Supporting Information:

Identification of the mechanism of NO reduction with ammonia (SCR) on zeolite catalysts

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Materials and methods

BEA with Si/Al ratio ~ 15 was synthesized in the presence of fluoride anions according to a procedure developed by Camblor et al. [S1] The gel composition was as follows SiO_2: xAl_2O_3:(0.54 + 2x)TEAOH:(0.54 + 2x)HF:(7 + 2x)H_2O. The absence of alkali cations requires only a calcination step (550 ºC in flowing air), decomposing the organic cation (TEA^+) to convert it into Brønsted acidic H-Form.

Na/SSZ-13 zeolite with Si/Al 12 was hydrothermally synthesized using the following recipe: 0.8 g of NaOH (Sigma Aldrich, ≥ 99%) was dissolved in 50 ml of deionized water. 17 g of TMAda-OH (Sachem Inc., 25% N,N,N-trimethyl-1-adamantyl ammonium hydroxide) was added as structure directing agent. 0.75 g of $Al(OH)_3$ (Sigma Aldrich, ~54% Al_2O_3) was slowly added to the solution and stirred at 400 rpm until it was completely dissolved. 20.0 g of LUDOX HS-30 colloidal silica (Sigma Aldrich, 30 wt% suspension in H_2O) was added slowly to the solution until a uniform gel was formed. The obtained gel was sealed in a 125 mL Teflon-lined stainless steel autoclave with a magnetic stirring bar. Hydrothermal synthesis was carried out at 160 °C under continuous stirring at 400 rpm for 4 days. After synthesis, the zeolite cake was separated from the suspension by centrifugation, and washed with deionized water. It was then dried at 80 °C under N_2 flow overnight, and calcined in air at 550 °C for 5 h in order to remove the SDA. NH_4/SSZ-13 was obtained by ion

exchange of the as-prepared Na/SSZ-13 zeolite with 1 M NH_4NO_3 solution at 80 °C for 5 h. The process was repeated three times. H-form of zeolite was obtained by calcining in air at 550 ºC for 5 hours. Ion-exchange with Cu(II) to produce Cu/SSZ-13 was performed in the presence of copper nitrate. The resulting sample was calcined at 550 ºC in air.

$NO[BF_4]$ nitrosyl tetrafluoroborate (99%) was purchased from Strem Chemicals and stored cold in the absence of moisture.

All the chemicals used were the highest-grade purity available.

HAADF-STEM analysis was performed with a FEI Titan 80–300 microscope operated at 300 kV. The instrument is equipped with a CEOS GmbH double-hexapole aberration corrector for the probe-forming lens, which allows for imaging with 0.1 nm resolution in scanning transmission electron microscopy mode (STEM). The images were acquired with a high angle annular dark field (HAADF) detector with inner collection angle set to 52 mrad.

Helium ion microscopy (HIM) images were obtained using 35 keV He ions with 0.1 pA beam current at normal incidence. Secondary electrons were detected using an Everhart–Thornley detector. For HIM imaging, a very thin layer of carbon (<1 nm) was coated using a carbon sputter deposition system as the samples were completely insulating. The instrument resolution was 0.35 nm.

The *in-situ* static transmission IR experiments were conducted in a home-built cell housed in the sample compartment of a Bruker Vertex 80 spectrometer, equipped with an MCT detector and operated at 4 cm^{-1} resolution. The powder sample was pressed onto a tungsten mesh which, in turn, was mounted onto a copper heating assembly attached to a ceramic feedthrough. The sample could be resistively heated, and the sample temperature was monitored by a thermocouple spot welded onto the top center of the W grid. The cold finger on the glass bulb containing CO (99.995%) was cooled with liquid nitrogen to eliminate any contamination originating from metal carbonyls, while NO (99.95%) was cleaned with multiple freeze–pump–thaw cycles. $^{15}NH_3$ (15N, 98%) was purchased from Cambridge Isotopes. Special research-grade oxygen (purity 99.995%) was purchased from Oxarc.

The NO reduction by ammonia (in the presence of oxygen) was carried out in a typical quartz the plug-flow reactor. 120 mg of H-zeolites was used for reaction tests. The composition of the gas flowing through the catalyst was ~ 360 ppm NH_3, 360 ppm NO, ~12 % O_2 balanced with nitrogen. The total flow rate was ~ 300 sscm/min. Concentrations of reactants and products were measured by the MKS FTIR analyzer.

Computational details

We performed periodic DFT calculations with VASP program [S2] using PBE functional [S3] with empirical correction D2 for the dispersion interactions [S4], as well as PAW pseudopotentials S5]. The cut-off energy was set to 700 eV. The *Brillouin zone was sampled* by using the Gamma point only. For the geometry optimization, the threshold for the relaxation of the forces acting on each atom is 5×10^{-2} eV/Å. The chabazite model contains in total 108 atoms per unit cell (36 T atoms and 72 O atoms) with the following dimensions: a = b = 13.675 Å, c = 14.767 Å; $\alpha = \beta = 90^{o}$, $\gamma = 120^{o}$. To create negative charge in the zeolite framework one or two Si are substituted with Al. The general location of the species sorbed in the pores of the periodic chabazite model is presented in Figure 7A.

The energies of the reactions are calculated as follows: $\Delta E=E_P-E_R$, where the E_p is the total energy of the products and E_R is the total energy of the reactants. Thus, negative value of ΔE indicates that the reaction is energetically favorable. In the same way, the activation barriers are calculated as the difference between the energies of the transition state and the initial state (reactants).

References:

S1 M.A. Camblor, A. Corma, S. Valencia Synthesis in fluoride media and characterisation of aluminosilicate zeolite beta, J. Mater. Chem., 8 (1998), pp. 2137-2145

S2 G. Kresse, J. Furthmüller, Comput. Mater. Sci. 1996, 6, 15.
S3 J. P. Perdew, K. Burke, M. Ernzerhof, Phys. Rev. Lett. 1996, 77, 3865.
S4 S. Grimme. J. Comput. Chem. 2006, 27, 1787−1799.
S5 P. E. Blöchl, Phys. Rev. B, 1994, 50, 17953.

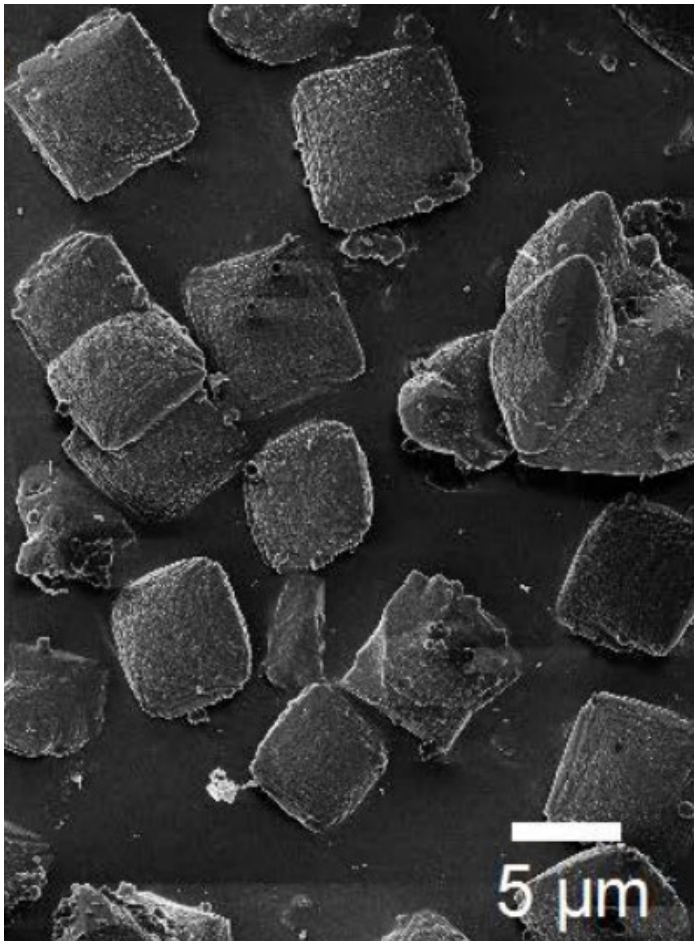


Figure S0. Typical Helium Ion Microscopy (HIM) image of H-BEA crystals with Si/Al ~ 15.

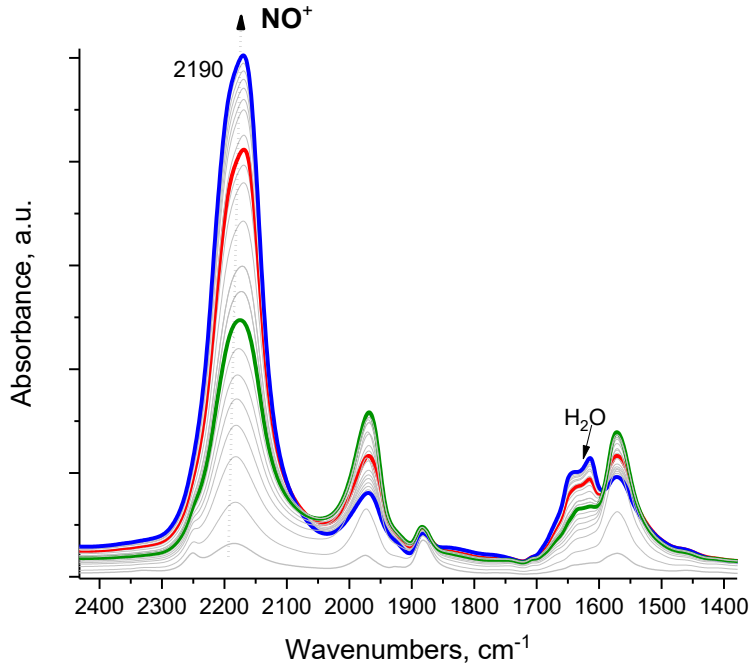


Figure S1. *In-situ* FTIR during sequential NO (0.5 Torr) and O_2 (0.1 Torr) co-adsorption on H-SSZ-13 with Si/Al~12 at room temperature.

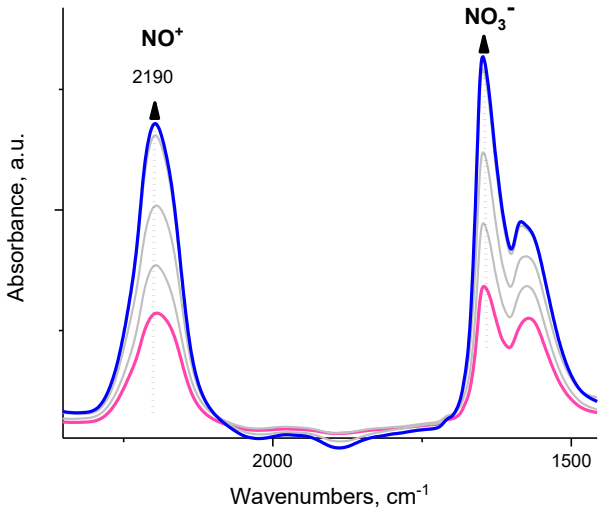


Figure S2. *In-situ* FTIR during sequential NO_2 (0.5 Torr) on H-SSZ-13 with Si/Al~12 at room temperature. NO_2 forms N_2O_4 in the pores and immediately reacts with H-SSZ-13 to form NO^+ and HNO_3.

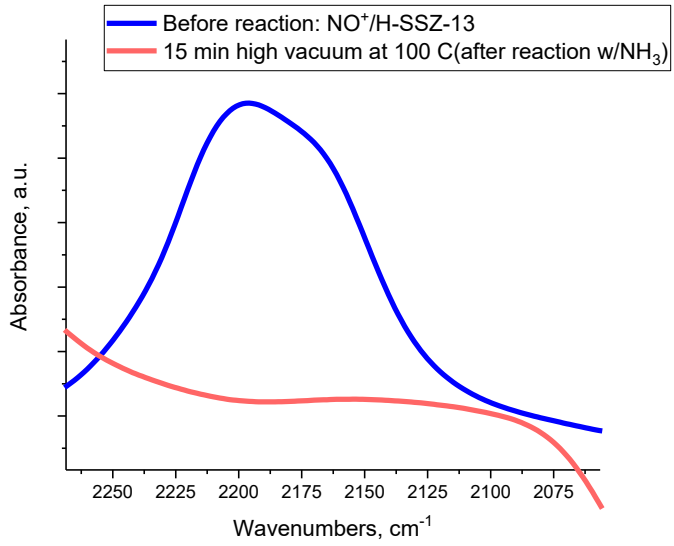
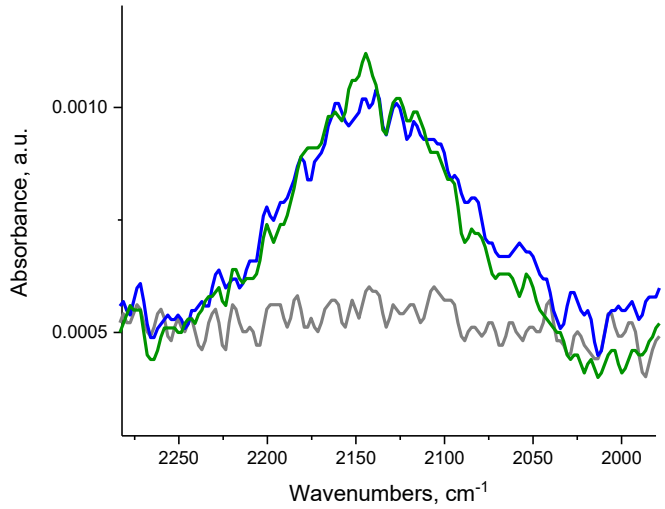
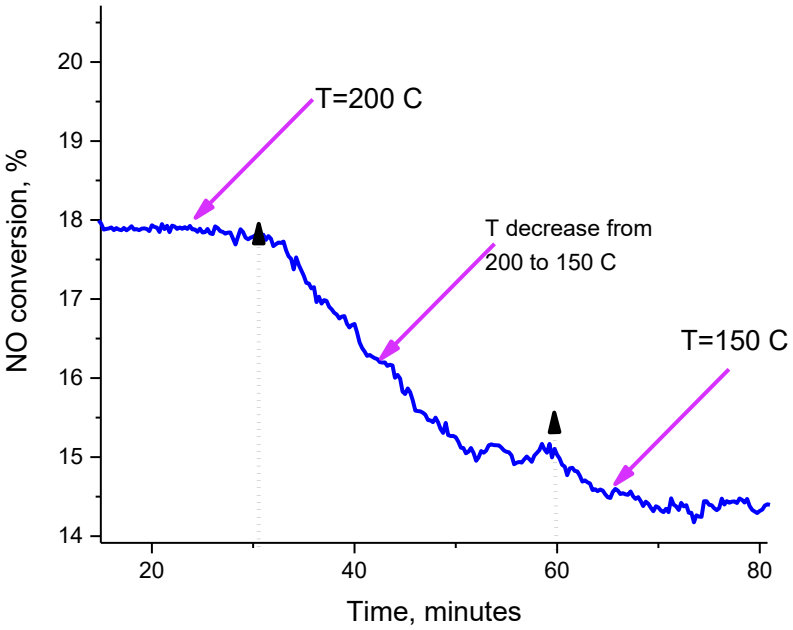


Figure S3. *Continuing from Fig 5 in the Main Text.* FTIR of the N-O stretching region of NO^+/H-SSZ-13 system before reaction with ammonia, and after reaction with ammonia (at room temperature), and after pulling high vacuum at 100 ºC for 15 minutes.



Figs. S4. *Continuing FTIR experiments after the ones performed in Fig 2A*. After reaction between NO^+/H-BEA with $^{15}NH_3$, the sample was vacuumed at room temperature and new baseline was collected (gray spectrum). 2 Torr NO + 0.7 Torr O_2 were then reacted with the sample: the resulting spectra (green and blue) show that because NH_3 occupied Brønsted acid sites of zeolite with the formation of NH_4-Zeolite (ammonia is strongly adsorbed and cannot be desorbed at room temperature even to a small extent), only extremely small amounts of NO^+ can be formed (intensities barely above the noise level).



