.090491	10.195853	10.945200	O	10.604074	2.179299	10.792399
O	4.689340	2.785043	7.269200	O	11.853820	9.559185	10.317201
O	4.895081	7.608168	8.053600	O	8.898306	5.963077	5.940400
O	8.191955	13.104727	3.340000	O	11.026072	5.876830	15.883056
O	8.886584	12.063254	9.446400	O	5.862259	11.234272	13.865200
O	11.266961	6.044127	13.289806	O	7.391491	9.295200	10.160399
O	5.428379	4.622051	4.457600	O	7.332047	11.494408	11.745600
O	7.530089	3.037289	13.183846	O	12.504366	6.544400	2.473200
O	12.478667	10.454661	12.866401	O	7.572567	7.657541	7.511200
O	8.152338	4.531535	3.923600	O	6.327748	4.867610	14.595264
O	7.701066	11.511662	6.972000	O	11.283936	4.368817	7.116000
O	7.028008	3.563591	6.182400	O	8.365394	7.133554	3.569600
O	12.430955	6.724504	7.685600	O	9.816282	10.696614	11.728000
O	6.210792	7.564768	11.869201	O	10.374769	10.180988	14.355600
O	10.927289	8.436353	12.674519	O	8.269634	6.424016	16.003830
O	12.123152	12.162531	14.865600	O	9.380091	1.932834	2.936000
O	8.150500	12.504423	14.143200	O	9.429130	4.863947	17.747246
O	7.080863	12.953290	16.639599	O	9.224873	3.993210	15.190592
O	10.048716	8.165867	6.658000	O	9.373579	10.650427	3.060400
O	10.281426	6.297355	11.021749	O	8.875794	12.074802	0.912400
O	11.700548	3.457016	3.255200	O	7.347367	8.026111	1.292000

O	12.749405	9.401511	15.374399	O	5.595158	0.513635	14.460401
O	5.868359	7.487992	14.867289	O	4.901489	12.889318	12.021600
O	3.312936	0.709533	6.626000	O	8.150242	1.779009	10.280000
O	2.978678	1.350449	11.330400	O	5.493874	1.418800	10.349999
O	1.068614	0.149711	8.228399	O	6.987936	0.560486	8.251600
O	0.204751	1.514095	14.714001	O	9.912067	2.121830	13.419600
O	0.721963	1.945575	10.135201	O	11.742654	0.508326	12.582001
O	1.122239	2.843706	12.597199	O	12.363857	0.680201	3.919200
O	0.463370	11.055894	8.455600	O	8.024569	1.615362	15.300400
O	2.104801	9.990797	14.309601	O	7.290307	1.459944	1.323600
O	2.886552	9.287635	4.802400	O	7.249025	8.781975	17.961767
O	2.586701	3.790945	10.562000	H	7.780772	13.063582	17.302401
O	0.464383	12.203410	5.936400	H	9.535483	2.888301	2.830400
O	1.159651	4.920012	6.494400	H	10.139410	4.276259	18.049116
O	3.494215	6.622971	4.619600	H	8.480283	12.870338	0.506400
O	0.788414	8.241385	11.837601	H	7.238176	8.941231	0.982400
O	1.783353	11.622352	3.714400	H	4.057253	3.237327	13.926906
O	3.994570	13.081898	9.267200	H	2.704204	2.173459	15.322400
O	1.786450	6.227858	10.691200	H	6.381372	1.760295	1.167600
O	3.047836	5.504786	8.475200	H	8.008012	8.469534	18.507616
O	2.093647	2.575607	7.928400	H	9.111414	9.090623	20.916618
O	0.145068	4.350900	14.561200	H	8.638910	7.294751	20.869522
O	2.930433	3.255809	5.437200	H	10.558781	8.755032	18.920195
O	2.750156	11.560105	7.304000	H	10.075133	6.957285	18.882284
O	0.516184	2.624980	5.283200	H	5.514124	8.866961	21.356255
O	4.207373	6.450256	13.010271	H	5.190322	7.042491	21.502232
O	0.916564	7.557336	4.547600	H	4.532283	8.867042	19.087030
O	3.206430	8.467013	10.895200	H	4.200971	7.042120	19.224277
O	2.383492	3.021952	14.969601	Ni	6.781608	8.003149	16.489183
O	1.437888	12.619760	13.326401	C	9.211641	8.116187	20.434275
O	0.612614	7.058433	14.690400	C	9.988719	7.934480	19.361021
O	2.190965	7.677449	6.776400	C	5.122520	7.953436	20.904510
O	0.550035	4.612362	9.024000	C	4.590471	7.954003	19.681494
O	2.995697	7.796822	15.069225	O	7.254618	13.832707	8.251600
O	1.279718	8.335619	9.109200	O	5.861839	13.785856	14.460401
O	2.861917	10.867428	12.039599	O	13.660769	4.858828	3.969200
O	3.622376	12.232078	14.337999	O	13.132569	11.055894	8.455600
O	0.991568	4.858828	3.969200	O	9.611659	13.306198	11.782000
O	4.117428	10.476163	2.896400	O	11.856470	-1.109691	14.865600
O	1.492396	9.134474	2.577600	O	13.840406	-0.652462	13.326401
O	4.394044	9.050728	13.239443	O	12.873951	1.514095	14.714001
O	10.672203	2.253358	5.550000	O	13.828851	4.920012	6.494400
O	12.131184	2.007291	7.788400	O	13.219235	4.612362	9.024000

O	12.814268	4.350900	14.561200	Si	8.689230	2.733149	14.299601
O	13.281814	7.058433	14.690400	Si	6.842045	3.766391	4.573600
O	-0.164834	6.544400	2.473200	Si	8.310841	11.745253	2.410400
O	-1.114942	8.938177	3.251200	Si	12.119840	5.856368	14.646000
O	13.457614	8.241385	11.837601	Si	9.575190	9.643729	12.966000
O	-0.538016	2.007291	7.788400	Si	6.228600	11.080315	6.326000
O	0.080205	9.401511	15.374399	Si	9.418234	2.664664	9.769600
O	-0.238245	6.724504	7.685600	Si	6.565253	10.646844	10.577200
O	-0.082879	9.084703	6.780000	Si	6.069852	7.946477	6.949200
O	-0.815364	11.571386	3.535200	Si	0.274987	8.055044	3.125600
O	-0.038661	13.952423	3.919200	Si	12.176368	9.218222	11.863199
O	1.335296	13.421932	8.228399	Si	10.824993	10.336671	3.770400
O	3.579617	13.981754	6.626000	Si	9.054027	5.850395	4.332000
O	3.727889	-0.190324	9.267200	Si	9.031193	7.028039	7.155600
O	4.634808	-0.382904	12.021600	Si	6.994024	7.723504	2.854400
O	7.925273	-0.167495	3.340000	Si	4.327672	7.681162	14.099809
O	7.883819	-0.767798	14.143200	Si	0.835714	1.705082	8.539599
O	6.814182	-0.318932	16.639599	Si	1.466075	8.518111	14.830400
O	13.185384	2.624980	5.283200	Si	3.888379	9.619175	11.809601
H	7.514091	-0.208639	17.302401	Si	0.805332	7.973685	7.592400
C-C TS (IV)				Si	1.759330	7.829018	10.581200
Si	6.166693	3.975059	13.393486	Si	1.840227	2.479251	11.191999
Si	7.621518	12.256366	8.442000	Si	0.911156	2.943912	14.214400
Si	11.955669	10.554867	14.462399	Si	2.459718	11.386902	13.536400
Si	9.999301	6.840302	12.592067	Si	2.016362	5.002964	9.659200
Si	5.030561	12.629448	13.642000	Si	1.452010	3.940390	5.250000
Si	12.121967	5.142588	3.396400	Si	2.550819	10.164133	3.446400
Si	5.089982	6.236086	4.428400	Si	0.383942	12.374090	4.288400
Si	4.560124	6.121016	8.649600	Si	3.235090	2.327151	6.777600
Si	9.211920	5.814295	9.909600	Si	1.197727	12.042020	7.403600
Si	11.746457	10.779698	9.227201	Si	3.876153	12.711868	7.652400
Si	9.812782	12.048257	10.795200	Si	2.418584	7.757083	5.170000
Si	12.541766	0.089189	13.925600	Si	4.199781	0.495187	10.704401
Si	9.597735	5.194267	16.242224	Si	7.831317	1.404997	2.890000
Si	6.005562	3.693925	7.441600	Si	10.379497	1.248518	12.132000
Si	10.892969	2.767524	7.109600	Si	7.089207	0.285220	15.146000
Si	7.535115	7.937319	11.023600	Si	11.886435	2.203720	4.395200
Si	10.984008	9.467341	6.729600	Si	6.783931	1.687563	9.423600
Si	5.731494	10.501911	3.363200	Al	7.414855	6.362441	14.731898
Si	5.269097	6.215779	11.762400	O	6.759162	11.154772	2.246000
Si	12.646716	5.129448	7.583200	O	10.662036	10.322471	8.084400
Si	7.398423	11.266921	13.382401	O	4.844227	3.038660	13.509034
				O	9.344977	0.033977	11.782000

O	6.799699	2.314676	3.812400	O	5.227203	12.081703	7.077200
O	5.597132	5.221026	7.776000	O	9.695821	6.302978	8.446400
O	8.718911	6.444673	13.540012	O	11.853836	11.571386	3.535200
O	5.090491	10.195853	10.945200	O	10.604074	2.179299	10.792399
O	4.689340	2.785043	7.269200	O	11.853820	9.559185	10.317201
O	4.895081	7.608168	8.053600	O	8.898306	5.963077	5.940400
O	8.191955	13.104727	3.340000	O	11.099360	5.840206	15.927138
O	8.886584	12.063254	9.446400	O	5.862259	11.234272	13.865200
O	11.262625	6.041082	13.297433	O	7.391491	9.295200	10.160399
O	5.428379	4.622051	4.457600	O	7.332047	11.494408	11.745600
O	7.530829	3.085922	13.212451	O	12.504366	6.544400	2.473200
O	12.478667	10.454661	12.866401	O	7.572567	7.657541	7.511200
O	8.152338	4.531535	3.923600	O	6.394277	4.961134	14.645361
O	7.701066	11.511662	6.972000	O	11.283936	4.368817	7.116000
O	7.028008	3.563591	6.182400	O	8.365394	7.133554	3.569600
O	12.430955	6.724504	7.685600	O	9.816282	10.696614	11.728000
O	6.210792	7.564768	11.869201	O	10.374769	10.180988	14.355600
O	10.929877	8.440380	12.680034	O	8.394897	6.284987	16.207970
O	12.123152	12.162531	14.865600	O	9.380091	1.932834	2.936000
O	8.150500	12.504423	14.143200	O	9.672124	4.648478	17.804169
O	7.080863	12.953290	16.639599	O	9.304428	3.932393	15.211473
O	10.048716	8.165867	6.658000	O	9.373579	10.650427	3.060400
O	10.243506	6.276332	11.066448	O	8.875794	12.074802	0.912400
O	11.700548	3.457016	3.255200	O	7.347367	8.026111	1.292000
O	8.077121	9.829805	13.651600	O	12.749405	9.401511	15.374399
O	5.990423	11.345361	4.736000	O	5.801875	7.528538	14.887341
O	5.921060	9.520032	6.624000	O	3.312936	0.709533	6.626000
O	4.723644	6.119025	10.254001	O	2.978678	1.350449	11.330400
O	5.736908	6.666637	2.982400	O	1.068614	0.149711	8.228399
O	11.297309	12.089932	10.074000	O	0.204751	1.514095	14.714001
O	8.859488	8.258439	11.960733	O	0.721963	1.945575	10.135201
O	6.404660	11.582667	9.290401	O	1.122239	2.843706	12.597199
O	5.882887	7.027509	5.610400	O	0.463370	11.055894	8.455600
O	6.387131	9.033073	3.624000	O	2.104801	9.990797	14.309601
O	7.798911	6.595498	10.155200	O	2.886552	9.287635	4.802400
O	6.732806	3.159585	8.763600	O	2.586701	3.790945	10.562000
O	10.657479	5.656886	3.996000	O	0.464383	12.203410	5.936400
O	12.586321	9.084703	6.780000	O	1.159651	4.920012	6.494400
O	9.089299	4.226274	9.981200	O	3.494215	6.622971	4.619600
O	9.669577	2.455892	8.148001	O	0.788414	8.241385	11.837601
O	6.084138	4.847899	12.000475	O	1.783353	11.622352	3.714400
O	11.554258	8.938177	3.251200	O	3.994570	13.081898	9.267200
O	10.626290	10.290086	5.385600	O	1.786450	6.227858	10.691200