Figs. S5. NO conversion (%) vs time-on-stream for H-BEA Si/Al ~ 15 sample under dry conditions (conditions specified in experimental section).

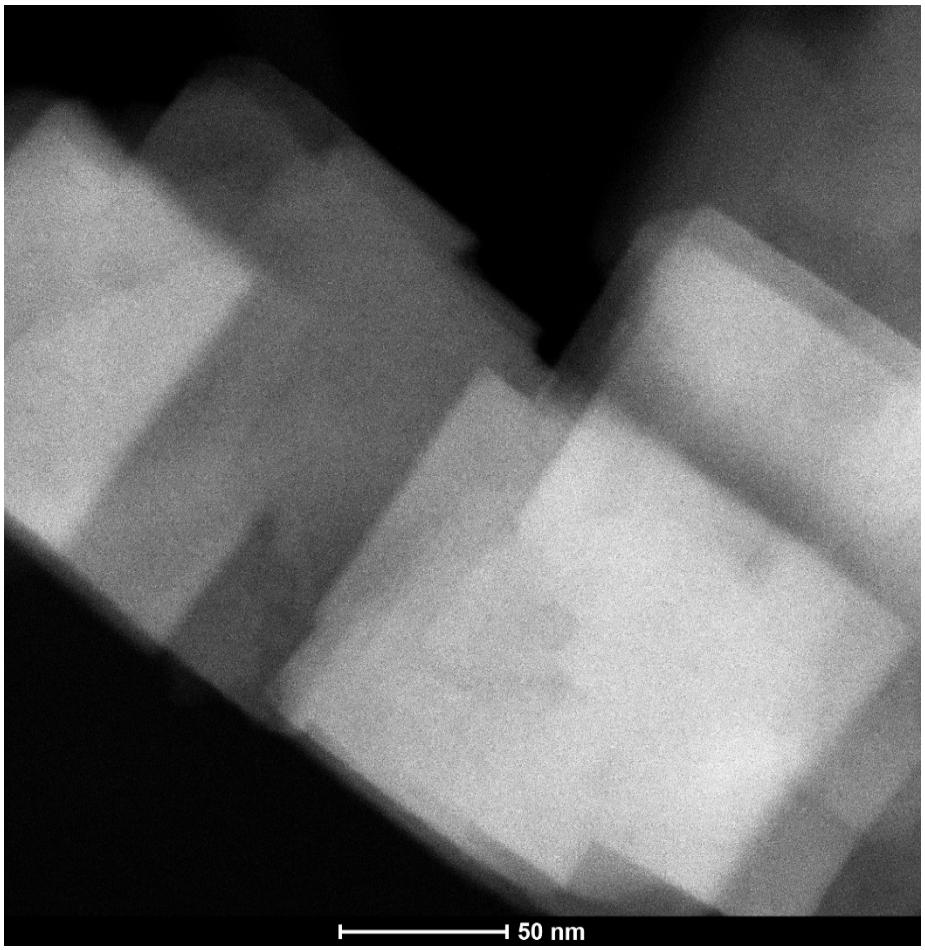
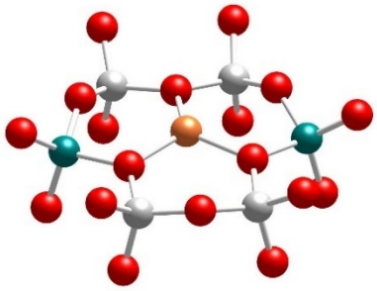
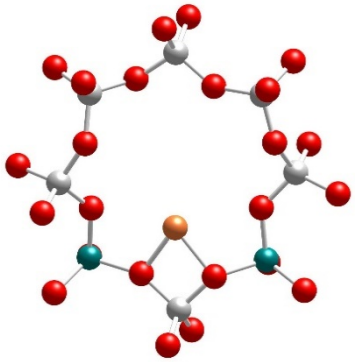


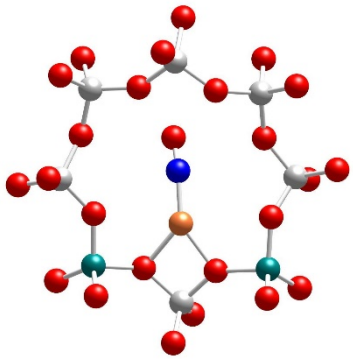
Figure S6. Typical HAADF-STEM images of SSZ-13 crystals.



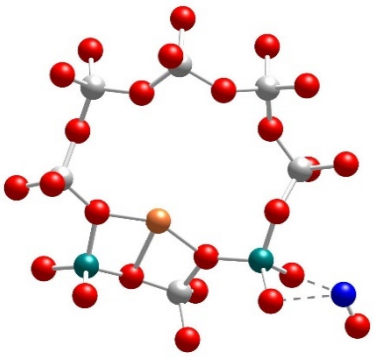
ZEO(2Al_6ring)/Cu^{2+}



ZEO(2Al_8ring)/Cu^{2+}



ZEO(2Al_8ring)/Cu^{2+}(NO)



ZEO(2Al_8ring)/(Cu^{+} + NO^{+})

Figure S7. Optimized structures of selected models. The models are visualized with VESTA program [34].