O	3.047836	5.504786	8.475200	H	7.615766	7.813290	18.584660
O	2.093647	2.575607	7.928400	H	8.743099	9.374758	20.875647
O	0.145068	4.350900	14.561200	H	9.037886	7.627727	21.416758
O	2.930433	3.255809	5.437200	H	9.541000	8.804358	18.587198
O	2.750156	11.560105	7.304000	H	9.775120	7.032018	19.104816
O	0.516184	2.624980	5.283200	H	6.482028	8.336188	21.772915
O	4.184248	6.453813	12.994781	H	6.734778	6.758637	20.832787
O	0.916564	7.557336	4.547600	H	6.078568	9.560758	19.638779
O	3.206430	8.467013	10.895200	H	4.948967	8.184926	19.490088
O	2.383492	3.021952	14.969601	Ni	6.106652	7.914701	16.635923
O	1.437888	12.619760	13.326401	C	8.945954	8.339831	20.596476
O	0.612614	7.058433	14.690400	C	9.443328	8.039479	19.361752
O	2.190965	7.677449	6.776400	C	6.630144	7.843863	20.808964
O	0.550035	4.612362	9.024000	C	6.011760	8.461542	19.615824
O	2.976368	7.790760	15.073517	O	7.254618	13.832707	8.251600
O	1.279718	8.335619	9.109200	O	5.861839	13.785856	14.460401
O	2.861917	10.867428	12.039599	O	13.660769	4.858828	3.969200
O	3.622376	12.232078	14.337999	O	13.132569	11.055894	8.455600
O	0.991568	4.858828	3.969200	O	9.611659	13.306198	11.782000
O	4.117428	10.476163	2.896400	O	11.856470	-1.109691	14.865600
O	1.492396	9.134474	2.577600	O	13.840406	-0.652462	13.326401
O	4.377143	9.054358	13.240448	O	12.873951	1.514095	14.714001
O	10.672203	2.253358	5.550000	O	13.828851	4.920012	6.494400
O	12.131184	2.007291	7.788400	O	13.219235	4.612362	9.024000
O	5.595158	0.513635	14.460401	O	12.814268	4.350900	14.561200
O	4.901489	12.889318	12.021600	O	13.281814	7.058433	14.690400
O	8.150242	1.779009	10.280000	O	-0.164834	6.544400	2.473200
O	5.493874	1.418800	10.349999	O	-1.114942	8.938177	3.251200
O	6.987936	0.560486	8.251600	O	13.457614	8.241385	11.837601
O	9.912067	2.121830	13.419600	O	-0.538016	2.007291	7.788400
O	11.742654	0.508326	12.582001	O	0.080205	9.401511	15.374399
O	12.363857	0.680201	3.919200	O	-0.238245	6.724504	7.685600
O	8.024569	1.615362	15.300400	O	-0.082879	9.084703	6.780000
O	7.290307	1.459944	1.323600	O	-0.815364	11.571386	3.535200
O	6.653438	7.972277	18.395630	O	-0.038661	13.952423	3.919200
H	7.780772	13.063582	17.302401	O	1.335296	13.421932	8.228399
H	9.535483	2.888301	2.830400	O	3.579617	13.981754	6.626000
H	10.460801	4.122105	18.007654	O	3.727889	-0.190324	9.267200
H	8.480283	12.870338	0.506400	O	4.634808	-0.382904	12.021600
H	7.238176	8.941231	0.982400	O	7.925273	-0.167495	3.340000
H	4.068878	3.333451	14.027687	O	7.883819	-0.767798	14.143200
H	2.704204	2.173459	15.322400	O	6.814182	-0.318932	16.639599
H	6.381372	1.760295	1.167600	O	13.185384	2.624980	5.283200

H 7.514091 -0.208639 17.302401

Butoxide* (V)

Si 6.146886 3.917605 13.333974
Si 7.621518 12.256366 8.442000
Si 11.955669 10.554867 14.462399
Si 10.024678 6.827692 12.552063
Si 5.030561 12.629448 13.642000
Si 12.121967 5.142588 3.396400
Si 5.089982 6.236086 4.428400
Si 4.560124 6.121016 8.649600
Si 9.211920 5.814295 9.909600
Si 11.746457 10.779698 9.227201
Si 9.812782 12.048257 10.795200
Si 12.541766 0.089189 13.925600
Si 9.502891 5.275004 16.196079
Si 6.005562 3.693925 7.441600
Si 10.892969 2.767524 7.109600
Si 7.535115 7.937319 11.023600
Si 10.984008 9.467341 6.729600
Si 5.731494 10.501911 3.363200
Si 5.269097 6.215779 11.762400
Si 12.646716 5.129448 7.583200
Si 7.398423 11.266921 13.382401
Si 8.689230 2.733149 14.299601
Si 6.842045 3.766391 4.573600
Si 8.310841 11.745253 2.410400
Si 12.119840 5.856368 14.646000
Si 9.575190 9.643729 12.966000
Si 6.228600 11.080315 6.326000
Si 9.418234 2.664664 9.769600
Si 6.565253 10.646844 10.577200
Si 6.069852 7.946477 6.949200
Si 0.274987 8.055044 3.125600
Si 12.176368 9.218222 11.863199
Si 10.824993 10.336671 3.770400
Si 9.054027 5.850395 4.332000
Si 9.031193 7.028039 7.155600
Si 6.994024 7.723504 2.854400
Si 4.353263 7.680171 14.110527
Si 0.835714 1.705082 8.539599
Si 1.466075 8.518111 14.830400
Si 3.888379 9.619175 11.809601

Si 0.805332 7.973685 7.592400
Si 1.759330 7.829018 10.581200
Si 1.840227 2.479251 11.191999
Si 0.911156 2.943912 14.214400
Si 2.459718 11.386902 13.536400
Si 2.016362 5.002964 9.659200
Si 1.452010 3.940390 5.250000
Si 2.550819 10.164133 3.446400
Si 0.383942 12.374090 4.288400
Si 3.235090 2.327151 6.777600
Si 1.197727 12.042020 7.403600
Si 3.876153 12.711868 7.652400
Si 2.418584 7.757083 5.170000
Si 4.199781 0.495187 10.704401
Si 7.831317 1.404997 2.890000
Si 10.379497 1.248518 12.132000
Si 7.089207 0.285220 15.146000
Si 11.886435 2.203720 4.395200
Si 6.783931 1.687563 9.423600
Al 7.360579 6.307755 14.521533
O 6.759162 11.154772 2.246000
O 10.662036 10.322471 8.084400
O 4.814638 2.991501 13.402511
O 9.344977 0.033977 11.782000
O 6.799699 2.314676 3.812400
O 5.597132 5.221026 7.776000
O 8.711951 6.334918 13.409121
O 5.090491 10.195853 10.945200
O 4.689340 2.785043 7.269200
O 4.895081 7.608168 8.053600
O 8.191955 13.104727 3.340000
O 8.886584 12.063254 9.446400
O 11.280232 6.042266 13.281347
O 5.428379 4.622051 4.457600
O 7.526674 3.048424 13.192476
O 12.478667 10.454661 12.866401
O 8.152338 4.531535 3.923600
O 7.701066 11.511662 6.972000
O 7.028008 3.563591 6.182400
O 12.430955 6.724504 7.685600
O 6.210792 7.564768 11.869201
O 10.929564 8.436225 12.675923
O 12.123152 12.162531 14.865600

O	8.150500	12.504423	14.143200	O	9.488457	4.803022	17.766132
O	7.080863	12.953290	16.639599	O	9.235291	3.981335	15.193611
O	10.048716	8.165867	6.658000	O	9.373579	10.650427	3.060400
O	10.279480	6.295816	11.024064	O	8.875794	12.074802	0.912400
O	11.700548	3.457016	3.255200	O	7.347367	8.026111	1.292000
O	8.077121	9.829805	13.651600	O	12.749405	9.401511	15.374399
O	5.990423	11.345361	4.736000	O	5.837551	7.494902	14.895158
O	5.921060	9.520032	6.624000	O	3.312936	0.709533	6.626000
O	4.723644	6.119025	10.254001	O	2.978678	1.350449	11.330400
O	5.736908	6.666637	2.982400	O	1.068614	0.149711	8.228399
O	11.297309	12.089932	10.074000	O	0.204751	1.514095	14.714001
O	8.857220	8.255006	11.969208	O	0.721963	1.945575	10.135201
O	6.404660	11.582667	9.290401	O	1.122239	2.843706	12.597199
O	5.882887	7.027509	5.610400	O	0.463370	11.055894	8.455600
O	6.387131	9.033073	3.624000	O	2.104801	9.990797	14.309601
O	7.798911	6.595498	10.155200	O	2.886552	9.287635	4.802400
O	6.732806	3.159585	8.763600	O	2.586701	3.790945	10.562000
O	10.657479	5.656886	3.996000	O	0.464383	12.203410	5.936400
O	12.586321	9.084703	6.780000	O	1.159651	4.920012	6.494400
O	9.089299	4.226274	9.981200	O	3.494215	6.622971	4.619600
O	9.669577	2.455892	8.148001	O	0.788414	8.241385	11.837601
O	6.092182	4.842991	11.971146	O	1.783353	11.622352	3.714400
O	11.554258	8.938177	3.251200	O	3.994570	13.081898	9.267200
O	10.626290	10.290086	5.385600	O	1.786450	6.227858	10.691200
O	5.227203	12.081703	7.077200	O	3.047836	5.504786	8.475200
O	9.695821	6.302978	8.446400	O	2.093647	2.575607	7.928400
O	11.853836	11.571386	3.535200	O	0.145068	4.350900	14.561200
O	10.604074	2.179299	10.792399	O	2.930433	3.255809	5.437200
O	11.853820	9.559185	10.317201	O	2.750156	11.560105	7.304000
O	8.898306	5.963077	5.940400	O	0.516184	2.624980	5.283200
O	11.027869	5.871749	15.881915	O	4.200576	6.451334	13.005294
O	5.862259	11.234272	13.865200	O	0.916564	7.557336	4.547600
O	7.391491	9.295200	10.160399	O	3.206430	8.467013	10.895200
O	7.332047	11.494408	11.745600	O	2.383492	3.021952	14.969601
O	12.504366	6.544400	2.473200	O	1.437888	12.619760	13.326401
O	7.572567	7.657541	7.511200	O	0.612614	7.058433	14.690400
O	6.341939	4.908763	14.590494	O	2.190965	7.677449	6.776400
O	11.283936	4.368817	7.116000	O	0.550035	4.612362	9.024000
O	8.365394	7.133554	3.569600	O	2.992561	7.797371	15.077051
O	9.816282	10.696614	11.728000	O	1.279718	8.335619	9.109200
O	10.374769	10.180988	14.355600	O	2.861917	10.867428	12.039599
O	8.266185	6.372925	16.052811	O	3.622376	12.232078	14.337999
O	9.380091	1.932834	2.936000	O	0.991568	4.858828	3.969200

O	4.117428	10.476163	2.896400	O	11.856470	-1.109691	14.865600
O	1.492396	9.134474	2.577600	O	13.840406	-0.652462	13.326401
O	4.391256	9.048319	13.239516	O	12.873951	1.514095	14.714001
O	10.672203	2.253358	5.550000	O	13.828851	4.920012	6.494400
O	12.131184	2.007291	7.788400	O	13.219235	4.612362	9.024000
O	5.595158	0.513635	14.460401	O	12.814268	4.350900	14.561200
O	4.901489	12.889318	12.021600	O	13.281814	7.058433	14.690400
O	8.150242	1.779009	10.280000	O	-0.164834	6.544400	2.473200
O	5.493874	1.418800	10.349999	O	-1.114942	8.938177	3.251200
O	6.987936	0.560486	8.251600	O	13.457614	8.241385	11.837601
O	9.912067	2.121830	13.419600	O	-0.538016	2.007291	7.788400
O	11.742654	0.508326	12.582001	O	0.080205	9.401511	15.374399
O	12.363857	0.680201	3.919200	O	-0.238245	6.724504	7.685600
O	8.024569	1.615362	15.300400	O	-0.082879	9.084703	6.780000
O	7.290307	1.459944	1.323600	O	-0.815364	11.571386	3.535200
O	6.543602	7.256905	18.453571	O	-0.038661	13.952423	3.919200
H	7.780772	13.063582	17.302401	O	1.335296	13.421932	8.228399
H	9.535483	2.888301	2.830400	O	3.579617	13.981754	6.626000
H	10.313303	4.419003	18.099957	O	3.727889	-0.190324	9.267200
H	8.480283	12.870338	0.506400	O	4.634808	-0.382904	12.021600
H	7.238176	8.941231	0.982400	O	7.925273	-0.167495	3.340000
H	4.056318	3.267664	13.956971	O	7.883819	-0.767798	14.143200
H	2.704204	2.173459	15.322400	O	6.814182	-0.318932	16.639599
H	6.381372	1.760295	1.167600	O	13.185384	2.624980	5.283200
H	8.620474	8.642807	18.869341	H	7.514091	-0.208639	17.302401
H	7.570839	9.815003	20.803288				
H	8.163858	8.591654	21.920137	Butene* (VI)			
H	9.832603	8.839075	20.148203	Si	6.148623	3.914789	13.328291
H	9.047155	7.261653	19.877754	Si	7.621518	12.256366	8.442000
H	5.752726	8.319911	21.508953	Si	11.955669	10.554867	14.462399
H	6.649001	6.884667	20.984163	Si	10.036707	6.828591	12.542752
H	5.736989	9.085585	19.053215	Si	5.030561	12.629448	13.642000
H	4.782146	7.630810	19.451929	Si	12.121967	5.142588	3.396400
Ni	6.368886	7.444735	16.728580	Si	5.089982	6.236086	4.428400
C	7.788522	8.736701	20.893736	Si	4.560124	6.121016	8.649600
C	8.881871	8.348369	19.894970	Si	9.211920	5.814295	9.909600
C	6.478466	7.951286	20.765049	Si	11.746457	10.779698	9.227201
C	5.813045	8.031593	19.390160	Si	9.812782	12.048257	10.795200
O	7.254618	13.832707	8.251600	Si	12.541766	0.089189	13.925600
O	5.861839	13.785856	14.460401	Si	9.491869	5.278672	16.180584
O	13.660769	4.858828	3.969200	Si	6.005562	3.693925	7.441600
O	13.132569	11.055894	8.455600	Si	10.892969	2.767524	7.109600
O	9.611659	13.306198	11.782000	Si	7.535115	7.937319	11.023600

Si	10.984008	9.467341	6.729600	Al	7.354225	6.325150	14.474392
Si	5.731494	10.501911	3.363200	O	6.759162	11.154772	2.246000
Si	5.269097	6.215779	11.762400	O	10.662036	10.322471	8.084400
Si	12.646716	5.129448	7.583200	O	4.813373	2.994855	13.403564
Si	7.398423	11.266921	13.382401	O	9.344977	0.033977	11.782000
Si	8.689230	2.733149	14.299601	O	6.799699	2.314676	3.812400
Si	6.842045	3.766391	4.573600	O	5.597132	5.221026	7.776000
Si	8.310841	11.745253	2.410400	O	8.722613	6.326149	13.391546
Si	12.119840	5.856368	14.646000	O	5.090491	10.195853	10.945200
Si	9.575190	9.643729	12.966000	O	4.689340	2.785043	7.269200
Si	6.228600	11.080315	6.326000	O	4.895081	7.608168	8.053600
Si	9.418234	2.664664	9.769600	O	8.191955	13.104727	3.340000
Si	6.565253	10.646844	10.577200	O	8.886584	12.063254	9.446400
Si	6.069852	7.946477	6.949200	O	11.287843	6.040668	13.275575
Si	0.274987	8.055044	3.125600	O	5.428379	4.622051	4.457600
Si	12.176368	9.218222	11.863199	O	7.526192	3.042510	13.189600
Si	10.824993	10.336671	3.770400	O	12.478667	10.454661	12.866401
Si	9.054027	5.850395	4.332000	O	8.152338	4.531535	3.923600
Si	9.031193	7.028039	7.155600	O	7.701066	11.511662	6.972000
Si	6.994024	7.723504	2.854400	O	7.028008	3.563591	6.182400
Si	4.358527	7.680243	14.119768	O	12.430955	6.724504	7.685600
Si	0.835714	1.705082	8.539599	O	6.210792	7.564768	11.869201
Si	1.466075	8.518111	14.830400	O	10.930665	8.434915	12.675650
Si	3.888379	9.619175	11.809601	O	12.123152	12.162531	14.865600
Si	0.805332	7.973685	7.592400	O	8.150500	12.504423	14.143200
Si	1.759330	7.829018	10.581200	O	7.080863	12.953290	16.639599
Si	1.840227	2.479251	11.191999	O	10.048716	8.165867	6.658000
Si	0.911156	2.943912	14.214400	O	10.287542	6.299657	11.014839
Si	2.459718	11.386902	13.536400	O	11.700548	3.457016	3.255200
Si	2.016362	5.002964	9.659200	O	8.077121	9.829805	13.651600
Si	1.452010	3.940390	5.250000	O	5.990423	11.345361	4.736000
Si	2.550819	10.164133	3.446400	O	5.921060	9.520032	6.624000
Si	0.383942	12.374090	4.288400	O	4.723644	6.119025	10.254001
Si	3.235090	2.327151	6.777600	O	5.736908	6.666637	2.982400
Si	1.197727	12.042020	7.403600	O	11.297309	12.089932	10.074000
Si	3.876153	12.711868	7.652400	O	8.858263	8.255623	11.967906
Si	2.418584	7.757083	5.170000	O	6.404660	11.582667	9.290401
Si	4.199781	0.495187	10.704401	O	5.882887	7.027509	5.610400
Si	7.831317	1.404997	2.890000	O	6.387131	9.033073	3.624000
Si	10.379497	1.248518	12.132000	O	7.798911	6.595498	10.155200
Si	7.089207	0.285220	15.146000	O	6.732806	3.159585	8.763600
Si	11.886435	2.203720	4.395200	O	10.657479	5.656886	3.996000
Si	6.783931	1.687563	9.423600	O	12.586321	9.084703	6.780000

O	9.089299	4.226274	9.981200	O	3.494215	6.622971	4.619600
O	9.669577	2.455892	8.148001	O	0.788414	8.241385	11.837601
O	6.094365	4.842470	11.966065	O	1.783353	11.622352	3.714400
O	11.554258	8.938177	3.251200	O	3.994570	13.081898	9.267200
O	10.626290	10.290086	5.385600	O	1.786450	6.227858	10.691200
O	5.227203	12.081703	7.077200	O	3.047836	5.504786	8.475200
O	9.695821	6.302978	8.446400	O	2.093647	2.575607	7.928400
O	11.853836	11.571386	3.535200	O	0.145068	4.350900	14.561200
O	10.604074	2.179299	10.792399	O	2.930433	3.255809	5.437200
O	11.853820	9.559185	10.317201	O	2.750156	11.560105	7.304000
O	8.898306	5.963077	5.940400	O	0.516184	2.624980	5.283200
O	11.014905	5.880821	15.872839	O	4.206684	6.451324	13.009749
O	5.862259	11.234272	13.865200	O	0.916564	7.557336	4.547600
O	7.391491	9.295200	10.160399	O	3.206430	8.467013	10.895200
O	7.332047	11.494408	11.745600	O	2.383492	3.021952	14.969601
O	12.504366	6.544400	2.473200	O	1.437888	12.619760	13.326401
O	7.572567	7.657541	7.511200	O	0.612614	7.058433	14.690400
O	6.353006	4.913602	14.577355	O	2.190965	7.677449	6.776400
O	11.283936	4.368817	7.116000	O	0.550035	4.612362	9.024000
O	8.365394	7.133554	3.569600	O	2.991374	7.796428	15.076927
O	9.816282	10.696614	11.728000	O	1.279718	8.335619	9.109200
O	10.374769	10.180988	14.355600	O	2.861917	10.867428	12.039599
O	8.248583	6.380849	16.022284	O	3.622376	12.232078	14.337999
O	9.380091	1.932834	2.936000	O	0.991568	4.858828	3.969200
O	9.465385	4.814404	17.749046	O	4.117428	10.476163	2.896400
O	9.232171	3.986022	15.184689	O	1.492396	9.134474	2.577600
O	9.373579	10.650427	3.060400	O	4.395587	9.044548	13.239388
O	8.875794	12.074802	0.912400	O	10.672203	2.253358	5.550000
O	7.347367	8.026111	1.292000	O	12.131184	2.007291	7.788400
O	12.749405	9.401511	15.374399	O	5.595158	0.513635	14.460401
O	5.837049	7.482698	14.919062	O	4.901489	12.889318	12.021600
O	3.312936	0.709533	6.626000	O	8.150242	1.779009	10.280000
O	2.978678	1.350449	11.330400	O	5.493874	1.418800	10.349999
O	1.068614	0.149711	8.228399	O	6.987936	0.560486	8.251600
O	0.204751	1.514095	14.714001	O	9.912067	2.121830	13.419600
O	0.721963	1.945575	10.135201	O	11.742654	0.508326	12.582001
O	1.122239	2.843706	12.597199	O	12.363857	0.680201	3.919200
O	0.463370	11.055894	8.455600	O	8.024569	1.615362	15.300400
O	2.104801	9.990797	14.309601	O	7.290307	1.459944	1.323600
O	2.886552	9.287635	4.802400	O	6.395298	6.486991	18.391743
O	2.586701	3.790945	10.562000	H	7.780772	13.063582	17.302401
O	0.464383	12.203410	5.936400	H	9.535483	2.888301	2.830400
O	1.159651	4.920012	6.494400	H	10.307154	4.509037	18.119143

H	8.480283	12.870338	0.506400
H	7.238176	8.941231	0.982400
H	4.057307	3.272291	13.960896
H	2.704204	2.173459	15.322400
H	6.381372	1.760295	1.167600
H	8.488313	6.571616	19.526995
H	7.974044	6.906126	22.544470
H	7.121862	5.784841	21.472921
H	9.269900	7.811843	20.542698
H	9.569651	6.087925	20.851097
H	6.998709	8.858955	21.141399
H	5.834635	6.957259	19.052235
H	4.816923	6.677373	21.222754
H	4.597088	8.507809	20.949276
Ni	6.352596	7.120565	16.760008
C	7.607316	6.772637	21.510324
C	8.802830	6.815256	20.549555
C	6.595168	7.843447	21.241173
C	5.271203	7.666684	21.118542
O	7.254618	13.832707	8.251600
O	5.861839	13.785856	14.460401
O	13.660769	4.858828	3.969200
O	13.132569	11.055894	8.455600
O	9.611659	13.306198	11.782000
O	11.856470	-1.109691	14.865600
O	13.840406	-0.652462	13.326401
O	12.873951	1.514095	14.714001
O	13.828851	4.920012	6.494400
O	13.219235	4.612362	9.024000
O	12.814268	4.350900	14.561200
O	13.281814	7.058433	14.690400
O	-0.164834	6.544400	2.473200
O	-1.114942	8.938177	3.251200
O	13.457614	8.241385	11.837601
O	-0.538016	2.007291	7.788400
O	0.080205	9.401511	15.374399
O	-0.238245	6.724504	7.685600
O	-0.082879	9.084703	6.780000
O	-0.815364	11.571386	3.535200
O	-0.038661	13.952423	3.919200
O	1.335296	13.421932	8.228399
O	3.579617	13.981754	6.626000
O	3.727889	-0.190324	9.267200

O	4.634808	-0.382904	12.021600
O	7.925273	-0.167495	3.340000
O	7.883819	-0.767798	14.143200
O	6.814182	-0.318932	16.639599
O	13.185384	2.624980	5.283200
H	7.514091	-0.208639	17.302401

C₄H₈(g)

H	7.828943	8.247104	22.074278
H	7.487035	8.785353	20.427361
H	9.380940	6.464003	21.207315
H	9.899497	8.085801	20.703720
H	9.083457	7.010026	19.544333
H	5.182578	8.064711	19.936096
H	6.852071	5.911448	21.383251
H	4.672035	6.328653	20.371006
C	5.440288	7.102959	20.387108
C	6.637294	6.893007	20.942486
C	7.746375	7.899508	21.028738
C	9.104423	7.334977	20.579302

Ni-H Bare

Si	6.140586	3.894142	13.326653
Si	7.621518	12.256366	8.442000
Si	11.955669	10.554867	14.462399
Si	10.012696	6.822002	12.546109
Si	5.030561	12.629448	13.642000
Si	12.121967	5.142588	3.396400
Si	5.089982	6.236086	4.428400
Si	4.560124	6.121016	8.649600
Si	9.211920	5.814295	9.909600
Si	11.746457	10.779698	9.227201
Si	9.812782	12.048257	10.795200
Si	12.541766	0.089189	13.925600
Si	9.492292	5.303754	16.163609
Si	6.005562	3.693925	7.441600
Si	10.892969	2.767524	7.109600
Si	7.535115	7.937319	11.023600
Si	10.984008	9.467341	6.729600
Si	5.731494	10.501911	3.363200
Si	5.269097	6.215779	11.762400
Si	12.646716	5.129448	7.583200
Si	7.398423	11.266921	13.382401