Geometry Coordinates

Direct participation of the chabazite

$NO^{+}(NH_3)$/ZEO

O	-4.812760	10.672171	1.894533
O	1.970147	6.763582	6.922444
O	8.956755	2.704412	11.577582
O	0.012091	2.348449	1.841707
O	0.056012	10.254211	6.820179
O	6.864757	6.289095	11.582950
O	4.823052	10.671385	1.895247
O	-2.095356	6.629193	6.774483
O	4.827638	2.691293	11.754954
O	11.646618	1.142530	12.871969
O	-2.022668	9.055925	3.049286
O	4.887120	5.080087	8.023171
O	6.866096	9.441485	12.921076
O	-0.003938	5.546252	2.852763
O	6.853324	1.395553	8.076541
O	2.109101	1.124675	12.787311

```
O    2.063421    9.086314    3.044599
O    8.820814    5.141383    8.017162
O   -4.445854    8.086383    2.470180
O    2.455756    4.039127    7.430955
O    9.236070    0.143751   12.331969
O    2.083754    3.991804    2.293957
O    8.989884    0.009705    7.316527
O    8.915799    7.817846   12.366186
O    2.397482   11.664625    2.436932
O    9.218654    7.714856    7.357362
O    2.402980    3.728982   12.258758
O   -2.393390   11.636159    2.472245
O    4.455190    7.653156    7.346431
O   11.338786    3.726916   12.230010
O    4.476742    8.097469    2.510693
O   11.118089    4.054376    7.195057
O    4.545305    0.111481   12.378118
O   -2.073367    3.947753    2.386569
O   -2.079747   11.759931    7.398277
O    4.814017    7.831874   12.351660
O    6.847665    8.996076    1.977010
O   -0.107956    4.928445    7.015654
O    6.888777    1.080178   11.736431
O    2.469108    1.423535    1.991592
O    2.535577    9.336893    6.857320
O    9.298825    5.304084   11.782908
O   11.226071    1.425310    1.915344
O   -2.368950    9.231183    6.888722
O    4.444371    5.304216   11.851328
O    0.031209    2.766275   12.672658
O    0.007275   10.724054    2.888028
O    6.837212    6.861947    7.995253
O    4.419249   10.382859   12.749074
O   -2.468151    6.465469    2.903691
O    4.503356    2.483163    7.893302
O   -4.342377   10.370105   12.761715
O    2.436262    6.507646    2.767099
O    9.183388    2.536773    7.957001
O   -5.024661    8.783819    0.019807
O    1.730670    4.868322    4.766219
O    8.726402    0.701039    9.833840
O    1.762256    2.947424   14.692878
O    1.747754   10.977287    4.888282
O    8.743066    7.065941    9.855107
O    3.338153   11.774243   14.753243
O   -3.533848    7.882362    4.907711
O    3.367664    3.893068    9.857631
O   -3.336761   11.821694    0.007314
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O   10.474692    3.999941    9.770919
O    5.056656    8.784897    0.021648
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O    4.989387    0.781384    9.880139
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Si	1.572941	2.683232	1.518960
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Si	8.444795	6.621086	11.388215
Si	3.741246	11.836866	1.557435
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Si	3.085570	7.852972	6.493601
Si	10.004403	3.921950	11.329556
Si	5.289997	9.142107	1.592843
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Si	-1.541727	2.698338	1.515566
Si	-1.515768	10.543201	6.490833
Si	5.283674	6.613463	11.398127
Si	-1.518130	2.662007	13.140253
Si	-1.535227	10.578827	3.345372
Si	5.268009	6.635623	8.299308
Si	5.300442	9.109467	13.218230
Si	-1.531686	5.198456	3.265489
Si	5.274457	1.142369	8.318156
Si	-3.681971	11.782892	13.191550
Si	3.098570	7.861620	3.328607
Si	9.899597	3.945872	8.239164
Si	3.752118	11.788262	13.189515
Si	-3.105397	7.876880	3.343531
Si	3.793307	3.886192	8.260967
Si	1.581367	2.625922	13.124035
Si	1.559212	10.601476	3.322391
Si	8.407497	6.688315	8.305812
Si	-5.243607	9.105962	13.215898
Si	1.559337	5.218261	3.225227
Si	8.434398	1.158894	8.300885
Al	1.537753	5.114453	6.448104
H	0.195155	5.054252	8.722089
H	1.427842	4.528364	9.793697
H	0.066869	5.332870	10.435361
N	1.699028	6.863129	9.356613
N	0.690058	5.225353	9.631614

TS $NO^+(NH_3)$/ZEO → $NONH_2/H^+$-ZEO

O	1.981658	1.196868	1.853798
O	8.707891	5.141585	6.654119
O	2.090210	9.158137	11.513103
O	11.621031	1.214012	1.881842
O	4.804426	5.211409	6.783937

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O   -2.008083    9.104586   11.658828
O    6.814589    9.578811    1.866007
O    6.831457    1.568979    6.710238
O    0.022365    5.566411   11.659249
O    4.810173   10.708976   12.907295
O    4.812517    2.827074    3.081482
O   -1.969892    6.796874    8.116677
O   -4.793739   10.732434   12.832390
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O    2.073660    6.721261    8.015793
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O    2.412521    4.159185    7.376887
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O    0.024438   10.771175   11.729839
O    4.332648   10.459960    1.879141
O    4.428474    2.604160    6.859775
O   -2.433768    6.518479   11.781657
O   11.254799    1.447305   12.643519
O    4.361121    5.411063    2.873590
O   -2.516273    9.365341    7.888046
O    6.854441    9.061561   12.715597
O    6.812027    1.117275    2.962304
O    0.034329    5.103565    7.947987
O    2.516266    1.486032   12.766546
O    9.272191    5.422496    2.933114
O    2.387113    9.304057    7.981938
O    3.495962    0.022602   14.763927
O   10.372991    3.762016    4.746386
O    3.677271    7.865870    9.812567
O   -1.683223    2.978385   14.699420
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O	5.004839	7.052435	4.870437
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O	5.124207	8.787256	14.733139
O	4.993234	0.882084	4.902006
O	-1.795665	4.768777	9.859001
O	1.704980	3.076755	14.761541
O	8.587491	7.150984	4.883147
O	1.790228	11.188142	9.768538
O	-5.103841	8.895777	14.747918
O	8.689605	1.080954	4.842777
O	1.858574	4.808147	9.864567
O	10.138609	0.138526	14.710585
O	3.297811	4.040344	4.906713
O	-3.614554	7.947782	9.853734
O	8.599335	4.479817	9.970252
Si	3.080487	0.034399	1.564940
Si	3.158323	7.937934	11.347328
Si	-1.564303	2.729287	1.531264
Si	5.269309	6.739550	6.439583
Si	-1.553050	10.642407	11.390436
Si	5.270173	9.193469	1.532366
Si	5.250574	1.278144	6.452889
Si	-1.542888	5.231589	11.399407
Si	1.516898	2.728909	1.571404
Si	8.356748	6.684637	6.435360
Si	1.578102	10.683048	11.312997
Si	-5.303161	9.210074	1.560706
Si	8.393575	1.236275	6.419164
Si	1.598830	5.241187	11.406386
Si	10.535727	0.056681	1.524903
Si	3.744195	4.016354	6.468729
Si	-3.111868	7.935572	11.394500
Si	10.579626	0.062261	13.155173
Si	3.718641	4.004838	3.337520
Si	-3.133411	7.922875	8.295173
Si	-5.275274	9.212506	13.171450
Si	8.382114	1.335941	3.261640
Si	1.595857	5.198285	8.305973
Si	1.588248	2.742943	13.180129
Si	8.382103	6.698378	3.340420
Si	1.510804	10.616203	8.255576
Si	5.310593	9.181420	13.174737
Si	5.258118	1.286732	3.350415
Si	-1.539206	5.231214	8.291578
Si	-1.508441	2.701141	13.126556
Si	5.255148	6.685792	3.312334
Si	-1.629102	10.645655	8.295333
Si	3.129747	0.050033	13.187802
Si	9.920007	3.969735	3.234363
Si	3.137824	7.911876	8.279584
Al	9.950750	3.970244	6.389986
H	9.520855	2.417156	8.341892
H	9.798225	1.652014	10.033803

H	10.594509	3.141799	9.649061
N	8.500866	3.313833	10.122273
N	9.747703	2.551344	9.539714

$NONH_2/H^+$-ZEO

O	-4.811407	10.712015	1.876695
O	1.999328	6.849259	6.507739
O	9.003945	2.750186	11.498055
O	0.033616	2.410380	1.907603
O	0.068443	10.292596	6.792477
O	6.879065	6.308843	11.675757
O	4.844749	10.696980	1.908495
O	-2.099079	6.702476	6.701592
O	4.825985	2.754096	11.724512
O	11.654260	1.203346	12.897439
O	-1.993765	9.084197	3.078474
O	4.877774	5.097918	8.082312
O	6.905778	9.507359	12.782641
O	0.025608	5.612742	2.781463
O	6.851074	1.545880	8.038767
O	2.118744	1.152865	12.714428
O	2.071475	9.100056	3.002669
O	8.883858	5.193046	8.016235
O	-4.395851	8.122422	2.399082
O	2.430539	4.144808	7.441447
O	9.256248	0.211894	12.315537
O	2.122119	4.073034	2.208510
O	8.957804	0.096253	7.268214
O	8.957139	7.855320	12.352012
O	2.420663	11.693460	2.421445
O	-4.439228	7.767905	7.376829
O	2.428023	3.782736	12.320878
O	-2.378199	11.649039	2.434477
O	4.425058	7.650471	7.356644
O	11.363051	3.779184	12.238927
O	4.439647	8.082744	2.341069
O	11.170410	4.108075	7.195115
O	4.576659	0.178620	12.381310
O	-2.062225	3.981687	2.408416
O	-2.040563	11.825085	7.384782
O	4.828392	7.883773	12.339879
O	6.860788	9.012528	2.023667
O	-0.086669	5.033199	7.063972
O	6.908624	1.181006	11.765334
O	2.486290	1.464347	2.042238
O	2.569838	9.408967	6.870276
O	9.326700	5.350795	11.740270
O	11.247759	1.457507	1.877502
O	-2.374508	9.305195	6.847929
O	4.441572	5.360409	11.803669

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 O    0.046085    2.799154   12.633818
 O    0.027359   10.754325    2.861299
 O    6.842400    6.839815    7.876626
 O    4.452576   10.450900   12.684512
 O   -2.461136    6.493037    2.975817
 O    4.430394    2.517892    7.906333
 O   -4.282286   10.401208   12.753448
 O    2.498757    6.504282    3.047541
 O    9.242673    2.580175    7.993985
 O   -5.098938    8.847817   14.753709
 O    1.540456    4.634438    4.729756
 O    8.669074    0.722420    9.809154
 O    1.735270    2.878860   14.691673
 O    1.766124   10.989702    4.862964
 O    8.646106    7.107657    9.845974
 O    3.365663   11.767580   14.737434
 O   -3.594863    7.956841    4.892021
 O    3.284898    3.903380    9.873078
 O    3.469536    0.071173   14.761151
 O    3.701398    8.080900    4.865070
 O   10.577566    4.066140    9.763861
 O    5.182634    8.905993   14.729502
 O   -1.512576    4.857926    4.838817
 O    5.050597    0.828348    9.873193
 O   -1.627086    3.123305   14.711328
 O   -1.685416   11.002269    4.901944
 O    5.082284    7.077332    9.850001
 O    1.460072    6.739048    9.917314
Si   -5.277615    9.185433    1.562489
Si    8.462213    1.220579   11.340650
Si    1.591121    2.711799    1.529103
Si    1.625084   10.637165    6.439812
Si    8.439494    6.660061   11.394724
Si   10.603050    0.014836    1.541822
Si   -3.132373    7.944011    6.445507
Si    3.768321    3.947914   11.422771
Si    3.109627    0.046212    1.578564
Si    3.146262    7.960479    6.403951
Si   10.047755    3.975327   11.312802
Si    5.322358    9.179042    1.554706
Si   -1.618428    5.193481    6.400628
Si    5.333583    1.237866   11.419642
Si   -1.512185    2.738634    1.525870
Si   -1.493387   10.609240    6.468249
Si    5.311279    6.661151   11.399274
Si   -1.489390    2.714339   13.148482
Si   -1.511418   10.619383    3.330741
Si    5.282309    6.660836    8.288583
Si    5.348900    9.184651   13.144485
Si   -1.481601    5.242687    3.245358
Si    5.283703    1.217207    8.309275
Si   -3.662931   11.835156   13.168440
Si    3.168690    7.937787    3.338148
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Si	9.945149	3.994191	8.256091
Si	3.768571	11.830700	13.170783
Si	-3.102675	7.926600	3.341279
Si	3.752339	3.934431	8.297460
Si	1.590570	2.641503	13.107322
Si	1.580058	10.619589	3.296793
Si	8.394575	6.725997	8.286634
Si	-5.226514	9.156610	13.169072
Si	1.556384	5.204579	3.235317
Si	8.419015	1.223685	8.282733
Al	1.623454	5.180950	6.347454
H	-0.045712	4.939503	8.085132
H	-0.510336	4.457851	10.233577
H	1.179954	4.404038	9.768664
N	0.354588	6.265325	10.090874
N	0.274152	4.903782	9.749541

$NONH_2$_rotated1/H^+-ZEO

O	2.04079	-1.20130	1.85272
O	8.81324	-5.03290	6.79258
O	8.94912	2.70844	11.53633
O	6.85176	-9.49022	1.81202
O	6.91352	-1.62526	6.75466
O	6.86524	6.28934	11.52798
O	11.66627	-1.19178	1.83928
O	4.75079	-5.17907	6.64022
O	4.84493	2.70677	11.64597
O	11.65684	1.14808	12.86267
O	4.82600	-2.81605	2.99107
O	4.90777	5.06209	7.94344
O	6.88456	9.45550	12.83820
O	6.82743	-6.29790	2.72257
O	6.86337	1.47568	8.00255
O	2.08191	1.10013	12.74316
O	8.91477	-2.76973	3.00000
O	8.84043	5.13498	7.92750
O	2.40901	-3.79598	2.38732
O	2.47864	4.06518	7.34426
O	9.25706	0.14364	12.25977
O	8.93636	-7.86886	2.25015
O	8.96873	0.01569	7.26619
O	8.92284	7.81621	12.30308
O	9.24195	-0.19199	2.37798
O	2.39623	-4.12945	7.32643
O	2.43628	3.70140	12.24423
O	4.45328	-0.22942	2.41687
O	4.46421	7.63829	7.29681
O	11.32544	3.71684	12.20656
O	11.31160	-3.77631	2.40002
O	11.16890	4.08787	7.18164
O	4.53970	0.13943	12.32931
O	4.75325	-7.92752	2.39126
O	4.81107	-0.06434	7.32749

O	4.82278	7.84921	12.27033
O	6.85640	8.97432	1.92907
O	6.75638	-6.81020	7.05873
O	6.89475	1.07398	11.71978
O	2.46119	1.39555	1.97150
O	9.41966	-2.48244	6.78864
O	9.29235	5.29671	11.76279
O	11.23543	1.40364	1.85547
O	4.47105	-2.59318	6.85948
O	4.44716	5.30762	11.83014
O	6.87118	-9.07682	12.66036
O	6.85384	-1.14601	2.82746
O	6.84874	6.85424	7.94103
O	11.27259	-1.45056	12.67799
O	4.35156	-5.41530	2.98076
O	4.46219	2.47022	7.87670
O	2.52840	-1.48610	12.70976
O	9.28293	-5.35414	2.76086
O	9.24202	2.52789	7.87560
O	1.80259	-3.06656	14.72253
O	8.44228	-7.00761	4.69921
O	8.70083	0.72463	9.77598
O	1.78122	2.91039	14.65906
O	8.59018	-0.86031	4.82752
O	8.75598	7.02711	9.80503
O	10.16985	-0.09901	14.69609
O	3.25369	-3.88019	4.86133
O	3.37073	3.95547	9.80644
O	3.49439	-0.02133	14.72769
O	10.36874	-4.05145	4.83654
O	10.44876	4.00282	9.73575
O	5.09083	8.79057	14.70879
O	5.33880	-7.06221	4.81836
O	5.05060	0.74690	9.82405
O	5.13233	-8.76225	14.67627
O	5.14362	-0.94422	4.86508
O	4.93559	6.97854	9.79930
O	6.73825	-6.52655	9.51060
Si	8.40832	9.12166	1.52161
Si	8.45210	1.17758	11.31761
Si	1.57983	2.66047	1.47896
Si	8.46089	-1.24522	6.39461
Si	8.44790	6.60801	11.34448
Si	10.58516	-0.02579	1.49527
Si	3.71222	-3.94385	6.41259
Si	3.77961	3.90591	11.36802
Si	3.11116	-0.01696	1.53874
Si	9.96727	-3.96271	6.40750
Si	10.00574	3.92271	11.30140
Si	5.30499	9.12840	1.51678
Si	5.24510	-6.69805	6.38203
Si	5.32241	1.17804	11.36800
Si	5.29642	-9.15265	1.47970

Si	5.34522	-1.30000	6.43593
Si	5.28173	6.60347	11.34606
Si	5.32480	-9.16885	13.11447
Si	5.31176	-1.28859	3.28509
Si	5.28004	6.61343	8.24393
Si	5.32073	9.12016	13.13754
Si	5.33372	-6.66940	3.22907
Si	5.29471	1.15908	8.26907
Si	3.15422	-0.05812	13.14098
Si	9.96195	-3.98666	3.26490
Si	9.91620	3.94782	8.20184
Si	10.59934	-0.05328	13.13496
Si	3.72181	-3.96871	3.30762
Si	3.78564	3.89634	8.22876
Si	1.58513	2.61434	13.08295
Si	8.40571	-1.25301	3.26429
Si	8.41642	6.67316	8.25678
Si	1.60619	-2.73732	13.14921
Si	8.37662	-6.63953	3.14981
Si	8.43489	1.18441	8.24062
Al	8.43794	-6.69667	6.36652
H	8.41061	-3.99672	9.98224
H	6.78683	-6.66488	8.16859
H	8.19330	-4.83581	8.40183
N	7.27552	-5.56543	10.13693
N	7.98298	-4.74054	9.43324

TS $NONH_2$_rotated1/H^+-ZEO → HN=NOH/H^+-ZEO

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O	2.165116	9.123139	11.482099
O	11.620525	1.193956	1.838048
O	4.808478	5.196223	6.762656
O	-2.038655	9.103974	11.478241
O	6.849160	9.511361	1.857561
O	6.910382	1.515161	6.760411
O	0.082212	5.499292	11.630349
O	4.827831	10.661805	12.855589
O	4.808531	2.772893	2.979909
O	-1.889604	6.810532	7.985482
O	-4.713602	10.662414	12.964552
O	8.892678	2.757894	2.733241
O	2.228914	6.627668	7.933903
O	0.087866	2.379247	12.732209
O	6.837645	6.333387	2.989824
O	-0.042518	10.194598	7.944286
O	4.458273	0.166611	2.472435
O	-2.239016	4.229827	7.306588
O	4.517118	8.083192	12.265911
O	11.290392	3.819173	2.251930
O	4.513929	7.813051	7.290376
O	-2.305197	11.626089	12.322766

O	4.770487	7.911259	2.389621
O	-2.058231	11.843437	7.305103
O	-2.009991	3.966048	12.260125
O	2.394265	3.764441	2.430495
O	-4.348948	7.627784	7.282365
O	2.438138	11.670656	12.201112
O	8.904230	7.950851	2.514782
O	2.052898	11.639678	7.124665
O	2.175195	3.993350	12.348472
O	9.216904	0.147416	2.372618
O	2.452510	4.059311	7.362125
O	-4.373902	8.095326	12.300606
O	-4.357728	10.430136	1.883333
O	9.369583	2.381798	7.027394
O	2.486545	6.528569	11.790144
O	0.009568	2.817679	1.981671
O	6.870956	6.842546	6.827731
O	0.060319	10.669977	11.751790
O	4.387317	10.436435	1.857996
O	4.533757	2.585677	6.878777
O	-2.340863	6.521134	11.834935
O	11.307794	1.404960	12.639005
O	4.388182	5.374634	2.886589
O	-2.553269	9.373831	7.994621
O	6.905292	9.048088	12.709035
O	6.849386	1.110981	2.868142
O	0.118901	5.110042	7.948600
O	2.531378	1.420997	12.729016
O	9.252137	5.364627	2.657094
O	2.410926	9.223914	7.957123
O	3.616435	0.095222	14.761933
O	10.246858	3.941815	4.687942
O	3.736119	7.796738	9.792600
O	-1.635043	2.969625	14.661784
O	5.079962	7.041477	4.849311
O	-1.703476	11.143710	9.806259
O	5.162920	8.761210	14.705846
O	5.112166	0.925561	4.880242
O	-1.776338	4.887348	9.810469
O	1.754356	3.006325	14.739845
O	8.695611	6.767573	4.859410
O	1.736804	11.095409	9.717844
O	8.582013	8.707269	14.757975
O	8.683305	1.056417	4.801055
O	1.955085	4.779609	9.850661
O	10.167168	0.076998	14.668130