Si	8.689230	2.733149	14.299601	O	6.799699	2.314676	3.812400
Si	6.842045	3.766391	4.573600	O	5.597132	5.221026	7.776000
Si	8.310841	11.745253	2.410400	O	8.689110	6.296940	13.374367
Si	12.119840	5.856368	14.646000	O	5.090491	10.195853	10.945200
Si	9.575190	9.643729	12.966000	O	4.689340	2.785043	7.269200
Si	6.228600	11.080315	6.326000	O	4.895081	7.608168	8.053600
Si	9.418234	2.664664	9.769600	O	8.191955	13.104727	3.340000
Si	6.565253	10.646844	10.577200	O	8.886584	12.063254	9.446400
Si	6.069852	7.946477	6.949200	O	11.262012	6.041566	13.292576
Si	0.274987	8.055044	3.125600	O	5.428379	4.622051	4.457600
Si	12.176368	9.218222	11.863199	O	7.526346	3.032399	13.185745
Si	10.824993	10.336671	3.770400	O	12.478667	10.454661	12.866401
Si	9.054027	5.850395	4.332000	O	8.152338	4.531535	3.923600
Si	9.031193	7.028039	7.155600	O	7.701066	11.511662	6.972000
Si	6.994024	7.723504	2.854400	O	7.028008	3.563591	6.182400
Si	4.373089	7.685688	14.124116	O	12.430955	6.724504	7.685600
Si	0.835714	1.705082	8.539599	O	6.210792	7.564768	11.869201
Si	1.466075	8.518111	14.830400	O	10.926948	8.435143	12.674623
Si	3.888379	9.619175	11.809601	O	12.123152	12.162531	14.865600
Si	0.805332	7.973685	7.592400	O	8.150500	12.504423	14.143200
Si	1.759330	7.829018	10.581200	O	7.080863	12.953290	16.639599
Si	1.840227	2.479251	11.191999	O	10.048716	8.165867	6.658000
Si	0.911156	2.943912	14.214400	O	10.283979	6.298435	11.019234
Si	2.459718	11.386902	13.536400	O	11.700548	3.457016	3.255200
Si	2.016362	5.002964	9.659200	O	8.077121	9.829805	13.651600
Si	1.452010	3.940390	5.250000	O	5.990423	11.345361	4.736000
Si	2.550819	10.164133	3.446400	O	5.921060	9.520032	6.624000
Si	0.383942	12.374090	4.288400	O	4.723644	6.119025	10.254001
Si	3.235090	2.327151	6.777600	O	5.736908	6.666637	2.982400
Si	1.197727	12.042020	7.403600	O	11.297309	12.089932	10.074000
Si	3.876153	12.711868	7.652400	O	8.853497	8.250352	11.977945
Si	2.418584	7.757083	5.170000	O	6.404660	11.582667	9.290401
Si	4.199781	0.495187	10.704401	O	5.882887	7.027509	5.610400
Si	7.831317	1.404997	2.890000	O	6.387131	9.033073	3.624000
Si	10.379497	1.248518	12.132000	O	7.798911	6.595498	10.155200
Si	7.089207	0.285220	15.146000	O	6.732806	3.159585	8.763600
Si	11.886435	2.203720	4.395200	O	10.657479	5.656886	3.996000
Si	6.783931	1.687563	9.423600	O	12.586321	9.084703	6.780000
Al	7.298660	6.287870	14.448700	O	9.089299	4.226274	9.981200
O	6.759162	11.154772	2.246000	O	9.669577	2.455892	8.148001
O	10.662036	10.322471	8.084400	O	6.102824	4.848650	11.980717
O	4.801217	2.978179	13.368986	O	11.554258	8.938177	3.251200
O	9.344977	0.033977	11.782000	O	10.626290	10.290086	5.385600

O	5.227203	12.081703	7.077200	O	3.047836	5.504786	8.475200
O	9.695821	6.302978	8.446400	O	2.093647	2.575607	7.928400
O	11.853836	11.571386	3.535200	O	0.145068	4.350900	14.561200
O	10.604074	2.179299	10.792399	O	2.930433	3.255809	5.437200
O	11.853820	9.559185	10.317201	O	2.750156	11.560105	7.304000
O	8.898306	5.963077	5.940400	O	0.516184	2.624980	5.283200
O	11.022256	5.878982	15.883038	O	4.214089	6.452224	13.014288
O	5.862259	11.234272	13.865200	O	0.916564	7.557336	4.547600
O	7.391491	9.295200	10.160399	O	3.206430	8.467013	10.895200
O	7.332047	11.494408	11.745600	O	2.383492	3.021952	14.969601
O	12.504366	6.544400	2.473200	O	1.437888	12.619760	13.326401
O	7.572567	7.657541	7.511200	O	0.612614	7.058433	14.690400
O	6.334984	4.862801	14.602379	O	2.190965	7.677449	6.776400
O	11.283936	4.368817	7.116000	O	0.550035	4.612362	9.024000
O	8.365394	7.133554	3.569600	O	2.993636	7.797057	15.066157
O	9.816282	10.696614	11.728000	O	1.279718	8.335619	9.109200
O	10.374769	10.180988	14.355600	O	2.861917	10.867428	12.039599
O	8.268087	6.442274	15.973049	O	3.622376	12.232078	14.337999
O	9.380091	1.932834	2.936000	O	0.991568	4.858828	3.969200
O	9.394938	4.896988	17.744123	O	4.117428	10.476163	2.896400
O	9.214659	4.000784	15.189038	O	1.492396	9.134474	2.577600
O	9.373579	10.650427	3.060400	O	4.393628	9.049450	13.238383
O	8.875794	12.074802	0.912400	O	10.672203	2.253358	5.550000
O	7.347367	8.026111	1.292000	O	12.131184	2.007291	7.788400
O	12.749405	9.401511	15.374399	O	5.595158	0.513635	14.460401
O	5.882169	7.501484	14.866074	O	4.901489	12.889318	12.021600
O	3.312936	0.709533	6.626000	O	8.150242	1.779009	10.280000
O	2.978678	1.350449	11.330400	O	5.493874	1.418800	10.349999
O	1.068614	0.149711	8.228399	O	6.987936	0.560486	8.251600
O	0.204751	1.514095	14.714001	O	9.912067	2.121830	13.419600
O	0.721963	1.945575	10.135201	O	11.742654	0.508326	12.582001
O	1.122239	2.843706	12.597199	O	12.363857	0.680201	3.919200
O	0.463370	11.055894	8.455600	O	8.024569	1.615362	15.300400
O	2.104801	9.990797	14.309601	O	7.290307	1.459944	1.323600
O	2.886552	9.287635	4.802400	H	7.780772	13.063582	17.302401
O	2.586701	3.790945	10.562000	H	9.535483	2.888301	2.830400
O	0.464383	12.203410	5.936400	H	10.199619	4.546521	18.155331
O	1.159651	4.920012	6.494400	H	8.480283	12.870338	0.506400
O	3.494215	6.622971	4.619600	H	7.238176	8.941231	0.982400
O	0.788414	8.241385	11.837601	H	4.053142	3.246238	13.942390
O	1.783353	11.622352	3.714400	H	2.704204	2.173459	15.322400
O	3.994570	13.081898	9.267200	H	6.381372	1.760295	1.167600
O	1.786450	6.227858	10.691200	H	6.091930	7.641634	17.904240

Ni	6.873578	7.736488	16.626135	Si	9.812782	12.048257	10.795200
O	7.254618	13.832707	8.251600	Si	12.541766	0.089189	13.925600
O	5.861839	13.785856	14.460401	Si	9.479825	5.301479	16.167776
O	13.660769	4.858828	3.969200	Si	6.005562	3.693925	7.441600
O	13.132569	11.055894	8.455600	Si	10.892969	2.767524	7.109600
O	9.611659	13.306198	11.782000	Si	7.535115	7.937319	11.023600
O	11.856470	-1.109691	14.865600	Si	10.984008	9.467341	6.729600
O	13.840406	-0.652462	13.326401	Si	5.731494	10.501911	3.363200
O	12.873951	1.514095	14.714001	Si	5.269097	6.215779	11.762400
O	13.828851	4.920012	6.494400	Si	12.646716	5.129448	7.583200
O	13.219235	4.612362	9.024000	Si	7.398423	11.266921	13.382401
O	12.814268	4.350900	14.561200	Si	8.689230	2.733149	14.299601
O	13.281814	7.058433	14.690400	Si	6.842045	3.766391	4.573600
O	-0.164834	6.544400	2.473200	Si	8.310841	11.745253	2.410400
O	-1.114942	8.938177	3.251200	Si	12.119840	5.856368	14.646000
O	13.457614	8.241385	11.837601	Si	9.575190	9.643729	12.966000
O	-0.538016	2.007291	7.788400	Si	6.228600	11.080315	6.326000
O	0.080205	9.401511	15.374399	Si	9.418234	2.664664	9.769600
O	-0.238245	6.724504	7.685600	Si	6.565253	10.646844	10.577200
O	-0.082879	9.084703	6.780000	Si	6.069852	7.946477	6.949200
O	-0.815364	11.571386	3.535200	Si	0.274987	8.055044	3.125600
O	-0.038661	13.952423	3.919200	Si	12.176368	9.218222	11.863199
O	1.335296	13.421932	8.228399	Si	10.824993	10.336671	3.770400
O	3.579617	13.981754	6.626000	Si	9.054027	5.850395	4.332000
O	3.727889	-0.190324	9.267200	Si	9.031193	7.028039	7.155600
O	4.634808	-0.382904	12.021600	Si	6.994024	7.723504	2.854400
O	7.925273	-0.167495	3.340000	Si	4.370661	7.678967	14.121452
O	7.883819	-0.767798	14.143200	Si	0.835714	1.705082	8.539599
O	6.814182	-0.318932	16.639599	Si	1.466075	8.518111	14.830400
O	13.185384	2.624980	5.283200	Si	3.888379	9.619175	11.809601
H	7.514091	-0.208639	17.302401	Si	0.805332	7.973685	7.592400
Ni-H Ethene*				Si	1.759330	7.829018	10.581200
Si	6.151890	3.908429	13.326317	Si	1.840227	2.479251	11.191999
Si	7.621518	12.256366	8.442000	Si	0.911156	2.943912	14.214400
Si	11.955669	10.554867	14.462399	Si	2.459718	11.386902	13.536400
Si	10.024274	6.824786	12.546663	Si	2.016362	5.002964	9.659200
Si	5.030561	12.629448	13.642000	Si	1.452010	3.940390	5.250000
Si	12.121967	5.142588	3.396400	Si	2.550819	10.164133	3.446400
Si	5.089982	6.236086	4.428400	Si	0.383942	12.374090	4.288400
Si	4.560124	6.121016	8.649600	Si	3.235090	2.327151	6.777600
Si	9.211920	5.814295	9.909600	Si	1.197727	12.042020	7.403600
Si	11.746457	10.779698	9.227201	Si	3.876153	12.711868	7.652400
				Si	2.418584	7.757083	5.170000

Si	4.199781	0.495187	10.704401	O	5.882887	7.027509	5.610400
Si	7.831317	1.404997	2.890000	O	6.387131	9.033073	3.624000
Si	10.379497	1.248518	12.132000	O	7.798911	6.595498	10.155200
Si	7.089207	0.285220	15.146000	O	6.732806	3.159585	8.763600
Si	11.886435	2.203720	4.395200	O	10.657479	5.656886	3.996000
Si	6.783931	1.687563	9.423600	O	12.586321	9.084703	6.780000
Al	7.328703	6.322418	14.475322	O	9.089299	4.226274	9.981200
O	6.759162	11.154772	2.246000	O	9.669577	2.455892	8.148001
O	10.662036	10.322471	8.084400	O	6.097899	4.844368	11.969481
O	4.815176	2.986660	13.390370	O	11.554258	8.938177	3.251200
O	9.344977	0.033977	11.782000	O	10.626290	10.290086	5.385600
O	6.799699	2.314676	3.812400	O	5.227203	12.081703	7.077200
O	5.597132	5.221026	7.776000	O	9.695821	6.302978	8.446400
O	8.709200	6.317090	13.390368	O	11.853836	11.571386	3.535200
O	5.090491	10.195853	10.945200	O	10.604074	2.179299	10.792399
O	4.689340	2.785043	7.269200	O	11.853820	9.559185	10.317201
O	4.895081	7.608168	8.053600	O	8.898306	5.963077	5.940400
O	8.191955	13.104727	3.340000	O	11.015806	5.877227	15.876140
O	8.886584	12.063254	9.446400	O	5.862259	11.234272	13.865200
O	11.279428	6.041273	13.281427	O	7.391491	9.295200	10.160399
O	5.428379	4.622051	4.457600	O	7.332047	11.494408	11.745600
O	7.529670	3.033971	13.183881	O	12.504366	6.544400	2.473200
O	12.478667	10.454661	12.866401	O	7.572567	7.657541	7.511200
O	8.152338	4.531535	3.923600	O	6.358700	4.887618	14.587683
O	7.701066	11.511662	6.972000	O	11.283936	4.368817	7.116000
O	7.028008	3.563591	6.182400	O	8.365394	7.133554	3.569600
O	12.430955	6.724504	7.685600	O	9.816282	10.696614	11.728000
O	6.210792	7.564768	11.869201	O	10.374769	10.180988	14.355600
O	10.929668	8.435651	12.675858	O	8.248750	6.405876	16.010441
O	12.123152	12.162531	14.865600	O	9.380091	1.932834	2.936000
O	8.150500	12.504423	14.143200	O	9.427253	4.876154	17.754803
O	7.080863	12.953290	16.639599	O	9.228226	3.984809	15.197529
O	10.048716	8.165867	6.658000	O	9.373579	10.650427	3.060400
O	10.284979	6.297839	11.018248	O	8.875794	12.074802	0.912400
O	11.700548	3.457016	3.255200	O	7.347367	8.026111	1.292000
O	8.077121	9.829805	13.651600	O	12.749405	9.401511	15.374399
O	5.990423	11.345361	4.736000	O	5.861920	7.481382	14.874041
O	5.921060	9.520032	6.624000	O	3.312936	0.709533	6.626000
O	4.723644	6.119025	10.254001	O	2.978678	1.350449	11.330400
O	5.736908	6.666637	2.982400	O	1.068614	0.149711	8.228399
O	11.297309	12.089932	10.074000	O	0.204751	1.514095	14.714001
O	8.857458	8.254171	11.969875	O	0.721963	1.945575	10.135201
O	6.404660	11.582667	9.290401	O	1.122239	2.843706	12.597199

O	0.463370	11.055894	8.455600	O	8.024569	1.615362	15.300400
O	2.104801	9.990797	14.309601	O	7.290307	1.459944	1.323600
O	2.886552	9.287635	4.802400	H	7.780772	13.063582	17.302401
O	2.586701	3.790945	10.562000	H	9.535483	2.888301	2.830400
O	0.464383	12.203410	5.936400	H	10.229674	4.460598	18.105833
O	1.159651	4.920012	6.494400	H	8.480283	12.870338	0.506400
O	3.494215	6.622971	4.619600	H	7.238176	8.941231	0.982400
O	0.788414	8.241385	11.837601	H	4.060779	3.268534	13.947086
O	1.783353	11.622352	3.714400	H	2.704204	2.173459	15.322400
O	3.994570	13.081898	9.267200	H	6.381372	1.760295	1.167600
O	1.786450	6.227858	10.691200	H	7.073126	7.312569	18.192406
O	3.047836	5.504786	8.475200	H	4.183622	7.564073	17.537891
O	2.093647	2.575607	7.928400	H	5.783948	7.079359	19.364889
O	0.145068	4.350900	14.561200	H	4.940376	9.227438	17.329695
O	2.930433	3.255809	5.437200	H	6.549713	8.712540	19.141029
O	2.750156	11.560105	7.304000	Ni	6.525678	7.389384	16.701611
O	0.516184	2.624980	5.283200	C	5.086597	8.178890	17.609131
O	4.205078	6.451845	13.006577	C	6.079247	7.854176	18.630922
O	0.916564	7.557336	4.547600	O	7.254618	13.832707	8.251600
O	3.206430	8.467013	10.895200	O	5.861839	13.785856	14.460401
O	2.383492	3.021952	14.969601	O	13.660769	4.858828	3.969200
O	1.437888	12.619760	13.326401	O	13.132569	11.055894	8.455600
O	0.612614	7.058433	14.690400	O	9.611659	13.306198	11.782000
O	2.190965	7.677449	6.776400	O	11.856470	-1.109691	14.865600
O	0.550035	4.612362	9.024000	O	13.840406	-0.652462	13.326401
O	2.990869	7.795805	15.071641	O	12.873951	1.514095	14.714001
O	1.279718	8.335619	9.109200	O	13.828851	4.920012	6.494400
O	2.861917	10.867428	12.039599	O	13.219235	4.612362	9.024000
O	3.622376	12.232078	14.337999	O	12.814268	4.350900	14.561200
O	0.991568	4.858828	3.969200	O	13.281814	7.058433	14.690400
O	4.117428	10.476163	2.896400	O	-0.164834	6.544400	2.473200
O	1.492396	9.134474	2.577600	O	-1.114942	8.938177	3.251200
O	4.389367	9.045936	13.239671	O	13.457614	8.241385	11.837601
O	10.672203	2.253358	5.550000	O	-0.538016	2.007291	7.788400
O	12.131184	2.007291	7.788400	O	0.080205	9.401511	15.374399
O	5.595158	0.513635	14.460401	O	-0.238245	6.724504	7.685600
O	4.901489	12.889318	12.021600	O	-0.082879	9.084703	6.780000
O	8.150242	1.779009	10.280000	O	-0.815364	11.571386	3.535200
O	5.493874	1.418800	10.349999	O	-0.038661	13.952423	3.919200
O	6.987936	0.560486	8.251600	O	1.335296	13.421932	8.228399
O	9.912067	2.121830	13.419600	O	3.579617	13.981754	6.626000
O	11.742654	0.508326	12.582001	O	3.727889	-0.190324	9.267200
O	12.363857	0.680201	3.919200	O	4.634808	-0.382904	12.021600

O	7.925273	-0.167495	3.340000
O	7.883819	-0.767798	14.143200
O	6.814182	-0.318932	16.639599
O	13.185384	2.624980	5.283200
H	7.514091	-0.208639	17.302401

Ni⁺ Bare

Si	6.150652	3.915017	13.332502
Si	7.621518	12.256366	8.442000
Si	11.955669	10.554867	14.462399
Si	10.015757	6.831888	12.556663
Si	5.030561	12.629448	13.642000
Si	12.121967	5.142588	3.396400
Si	5.089982	6.236086	4.428400
Si	4.560124	6.121016	8.649600
Si	9.211920	5.814295	9.909600
Si	11.746457	10.779698	9.227201
Si	9.812782	12.048257	10.795200
Si	12.541766	0.089189	13.925600
Si	9.530469	5.255010	16.201664
Si	6.005562	3.693925	7.441600
Si	10.892969	2.767524	7.109600
Si	7.535115	7.937319	11.023600
Si	10.984008	9.467341	6.729600
Si	5.731494	10.501911	3.363200
Si	5.269097	6.215779	11.762400
Si	12.646716	5.129448	7.583200
Si	7.398423	11.266921	13.382401
Si	8.689230	2.733149	14.299601
Si	6.842045	3.766391	4.573600
Si	8.310841	11.745253	2.410400
Si	12.119840	5.856368	14.646000
Si	9.575190	9.643729	12.966000
Si	6.228600	11.080315	6.326000
Si	9.418234	2.664664	9.769600
Si	6.565253	10.646844	10.577200
Si	6.069852	7.946477	6.949200
Si	0.274987	8.055044	3.125600
Si	12.176368	9.218222	11.863199
Si	10.824993	10.336671	3.770400
Si	9.054027	5.850395	4.332000
Si	9.031193	7.028039	7.155600
Si	6.994024	7.723504	2.854400

Si	4.361188	7.685013	14.123794
Si	0.835714	1.705082	8.539599
Si	1.466075	8.518111	14.830400
Si	3.888379	9.619175	11.809601
Si	0.805332	7.973685	7.592400
Si	1.759330	7.829018	10.581200
Si	1.840227	2.479251	11.191999
Si	0.911156	2.943912	14.214400
Si	2.459718	11.386902	13.536400
Si	2.016362	5.002964	9.659200
Si	1.452010	3.940390	5.250000
Si	2.550819	10.164133	3.446400
Si	0.383942	12.374090	4.288400
Si	3.235090	2.327151	6.777600
Si	1.197727	12.042020	7.403600
Si	3.876153	12.711868	7.652400
Si	2.418584	7.757083	5.170000
Si	4.199781	0.495187	10.704401
Si	7.831317	1.404997	2.890000
Si	10.379497	1.248518	12.132000
Si	7.089207	0.285220	15.146000
Si	11.886435	2.203720	4.395200
Si	6.783931	1.687563	9.423600
Al	7.333287	6.315354	14.511728
O	6.759162	11.154772	2.246000
O	10.662036	10.322471	8.084400
O	4.818040	2.990102	13.400784
O	9.344977	0.033977	11.782000
O	6.799699	2.314676	3.812400
O	5.597132	5.221026	7.776000
O	8.707648	6.346000	13.426720
O	5.090491	10.195853	10.945200
O	4.689340	2.785043	7.269200
O	4.895081	7.608168	8.053600
O	8.191955	13.104727	3.340000
O	8.886584	12.063254	9.446400
O	11.266127	6.042868	13.293061
O	5.428379	4.622051	4.457600
O	7.531432	3.045549	13.188301
O	12.478667	10.454661	12.866401
O	8.152338	4.531535	3.923600
O	7.701066	11.511662	6.972000
O	7.028008	3.563591	6.182400

O	12.430955	6.724504	7.685600	O	9.816282	10.696614	11.728000
O	6.210792	7.564768	11.869201	O	10.374769	10.180988	14.355600
O	10.928983	8.436381	12.677073	O	8.299191	6.363756	16.062981
O	12.123152	12.162531	14.865600	O	9.380091	1.932834	2.936000
O	8.150500	12.504423	14.143200	O	9.490504	4.793135	17.773718
O	7.080863	12.953290	16.639599	O	9.239206	3.981164	15.196011
O	10.048716	8.165867	6.658000	O	9.373579	10.650427	3.060400
O	10.273939	6.291460	11.031943	O	8.875794	12.074802	0.912400
O	11.700548	3.457016	3.255200	O	7.347367	8.026111	1.292000
O	8.077121	9.829805	13.651600	O	12.749405	9.401511	15.374399
O	5.990423	11.345361	4.736000	O	5.841494	7.510423	14.886793
O	5.921060	9.520032	6.624000	O	3.312936	0.709533	6.626000
O	4.723644	6.119025	10.254001	O	2.978678	1.350449	11.330400
O	5.736908	6.666637	2.982400	O	1.068614	0.149711	8.228399
O	11.297309	12.089932	10.074000	O	0.204751	1.514095	14.714001
O	8.857594	8.253839	11.969361	O	0.721963	1.945575	10.135201
O	6.404660	11.582667	9.290401	O	1.122239	2.843706	12.597199
O	5.882887	7.027509	5.610400	O	0.463370	11.055894	8.455600
O	6.387131	9.033073	3.624000	O	2.104801	9.990797	14.309601
O	7.798911	6.595498	10.155200	O	2.886552	9.287635	4.802400
O	6.732806	3.159585	8.763600	O	2.586701	3.790945	10.562000
O	10.657479	5.656886	3.996000	O	0.464383	12.203410	5.936400
O	12.586321	9.084703	6.780000	O	1.159651	4.920012	6.494400
O	9.089299	4.226274	9.981200	O	3.494215	6.622971	4.619600
O	9.669577	2.455892	8.148001	O	0.788414	8.241385	11.837601
O	6.096066	4.843940	11.972522	O	1.783353	11.622352	3.714400
O	11.554258	8.938177	3.251200	O	3.994570	13.081898	9.267200
O	10.626290	10.290086	5.385600	O	1.786450	6.227858	10.691200
O	5.227203	12.081703	7.077200	O	3.047836	5.504786	8.475200
O	9.695821	6.302978	8.446400	O	2.093647	2.575607	7.928400
O	11.853836	11.571386	3.535200	O	0.145068	4.350900	14.561200
O	10.604074	2.179299	10.792399	O	2.930433	3.255809	5.437200
O	11.853820	9.559185	10.317201	O	2.750156	11.560105	7.304000
O	8.898306	5.963077	5.940400	O	0.516184	2.624980	5.283200
O	11.043491	5.862247	15.897874	O	4.209446	6.453253	13.011353
O	5.862259	11.234272	13.865200	O	0.916564	7.557336	4.547600
O	7.391491	9.295200	10.160399	O	3.206430	8.467013	10.895200
O	7.332047	11.494408	11.745600	O	2.383492	3.021952	14.969601
O	12.504366	6.544400	2.473200	O	1.437888	12.619760	13.326401
O	7.572567	7.657541	7.511200	O	0.612614	7.058433	14.690400
O	6.357223	4.893321	14.597139	O	2.190965	7.677449	6.776400
O	11.283936	4.368817	7.116000	O	0.550035	4.612362	9.024000
O	8.365394	7.133554	3.569600	O	2.986172	7.797700	15.073734

O	1.279718	8.335619	9.109200	O	-0.538016	2.007291	7.788400
O	2.861917	10.867428	12.039599	O	0.080205	9.401511	15.374399
O	3.622376	12.232078	14.337999	O	-0.238245	6.724504	7.685600
O	0.991568	4.858828	3.969200	O	-0.082879	9.084703	6.780000
O	4.117428	10.476163	2.896400	O	-0.815364	11.571386	3.535200
O	1.492396	9.134474	2.577600	O	-0.038661	13.952423	3.919200
O	4.384195	9.049695	13.239582	O	1.335296	13.421932	8.228399
O	10.672203	2.253358	5.550000	O	3.579617	13.981754	6.626000
O	12.131184	2.007291	7.788400	O	3.727889	-0.190324	9.267200
O	5.595158	0.513635	14.460401	O	4.634808	-0.382904	12.021600
O	4.901489	12.889318	12.021600	O	7.925273	-0.167495	3.340000
O	8.150242	1.779009	10.280000	O	7.883819	-0.767798	14.143200
O	5.493874	1.418800	10.349999	O	6.814182	-0.318932	16.639599
O	6.987936	0.560486	8.251600	O	13.185384	2.624980	5.283200
O	9.912067	2.121830	13.419600	H	7.514091	-0.208639	17.302401
O	11.742654	0.508326	12.582001				
O	12.363857	0.680201	3.919200	Ni+ Ethene			
O	8.024569	1.615362	15.300400	Si	6.171015	3.953674	13.381361
O	7.290307	1.459944	1.323600	Si	7.621518	12.256366	8.442000
H	7.780772	13.063582	17.302401	Si	11.955669	10.554867	14.462399
H	9.535483	2.888301	2.830400	Si	9.967922	6.841955	12.598854
H	10.307095	4.413175	18.132017	Si	5.030561	12.629448	13.642000
H	8.480283	12.870338	0.506400	Si	12.121967	5.142588	3.396400
H	7.238176	8.941231	0.982400	Si	5.089982	6.236086	4.428400
H	4.060141	3.268242	13.955350	Si	4.560124	6.121016	8.649600
H	2.704204	2.173459	15.322400	Si	9.211920	5.814295	9.909600
H	6.381372	1.760295	1.167600	Si	11.746457	10.779698	9.227201
Ni	6.906331	7.673528	16.514055	Si	9.812782	12.048257	10.795200
O	7.254618	13.832707	8.251600	Si	12.541766	0.089189	13.925600
O	5.861839	13.785856	14.460401	Si	9.585712	5.211175	16.197926
O	13.660769	4.858828	3.969200	Si	6.005562	3.693925	7.441600
O	13.132569	11.055894	8.455600	Si	10.892969	2.767524	7.109600
O	9.611659	13.306198	11.782000	Si	7.535115	7.937319	11.023600
O	11.856470	-1.109691	14.865600	Si	10.984008	9.467341	6.729600
O	13.840406	-0.652462	13.326401	Si	5.731494	10.501911	3.363200
O	12.873951	1.514095	14.714001	Si	5.269097	6.215779	11.762400
O	13.828851	4.920012	6.494400	Si	12.646716	5.129448	7.583200
O	13.219235	4.612362	9.024000	Si	7.398423	11.266921	13.382401
O	12.814268	4.350900	14.561200	Si	8.689230	2.733149	14.299601
O	13.281814	7.058433	14.690400	Si	6.842045	3.766391	4.573600
O	-0.164834	6.544400	2.473200	Si	8.310841	11.745253	2.410400
O	-1.114942	8.938177	3.251200	Si	12.119840	5.856368	14.646000
O	13.457614	8.241385	11.837601	Si	9.575190	9.643729	12.966000