O	3.364540	3.945443	4.889840
O	-3.612738	7.723178	9.809601
O	9.115826	2.587764	9.631712
Si	3.146018	0.014127	1.546247
Si	3.214593	7.894347	11.329815
Si	-1.524815	2.693583	1.485872
Si	5.306577	6.708765	6.416176

Si	-1.501543	10.630689	11.336243
Si	5.300153	9.158262	1.505267
Si	5.338799	1.253669	6.447795
Si	-1.498645	5.216554	11.370198
Si	1.559008	2.689285	1.553494
Si	8.419648	6.590944	6.437885
Si	1.607496	10.637745	11.277530
Si	-5.269884	9.146720	1.548475
Si	8.467930	1.186857	6.402577
Si	1.660593	5.196186	11.394882
Si	10.559644	0.014736	1.478608
Si	3.788988	3.955103	6.456991
Si	-3.085566	7.870296	11.348433
Si	10.603424	0.027131	13.103445
Si	3.739498	3.955540	3.307400
Si	-3.082529	7.872972	8.270139
Si	-5.228533	9.136873	13.195627
Si	8.418114	1.282371	3.210927
Si	1.682468	5.142557	8.288900
Si	1.628512	2.697090	13.151084
Si	8.417949	6.600073	3.260260
Si	1.528948	10.546964	8.196006
Si	5.350400	9.152149	13.144288
Si	5.307105	1.257557	3.306489
Si	-1.462858	5.243365	8.246109
Si	-1.475954	2.678620	13.080088
Si	5.275639	6.663104	3.282202
Si	-1.578827	10.633437	8.266087
Si	3.194682	0.022448	13.197818
Si	9.930242	3.962358	3.126197
Si	3.215213	7.867058	8.255528
Al	10.061397	3.859837	6.372871
H	7.551533	5.214941	9.734620
H	9.239480	2.583557	8.598043
H	8.409005	4.711620	8.024163
N	8.417696	3.604762	10.088319
N	8.088068	4.489406	9.244728

HN=NOH /H^+-ZEO

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O	8.759340	5.054689	6.883296
O	2.162763	9.122781	11.485705
O	11.618822	1.194693	1.834134
O	4.818033	5.199914	6.761719
O	-2.037959	9.103916	11.474678
O	6.852561	9.505601	1.865947
O	6.902585	1.496751	6.721968
O	0.082401	5.500002	11.627247
O	4.828527	10.661891	12.851725
O	4.810481	2.765468	2.970991
O	-1.891185	6.811689	7.985306
O	-4.720690	10.666352	12.940112

O	8.892822	2.751700	2.726621
O	2.226760	6.629835	7.952001
O	0.088262	2.382247	12.730664
O	6.840467	6.347611	3.004088
O	-0.043751	10.205746	7.929669
O	4.473410	0.161596	2.447866
O	-2.247056	4.235757	7.303092
O	4.511966	8.080639	12.270197
O	11.292936	3.817442	2.256864
O	4.507104	7.815629	7.283613
O	-2.305684	11.626164	12.319563
O	4.767379	7.909787	2.379590
O	4.767486	0.006060	7.310375
O	-2.009619	3.967247	12.259303
O	2.397497	3.766565	2.425812
O	-4.349724	7.637182	7.282921
O	2.440877	11.672495	12.196178
O	8.915101	7.946579	2.496962
O	2.059722	11.647620	7.131193
O	2.175130	3.999435	12.351756
O	9.215353	0.142416	2.366831
O	2.455595	4.068525	7.349289
O	-4.371998	8.093901	12.300397
O	-4.356207	10.431027	1.888143
O	9.348519	2.393693	7.025940
O	2.488212	6.526773	11.765387
O	0.012149	2.814377	1.980965
O	6.868075	6.867443	6.796061
O	0.060824	10.670163	11.759415
O	4.392460	10.437635	1.852815
O	4.538099	2.590653	6.872734
O	-2.339896	6.520396	11.828783
O	11.310476	1.406143	12.640954
O	4.401968	5.367866	2.865975
O	-2.550390	9.376097	7.996739
O	6.903824	9.044570	12.693911
O	6.853208	1.102360	2.903117
O	0.117283	5.109288	7.936137
O	2.532338	1.425651	12.714792
O	9.244588	5.358589	2.647290
O	2.404198	9.225133	7.949031
O	3.597932	0.091523	14.751182
O	10.234618	3.945640	4.684526
O	3.745703	7.819160	9.789242
O	-1.633275	2.974438	14.662030
O	5.052581	7.039372	4.839562
O	-1.694220	11.144599	9.806208
O	5.176282	8.764700	14.702118
O	5.067265	0.914122	4.874675
O	-1.771135	4.883661	9.806598
O	1.757177	2.996259	14.738323
O	8.721647	6.776354	4.848146
O	1.730262	11.089259	9.718185

O	8.578035	8.724800	14.749085
O	8.719647	1.053451	4.800783
O	1.944013	4.759275	9.844872
O	10.166405	0.075250	14.664220
O	3.378984	3.955381	4.880736
O	-3.615968	7.724842	9.808675
O	9.078627	2.599893	9.647020
Si	3.147349	0.012800	1.540536
Si	3.215695	7.898126	11.324765
Si	-1.523119	2.694016	1.485850
Si	5.298700	6.715477	6.404824
Si	-1.498955	10.630536	11.336311
Si	5.304569	9.158576	1.502381
Si	5.324752	1.248805	6.436981
Si	-1.497793	5.215197	11.366539
Si	1.562292	2.686985	1.553427
Si	8.418501	6.620441	6.420712
Si	1.606108	10.637187	11.279137
Si	-5.267324	9.149609	1.543660
Si	8.469566	1.186352	6.397259
Si	1.659115	5.192504	11.386650
Si	10.559760	0.013921	1.474320
Si	3.795892	3.961284	6.450148
Si	-3.085023	7.870341	11.346581
Si	10.604759	0.027809	13.100214
Si	3.747750	3.954193	3.296705
Si	-3.081034	7.876527	8.271859
Si	-5.231755	9.141497	13.183440
Si	8.426722	1.276614	3.215818
Si	1.680067	5.139908	8.285452
Si	1.629719	2.698409	13.147597
Si	8.425024	6.603206	3.251302
Si	1.527392	10.550325	8.193285
Si	5.351721	9.152206	13.138980
Si	5.302044	1.249441	3.306086
Si	-1.462989	5.244083	8.242808
Si	-1.474842	2.681244	13.080564
Si	5.272222	6.663955	3.274725
Si	-1.578485	10.638607	8.264618
Si	3.188339	0.023996	13.184371
Si	9.925889	3.959064	3.120814
Si	3.213479	7.872896	8.255457
Al	10.060538	3.853558	6.368149
H	7.596533	5.267006	9.778366
H	9.196390	2.605787	8.619395
H	8.422501	4.768314	7.937132
N	8.415016	3.642514	10.115944
N	8.100691	4.528681	9.271774

HN=NOH_rotated1/H^+-ZEO

O	2.040793	1.164377	1.807795

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O    8.695867    4.994955    6.773075
O    2.090463    9.053255   11.611592
O   11.621902    1.167143    1.826325
O    4.838920    5.158474    6.729951
O   -2.016407    9.076140   11.521384
O    6.829107    9.505891    1.815332
O    6.908144    1.530302    6.712875
O    0.097801    5.522440   11.776833
O    4.854151   10.641736   12.797108
O    4.793691    2.765120    3.012389
O   -1.863084    6.819256    8.003294
O   -4.753981   10.657330   12.841199
O    8.904608    2.737769    2.871883
O    2.232434    6.594742    8.028976
O    0.095085    2.358793   12.685184
O    6.817434    6.309691    3.038756
O   -0.060561   10.164525    7.954385
O    4.447986    0.180096    2.419440
O   -2.327607    4.244956    7.396053
O    4.503106    8.053720   12.250350
O   11.250089    3.795074    2.171769
O    4.510870    7.759371    7.305338
O   -2.317803   11.615920   12.302787
O    4.770670    7.889212    2.360216
O   -2.045553   11.839241    7.297446
O   -2.009197    3.941950   12.228190
O    2.381837    3.739548    2.413083
O   -4.341949    7.552185    7.287762
O    2.447138   11.630179   12.176991
O    8.869600    7.909658    2.439105
O    2.028233   11.653365    7.184100
O    2.197713    3.962443   12.313025
O    9.189810    0.157818    2.293587
O    2.479626    4.048343    7.377873
O   -4.372489    8.070232   12.293297
O   -4.386281   10.421691    1.958229
O    9.402639    2.343816    6.895509
O    2.548725    6.459506   11.657083
O   -0.008500    2.810783    1.964050
O    6.863288    6.860581    6.741628
O    0.047212   10.699803   11.721951
O    4.358010   10.414468    1.857048
O    4.510597    2.552250    6.811468
O   -2.358724    6.492127   11.809681
O   11.310901    1.381326   12.571154
O    4.369524    5.358186    2.856426
O   -2.577210    9.362235    7.912834
O    6.896393    8.984482   12.697783
O    6.838374    1.123612    2.826389
O    0.109419    5.097754    7.773316
O    2.540794    1.411737   12.752479
O    9.219607    5.327933    2.638297
O    2.368292    9.178098    7.788171
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O	-3.274592	11.804832	14.735520
O	10.386451	4.040605	4.669824
O	3.691610	7.977301	9.775910
O	-1.629655	2.907036	14.619601
O	5.001447	7.033340	4.831916
O	-1.759829	11.080147	9.790563
O	5.124291	8.764241	14.680989
O	5.117752	0.856856	4.849316
O	-1.590743	4.893970	9.818091
O	1.718312	3.035059	14.714686
O	8.746160	6.795130	4.815610
O	1.795155	10.926095	9.718753
O	-5.061746	8.785768	14.728525
O	8.634750	0.872247	4.779782
O	1.750067	4.690590	9.831468
O	10.212797	0.053628	14.625760
O	3.319014	3.972597	4.878032
O	-3.593583	7.767372	9.801025
O	8.066903	4.564843	9.255179
Si	-3.717656	11.825820	1.528090
Si	3.193644	7.895045	11.319945
Si	-1.535492	2.664673	1.449394
Si	5.286430	6.685881	6.386206
Si	-1.515859	10.610335	11.327082
Si	5.278196	9.147173	1.480997
Si	5.343985	1.230295	6.409387
Si	-1.456503	5.216276	11.394221
Si	1.538718	2.684137	1.522561
Si	8.409320	6.610573	6.373951
Si	1.599620	10.574877	11.294849
Si	-5.284143	9.154383	1.527846
Si	8.463151	1.154523	6.373976
Si	1.635391	5.160567	11.382072
Si	3.719102	11.840729	1.446625
Si	3.786428	3.940349	6.434181
Si	-3.079428	7.860226	11.345865
Si	3.786611	11.842789	13.056343
Si	3.716500	3.947298	3.300469
Si	-3.074727	7.864541	8.258738
Si	-5.234883	9.133879	13.151838
Si	8.403582	1.235895	3.213570
Si	1.639031	5.107703	8.265548
Si	1.626937	2.688211	13.131651
Si	8.406344	6.580978	3.228133
Si	1.519054	10.491271	8.173851
Si	5.342127	9.125939	13.116930
Si	5.299811	1.242541	3.285220
Si	-1.436450	5.250070	8.234949
Si	-1.469965	2.646702	13.034501
Si	5.246882	6.646522	3.272359
Si	-1.599208	10.608354	8.242743
Si	-3.667506	11.827180	13.163794
Si	9.954030	3.961087	3.132822

Si	3.192896	7.873793	8.236167
Al	10.095861	3.818058	6.333055
H	9.402072	2.555454	9.058551
H	7.439544	5.156794	9.712335
H	8.345141	4.754105	7.711649
N	8.130514	3.332779	10.299243
N	8.887337	2.477855	9.965694

TS HN=NOH_rotated1 → (N_2 + H_2O)/H^+-ZEO

O	2.057678	1.172547	1.832506
O	8.727504	5.033446	6.802157
O	2.100302	9.047461	11.664136
O	11.612739	1.178719	1.867976
O	4.830551	5.157110	6.711927
O	-2.045937	9.096324	11.485121
O	6.835373	9.486679	1.821929
O	6.908846	1.475809	6.760192
O	0.108544	5.521101	11.848028
O	4.839323	10.634856	12.785733
O	4.767354	2.782053	3.023028
O	-1.900132	6.758418	7.974738
O	-4.742104	10.648242	12.833072
O	8.986856	2.716939	3.064171
O	2.199036	6.577317	8.056124
O	0.088994	2.378032	12.687439
O	6.802137	6.320568	2.963074
O	-0.050304	10.227846	7.950462
O	4.471783	0.192252	2.409011
O	-2.383321	4.145631	7.527133
O	4.516002	8.041945	12.248422
O	11.254978	3.808561	2.187905
O	4.475187	7.742181	7.304151
O	-2.311137	11.625939	12.309254
O	4.744678	7.906541	2.372816
O	-2.086053	11.821473	7.267983
O	-2.022087	3.959494	12.263382
O	2.368353	3.761260	2.411066
O	-4.341183	7.603725	7.258048
O	2.432534	11.639534	12.192813
O	8.888591	7.899924	2.439328
O	2.089382	11.676312	7.239378
O	2.214220	3.955932	12.322583
O	9.176047	0.174519	2.271757
O	2.491624	4.033599	7.413914
O	-4.380860	8.063258	12.287674
O	-4.380995	10.424662	1.973202
O	9.393362	2.344584	6.751821
O	2.559671	6.448089	11.645280
O	-0.007915	2.804657	1.975793
O	6.856794	6.857877	6.815813
O	0.040870	10.685337	11.710887

O	4.370418	10.430807	1.864968
O	4.527035	2.551069	6.795127
O	-2.340405	6.515992	11.830385
O	11.311606	1.385756	12.559519
O	4.342075	5.380654	2.901751
O	-2.528734	9.333950	7.946141
O	6.896767	8.991246	12.716816
O	6.849509	1.213548	2.787176
O	0.085783	5.045434	7.757775
O	2.527059	1.402439	12.752558
O	9.196751	5.305721	2.672816
O	2.332953	9.159090	7.774050
O	-3.285994	11.804027	14.740014
O	10.495774	4.178026	4.711164
O	3.664182	7.995594	9.776123
O	-1.638694	2.882991	14.636915
O	5.071435	7.056565	4.840999
O	-1.761601	11.121917	9.783090
O	5.114057	8.774538	14.687610
O	5.164713	0.863657	4.834293
O	-1.538614	4.911788	9.861846
O	1.712544	3.021159	14.721518
O	8.657176	6.810887	4.817496
O	1.824711	10.886481	9.740613
O	-5.045367	8.792615	14.734425
O	8.540086	0.712852	4.780903
O	1.692678	4.676759	9.849342
O	10.241172	0.072827	14.629834
O	3.277295	3.963858	4.893158
O	-3.596054	7.729871	9.792249
O	8.153958	4.667833	9.170055
Si	-3.708953	11.828345	1.538574
Si	3.196410	7.891820	11.328327
Si	-1.538097	2.667693	1.471205
Si	5.294556	6.687598	6.400892
Si	-1.524777	10.624940	11.314255
Si	5.277395	9.152426	1.489277
Si	5.346382	1.215240	6.405084
Si	-1.442675	5.231369	11.438582
Si	1.539163	2.684478	1.532939
Si	8.397638	6.620994	6.391945
Si	1.601752	10.560046	11.316953
Si	-5.272005	9.150219	1.537190
Si	8.453588	1.110821	6.357700
Si	1.631504	5.153639	11.401512
Si	10.561012	0.009888	1.455084
Si	3.778935	3.933956	6.439634
Si	-3.088873	7.859448	11.335980
Si	10.625352	0.004518	13.055414
Si	3.690679	3.961795	3.318359
Si	-3.075348	7.844116	8.250382
Si	-5.229848	9.129950	13.156468
Si	8.403611	1.219156	3.241114

Si	1.611572	5.083665	8.277716
Si	1.625301	2.685605	13.136467
Si	8.384604	6.579110	3.223961
Si	1.534976	10.496798	8.187195
Si	5.338936	9.124236	13.121300
Si	5.312764	1.270035	3.271472
Si	-1.451644	5.204228	8.263659
Si	-1.476266	2.651259	13.047488
Si	5.246377	6.663333	3.273752
Si	-1.600327	10.623061	8.241166
Si	-3.667595	11.824371	13.165795
Si	9.999522	3.990126	3.200782
Si	3.161235	7.861278	8.238479
Al	10.092346	3.865653	6.340701
H	9.600127	2.588806	8.850517
H	7.335116	5.087345	9.496855
H	8.394404	4.816497	7.828543
N	8.093300	3.146626	9.995807
N	8.936304	2.413669	9.641882

$(N_2 + H_2O)/H^+$-ZEO

O	2.071930	1.155974	1.826382
O	8.721009	5.159623	6.724072
O	2.098627	9.072549	11.520309
O	11.606823	1.179296	1.818148
O	4.863944	5.191823	6.743743
O	-2.038315	9.098200	11.499994
O	6.854285	9.514584	1.880576
O	6.843027	1.461019	6.563913
O	0.082258	5.534984	11.717433
O	4.841292	10.666645	12.834925
O	4.833181	2.750149	2.956994
O	-1.994406	6.755261	7.938601
O	-4.757490	10.681921	12.737179
O	8.870463	2.734250	2.709746
O	2.167074	6.659523	8.058021
O	0.075558	2.366747	12.742841
O	6.840418	6.353623	3.103597
O	-0.046613	10.246423	7.888294
O	4.507842	0.171483	2.337393
O	-2.330491	4.147864	7.382107
O	4.462611	8.079903	12.285336
O	11.279596	3.794725	2.268809
O	4.454817	7.786777	7.247709
O	-2.312607	11.645872	12.289300
O	4.783552	7.882657	2.328783
O	4.736310	0.006832	7.312061
O	-2.010857	3.957796	12.237759
O	2.401578	3.728551	2.424032
O	-4.433500	7.714294	7.298624
O	2.447781	11.642066	12.180975

O	8.900717	7.855807	2.302056
O	2.057711	11.715766	7.200397
O	2.162807	3.983329	12.308101
O	9.203883	0.121700	2.356078
O	2.458472	4.135236	7.306732
O	-4.379714	8.077391	12.294072
O	-4.347518	10.405587	1.969129
O	9.261539	2.421962	7.033345
O	2.528125	6.475329	11.624519
O	0.008677	2.789123	1.959881
O	6.833692	6.994115	6.604677
O	0.046407	10.687336	11.761819
O	4.381990	10.416108	1.840545
O	4.498966	2.586269	6.845272
O	-2.359443	6.510029	11.799256
O	11.285878	1.409325	12.638001
O	4.431693	5.334496	2.772876
O	-2.516873	9.343569	7.951551
O	6.881240	9.021629	12.607411
O	6.853560	1.047546	3.035342
O	0.069034	5.125612	7.781569
O	2.533432	1.437213	12.722754
O	9.239022	5.330272	2.766748
O	2.390613	9.242063	7.862992
O	-3.328487	11.785811	14.698923
O	10.257637	3.776348	4.712454
O	3.749733	7.958658	9.765714
O	-1.659603	2.978726	14.659739
O	4.878419	6.999106	4.792644
O	-1.698637	11.108622	9.790281
O	5.222070	8.780512	14.679523
O	4.906517	0.866411	4.838743
O	-1.647046	4.883958	9.804981
O	1.752401	3.027748	14.723348
O	8.795230	7.023560	4.795380
O	1.733008	11.038645	9.729183
O	-5.123321	8.893855	14.682362
O	8.830489	1.062831	4.800930
O	1.756744	4.684766	9.799615
O	10.153943	0.052770	14.653989
O	3.412102	3.985840	4.849106
O	-3.620618	7.772663	9.799089
O	7.997927	5.283526	9.578036
Si	-3.702675	11.811450	1.507479
Si	3.204450	7.897338	11.294712
Si	-1.533849	2.683109	1.481772
Si	5.269481	6.723110	6.343740
Si	-1.511395	10.624113	11.331142
Si	5.318038	9.151652	1.486158
Si	5.233277	1.229386	6.383302
Si	-1.478926	5.222225	11.373994
Si	1.561450	2.672951	1.530049
Si	8.404974	6.695813	6.344923

Si	1.589441	10.596872	11.296551
Si	-5.274226	9.165187	1.507147
Si	8.403432	1.138962	6.342040
Si	1.623789	5.168934	11.346926
Si	3.716254	11.836104	1.463060
Si	3.807843	3.991164	6.425331
Si	-3.092437	7.871027	11.338307
Si	10.605253	0.015308	13.094127
Si	3.767963	3.945655	3.263554
Si	-3.131657	7.874169	8.241341
Si	-5.258495	9.174191	13.093474
Si	8.438709	1.259954	3.215880
Si	1.610266	5.147336	8.245398
Si	1.620499	2.704572	13.137416
Si	8.435853	6.636989	3.257849
Si	1.518359	10.543177	8.194744
Si	5.349094	9.146332	13.108916
Si	5.272033	1.222473	3.293272
Si	-1.493414	5.215914	8.217038
Si	-1.487037	2.680713	13.080168
Si	5.251817	6.643853	3.254505
Si	-1.592910	10.626583	8.243415
Si	3.152476	0.001887	13.120603
Si	9.923268	3.915637	3.157626
Si	3.193056	7.893380	8.241970
Al	9.976611	4.015867	6.372208
H	9.317271	2.373710	8.023012
H	8.209929	6.214578	9.764617
H	8.120982	5.194952	8.610510
N	9.060711	2.448910	9.878469
N	8.799235	2.585713	10.949046

$(NNH^+ + H_2O)$/ZEO

O	2.031454	1.133258	1.855701
O	8.829510	5.011196	6.875780
O	2.138254	9.062682	11.548633
O	11.626253	1.144382	1.829464
O	4.805396	5.135473	6.724394
O	-2.038362	9.074415	11.491865
O	6.839927	9.472213	1.818138
O	6.927422	1.533872	6.694059
O	0.081416	5.416078	11.448015
O	4.844363	10.611534	12.749079
O	4.784396	2.753830	2.950691
O	-1.887534	6.763368	7.933378
O	-4.739703	10.619402	12.876735
O	8.946049	2.684721	3.045279
O	2.189311	6.614982	7.907374
O	0.080042	2.309087	12.670654
O	6.800675	6.301522	3.051128
O	-0.020659	10.124578	7.969528