Si	6.228600	11.080315	6.326000	O	4.895081	7.608168	8.053600
Si	9.418234	2.664664	9.769600	O	8.191955	13.104727	3.340000
Si	6.565253	10.646844	10.577200	O	8.886584	12.063254	9.446400
Si	6.069852	7.946477	6.949200	O	11.218328	6.037754	13.329140
Si	0.274987	8.055044	3.125600	O	5.428379	4.622051	4.457600
Si	12.176368	9.218222	11.863199	O	7.539625	3.066679	13.198551
Si	10.824993	10.336671	3.770400	O	12.478667	10.454661	12.866401
Si	9.054027	5.850395	4.332000	O	8.152338	4.531535	3.923600
Si	9.031193	7.028039	7.155600	O	7.701066	11.511662	6.972000
Si	6.994024	7.723504	2.854400	O	7.028008	3.563591	6.182400
Si	4.381183	7.683606	14.118825	O	12.430955	6.724504	7.685600
Si	0.835714	1.705082	8.539599	O	6.210792	7.564768	11.869201
Si	1.466075	8.518111	14.830400	O	10.926104	8.438611	12.683082
Si	3.888379	9.619175	11.809601	O	12.123152	12.162531	14.865600
Si	0.805332	7.973685	7.592400	O	8.150500	12.504423	14.143200
Si	1.759330	7.829018	10.581200	O	7.080863	12.953290	16.639599
Si	1.840227	2.479251	11.191999	O	10.048716	8.165867	6.658000
Si	0.911156	2.943912	14.214400	O	10.233204	6.269186	11.080585
Si	2.459718	11.386902	13.536400	O	11.700548	3.457016	3.255200
Si	2.016362	5.002964	9.659200	O	8.077121	9.829805	13.651600
Si	1.452010	3.940390	5.250000	O	5.990423	11.345361	4.736000
Si	2.550819	10.164133	3.446400	O	5.921060	9.520032	6.624000
Si	0.383942	12.374090	4.288400	O	4.723644	6.119025	10.254001
Si	3.235090	2.327151	6.777600	O	5.736908	6.666637	2.982400
Si	1.197727	12.042020	7.403600	O	11.297309	12.089932	10.074000
Si	3.876153	12.711868	7.652400	O	8.857047	8.252730	11.967336
Si	2.418584	7.757083	5.170000	O	6.404660	11.582667	9.290401
Si	4.199781	0.495187	10.704401	O	5.882887	7.027509	5.610400
Si	7.831317	1.404997	2.890000	O	6.387131	9.033073	3.624000
Si	10.379497	1.248518	12.132000	O	7.798911	6.595498	10.155200
Si	7.089207	0.285220	15.146000	O	6.732806	3.159585	8.763600
Si	11.886435	2.203720	4.395200	O	10.657479	5.656886	3.996000
Si	6.783931	1.687563	9.423600	O	12.586321	9.084703	6.780000
Al	7.235239	6.420115	14.617075	O	9.089299	4.226274	9.981200
O	6.759162	11.154772	2.246000	O	9.669577	2.455892	8.148001
O	10.662036	10.322471	8.084400	O	6.114295	4.862643	12.009851
O	4.840294	3.024235	13.457100	O	11.554258	8.938177	3.251200
O	9.344977	0.033977	11.782000	O	10.626290	10.290086	5.385600
O	6.799699	2.314676	3.812400	O	5.227203	12.081703	7.077200
O	5.597132	5.221026	7.776000	O	9.695821	6.302978	8.446400
O	8.679100	6.445300	13.551756	O	11.853836	11.571386	3.535200
O	5.090491	10.195853	10.945200	O	10.604074	2.179299	10.792399
O	4.689340	2.785043	7.269200	O	11.853820	9.559185	10.317201

O	8.898306	5.963077	5.940400	O	0.516184	2.624980	5.283200
O	11.081738	5.851687	15.934276	O	4.187446	6.455822	12.988121
O	5.862259	11.234272	13.865200	O	0.916564	7.557336	4.547600
O	7.391491	9.295200	10.160399	O	3.206430	8.467013	10.895200
O	7.332047	11.494408	11.745600	O	2.383492	3.021952	14.969601
O	12.504366	6.544400	2.473200	O	1.437888	12.619760	13.326401
O	7.572567	7.657541	7.511200	O	0.612614	7.058433	14.690400
O	6.415838	4.892231	14.667062	O	2.190965	7.677449	6.776400
O	11.283936	4.368817	7.116000	O	0.550035	4.612362	9.024000
O	8.365394	7.133554	3.569600	O	2.979235	7.795411	15.056697
O	9.816282	10.696614	11.728000	O	1.279718	8.335619	9.109200
O	10.374769	10.180988	14.355600	O	2.861917	10.867428	12.039599
O	8.355555	6.353331	16.111116	O	3.622376	12.232078	14.337999
O	9.380091	1.932834	2.936000	O	0.991568	4.858828	3.969200
O	9.519732	4.772870	17.781395	O	4.117428	10.476163	2.896400
O	9.282311	3.954735	15.206999	O	1.492396	9.134474	2.577600
O	9.373579	10.650427	3.060400	O	4.373235	9.056083	13.236369
O	8.875794	12.074802	0.912400	O	10.672203	2.253358	5.550000
O	7.347367	8.026111	1.292000	O	12.131184	2.007291	7.788400
O	12.749405	9.401511	15.374399	O	5.595158	0.513635	14.460401
O	5.831600	7.520323	14.861353	O	4.901489	12.889318	12.021600
O	3.312936	0.709533	6.626000	O	8.150242	1.779009	10.280000
O	2.978678	1.350449	11.330400	O	5.493874	1.418800	10.349999
O	1.068614	0.149711	8.228399	O	6.987936	0.560486	8.251600
O	0.204751	1.514095	14.714001	O	9.912067	2.121830	13.419600
O	0.721963	1.945575	10.135201	O	11.742654	0.508326	12.582001
O	1.122239	2.843706	12.597199	O	12.363857	0.680201	3.919200
O	0.463370	11.055894	8.455600	O	8.024569	1.615362	15.300400
O	2.104801	9.990797	14.309601	O	7.290307	1.459944	1.323600
O	2.886552	9.287635	4.802400	H	7.780772	13.063582	17.302401
O	2.586701	3.790945	10.562000	H	9.535483	2.888301	2.830400
O	0.464383	12.203410	5.936400	H	10.289710	4.290699	18.120995
O	1.159651	4.920012	6.494400	H	8.480283	12.870338	0.506400
O	3.494215	6.622971	4.619600	H	7.238176	8.941231	0.982400
O	0.788414	8.241385	11.837601	H	4.071962	3.312867	13.989946
O	1.783353	11.622352	3.714400	H	2.704204	2.173459	15.322400
O	3.994570	13.081898	9.267200	H	6.381372	1.760295	1.167600
O	1.786450	6.227858	10.691200	H	7.210077	9.357668	18.973660
O	3.047836	5.504786	8.475200	H	7.595781	7.670479	19.636459
O	2.093647	2.575607	7.928400	H	9.622254	9.632107	18.266880
O	0.145068	4.350900	14.561200	H	10.011154	7.946662	18.926600
O	2.930433	3.255809	5.437200	Ni	8.200200	7.846835	17.182411
O	2.750156	11.560105	7.304000	C	7.910619	8.518062	19.023079

C	9.247727	8.672894	18.637608	Si	9.812782	12.048257	10.795200
O	7.254618	13.832707	8.251600	Si	12.541766	0.089189	13.925600
O	5.861839	13.785856	14.460401	Si	9.598348	5.188246	16.201595
O	13.660769	4.858828	3.969200	Si	6.005562	3.693925	7.441600
O	13.132569	11.055894	8.455600	Si	10.892969	2.767524	7.109600
O	9.611659	13.306198	11.782000	Si	7.535115	7.937319	11.023600
O	11.856470	-1.109691	14.865600	Si	10.984008	9.467341	6.729600
O	13.840406	-0.652462	13.326401	Si	5.731494	10.501911	3.363200
O	12.873951	1.514095	14.714001	Si	5.269097	6.215779	11.762400
O	13.828851	4.920012	6.494400	Si	12.646716	5.129448	7.583200
O	13.219235	4.612362	9.024000	Si	7.398423	11.266921	13.382401
O	12.814268	4.350900	14.561200	Si	8.689230	2.733149	14.299601
O	13.281814	7.058433	14.690400	Si	6.842045	3.766391	4.573600
O	-0.164834	6.544400	2.473200	Si	8.310841	11.745253	2.410400
O	-1.114942	8.938177	3.251200	Si	12.119840	5.856368	14.646000
O	13.457614	8.241385	11.837601	Si	9.575190	9.643729	12.966000
O	-0.538016	2.007291	7.788400	Si	6.228600	11.080315	6.326000
O	0.080205	9.401511	15.374399	Si	9.418234	2.664664	9.769600
O	-0.238245	6.724504	7.685600	Si	6.565253	10.646844	10.577200
O	-0.082879	9.084703	6.780000	Si	6.069852	7.946477	6.949200
O	-0.815364	11.571386	3.535200	Si	0.274987	8.055044	3.125600
O	-0.038661	13.952423	3.919200	Si	12.176368	9.218222	11.863199
O	1.335296	13.421932	8.228399	Si	10.824993	10.336671	3.770400
O	3.579617	13.981754	6.626000	Si	9.054027	5.850395	4.332000
O	3.727889	-0.190324	9.267200	Si	9.031193	7.028039	7.155600
O	4.634808	-0.382904	12.021600	Si	6.994024	7.723504	2.854400
O	7.925273	-0.167495	3.340000	Si	4.389287	7.684674	14.123740
O	7.883819	-0.767798	14.143200	Si	0.835714	1.705082	8.539599
O	6.814182	-0.318932	16.639599	Si	1.466075	8.518111	14.830400
O	13.185384	2.624980	5.283200	Si	3.888379	9.619175	11.809601
H	7.514091	-0.208639	17.302401	Si	0.805332	7.973685	7.592400
Ni+ 2Ethene				Si	1.759330	7.829018	10.581200
Si	6.182641	3.978000	13.403889	Si	1.840227	2.479251	11.191999
Si	7.621518	12.256366	8.442000	Si	0.911156	2.943912	14.214400
Si	11.955669	10.554867	14.462399	Si	2.459718	11.386902	13.536400
Si	9.968308	6.846851	12.616838	Si	2.016362	5.002964	9.659200
Si	5.030561	12.629448	13.642000	Si	1.452010	3.940390	5.250000
Si	12.121967	5.142588	3.396400	Si	2.550819	10.164133	3.446400
Si	5.089982	6.236086	4.428400	Si	0.383942	12.374090	4.288400
Si	4.560124	6.121016	8.649600	Si	3.235090	2.327151	6.777600
Si	9.211920	5.814295	9.909600	Si	1.197727	12.042020	7.403600
Si	11.746457	10.779698	9.227201	Si	3.876153	12.711868	7.652400
				Si	2.418584	7.757083	5.170000