```
O    4.449833    0.150937    2.428301
O   -2.198710    4.160438    7.309385
O    4.506287    8.018030   12.268201
O   11.217550    3.767015    2.147651
O    4.530355    7.738178    7.332060
O   -2.318036   11.600081   12.308379
O    4.762125    7.875223    2.366205
O   -1.996660   11.803366    7.271875
O   -1.997204    3.936260   12.253194
O    2.372972    3.730152    2.392253
O   -4.356375    7.599301    7.283518
O    2.430547   11.635689   12.194067
O    8.873449    7.883658    2.480590
O    2.045528   11.668072    7.222583
O    2.145280    3.948249   12.340416
O    9.175465    0.151843    2.245758
O    2.426849    4.043121    7.318301
O   -4.372363    8.042448   12.284246
O   -4.371045   10.385520    1.937092
O    9.460024    2.301289    6.621568
O    2.447862    6.482808   11.830751
O   -0.018211    2.795479    1.984600
O    6.870129    6.788235    6.749289
O    0.043696   10.645010   11.768663
O    4.372093   10.401772    1.901582
O    4.494594    2.524048    6.834455
O   -2.303936    6.500778   11.856404
O   11.293789    1.365663   12.579685
O    4.350450    5.353993    2.868686
O   -2.537485    9.338552    7.957027
O    6.900285    8.965721   12.719896
O    6.834299    1.143797    2.772250
O    0.119838    5.047028    8.121548
O    2.528931    1.382553   12.719817
O    9.158797    5.277490    2.605447
O    2.452590    9.213659    7.939311
O   -3.284943   11.834209   14.742680
O   10.457645    4.197884    4.645529
O    3.669130    7.753452    9.808904
O   -1.614055    2.881444   14.622969
O    4.996361    7.026896    4.850392
O   -1.703296   11.094266    9.791614
O    5.107997    8.785704   14.689742
O    5.129875    0.890251    4.834116
O   -1.956854    4.878453    9.799687
O    1.694925    2.954086   14.718306
O    8.740094    6.711180    4.835662
O    1.746581   11.029026    9.756119
O    8.622910    8.717591   14.741271
O    8.526221    0.639777    4.749912
O    2.111010    4.755051    9.836181
O    3.410235   11.835139   14.627017
O    3.330168    3.909139    4.858797
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O	-3.557889	7.683440	9.796658
O	8.912514	4.281482	9.364642
Si	-3.719286	11.807225	1.539664
Si	3.188601	7.835077	11.355805
Si	12.134967	2.643778	1.454804
Si	5.288118	6.655830	6.401280
Si	-1.513827	10.600497	11.329413
Si	5.281491	9.134272	1.496808
Si	5.362881	1.227962	6.403454
Si	-1.518552	5.181290	11.343509
Si	1.526899	2.647472	1.537436
Si	8.427524	6.582156	6.407152
Si	1.590021	10.567707	11.315947
Si	8.401821	9.110303	1.538651
Si	8.463779	1.106723	6.313444
Si	1.682668	5.141246	11.356135
Si	3.729643	11.814108	1.452907
Si	3.770292	3.906453	6.421934
Si	-3.072302	7.833246	11.346931
Si	3.793859	11.814792	13.055904
Si	3.711261	3.927489	3.279111
Si	-3.065518	7.840921	8.248344
Si	-5.227201	9.093501	13.168996
Si	8.387943	1.174897	3.224051
Si	1.711131	5.112560	8.299462
Si	1.606124	2.643832	13.129511
Si	8.393099	6.540937	3.244008
Si	1.542288	10.511260	8.212959
Si	5.341933	9.106294	13.119528
Si	5.302757	1.242357	3.260994
Si	-1.475421	5.203410	8.251669
Si	-1.473685	2.621465	13.038317
Si	5.233069	6.637675	3.289323
Si	-1.557625	10.593777	8.247472
Si	-3.669661	11.811395	13.169454
Si	9.956877	3.962786	3.149610
Si	3.204559	7.828751	8.256100
Al	10.166268	3.810861	6.277557
H	9.102852	1.271523	10.074692
H	9.880967	4.327433	9.619426
H	8.686876	4.775435	7.866036
N	8.511916	2.900743	9.530521
N	9.442377	2.247363	9.986791