Si	4.199781	0.495187	10.704401	O	5.882887	7.027509	5.610400
Si	7.831317	1.404997	2.890000	O	6.387131	9.033073	3.624000
Si	10.379497	1.248518	12.132000	O	7.798911	6.595498	10.155200
Si	7.089207	0.285220	15.146000	O	6.732806	3.159585	8.763600
Si	11.886435	2.203720	4.395200	O	10.657479	5.656886	3.996000
Si	6.783931	1.687563	9.423600	O	12.586321	9.084703	6.780000
Al	7.268751	6.448573	14.700949	O	9.089299	4.226274	9.981200
O	6.759162	11.154772	2.246000	O	9.669577	2.455892	8.148001
O	10.662036	10.322471	8.084400	O	6.112719	4.863828	12.018425
O	4.852738	3.048832	13.507606	O	11.554258	8.938177	3.251200
O	9.344977	0.033977	11.782000	O	10.626290	10.290086	5.385600
O	6.799699	2.314676	3.812400	O	5.227203	12.081703	7.077200
O	5.597132	5.221026	7.776000	O	9.695821	6.302978	8.446400
O	8.707576	6.497150	13.620940	O	11.853836	11.571386	3.535200
O	5.090491	10.195853	10.945200	O	10.604074	2.179299	10.792399
O	4.689340	2.785043	7.269200	O	11.853820	9.559185	10.317201
O	4.895081	7.608168	8.053600	O	8.898306	5.963077	5.940400
O	8.191955	13.104727	3.340000	O	11.085461	5.852015	15.934488
O	8.886584	12.063254	9.446400	O	5.862259	11.234272	13.865200
O	11.229798	6.036629	13.322025	O	7.391491	9.295200	10.160399
O	5.428379	4.622051	4.457600	O	7.332047	11.494408	11.745600
O	7.537170	3.072072	13.205036	O	12.504366	6.544400	2.473200
O	12.478667	10.454661	12.866401	O	7.572567	7.657541	7.511200
O	8.152338	4.531535	3.923600	O	6.452952	4.914595	14.684972
O	7.701066	11.511662	6.972000	O	11.283936	4.368817	7.116000
O	7.028008	3.563591	6.182400	O	8.365394	7.133554	3.569600
O	12.430955	6.724504	7.685600	O	9.816282	10.696614	11.728000
O	6.210792	7.564768	11.869201	O	10.374769	10.180988	14.355600
O	10.926600	8.442198	12.686089	O	8.374947	6.323570	16.208227
O	12.123152	12.162531	14.865600	O	9.380091	1.932834	2.936000
O	8.150500	12.504423	14.143200	O	9.596231	4.625309	17.756027
O	7.080863	12.953290	16.639599	O	9.303273	3.951582	15.184956
O	10.048716	8.165867	6.658000	O	9.373579	10.650427	3.060400
O	10.217791	6.264072	11.096349	O	8.875794	12.074802	0.912400
O	11.700548	3.457016	3.255200	O	7.347367	8.026111	1.292000
O	8.077121	9.829805	13.651600	O	12.749405	9.401511	15.374399
O	5.990423	11.345361	4.736000	O	5.831095	7.527285	14.877941
O	5.921060	9.520032	6.624000	O	3.312936	0.709533	6.626000
O	4.723644	6.119025	10.254001	O	2.978678	1.350449	11.330400
O	5.736908	6.666637	2.982400	O	1.068614	0.149711	8.228399
O	11.297309	12.089932	10.074000	O	0.204751	1.514095	14.714001
O	8.856462	8.253284	11.966877	O	0.721963	1.945575	10.135201
O	6.404660	11.582667	9.290401	O	1.122239	2.843706	12.597199

O	0.463370	11.055894	8.455600	O	8.024569	1.615362	15.300400
O	2.104801	9.990797	14.309601	O	7.290307	1.459944	1.323600
O	2.886552	9.287635	4.802400	H	7.780772	13.063582	17.302401
O	2.586701	3.790945	10.562000	H	9.535483	2.888301	2.830400
O	0.464383	12.203410	5.936400	H	10.260380	3.944360	17.946472
O	1.159651	4.920012	6.494400	H	8.480283	12.870338	0.506400
O	3.494215	6.622971	4.619600	H	7.238176	8.941231	0.982400
O	0.788414	8.241385	11.837601	H	4.075233	3.352021	14.017759
O	1.783353	11.622352	3.714400	H	2.704204	2.173459	15.322400
O	3.994570	13.081898	9.267200	H	6.381372	1.760295	1.167600
O	1.786450	6.227858	10.691200	H	6.943638	9.973174	17.451582
O	3.047836	5.504786	8.475200	H	7.581084	9.698998	19.172470
O	2.093647	2.575607	7.928400	H	9.287757	9.904334	16.557001
O	0.145068	4.350900	14.561200	H	9.939772	9.620575	18.273933
O	2.930433	3.255809	5.437200	H	7.384235	5.588810	18.775578
O	2.750156	11.560105	7.304000	H	6.592768	7.079384	19.573957
O	0.516184	2.624980	5.283200	H	9.627137	6.412465	19.388958
O	4.190455	6.457521	12.991934	H	8.876268	7.914565	20.205000
O	0.916564	7.557336	4.547600	Ni	8.290647	7.775716	17.498135
O	3.206430	8.467013	10.895200	C	7.780614	9.695222	18.098604
O	2.383492	3.021952	14.969601	C	9.075979	9.662625	17.605015
O	1.437888	12.619760	13.326401	C	7.499875	6.559843	19.260189
O	0.612614	7.058433	14.690400	C	8.743122	7.018530	19.596308
O	2.190965	7.677449	6.776400	O	7.254618	13.832707	8.251600
O	0.550035	4.612362	9.024000	O	5.861839	13.785856	14.460401
O	2.980275	7.798162	15.058173	O	13.660769	4.858828	3.969200
O	1.279718	8.335619	9.109200	O	13.132569	11.055894	8.455600
O	2.861917	10.867428	12.039599	O	9.611659	13.306198	11.782000
O	3.622376	12.232078	14.337999	O	11.856470	-1.109691	14.865600
O	0.991568	4.858828	3.969200	O	13.840406	-0.652462	13.326401
O	4.117428	10.476163	2.896400	O	12.873951	1.514095	14.714001
O	1.492396	9.134474	2.577600	O	13.828851	4.920012	6.494400
O	4.374064	9.056627	13.236771	O	13.219235	4.612362	9.024000
O	10.672203	2.253358	5.550000	O	12.814268	4.350900	14.561200
O	12.131184	2.007291	7.788400	O	13.281814	7.058433	14.690400
O	5.595158	0.513635	14.460401	O	-0.164834	6.544400	2.473200
O	4.901489	12.889318	12.021600	O	-1.114942	8.938177	3.251200
O	8.150242	1.779009	10.280000	O	13.457614	8.241385	11.837601
O	5.493874	1.418800	10.349999	O	-0.538016	2.007291	7.788400
O	6.987936	0.560486	8.251600	O	0.080205	9.401511	15.374399
O	9.912067	2.121830	13.419600	O	-0.238245	6.724504	7.685600
O	11.742654	0.508326	12.582001	O	-0.082879	9.084703	6.780000
O	12.363857	0.680201	3.919200	O	-0.815364	11.571386	3.535200

O	-0.038661	13.952423	3.919200
O	1.335296	13.421932	8.228399
O	3.579617	13.981754	6.626000
O	3.727889	-0.190324	9.267200
O	4.634808	-0.382904	12.021600
O	7.925273	-0.167495	3.340000
O	7.883819	-0.767798	14.143200
O	6.814182	-0.318932	16.639599
O	13.185384	2.624980	5.283200
H	7.514091	-0.208639	17.302401

Ni²⁺

Si	6.144834	3.861380	13.270999
Si	11.746457	10.779698	9.227201
Si	9.812782	12.048257	10.795200
Si	12.541766	0.089189	13.925600
Si	9.493255	5.319486	16.171480
Si	6.005562	3.693925	7.441600
Si	10.892969	2.767524	7.109600
Si	7.535115	7.937319	11.023600
Si	10.984008	9.467341	6.729600
Si	5.731494	10.501911	3.363200
Si	5.269097	6.215779	11.762400
Si	7.621518	12.256366	8.442000
Si	12.646716	5.129448	7.583200
Si	7.398423	11.266921	13.382401
Si	8.689230	2.733149	14.299601
Si	6.842045	3.766391	4.573600
Si	8.310841	11.745253	2.410400
Si	12.122548	5.855271	14.650063
Si	9.575190	9.643729	12.966000
Si	6.228600	11.080315	6.326000
Si	9.418234	2.664664	9.769600
Si	6.565253	10.646844	10.577200
Si	11.945290	10.570264	14.460822
Si	6.069852	7.946477	6.949200
Si	0.274987	8.055044	3.125600
Si	12.176368	9.218222	11.863199
Si	10.824993	10.336671	3.770400
Si	9.054027	5.850395	4.332000
Si	9.031193	7.028039	7.155600
Si	6.994024	7.723504	2.854400

Si	4.388190	7.736894	14.105734
Si	0.835714	1.705082	8.539599
Si	10.004989	6.796566	12.547791
Si	3.888379	9.619175	11.809601
Si	0.805332	7.973685	7.592400
Si	1.759330	7.829018	10.581200
Si	1.840227	2.479251	11.191999
Si	0.911156	2.943912	14.214400
Si	2.458287	11.393605	13.545321
Si	2.016362	5.002964	9.659200
Si	1.452010	3.940390	5.250000
Si	2.550819	10.164133	3.446400
Si	0.383942	12.374090	4.288400
Si	5.030561	12.629448	13.642000
Si	3.235090	2.327151	6.777600
Si	1.197727	12.042020	7.403600
Si	3.876153	12.711868	7.652400
Si	2.418584	7.757083	5.170000
Si	4.199781	0.495187	10.704401
Si	7.831317	1.404997	2.890000
Si	10.379497	1.248518	12.132000
Si	7.089207	0.285220	15.146000
Si	11.886435	2.203720	4.395200
Si	6.783931	1.687563	9.423600
Si	12.121967	5.142588	3.396400
Si	5.089982	6.236086	4.428400
Si	4.560124	6.121016	8.649600
Si	9.211920	5.814295	9.909600
Al	7.328919	6.298514	14.464025
Al	1.466075	8.518111	14.830400
O	6.759162	11.154772	2.246000
O	4.895081	7.608168	8.053600
O	2.383492	3.021952	14.969601
O	1.437888	12.619760	13.326401
O	0.601299	6.983470	14.769146
O	2.190965	7.677449	6.776400
O	0.550035	4.612362	9.024000
O	3.147954	7.635036	15.141673
O	1.279718	8.335619	9.109200
O	2.861917	10.867428	12.039599
O	3.622376	12.232078	14.337999
O	0.991568	4.858828	3.969200
O	8.191955	13.104727	3.340000

O	4.117428	10.476163	2.896400	O	6.387131	9.033073	3.624000
O	1.492396	9.134474	2.577600	O	7.798911	6.595498	10.155200
O	4.396040	9.048841	13.239684	O	9.344977	0.033977	11.782000
O	10.672203	2.253358	5.550000	O	6.732806	3.159585	8.763600
O	12.131184	2.007291	7.788400	O	10.657479	5.656886	3.996000
O	5.595158	0.513635	14.460401	O	12.586321	9.084703	6.780000
O	4.901489	12.889318	12.021600	O	9.089299	4.226274	9.981200
O	8.150242	1.779009	10.280000	O	9.669577	2.455892	8.148001
O	5.493874	1.418800	10.349999	O	6.093790	4.842000	11.966909
O	6.987936	0.560486	8.251600	O	11.554258	8.938177	3.251200
O	8.886584	12.063254	9.446400	O	10.626290	10.290086	5.385600
O	9.912067	2.121830	13.419600	O	5.227203	12.081703	7.077200
O	11.742654	0.508326	12.582001	O	9.695821	6.302978	8.446400
O	12.363857	0.680201	3.919200	O	6.799699	2.314676	3.812400
O	8.024569	1.615362	15.300400	O	11.853836	11.571386	3.535200
O	7.290307	1.459944	1.323600	O	10.604074	2.179299	10.792399
O	11.269333	6.043298	13.288025	O	11.853820	9.559185	10.317201
O	5.428379	4.622051	4.457600	O	8.898306	5.963077	5.940400
O	7.528183	3.043933	13.188847	O	11.024648	5.873256	15.882025
O	12.478667	10.454661	12.866401	O	5.862259	11.234272	13.865200
O	8.152338	4.531535	3.923600	O	7.391491	9.295200	10.160399
O	7.701066	11.511662	6.972000	O	7.332047	11.494408	11.745600
O	7.028008	3.563591	6.182400	O	12.504366	6.544400	2.473200
O	10.662036	10.322471	8.084400	O	7.572567	7.657541	7.511200
O	12.430955	6.724504	7.685600	O	5.597132	5.221026	7.776000
O	6.210792	7.564768	11.869201	O	6.244343	4.824239	14.622385
O	10.928246	8.435102	12.674246	O	11.283936	4.368817	7.116000
O	12.123152	12.162531	14.865600	O	8.365394	7.133554	3.569600
O	8.150500	12.504423	14.143200	O	9.816282	10.696614	11.728000
O	7.080863	12.953290	16.639599	O	10.374769	10.180988	14.355600
O	10.048716	8.165867	6.658000	O	8.289506	6.365214	15.914530
O	10.287496	6.299891	11.015220	O	9.380091	1.932834	2.936000
O	11.700548	3.457016	3.255200	O	9.403315	4.917802	17.758797
O	8.077121	9.829805	13.651600	O	9.222651	3.988538	15.201822
O	4.808184	2.980041	13.377386	O	9.373579	10.650427	3.060400
O	5.990423	11.345361	4.736000	O	8.616629	6.224320	13.257450
O	5.921060	9.520032	6.624000	O	8.875794	12.074802	0.912400
O	4.723644	6.119025	10.254001	O	7.347367	8.026111	1.292000
O	5.736908	6.666637	2.982400	O	12.713439	9.507992	15.418600
O	11.297309	12.089932	10.074000	O	5.819493	7.331955	14.833424
O	8.855690	8.253445	11.973213	O	3.312936	0.709533	6.626000
O	6.404660	11.582667	9.290401	O	2.978678	1.350449	11.330400
O	5.882887	7.027509	5.610400	O	1.068614	0.149711	8.228399

O	0.204751	1.514095	14.714001	O	13.270498	6.983470	14.769146
O	0.721963	1.945575	10.135201	O	-0.164834	6.544400	2.473200
O	1.122239	2.843706	12.597199	O	-1.114942	8.938177	3.251200
O	5.090491	10.195853	10.945200	O	13.457614	8.241385	11.837601
O	0.463370	11.055894	8.455600	O	-0.538016	2.007291	7.788400
O	2.171859	10.056838	14.383247	O	-0.238245	6.724504	7.685600
O	2.886552	9.287635	4.802400	O	-0.082879	9.084703	6.780000
O	2.586701	3.790945	10.562000	O	-0.815364	11.571386	3.535200
O	0.464383	12.203410	5.936400	O	-0.038661	13.952423	3.919200
O	1.159651	4.920012	6.494400	O	5.861839	13.785856	14.460401
O	3.494215	6.622971	4.619600	O	1.335296	13.421932	8.228399
O	0.788414	8.241385	11.837601	O	3.579617	13.981754	6.626000
O	1.783353	11.622352	3.714400	O	4.634808	-0.382904	12.021600
O	3.994570	13.081898	9.267200	O	3.727889	-0.190324	9.267200
O	4.689340	2.785043	7.269200	O	7.925273	-0.167495	3.340000
O	1.786450	6.227858	10.691200	O	7.883819	-0.767798	14.143200
O	3.047836	5.504786	8.475200	O	6.814182	-0.318932	16.639599
O	2.093647	2.575607	7.928400	O	13.185384	2.624980	5.283200
O	0.145068	4.350900	14.561200	O	13.660769	4.858828	3.969200
O	2.930433	3.255809	5.437200	O	0.044239	9.507992	15.418600
O	2.750156	11.560105	7.304000	H	7.514091	-0.208639	17.302401
O	0.516184	2.624980	5.283200				
O	4.215781	6.452354	13.017757	Ni2+ Ethene			
O	0.916564	7.557336	4.547600	Si	6.140720	3.865924	13.274077
O	3.206430	8.467013	10.895200	Si	11.746457	10.779698	9.227201
H	7.780772	13.063582	17.302401	Si	9.812782	12.048257	10.795200
H	9.535483	2.888301	2.830400	Si	12.541766	0.089189	13.925600
H	10.174930	4.472808	18.141293	Si	9.493484	5.319587	16.166517
H	8.480283	12.870338	0.506400	Si	6.005562	3.693925	7.441600
H	7.238176	8.941231	0.982400	Si	10.892969	2.767524	7.109600
H	4.055346	3.249006	13.943416	Si	7.535115	7.937319	11.023600
H	2.704204	2.173459	15.322400	Si	10.984008	9.467341	6.729600
H	6.381372	1.760295	1.167600	Si	5.731494	10.501911	3.363200
Ni	4.632463	5.706514	15.251569	Si	5.269097	6.215779	11.762400
O	13.132569	11.055894	8.455600	Si	7.621518	12.256366	8.442000
O	9.611659	13.306198	11.782000	Si	12.646716	5.129448	7.583200
O	11.856470	-1.109691	14.865600	Si	7.398423	11.266921	13.382401
O	13.840406	-0.652462	13.326401	Si	8.689230	2.733149	14.299601
O	12.873951	1.514095	14.714001	Si	6.842045	3.766391	4.573600
O	7.254618	13.832707	8.251600	Si	8.310841	11.745253	2.410400
O	13.219235	4.612362	9.024000	Si	12.123894	5.853727	14.646906
O	13.828851	4.920012	6.494400	Si	9.575190	9.643729	12.966000
O	12.814268	4.350900	14.561200	Si	6.228600	11.080315	6.326000

Si	9.418234	2.664664	9.769600	O	1.437888	12.619760	13.326401
Si	6.565253	10.646844	10.577200	O	0.596014	6.983466	14.777303
Si	11.948016	10.567852	14.461132	O	2.190965	7.677449	6.776400
Si	6.069852	7.946477	6.949200	O	0.550035	4.612362	9.024000
Si	0.274987	8.055044	3.125600	O	3.129683	7.705138	15.145788
Si	12.176368	9.218222	11.863199	O	1.279718	8.335619	9.109200
Si	10.824993	10.336671	3.770400	O	2.861917	10.867428	12.039599
Si	9.054027	5.850395	4.332000	O	3.622376	12.232078	14.337999
Si	9.031193	7.028039	7.155600	O	0.991568	4.858828	3.969200
Si	6.994024	7.723504	2.854400	O	8.191955	13.104727	3.340000
Si	4.364360	7.707510	14.103213	O	4.117428	10.476163	2.896400
Si	0.835714	1.705082	8.539599	O	1.492396	9.134474	2.577600
Si	10.009135	6.802924	12.546367	O	4.396040	9.048841	13.239684
Si	3.888379	9.619175	11.809601	O	10.672203	2.253358	5.550000
Si	0.805332	7.973685	7.592400	O	12.131184	2.007291	7.788400
Si	1.759330	7.829018	10.581200	O	5.595158	0.513635	14.460401
Si	1.840227	2.479251	11.191999	O	4.901489	12.889318	12.021600
Si	0.911156	2.943912	14.214400	O	8.150242	1.779009	10.280000
Si	2.458304	11.396377	13.541894	O	5.493874	1.418800	10.349999
Si	2.016362	5.002964	9.659200	O	6.987936	0.560486	8.251600
Si	1.452010	3.940390	5.250000	O	8.886584	12.063254	9.446400
Si	2.550819	10.164133	3.446400	O	9.912067	2.121830	13.419600
Si	0.383942	12.374090	4.288400	O	11.742654	0.508326	12.582001
Si	5.030561	12.629448	13.642000	O	12.363857	0.680201	3.919200
Si	3.235090	2.327151	6.777600	O	8.024569	1.615362	15.300400
Si	1.197727	12.042020	7.403600	O	7.290307	1.459944	1.323600
Si	3.876153	12.711868	7.652400	O	11.269333	6.043298	13.288025
Si	2.418584	7.757083	5.170000	O	5.428379	4.622051	4.457600
Si	4.199781	0.495187	10.704401	O	7.528183	3.043933	13.188847
Si	7.831317	1.404997	2.890000	O	12.478667	10.454661	12.866401
Si	10.379497	1.248518	12.132000	O	8.152338	4.531535	3.923600
Si	7.089207	0.285220	15.146000	O	7.701066	11.511662	6.972000
Si	11.886435	2.203720	4.395200	O	7.028008	3.563591	6.182400
Si	6.783931	1.687563	9.423600	O	10.662036	10.322471	8.084400
Si	12.121967	5.142588	3.396400	O	12.430955	6.724504	7.685600
Si	5.089982	6.236086	4.428400	O	6.210792	7.564768	11.869201
Si	4.560124	6.121016	8.649600	O	10.928246	8.435102	12.674246
Si	9.211920	5.814295	9.909600	O	12.123152	12.162531	14.865600
Al	7.328919	6.298514	14.464025	O	8.150500	12.504423	14.143200
Al	1.466075	8.518111	14.830400	O	7.080863	12.953290	16.639599
O	6.759162	11.154772	2.246000	O	10.048716	8.165867	6.658000
O	4.895081	7.608168	8.053600	O	10.287496	6.299891	11.015220
O	2.383492	3.021952	14.969601	O	11.700548	3.457016	3.255200

O	8.077121	9.829805	13.651600	O	9.222651	3.988538	15.201822
O	4.808184	2.980041	13.377386	O	9.373579	10.650427	3.060400
O	5.990423	11.345361	4.736000	O	8.631283	6.235976	13.276519
O	5.921060	9.520032	6.624000	O	8.875794	12.074802	0.912400
O	4.723644	6.119025	10.254001	O	7.347367	8.026111	1.292000
O	5.736908	6.666637	2.982400	O	12.703553	9.499927	15.421685
O	11.297309	12.089932	10.074000	O	5.815352	7.336853	14.843675
O	8.855690	8.253445	11.973213	O	3.312936	0.709533	6.626000
O	6.404660	11.582667	9.290401	O	2.978678	1.350449	11.330400
O	5.882887	7.027509	5.610400	O	1.068614	0.149711	8.228399
O	6.387131	9.033073	3.624000	O	0.204751	1.514095	14.714001
O	7.798911	6.595498	10.155200	O	0.721963	1.945575	10.135201
O	9.344977	0.033977	11.782000	O	1.122239	2.843706	12.597199
O	6.732806	3.159585	8.763600	O	5.090491	10.195853	10.945200
O	10.657479	5.656886	3.996000	O	0.463370	11.055894	8.455600
O	12.586321	9.084703	6.780000	O	2.140918	10.078265	14.389050
O	9.089299	4.226274	9.981200	O	2.886552	9.287635	4.802400
O	9.669577	2.455892	8.148001	O	2.586701	3.790945	10.562000
O	6.093790	4.842000	11.966909	O	0.464383	12.203410	5.936400
O	11.554258	8.938177	3.251200	O	1.159651	4.920012	6.494400
O	10.626290	10.290086	5.385600	O	3.494215	6.622971	4.619600
O	5.227203	12.081703	7.077200	O	0.788414	8.241385	11.837601
O	9.695821	6.302978	8.446400	O	1.783353	11.622352	3.714400
O	6.799699	2.314676	3.812400	O	3.994570	13.081898	9.267200
O	11.853836	11.571386	3.535200	O	4.689340	2.785043	7.269200
O	10.604074	2.179299	10.792399	O	1.786450	6.227858	10.691200
O	11.853820	9.559185	10.317201	O	3.047836	5.504786	8.475200
O	8.898306	5.963077	5.940400	O	2.093647	2.575607	7.928400
O	11.024648	5.873256	15.882025	O	0.145068	4.350900	14.561200
O	5.862259	11.234272	13.865200	O	2.930433	3.255809	5.437200
O	7.391491	9.295200	10.160399	O	2.750156	11.560105	7.304000
O	7.332047	11.494408	11.745600	O	0.516184	2.624980	5.283200
O	12.504366	6.544400	2.473200	O	4.215781	6.452354	13.017757
O	7.572567	7.657541	7.511200	O	0.916564	7.557336	4.547600
O	5.597132	5.221026	7.776000	O	3.206430	8.467013	10.895200
O	6.276107	4.829976	14.618516	H	7.780772	13.063582	17.302401
O	11.283936	4.368817	7.116000	H	9.535483	2.888301	2.830400
O	8.365394	7.133554	3.569600	H	10.174930	4.472808	18.141293
O	9.816282	10.696614	11.728000	H	8.480283	12.870338	0.506400
O	10.374769	10.180988	14.355600	H	7.238176	8.941231	0.982400
O	8.274082	6.356951	15.934295	H	4.055346	3.249006	13.943416
O	9.380091	1.932834	2.936000	H	2.704204	2.173459	15.322400
O	9.403315	4.917802	17.758797	H	6.381372	1.760295	1.167600

H	3.550224	4.423213	17.401621
H	5.361971	3.984561	17.522467
H	4.117005	6.834506	17.806078
H	5.925240	6.392643	17.932026
Ni	4.893650	5.732967	15.665262
C	4.590864	4.756296	17.465034
C	4.903032	6.080451	17.702721
O	13.132569	11.055894	8.455600
O	9.611659	13.306198	11.782000
O	11.856470	-1.109691	14.865600
O	13.840406	-0.652462	13.326401
O	12.873951	1.514095	14.714001
O	7.254618	13.832707	8.251600
O	13.219235	4.612362	9.024000
O	13.828851	4.920012	6.494400
O	12.814268	4.350900	14.561200
O	13.265214	6.983466	14.777303
O	-0.164834	6.544400	2.473200
O	-1.114942	8.938177	3.251200
O	13.457614	8.241385	11.837601
O	-0.538016	2.007291	7.788400
O	-0.238245	6.724504	7.685600
O	-0.082879	9.084703	6.780000
O	-0.815364	11.571386	3.535200
O	-0.038661	13.952423	3.919200
O	5.861839	13.785856	14.460401
O	1.335296	13.421932	8.228399
O	3.579617	13.981754	6.626000
O	4.634808	-0.382904	12.021600
O	3.727889	-0.190324	9.267200
O	7.925273	-0.167495	3.340000
O	7.883819	-0.767798	14.143200
O	6.814182	-0.318932	16.639599
O	13.185384	2.624980	5.283200
O	13.660769	4.858828	3.969200
O	0.034353	9.499927	15.421685
H	7.514091	-0.208639	17.302401