TS ($NNH^+ + H_2O$)/ZEO → (NNH^+_rotated + H_2O)/ZEO

O	2.023704	1.127038	1.816671
O	8.852832	5.030967	6.937834
O	2.132851	9.076178	11.465884
O	11.653554	1.131509	1.801559
O	4.829511	5.129111	6.712989
O	-2.000177	9.055611	11.506344
O	6.843045	9.476303	1.793739

```
O     6.924969    1.526744    6.675061
O     0.067735    5.436650   11.439013
O     4.861526   10.622286   12.781219
O     4.813142    2.758339    2.966315
O    -1.897657    6.744649    7.948598
O    -4.758482   10.630075   12.885942
O     8.903259    2.707193    2.977556
O     2.157546    6.643192    7.921899
O     0.080295    2.296223   12.723809
O     6.814524    6.280506    3.041452
O     0.005079   10.150695    8.027670
O     4.438993    0.160873    2.425213
O    -2.189350    4.139980    7.288176
O     4.484917    8.043985   12.265773
O    11.229829    3.747820    2.184570
O     4.511292    7.729352    7.310493
O    -2.324544   11.584454   12.303370
O     4.778626    7.869466    2.372672
O    -1.983712   11.799534    7.273651
O    -1.988572    3.923564   12.235464
O     2.389628    3.711069    2.405237
O    -4.354181    7.626376    7.275313
O     2.442800   11.631149   12.202861
O     8.868104    7.888871    2.488709
O     2.055139   11.671290    7.197508
O     2.123900    3.951154   12.320204
O     9.195755    0.155356    2.260911
O     2.446015    4.067169    7.321503
O    -4.361302    8.063246   12.276586
O    -4.371450   10.384306    1.926287
O     9.445067    2.315805    6.685821
O     2.432532    6.497921   11.817063
O    -0.005876    2.801665    1.950214
O     6.877414    6.799680    6.774098
O     0.051972   10.675375   11.713773
O     4.374955   10.392250    1.888379
O     4.494937    2.519411    6.837375
O    -2.333319    6.481289   11.817253
O    11.291595    1.370295   12.598361
O     4.355705    5.352689    2.880482
O    -2.488020    9.320151    7.920679
O     6.898754    8.955557   12.728567
O     6.833499    1.103835    2.786180
O     0.118863    5.041417    8.093546
O     2.535656    1.387787   12.730506
O     9.195970    5.300455    2.623366
O     2.475750    9.237273    7.991441
O    -3.262623   11.819709   14.736284
O    10.420586    4.131980    4.659783
O     3.703395    7.729223    9.800951
O    -1.653472    2.923367   14.629982
O     5.024785    7.028776    4.850030
O    -1.749679   11.083885    9.788796
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O	5.098401	8.756963	14.690431
O	5.110867	0.874838	4.834828
O	-1.951453	4.830502	9.781264
O	1.740958	2.995257	14.715756
O	8.723390	6.722948	4.854604
O	1.802578	11.131766	9.749093
O	8.637716	8.705182	14.737785
O	8.570670	0.691256	4.743888
O	2.092498	4.761045	9.828730
O	3.383625	11.834635	14.635291
O	3.332093	3.900530	4.864192
O	-3.556905	7.732929	9.786313
O	8.912812	4.353418	9.283879
Si	-3.719348	11.803092	1.527033
Si	3.187546	7.839880	11.333292
Si	12.137992	2.646168	1.454822
Si	5.308958	6.654559	6.401453
Si	-1.517883	10.593037	11.320146
Si	5.285756	9.123322	1.492640
Si	5.358539	1.223631	6.397974
Si	-1.526067	5.170852	11.321295
Si	1.543323	2.652950	1.524408
Si	8.438580	6.556984	6.438237
Si	1.604465	10.593184	11.294109
Si	8.405518	9.104749	1.533299
Si	8.470412	1.127267	6.308740
Si	1.666969	5.153312	11.345574
Si	3.738389	11.810013	1.454220
Si	3.783975	3.909513	6.422899
Si	-3.067439	7.841918	11.334965
Si	3.799255	11.816277	13.075475
Si	3.726469	3.922664	3.288975
Si	-3.063215	7.843760	8.233538
Si	-5.226440	9.095470	13.171218
Si	8.391555	1.189415	3.211254
Si	1.704786	5.126230	8.291308
Si	1.614698	2.652509	13.137147
Si	8.402077	6.545852	3.264510
Si	1.568655	10.540909	8.220149
Si	5.341428	9.104876	13.129022
Si	5.302299	1.234917	3.265725
Si	-1.476277	5.183863	8.232273
Si	-1.476057	2.628262	13.057277
Si	5.252761	6.629988	3.292392
Si	-1.550335	10.591116	8.249088
Si	-3.671152	11.808632	13.170012
Si	9.946222	3.955011	3.153706
Si	3.208575	7.829208	8.258152
Al	10.116403	3.842009	6.308164
H	9.089691	1.112272	9.911654
H	9.879569	4.383683	9.534603
H	8.793986	4.730595	8.097962
N	8.471085	2.761154	9.367792

N	9.348117	2.136004	9.871103

TS (NNH^+_rotated + H_2O)/ZEO → (N_2 + H_2O)/H^+-ZEO

O	2.045729	1.150513	1.816290
O	8.701015	5.095859	6.802051
O	2.150867	9.108997	11.443021
O	11.611621	1.164498	1.789933
O	4.816596	5.211729	6.716240
O	-2.037807	9.088012	11.439875
O	6.835335	9.506613	1.882688
O	6.875655	1.419879	6.607178
O	0.075763	5.474550	11.713481
O	4.823989	10.641740	12.756065
O	4.816902	2.745209	2.918251
O	-1.944269	6.785086	7.992092
O	-4.766219	10.666550	12.721547
O	8.866928	2.729818	2.723965
O	2.241355	6.595064	8.044963
O	0.072781	2.405178	12.734264
O	6.828291	6.330869	3.034209
O	-0.070443	10.214807	7.947376
O	4.485066	0.169672	2.335405
O	-2.326472	4.187103	7.349648
O	4.454330	8.041851	12.288106
O	11.271316	3.775421	2.289620
O	4.456473	7.819013	7.205223
O	-2.308450	11.616352	12.301898
O	4.764368	7.859863	2.278487
O	-2.104961	11.835644	7.272746
O	-2.057714	3.933793	12.201333
O	2.382649	3.727562	2.410459
O	-4.402736	7.655292	7.262161
O	2.435322	11.674719	12.151201
O	8.887210	7.857896	2.319514
O	2.052278	11.613464	7.100967
O	2.192602	3.984543	12.301247
O	9.192854	0.135720	2.331253
O	2.458160	4.068114	7.300573
O	-4.358743	8.064392	12.305398
O	-4.368253	10.402357	1.957755
O	9.285308	2.373822	7.138228
O	2.479869	6.495968	11.587768
O	-0.005080	2.799653	1.908698
O	6.834222	6.951193	6.630321
O	0.049951	10.679381	11.694618
O	4.357623	10.404156	1.834913
O	4.549277	2.589622	6.832150
O	-2.358184	6.492889	11.758208
O	11.290740	1.399450	12.606834
O	4.402244	5.332216	2.773681
O	-2.564123	9.353990	7.979902
O	6.882113	8.995157	12.576218
O	6.849531	1.050585	2.974149

O	0.089848	5.131230	7.784506
O	2.517263	1.419647	12.691249
O	9.238174	5.318059	2.711686
O	2.342611	9.184719	7.950764
O	-3.356653	11.786964	14.691027
O	10.217769	3.831973	4.740275
O	3.817391	7.900305	9.750332
O	-1.710506	2.979026	14.643998
O	4.921703	7.022103	4.762272
O	-1.752742	11.149975	9.778016
O	5.226811	8.815517	14.654995
O	4.943566	0.887310	4.824475
O	-1.659452	4.832319	9.782250
O	1.773099	3.016477	14.705574
O	8.754823	6.919141	4.792701
O	1.751178	11.118641	9.686899
O	8.522958	8.885942	14.679366
O	8.796813	1.046455	4.808676
O	1.763570	4.645369	9.792093
O	10.176514	0.030236	14.626841
O	3.399591	3.950805	4.835857
O	-3.667420	7.723590	9.788607
O	8.329410	4.731949	9.484197
Si	-3.721847	11.809955	1.505005
Si	3.219002	7.889517	11.259565
Si	12.117871	2.680920	1.473760
Si	5.269098	6.730658	6.320590
Si	-1.521756	10.624461	11.296604
Si	5.302480	9.150012	1.472551
Si	5.287600	1.224203	6.374950
Si	-1.480218	5.198200	11.344497
Si	1.552737	2.670320	1.512877
Si	8.401084	6.617671	6.355064
Si	1.599086	10.619199	11.234561
Si	8.382106	9.156627	1.510585
Si	8.477498	1.183907	6.403368
Si	1.626849	5.151312	11.328779
Si	3.704794	11.830208	1.454219
Si	3.810257	3.964704	6.408881
Si	-3.096619	7.862674	11.311352
Si	3.772295	11.837435	13.067587
Si	3.752827	3.931939	3.250234
Si	-3.134836	7.862943	8.236722
Si	-5.262618	9.159188	13.087568
Si	8.430979	1.254652	3.237221
Si	1.634827	5.106018	8.231796
Si	1.633112	2.704583	13.122159
Si	8.422257	6.602214	3.234746
Si	1.508135	10.537330	8.166777
Si	5.348343	9.130620	13.077807
Si	5.277931	1.224038	3.272119
Si	-1.479133	5.222387	8.192402
Si	-1.492800	2.682032	13.074235

Si	5.247193	6.636051	3.220688
Si	-1.617803	10.633500	8.236535
Si	-3.695191	11.831081	13.110561
Si	9.909526	3.913677	3.182367
Si	3.217284	7.866264	8.235321
Al	9.923979	3.866229	6.436520
H	9.501259	2.794196	9.411810
H	8.530469	5.610866	9.857706
H	8.359515	4.859614	8.492713
N	9.229007	2.727722	10.430442
N	8.934988	2.582872	11.492383

No direct participation of the chabazite at some reaction steps

TS $NO^{+}(NH_3)$/ZEO → $NONH_2$_rotated3/H^{+}-ZEO

O	11.578798	1.007139	1.813775
O	4.876089	4.787291	6.547828
O	-2.258879	8.986754	11.360850
O	6.773522	9.285970	1.830955
O	6.670661	1.381893	6.782717
O	-0.085788	5.350128	11.556043
O	1.956838	0.992930	1.890359
O	8.834507	5.032872	6.699952
O	1.966927	8.949350	11.605202
O	-4.825809	10.469712	12.979401
O	8.789017	2.616192	3.018409
O	1.794321	6.626577	8.040480
O	-0.151188	2.208780	12.743431
O	6.788471	6.135444	2.698681
O	-0.066854	10.171369	7.930925
O	4.653756	10.568463	12.689037
O	4.686392	2.557783	2.924391
O	-2.056197	6.503006	7.852548
O	11.204291	3.584751	2.398122
O	4.259365	7.495174	7.343032
O	-2.486299	11.505481	12.240276
O	4.667050	7.654531	2.181301
O	-2.219829	11.568384	7.190175
O	-2.190336	3.857649	12.296623
O	-2.465827	11.798832	2.373943
O	11.177855	3.925108	7.346405
O	4.357657	7.945096	12.252334
O	9.175043	0.037563	2.426657
O	2.374263	4.112852	7.266867
O	9.088345	7.938008	12.142421
O	2.333510	3.614684	2.287505
O	-4.368019	7.627588	7.148140
O	2.191688	11.514400	12.339147
O	8.888313	7.755782	2.383605
O	1.992279	11.735584	7.332322
O	1.952302	3.802981	12.296973

O	-0.073170	2.670860	1.968497
O	6.862331	6.801411	7.001680
O	-0.138822	10.487650	11.751369
O	4.330680	10.255005	1.990486
O	4.149568	2.254603	6.776077
O	-2.481023	6.399678	11.796035
O	-4.444876	10.239472	1.667452
O	9.083164	2.430602	6.811920
O	2.334199	6.339743	11.790659
O	6.738899	8.951563	12.596636
O	6.761274	0.947943	2.781983
O	-0.072796	4.760585	7.913288
O	2.275831	1.219427	12.591225
O	9.251084	5.215893	2.897122
O	2.359496	9.202029	7.920407
O	11.029319	1.320005	12.743353
O	4.345059	5.160454	2.845773
O	-2.441294	9.111648	8.036317
O	11.867294	2.899314	14.717903
O	5.208866	6.941149	4.671249
O	-1.808569	11.051694	9.745346
O	5.035768	8.809768	14.639782
O	5.043217	0.692331	4.797753
O	-1.974307	4.688395	9.803344
O	3.474901	0.073642	14.673143
O	10.317989	3.786551	4.866688
O	3.498787	7.695333	9.806553
O	3.275164	11.627639	14.729064
O	3.160954	3.727104	4.789154
O	-3.719455	7.471419	9.705437
O	1.607880	2.745208	14.676083
O	8.315636	6.832975	4.787430
O	1.663260	10.927264	9.826129
O	8.388467	8.446056	14.643372
O	8.421450	0.729069	4.863636
O	1.803642	4.632297	9.798479
O	7.844178	9.687877	9.495083
Si	12.058806	2.531134	1.520298
Si	-1.679850	10.503697	11.269602
Si	5.208322	8.997034	1.472676
Si	5.124999	1.034964	6.379176
Si	-1.670931	5.066124	11.355792
Si	-3.795255	11.700405	1.457512
Si	9.860451	3.782988	6.421179
Si	3.019234	7.738677	11.363749
Si	3.670310	11.658826	1.538156
Si	3.667311	3.748923	6.347366
Si	-3.252097	7.713358	11.256912
Si	1.465763	2.500560	1.506167
Si	8.407107	6.549377	6.359589
Si	1.429929	10.467545	11.367579
Si	8.311771	8.936833	1.430735
Si	8.236536	1.103712	6.433992

Si	1.494711	5.027238	11.345079
Si	8.276348	8.960689	13.104243
Si	8.291007	1.086733	3.283087
Si	1.492428	5.034752	8.247267
Si	1.415011	2.496693	13.087985
Si	8.292729	6.478889	3.185722
Si	1.487338	10.509585	8.262436
Si	3.585440	11.716308	13.138460
Si	3.638763	3.767501	3.237822
Si	-3.121944	7.677000	8.200234
Si	-3.815475	11.730949	13.126450
Si	9.881794	3.786154	3.298990
Si	2.973163	7.742899	8.244586
Si	5.192464	9.077539	13.058642
Si	5.207841	1.051736	3.227811
Si	-1.637621	4.969967	8.238628
Si	11.984608	2.565243	13.134692
Si	5.240722	6.474209	3.143676
Si	-1.628440	10.488451	8.230731
Al	5.150530	6.468729	6.308819
H	5.531946	7.808390	9.560749
H	7.792017	8.346595	9.707322
H	6.827294	7.323084	7.857511
N	6.583716	9.457298	9.318975
N	6.495263	8.174298	9.452270

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O	0.032497	2.430246	1.660688
O	0.119790	10.308649	6.640811
O	6.906648	6.399413	11.388005
O	4.896273	10.710669	1.734170
O	-2.201835	6.647851	6.382685
O	4.906574	2.728013	11.660164
O	11.622614	1.228983	12.670236
O	-1.970676	9.086947	2.862798
O	4.959506	5.117289	7.795891
O	6.949942	9.467093	12.546836
O	0.037794	5.609630	2.673619
O	6.857704	1.407115	8.063157
O	2.155071	1.138879	12.604133
O	2.062737	9.090177	2.851115
O	8.911861	5.260857	7.781692
O	-4.347698	8.072549	2.177605
O	2.478979	4.170957	7.325297
O	9.246937	0.138458	12.145539
O	2.120866	4.051857	2.101241
O	8.995456	0.113808	7.104737
O	9.036875	7.838012	12.206076

O	2.451610	11.669090	2.232496
O	-4.438355	7.842754	7.204271
O	2.471529	3.744667	12.096428
O	-2.377073	11.672044	2.317615
O	4.504213	7.696476	7.172611
O	11.394751	3.809609	12.029222
O	4.423542	8.100416	2.131860
O	-2.468915	4.100598	7.096442
O	4.626646	0.152815	12.249656
O	-2.052629	4.016392	2.201564
O	4.805403	-0.051857	7.234022
O	4.837508	7.887500	12.171332
O	6.882373	8.979098	1.884689
O	-0.090259	5.152591	6.923347
O	6.927254	1.061576	11.392863
O	2.462494	1.446204	1.845133
O	2.629784	9.434899	6.686371
O	9.314635	5.330630	11.631752
O	11.252788	1.472651	1.697549
O	-2.277513	9.247474	6.718989
O	4.528448	5.331511	11.749677
O	0.073594	2.783764	12.515749
O	0.043146	10.775523	2.699899
O	6.879193	6.933887	7.901586
O	4.515246	10.464496	12.499580
O	-2.442328	6.486989	2.970072
O	4.517084	2.529202	7.655525
O	-4.237638	10.387072	12.580192
O	2.516467	6.495517	2.889871
O	9.113775	2.653076	7.661798
O	-5.116022	8.868522	14.582411
O	1.570691	4.660230	4.626182
O	8.930281	0.868033	9.632261
O	1.813879	2.951229	14.518094
O	1.794748	11.011943	4.689967
O	8.857913	7.100428	9.696305
O	10.252501	-0.082238	14.555562
O	-3.636021	8.125872	4.708512
O	3.552889	3.920511	9.705541
O	3.506302	0.007054	14.623537
O	3.739120	8.088236	4.680622
O	10.383099	3.972910	9.605897
O	5.262608	8.933792	14.549062
O	-1.486456	4.705269	4.689674
O	4.858293	0.869603	9.719614
O	-1.681596	3.136115	14.508244
O	-1.661406	10.951058	4.754637
O	4.925046	6.994651	9.690002
O	-0.344355	5.403709	9.406661
Si	-5.259543	9.162395	1.405507
Si	8.514857	1.198789	11.167930
Si	1.604934	2.727004	1.344722
Si	1.671104	10.656560	6.268899

Si	8.491341	6.666641	11.221149
Si	10.637793	0.015512	1.364399
Si	-3.140169	7.968946	6.247010
Si	3.866006	3.927786	11.282944
Si	3.119040	0.028458	1.436348
Si	3.206502	7.979729	6.230689
Si	10.001603	3.934574	11.185818
Si	5.354412	9.184049	1.383621
Si	-1.607605	5.156673	6.229091
Si	5.327394	1.213296	11.239979
Si	-1.521370	2.761156	1.322797
Si	-1.451112	10.582899	6.323925
Si	5.301011	6.654203	11.230684
Si	-1.482184	2.719844	12.951775
Si	-1.494194	10.617031	3.172166
Si	5.295142	6.672268	8.130443
Si	5.394282	9.186696	12.956608
Si	-1.465847	5.212239	3.131196
Si	5.254379	1.193819	8.168390
Si	3.215615	-0.024139	13.028997
Si	3.178087	7.936513	3.163712
Si	9.895526	4.000645	8.049506
Si	10.624161	-0.019224	12.981813
Si	-3.088448	7.948208	3.184681
Si	3.846917	3.946052	8.100870
Si	1.635188	2.647811	12.941240
Si	1.597736	10.622064	3.128963
Si	8.457699	6.780396	8.144749
Si	-5.193524	9.151145	12.993113
Si	1.572433	5.199077	3.123180
Si	8.462395	1.245610	8.117218
Al	1.633240	5.204129	6.253909
H	-0.141513	5.269865	7.985590
H	-1.252305	5.773435	11.533516
H	-2.013712	7.337500	11.085514
N	-1.028824	6.440047	9.632820
N	-1.419957	6.539879	10.865082

TS $NONH_2$_rotated3/H^+-ZEO → HN=NOH_rotated3/H^+-ZEO

O	2.004076	1.283407	1.752936
O	8.863490	5.345919	6.688561
O	2.037628	9.140546	11.533349
O	11.656848	1.283271	1.729435
O	4.812655	5.221997	6.659386
O	-2.042914	9.182453	11.434161
O	6.821248	9.633171	1.691966
O	6.807000	1.591819	6.687492
O	0.062190	5.684463	11.763558
O	4.816260	10.764896	12.756287

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O    4.756818    2.890529    2.954031
O   -2.139386    6.761259    7.671934
O   -4.810111   10.790215   12.720711
O    8.922942    2.890116    3.079472
O    2.048070    6.775601    7.982986
O    0.044132    2.439290   12.675129
O    6.813010    6.406229    2.920566
O   -0.045287   10.377772    7.906900
O    4.447217    0.323685    2.289201
O   11.261678    4.097124    7.570596
O    4.453719    8.183395   12.172761
O   11.204226    3.896154    2.141771
O    4.378988    7.805796    7.184645
O   -2.349579   11.719854   12.231665
O    4.772436    8.022631    2.320220
O    4.695939    0.056458    7.192520
O   -2.015365    4.039690   12.115264
O    2.360974    3.869328    2.317178
O   -4.510545    7.930948    7.239442
O    2.396250   11.723777   12.157102
O    8.855145    7.993878    2.288581
O    8.895026    0.031509    7.208660
O    2.122918    4.056728   12.188060
O    9.206332    0.357454    2.261079
O    2.414779    4.220642    7.286108
O   -4.439623    8.218948   12.142322
O   -4.392285   10.534728    1.874269
O    9.265994    2.539931    6.673282
O    2.534039    6.547036   11.552079
O   -0.026210    2.977861    1.827992
O    6.792221    6.986197    6.741759
O    0.009167   10.820699   11.627634
O    4.341884   10.540678    1.800107
O    4.376533    2.614268    6.698562
O   -2.417072    6.615115   11.840889
O   11.237764    1.506463   12.525984
O    4.352228    5.480496    2.749839
O   -2.451391    9.383090    7.870947
O    6.844057    9.101259   12.641807
O    6.830857    1.311678    2.730874
O   -0.002726    5.186293    7.625776
O    2.509397    1.530266   12.613084
O    9.260632    5.477540    2.818266
O    2.355449    9.349099    7.725317
O    3.483605    0.103725   14.637353
O   10.627707    4.174238    4.715889
O    3.640059    8.079255    9.682605
O   -1.730473    3.083785   14.550940
O    5.002421    7.088742    4.759543
O   -1.813285   11.206821    9.711270
O    5.059304    8.869541   14.621071
O    5.091831    0.944864    4.746802
O   -1.589517    5.176201    9.773860
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O	1.753594	3.131290	14.619845
O	8.567694	7.202292	4.773163
O	1.824670	11.073255	9.689805
O	-5.048404	8.926807	14.615835
O	8.482985	0.836652	4.747204
O	1.584291	4.827951	9.730456
O	10.165429	0.178223	14.590313
O	3.261672	4.122444	4.786734
O	-3.518510	7.778113	9.706372
O	10.397532	2.551291	9.436624
Si	3.088776	0.108642	1.444706
Si	3.159906	7.996446	11.229358
Si	-1.569123	2.808648	1.377186
Si	5.258288	6.758038	6.325098
Si	-1.558271	10.720806	11.241301
Si	5.259812	9.267861	1.417337
Si	5.255011	1.307731	6.319777
Si	-1.488141	5.379201	11.381182
Si	1.527841	2.806697	1.431138
Si	8.359181	6.821268	6.348510
Si	1.569840	10.671407	11.245446
Si	-5.288936	9.267142	1.422791
Si	8.372044	1.283536	6.311764
Si	1.571553	5.283215	11.293450
Si	10.553570	0.134051	1.404764
Si	3.727113	4.049585	6.343195
Si	-3.107779	7.965278	11.266705
Si	10.581188	0.110969	13.027720
Si	3.687935	4.083526	3.215664
Si	-3.168038	7.964234	8.126678
Si	-5.277019	9.264968	13.047358
Si	8.377580	1.370594	3.218671
Si	1.535028	5.252030	8.161012
Si	1.593891	2.788685	13.043516
Si	8.377138	6.759969	3.224368
Si	1.534024	10.671848	8.132446
Si	5.292387	9.238471	13.062157
Si	5.284980	1.372109	3.192196
Si	-1.504040	5.367627	8.181198
Si	-1.520552	2.763335	12.983424
Si	5.251362	6.749039	3.195226
Si	-1.610199	10.723706	8.167665
Si	3.118854	0.104389	13.062041
Si	10.018097	4.102116	3.234113
Si	3.109376	7.993024	8.148924
Al	9.926041	4.062838	6.281252
H	11.007343	3.402502	8.293518
H	9.505118	1.629086	9.771699
H	7.910490	2.734626	11.072424
N	9.526115	3.289144	10.127991
N	8.675616	2.420950	10.462855

HNNOH_rotated3/H^+-ZEO

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O	11.588223	1.300676	1.722167
O	4.758157	5.296456	6.655896
O	-2.088199	9.190702	11.469359
O	6.833993	9.593404	1.775432
O	6.838376	1.550908	6.498521
O	0.066641	5.649394	11.686304
O	4.744036	10.710887	12.707812
O	4.801026	2.873791	2.920922
O	-1.952967	6.899689	7.825127
O	-4.747906	10.784883	12.608456
O	8.827560	2.876671	2.685917
O	2.216570	6.670662	8.080339
O	0.087357	2.463082	12.602289
O	6.818664	6.389640	2.835931
O	-0.107894	10.367262	7.929125
O	4.456260	0.308434	2.245569
O	-2.368061	4.282171	7.332176
O	4.471753	8.111374	12.194999
O	11.195911	3.928280	2.068863
O	4.385900	7.896435	7.107927
O	-2.275026	11.739848	12.285400
O	4.749096	7.998813	2.271200
O	4.712424	0.125730	7.246456
O	-2.018113	4.032780	12.108183
O	2.375596	3.825951	2.314691
O	-4.428256	7.736079	7.205607
O	2.389206	11.782700	12.086398
O	8.888484	7.921746	2.180675
O	8.849040	-0.080474	7.092396
O	2.166150	4.119502	12.276281
O	9.175642	0.264939	2.224399
O	2.419782	4.153282	7.268599
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O	-4.371418	10.492188	1.913760
O	9.285253	2.476984	6.903374
O	2.519148	6.568785	11.425335
O	-0.038556	2.943153	1.863553
O	6.803398	6.976770	6.748091
O	0.026058	10.726681	11.586255
O	4.364822	10.535136	1.739729
O	4.498366	2.687241	6.733669
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O	11.307417	1.471354	12.499271
O	4.353116	5.461876	2.745922
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O	6.852018	9.159781	12.543811
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 O    2.262000    9.257343    7.768937
 O    3.397531    0.078086   14.632963
 O   10.454565    3.711976    4.611754
 O    3.768760    8.139015    9.659796
 O   -1.652594    3.042839   14.520783
 O    5.062543    7.100474    4.716845
 O   -1.856887   11.208881    9.744181
 O    5.170796    8.869099   14.596141
 O    4.921098    0.938644    4.752941
 O   -1.627322    5.064052    9.722545
 O    1.730748    3.045958   14.637317
 O    8.485889    7.307864    4.717125
 O    1.821604   11.131383    9.632560
 O   -5.114946    9.033111   14.585532
 O    8.775836    1.096725    4.691387
 O    1.657982    4.682290    9.749446
 O   10.152349    0.175654   14.544576
 O    3.305071    4.067084    4.777076
 O   -3.586853    7.845875    9.710772
 O    8.971232    2.176411    9.473622
Si    3.066470    0.075582    1.452364
Si    3.217324    7.998162   11.183893
Si   -1.570426    2.804403    1.354316
Si    5.268973    6.803873    6.296573
Si   -1.557401   10.707325   11.264209
Si    5.286997    9.251595    1.402668
Si    5.232676    1.322703    6.295740
Si   -1.490155    5.338511   11.302707
Si    1.513997    2.760343    1.455396
Si    8.345122    6.765764    6.260660
Si    1.586403   10.686408   11.204583
Si   -5.287398    9.252303    1.417419
Si    8.394764    1.214979    6.241573
Si    1.591081    5.257750   11.271747
Si   10.538808    0.114318    1.358493
Si    3.743960    4.066856    6.342066
Si   -3.126375    7.953167   11.263758
Si   10.575703    0.111541   12.980409
Si    3.710056    4.052940    3.200975
Si   -3.140383    7.963044    8.144727
Si   -5.275279    9.289315   12.995131
Si    8.403601    1.375513    3.116387
Si    1.582574    5.182976    8.198268
Si    1.622227    2.794986   13.039239
Si    8.370640    6.760620    3.191569
Si    1.478915   10.611448    8.110433
Si    5.310871    9.220399   13.023250
Si    5.245591    1.336796    3.206875
Si   -1.497311    5.351401    8.124073
Si   -1.481239    2.755846   12.940465
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Si	5.263309	6.737498	3.150743
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Si	3.139942	0.110061	13.037429
Si	9.952478	4.001395	3.120951
Si	3.166245	7.971765	8.156579
Al	10.018584	4.058814	6.233820
H	9.275913	2.432264	7.922411
H	8.931182	1.208645	9.725956
H	6.080993	2.434196	10.513075
N	7.707567	2.757798	9.773680
N	6.970207	1.939554	10.326402

$(N_2 + H_2O)/H^+$-ZEO

O	2.003002	1.262494	1.813906
O	8.588102	5.059647	6.685731
O	2.045057	9.154303	11.606967
O	11.557539	1.268994	1.678979
O	4.762688	5.320270	6.642248
O	-1.975516	9.147471	11.385949
O	6.784062	9.600584	1.795535
O	6.906374	1.565065	6.567554
O	0.067901	5.647974	11.698081
O	4.818899	10.705866	12.715949
O	4.748192	2.866053	2.897675
O	-1.837681	7.025768	7.951093
O	-4.856361	10.802093	12.809875
O	8.862598	2.819515	2.762041
O	2.340072	6.600592	8.139063
O	0.087272	2.479210	12.654461
O	6.767773	6.424236	2.939855
O	-0.165931	10.302312	7.818659
O	4.424730	0.267922	2.336069
O	-2.361353	4.492854	7.250737
O	4.446882	8.111948	12.189316
O	11.218286	3.885324	2.130969
O	4.449917	7.920923	7.213655
O	-2.379000	11.645741	12.256887
O	4.704935	7.992868	2.265821
O	4.710262	0.164034	7.243375
O	-2.014714	4.020780	12.082774
O	2.320771	3.850270	2.359980
O	-4.350456	7.595892	7.212112
O	2.471368	11.756671	11.979211
O	8.838789	8.005714	2.368952
O	8.849341	-0.160244	7.078441
O	2.171248	4.120828	12.288044
O	9.131120	0.246349	2.163694
O	2.447599	4.112036	7.298872
O	-4.340976	8.239253	12.247618
O	-4.419494	10.515126	1.870636
O	9.405983	2.393309	6.809494

O	2.523500	6.554629	11.377337
O	-0.057208	2.899313	1.834960
O	6.809889	6.979537	6.693628
O	0.024883	10.847379	11.650276
O	4.311083	10.514780	1.704191
O	4.588477	2.729157	6.755737
O	-2.406478	6.577193	11.716102
O	11.325482	1.464818	12.477490
O	4.318931	5.468245	2.809188
O	-2.700263	9.526670	7.849996
O	6.868563	9.053127	12.562022
O	6.799642	1.208447	2.816759
O	0.114244	5.284349	7.654035
O	2.538242	1.541030	12.623957
O	9.169591	5.418982	2.575422
O	2.174799	9.155425	7.644131
O	3.483859	0.125303	14.667852
O	10.284662	4.113080	4.611640
O	3.666979	8.286512	9.692209
O	-1.716591	3.061279	14.519407
O	4.984396	7.185531	4.747364
O	-1.796607	11.211280	9.724295
O	5.165162	8.834003	14.593229
O	5.004023	0.993781	4.778451
O	-1.573140	5.041869	9.696730
O	1.758044	3.086788	14.659368
O	8.674170	6.886126	4.749810
O	1.731268	10.904782	9.600079
O	-5.160376	8.888743	14.657745
O	8.687755	0.938635	4.677897
O	1.622074	4.635644	9.762734
O	10.132611	0.147881	14.487350
O	3.296436	4.039180	4.806820
O	-3.645073	7.879093	9.729310
O	9.229866	2.423235	9.735343
Si	3.075481	0.090116	1.468747
Si	3.156946	8.026519	11.217253
Si	-1.593916	2.775541	1.344495
Si	5.231506	6.840717	6.307956
Si	-1.536465	10.708310	11.249487
Si	5.247553	9.242647	1.391661
Si	5.317547	1.351468	6.327076
Si	-1.478562	5.324039	11.282117
Si	1.507570	2.772097	1.464391
Si	8.347566	6.706183	6.309974
Si	1.565544	10.661641	11.195747
Si	-5.334640	9.251678	1.464846
Si	8.474391	1.199169	6.273462
Si	1.588874	5.244321	11.274628
Si	10.494306	0.094976	1.307343
Si	3.763857	4.056410	6.360480
Si	-3.090163	7.968229	11.262834
Si	10.606009	0.085389	12.935650

Si	3.674300	4.044652	3.224480
Si	-3.112727	7.998979	8.192653
Si	-5.284049	9.252459	13.078159
Si	8.381234	1.315827	3.126944
Si	1.618648	5.157193	8.220261
Si	1.629337	2.805974	13.066955
Si	8.357612	6.678465	3.153647
Si	1.427817	10.530646	8.047956
Si	5.321555	9.188452	13.020325
Si	5.247090	1.346242	3.213141
Si	-1.435757	5.438862	8.123562
Si	-1.489680	2.759838	12.946011
Si	5.199912	6.765232	3.190441
Si	-1.688013	10.754697	8.166725
Si	3.109708	0.101545	13.091184
Si	9.898409	4.045673	3.064771
Si	3.150668	7.990503	8.180412
Al	10.051105	3.903666	6.286478
H	9.584075	2.228463	8.845558
H	9.821638	1.976151	10.364449
H	7.991289	4.707142	7.395230
N	6.897944	4.042328	8.768021
N	6.263967	3.588297	9.558468

$PhNH_2$ transformation in the pores of ZEO/NO^+

($PhNH_2$-NO^+)/ZEO

O	-4.718360	10.758133	1.849157
O	2.100567	6.923625	6.693562
O	9.071939	2.741588	11.385096
O	0.089579	2.477003	1.752678
O	0.129702	10.367232	6.765177
O	6.913547	6.442880	11.425554
O	4.896084	10.768064	1.797501
O	-2.162916	6.700352	6.681359
O	4.918658	2.775113	11.889764
O	11.681319	1.256778	12.756494
O	-1.983099	9.206180	2.999223
O	4.929762	5.197244	7.801811
O	6.941281	9.536492	12.765630
O	0.114377	5.610426	2.916567
O	6.876121	1.577442	8.036141
O	2.200025	1.213793	12.793252
O	2.109854	9.156640	2.864368
O	8.915483	5.283584	7.868405
O	-4.350034	8.153987	2.338986
O	2.406148	4.243738	7.609006
O	9.287620	0.212530	12.243276
O	2.181171	4.086663	2.254266
O	8.996331	0.224615	7.132935

O	8.991522	7.883397	12.313912
O	2.477071	11.758207	2.365827
O	-4.449074	7.887797	7.293218
O	2.468086	3.788673	12.124451
O	-2.325650	11.786754	2.431285
O	4.565780	7.808422	7.276117
O	11.411339	3.833918	12.134247
O	4.522242	8.172909	2.363224
O	11.222366	4.119872	7.161403
O	4.621407	0.170783	12.275923
O	-1.984744	4.092687	2.265944
O	4.831820	0.003416	7.386063
O	4.863719	7.956903	12.237485
O	6.920391	9.096126	1.932731
O	-0.073119	5.175547	6.909795
O	6.957439	1.161580	11.620364
O	2.532142	1.520952	1.824783
O	2.630277	9.506936	6.894623
O	9.287198	5.345928	11.768436
O	11.306048	1.535888	1.836656
O	-2.296539	9.324727	6.789048
O	4.547187	5.396091	11.917541
O	0.105658	2.826225	12.585879
O	0.071373	10.838411	2.812776
O	6.894231	6.961640	8.062007
O	4.496794	10.497484	12.670945
O	-2.325205	6.608756	2.868169
O	4.478222	2.592434	7.689322
O	-4.266607	10.453979	12.659244
O	2.558048	6.562755	2.934714
O	9.235721	2.673169	8.023278
O	-5.002866	8.919023	14.699191
O	1.835778	4.767194	4.800503
O	8.754137	0.688083	9.714219
O	1.818561	3.139454	14.605826
O	1.835154	10.969143	4.795259
O	8.919943	7.107519	9.795783
O	10.243951	0.055113	14.672237
O	-3.529926	8.016256	4.818539
O	3.753781	3.953524	9.832382
O	-3.213895	11.828543	14.702306
O	3.616286	8.150073	4.835993
O	10.560730	4.243088	9.708544
O	5.191089	8.895075	14.684738
O	-1.689310	4.867668	4.762889
O	4.976903	1.055052	9.817323
O	-1.635475	3.151672	14.604805
O	-1.619826	11.070670	4.878553
O	4.874214	6.981318	9.782749
O	0.280749	3.264312	9.598791
Si	-5.205688	9.243037	1.509317
Si	8.519744	1.213912	11.234693
Si	1.651528	2.815592	1.427606

Si	1.682012	10.706855	6.385354
Si	8.509780	6.703823	11.317551
Si	10.654566	0.099957	1.480494
Si	-3.105232	7.983833	6.384399
Si	3.928930	3.983344	11.428577
Si	3.194064	0.088463	1.503611
Si	3.198401	8.048525	6.415309
Si	10.057229	4.019993	11.253623
Si	5.369827	9.236330	1.499802
Si	-1.564292	5.218005	6.339041
Si	5.366778	1.294480	11.375923
Si	-1.466135	2.813798	1.426735
Si	-1.441536	10.653432	6.442124
Si	5.308663	6.700095	11.322566
Si	-1.448189	2.757488	13.047935
Si	-1.467628	10.719816	3.297090
Si	5.300591	6.728060	8.221954
Si	5.381676	9.215185	13.107982
Si	-1.444515	5.296543	3.215120
Si	5.287661	1.306541	8.235299
Si	3.248894	0.006481	13.122889
Si	3.191121	7.999025	3.278373
Si	9.970211	4.087945	8.173980
Si	10.648280	0.048039	13.105885
Si	-3.037479	7.997626	3.269902
Si	3.870027	4.013256	8.207312
Si	1.662807	2.728537	13.053016
Si	1.629100	10.667201	3.218309
Si	8.482133	6.810968	8.250262
Si	-5.181036	9.200864	13.117049
Si	1.675712	5.245100	3.288357
Si	8.454707	1.281102	8.221160
Al	1.611314	5.269789	6.440788
H	0.734363	10.013173	12.579263
H	-0.916956	8.324838	13.389859
H	-1.464677	6.344273	11.983030
H	1.250686	7.763542	8.927463
H	-0.272044	5.899807	8.557273
H	-1.338516	5.361094	9.786052
H	1.829270	9.723240	10.365466
C	0.491443	9.146045	11.964685
C	-0.435564	8.198824	12.419439
C	-0.747915	7.091270	11.635909
C	-0.141108	6.946076	10.373887
C	0.794173	7.891060	9.911783
C	1.106300	8.985562	10.715533
N	0.839414	4.247192	9.751256
N	-0.455749	5.843525	9.578080

TS ($PhNH_2$-NO^+)/ZEO → PhNH=NO/H^+-ZEO

O	-4.808481	10.782444	1.870828

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O     2.042703    6.970358    6.480534
O     8.965501    2.817784   11.451736
O     0.022364    2.547177    1.722684
O     0.075892   10.401253    6.750582
O     6.864318    6.462002   11.453715
O     4.855026   10.788871    1.843239
O    -2.202381    6.769242    6.540991
O     4.909043    2.836180   11.836804
O    11.665065    1.286377   12.758123
O    -2.014854    9.205755    3.032521
O     4.940588    5.218945    7.869339
O     6.904283    9.617953   12.691150
O     0.037084    5.695603    2.823059
O     6.825779    1.586490    8.127183
O     2.100898    1.218495   12.721972
O     2.036593    9.173657    2.917569
O     8.840074    5.334196    7.885767
O    -4.375397    8.178756    2.291842
O     2.417402    4.335242    7.539430
O     9.239880    0.288153   12.280539
O     2.116389    4.147535    2.227547
O     8.936073    0.243291    7.162906
O     8.938290    7.927829   12.329772
O     2.422997   11.765973    2.350243
O    -4.468902    7.922456    7.325492
O     2.458495    3.812327   12.198360
O    -2.393145   11.776259    2.414151
O     4.465947    7.803632    7.294484
O    11.361164    3.852475   12.127379
O     4.412418    8.177550    2.268465
O    11.163549    4.218118    7.186978
O     4.578212    0.247509   12.339187
O    -2.062741    4.123037    2.293438
O     4.786348    0.053204    7.375251
O     4.832985    7.994153   12.266431
O     6.855666    9.083467    2.004667
O    -0.123992    5.236931    6.991262
O     6.903290    1.155113   11.565808
O     2.438445    1.540912    1.972470
O     2.582985    9.538062    6.851978
O     9.265932    5.409375   11.777295
O    11.263612    1.555777    1.889221
O    -2.348637    9.376168    6.786597
O     4.487941    5.440938   11.912069
O     0.057806    2.913497   12.702037
O     0.014240   10.866017    2.813048
O     6.841641    7.053100    8.047363
O     4.435358   10.536612   12.646792
O    -2.439871    6.606433    3.017407
O     4.443065    2.632095    7.731954
O    -4.259223   10.467858   12.685974
O     2.511035    6.581445    3.054724
O     9.161870    2.721216    7.935856
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 O   -5.149684    8.977538   14.700947
 O    1.587430    4.717554    4.762475
 O    8.800035    0.793829    9.733314
 O    1.872135    3.051409   14.638930
 O    1.776273   11.049004    4.794587
 O    8.844548    7.158214    9.814880
 O   10.250813    0.087416   14.685958
 O   -3.680576    8.145225    4.820838
 O    3.634372    4.011734    9.838757
 O    3.471078    0.104859   14.729849
 O    3.691465    8.248097    4.805242
 O   10.461793    4.232864    9.712958
 O    5.226364    8.994133   14.672644
 O   -1.572990    4.829191    4.779136
 O    4.870838    1.035982    9.836270
 O   -1.785716    3.177053   14.626637
 O   -1.680571   11.114569    4.871592
 O    4.845743    7.054547    9.801770
 O    0.361352    3.329717    9.829268
Si   -5.287773    9.267851    1.522264
Si    8.478829    1.272497   11.254379
Si    1.605098    2.830512    1.456584
Si    1.626835   10.746015    6.379143
Si    8.452753    6.746196   11.339778
Si   10.621252    0.122210    1.500985
Si   -3.176211    8.060789    6.361514
Si    3.868876    4.025500   11.428317
Si    3.093822    0.128160    1.545854
Si    3.168771    8.096927    6.352752
Si    9.994981    4.056192   11.279180
Si    5.325765    9.265172    1.504095
Si   -1.633963    5.272049    6.321059
Si    5.308729    1.329317   11.374873
Si   -1.547139    2.847871    1.438932
Si   -1.491096   10.702185    6.434555
Si    5.262818    6.741552   11.341466
Si   -1.509325    2.799057   13.075028
Si   -1.522555   10.736090    3.296580
Si    5.257649    6.770542    8.243855
Si    5.356612    9.283081   13.086041
Si   -1.487346    5.322087    3.221280
Si    5.227513    1.328775    8.270303
Si    3.176243    0.063494   13.135581
Si    3.153288    8.036638    3.285141
Si    9.883269    4.127894    8.175969
Si   10.615268    0.092854   13.110290
Si   -3.117766    8.041237    3.295678
Si    3.829791    4.060037    8.223584
Si    1.626774    2.739789   13.074376
Si    1.570431   10.699508    3.226036
Si    8.421318    6.866739    8.267878
Si   -5.241005    9.254489   13.112640
Si    1.570238    5.279311    3.265947
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Si	8.415836	1.321510	8.237718
Al	1.596684	5.303565	6.377862
H	0.019740	10.445532	11.137233
H	-2.107824	9.206074	11.506921
H	-2.305378	6.837436	10.765188
H	1.691794	6.996057	9.152629
H	-0.223378	5.337622	8.147226
H	-1.359659	5.005930	9.650046
H	1.921856	9.343289	9.959875
C	-0.074474	9.416773	10.791025
C	-1.267711	8.720312	11.009486
C	-1.384839	7.394264	10.592118
C	-0.312415	6.784490	9.932243
C	0.877718	7.479326	9.692190
C	0.995618	8.796628	10.137627
N	0.665735	4.457158	10.019462
N	-0.436301	5.438829	9.470658

PhNH=NO/H^+-ZEO

O	6.941696	9.545913	1.752720
O	6.945575	1.883892	6.451077
O	0.094117	5.403457	11.309861
O	2.170460	1.241067	1.769577
O	9.066246	5.114046	6.696222
O	2.152299	9.113071	11.482792
O	11.755773	1.214353	1.835825
O	4.800623	5.091693	6.674549
O	-1.968936	9.078081	11.740795
O	0.085411	2.437327	12.775291
O	6.952547	6.333867	2.989173
O	0.130172	10.007318	7.993129
O	4.924593	10.641159	12.730311
O	4.910837	2.821164	2.686604
O	-2.088352	6.679502	7.931190
O	-4.732069	10.597065	12.622903
O	8.985254	2.817799	2.855367
O	2.094014	6.872909	7.858226
O	4.904009	7.943394	2.386212
O	5.055738	-0.074595	7.300359
O	-1.998089	3.978682	12.229640
O	4.643012	0.245157	2.089107
O	-2.174324	4.123521	7.165841
O	4.493751	8.049536	12.264137
O	11.409791	3.818297	2.318916
O	4.567979	7.686950	7.288711
O	-2.307143	11.666247	12.183712
O	8.985799	7.950563	2.387322
O	1.914564	11.868215	7.224758
O	2.188672	3.932572	12.094676
O	9.302537	0.241294	2.278926
O	2.291304	4.326109	7.058771

O	-4.341135	7.976808	12.290187
O	2.479182	3.848457	2.258332
O	-4.469691	7.699424	7.370788
O	2.488817	11.638919	12.245621
O	4.483023	10.467355	1.933390
O	4.141119	2.511635	6.885331
O	-2.274795	6.494972	11.677417
O	-4.278369	10.488112	1.939242
O	9.491523	2.497819	6.829585
O	2.463513	6.509325	11.723084
O	0.116548	2.894036	1.744668
O	6.916179	6.623006	6.780946
O	0.093073	10.721932	11.768177
O	2.470593	1.378475	12.526772
O	9.417683	5.420273	2.837574
O	2.711338	9.453099	7.886212
O	11.357698	1.396950	12.577804
O	4.489288	5.414707	2.789314
O	-2.392381	9.266406	7.733286
O	6.924301	8.895625	12.729040
O	6.943364	1.158786	2.862731
O	0.050999	5.197787	8.021067
O	5.127673	8.837530	14.691157
O	4.908679	0.999157	4.619341
O	-1.925653	4.710301	9.721206
O	-3.415849	11.812095	14.566958
O	10.470532	3.918012	4.772902
O	3.708812	7.807077	9.757710
O	-1.759355	2.997820	14.636487
O	5.130964	6.993621	4.826501
O	-1.669138	10.814144	9.760050
O	-4.932034	8.880193	14.683746
O	8.822049	0.953622	4.771405
O	2.139161	4.889950	9.644167
O	3.539410	11.874694	14.648288
O	3.470996	3.864438	4.698173
O	-3.478916	7.972436	9.804397
O	1.956219	3.038165	14.570977
O	8.724685	7.026927	4.856793
O	1.806679	11.123052	9.748698
O	3.448870	1.707340	9.141975
Si	5.376346	9.200165	1.489728
Si	-1.511909	5.147893	11.231379
Si	3.202335	0.031568	1.401339
Si	10.110608	3.910240	6.353097
Si	3.201359	7.894688	11.299956
Si	-1.459074	2.724395	1.442111
Si	5.358939	6.605856	6.382589
Si	-1.460827	10.575747	11.336557
Si	-5.162398	9.212704	1.492396
Si	8.453645	1.343871	6.318999
Si	1.692701	5.186478	11.203203
Si	10.685909	0.038499	1.475804

Si	3.670680	3.997818	6.282750
Si	-3.013189	7.898893	11.356838
Si	1.682367	2.742374	1.383775
Si	8.491498	6.608214	6.412250
Si	1.634662	10.648864	11.293764
Si	1.669129	2.691597	13.011696
Si	8.516544	6.684967	3.279691
Si	1.621660	10.623038	8.202122
Si	3.867129	11.839839	13.063133
Si	3.852768	3.967847	3.108789
Si	-3.106633	7.913215	8.220934
Si	-5.184608	9.105442	13.096041
Si	8.504365	1.298261	3.217080
Si	1.635630	5.342570	8.142993
Si	-1.489579	2.694525	13.070608
Si	5.385487	6.671297	3.253714
Si	-1.430977	10.499388	8.179717
Si	-3.703923	11.814831	12.979360
Si	10.061382	3.982707	3.205393
Si	3.261080	7.970124	8.199576
Si	5.367792	9.122131	13.112802
Si	5.350549	1.293836	3.114255
Si	-1.549833	5.183303	8.207469
Al	5.348666	1.235517	6.258604
H	9.269999	5.278924	11.551968
H	7.148986	6.303929	12.305892
H	4.967382	5.351191	11.562235
H	7.063870	2.482812	9.109654
H	3.694905	2.218291	7.803735
H	3.880561	3.927638	9.636554
H	9.254919	3.382096	9.931916
C	8.326565	4.877670	11.190367
C	7.128915	5.452076	11.628655
C	5.908308	4.936105	11.200085
C	5.912317	3.844344	10.324968
C	7.104129	3.282581	9.848895
C	8.317217	3.802009	10.297054
N	4.502828	2.021584	9.789955
N	4.679277	3.314087	9.882368

TS PhNH=NO/H^+-ZEO → PhNH=NOH^+/ZEO

O	6.941146	9.548068	1.746154
O	6.932551	1.899249	6.466813
O	0.098028	5.395623	11.291624
O	2.166610	1.238900	1.763444
O	9.068468	5.112869	6.700335
O	2.146416	9.112125	11.490052
O	11.753910	1.215422	1.833137
O	4.795344	5.078138	6.701685
O	-1.966813	9.079446	11.738260
O	0.087748	2.441182	12.784928

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O     6.949626    6.329010    2.990812
O     0.132077    9.991556    8.008702
O     4.922609   10.638646   12.741146
O     4.905133    2.821232    2.689337
O    -2.085944    6.679229    7.917160
O    -4.733792   10.597495   12.625264
O     8.987253    2.817379    2.850914
O     2.084709    6.877109    7.872238
O     4.907552    7.946862    2.399796
O    -1.763370   11.764109    7.295553
O    -1.994851    3.976060   12.223486
O     4.639322    0.245702    2.098280
O    -2.173787    4.118638    7.166534
O     4.492160    8.049035   12.263171
O    11.411782    3.819696    2.321413
O     4.564632    7.677539    7.289410
O    -2.310671   11.667154   12.178856
O     8.979890    7.949483    2.389318
O     8.733182    0.026344    7.223031
O     2.192115    3.929170   12.090218
O     9.302507    0.240208    2.286198
O     2.281715    4.331773    7.049573
O    -4.341844    7.978536   12.284230
O     2.473140    3.844512    2.272137
O     9.200873    7.696464    7.374250
O     2.490535   11.640546   12.242127
O     4.481499   10.467017    1.925436
O     4.124268    2.504235    6.929057
O    -2.270036    6.495140   11.686561
O    -4.277924   10.486192    1.936153
O     9.485493    2.495885    6.832932
O     2.465170    6.506503   11.713158
O     0.115380    2.893943    1.732669
O     6.912384    6.613413    6.784705
O     0.092056   10.731043   11.757920
O     2.470329    1.378551   12.528341
O     9.417931    5.420735    2.839876
O     2.715156    9.455232    7.875600
O    11.362082    1.394826   12.577754
O     4.483353    5.412986    2.782562
O    -2.395156    9.266043    7.731142
O     6.922960    8.893061   12.731559
O     6.939456    1.163910    2.854089
O     0.050036    5.192725    8.042495
O     5.125942    8.823539   14.694705
O     4.914380    1.004665    4.629844
O    -1.943176    4.720663    9.720227
O    -3.409306   11.811407   14.567895
O    10.467610    3.914478    4.774338
O     3.708654    7.818657    9.757258
O    11.905847    3.002079   14.635262
O     5.125896    6.970346    4.832998
O    -1.677695   10.818627    9.755593
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O	-4.928738	8.875719	14.682806
O	8.804271	0.962609	4.774369
O	2.157968	4.875310	9.637562
O	10.367722	0.038181	14.648953
O	3.479586	3.868559	4.711190
O	-3.470028	7.962357	9.802520
O	1.967520	3.045080	14.573058
O	8.720481	7.024568	4.859514
O	1.817701	11.119205	9.745773
O	3.477856	1.668458	9.099708
Si	5.375543	9.196824	1.492002
Si	-1.511092	5.148856	11.227706
Si	3.203432	0.031509	1.403245
Si	10.108934	3.905976	6.354789
Si	3.198866	7.897778	11.298497
Si	-1.461596	2.725923	1.440163
Si	5.352248	6.585537	6.390476
Si	-1.462636	10.577731	11.330938
Si	-5.162926	9.211249	1.491404
Si	8.434773	1.350283	6.322481
Si	1.698249	5.180978	11.193443
Si	10.682296	0.039968	1.476372
Si	3.675686	3.965244	6.304604
Si	-3.009170	7.897726	11.356441
Si	1.684429	2.744003	1.385450
Si	8.487088	6.604487	6.414722
Si	1.635985	10.649643	11.290835
Si	1.672339	2.693874	13.016825
Si	8.512532	6.682830	3.282057
Si	1.621217	10.619630	8.198954
Si	3.865823	11.840475	13.065905
Si	3.849386	3.967039	3.121923
Si	-3.105507	7.910110	8.215937
Si	-5.184835	9.104365	13.096437
Si	8.498201	1.300860	3.216887
Si	1.636708	5.340442	8.139562
Si	-1.489565	2.695148	13.072145
Si	5.381591	6.663904	3.257970
Si	-1.427654	10.495475	8.175779
Si	-3.703786	11.814072	12.982197
Si	10.061272	3.982285	3.206071
Si	3.259206	7.971271	8.197197
Si	5.365754	9.118122	13.118155
Si	5.347877	1.296564	3.123261
Si	-1.552667	5.183151	8.205888
Al	5.321491	1.265838	6.278839
H	9.250212	5.275193	11.550290
H	7.125112	6.310079	12.279206
H	4.947235	5.362977	11.520564
H	7.060203	2.459252	9.116810
H	3.649294	2.160329	7.992169
H	3.892383	3.911438	9.558087
H	9.247049	3.364557	9.947749

C	8.308487	4.870174	11.186914
C	7.107691	5.452083	11.609558
C	5.889339	4.939130	11.172380
C	5.903256	3.835138	10.311838
C	7.097165	3.261796	9.853463
C	8.306893	3.785922	10.304152
N	4.499803	2.013818	9.819970
N	4.677607	3.297529	9.853523

PhNH=NOH^{+}/ZEO

O	6.948760	9.460759	1.783362
O	6.988818	1.488354	6.688254
O	0.080359	5.413438	11.579560
O	2.177142	1.157690	1.610963
O	9.011441	5.099884	6.663329
O	2.168139	9.040889	11.354255
O	11.777084	1.129800	1.750718
O	4.779071	5.148789	6.717509
O	-1.960375	8.969772	11.782958
O	0.081055	2.387883	12.691493
O	6.993193	6.319630	2.933510
O	0.109885	10.277625	7.683795
O	4.928849	10.608621	12.754250
O	4.849725	2.663123	3.071861
O	-2.116378	6.601715	8.105772
O	-4.705931	10.552112	12.624232
O	9.009169	2.755807	2.847192
O	2.170912	6.738689	7.808748
O	4.888755	7.837787	2.306831
O	-2.124153	11.818685	7.518773
O	-2.045387	3.928503	12.214618
O	4.636659	0.198388	2.112837
O	-2.243981	4.100515	7.183216
O	4.490722	8.024278	12.224679
O	11.434059	3.728629	2.318284
O	4.560283	7.764728	7.179499
O	-2.316735	11.609276	12.047594
O	9.047176	7.893117	2.322934
O	2.267095	11.791100	7.207728
O	2.224081	3.848906	12.027016
O	9.334647	0.174986	2.297882
O	2.370146	4.144066	7.160133
O	-4.351333	7.917130	12.254176
O	2.556981	3.737483	2.220371
O	-4.423513	7.677041	7.310639
O	2.515424	11.570254	12.154945
O	4.481219	10.380807	1.834509
O	4.354807	2.535231	6.610264
O	-2.384610	6.390994	11.457802
O	-4.264335	10.425517	1.835478
O	9.433023	2.493310	6.788167

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 O    2.507809    6.438939   11.687067
 O    0.145950    2.815016    1.768497
 O    6.913887    6.701818    6.701702
 O    0.111731   10.618750   11.831541
 O    2.512046    1.339704   12.554765
 O    9.443166    5.360928    2.780186
 O    2.579404    9.319781    7.955389
 O   11.338331    1.357767   12.590219
 O    4.613110    5.262583    2.688944
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 O    6.926666    8.890650   12.602513
 O    6.955798    1.127974    2.796676
 O    0.057675    5.203005    7.732619
 O    5.228116    8.736487   14.639536
 O    5.151356    0.541214    4.698149
 O   -1.605714    4.541020    9.700084
 O   -3.249424   11.729098   14.514452
 O   10.465870    3.913971    4.762285
 O    3.776545    7.699729    9.701813
 O   -1.685258    2.975166   14.620884
 O    5.122776    6.917175    4.746038
 O   -1.536022   10.609095    9.746741
 O   -5.012698    8.796549   14.633017
 O    8.787683    0.904074    4.765054
 O    1.873468    4.834124    9.649573
 O    3.449613   11.826379   14.616806
 O    3.322510    4.142499    4.715128
 O   -3.512696    8.124823    9.760001
 O    1.898919    3.054779   14.532585
 O    8.777830    6.993538    4.799309
 O    1.653813   11.087478    9.703336
 O    3.660824    1.396264    9.286781
Si    5.394715    9.107876    1.448640
Si   -1.478935    5.078499   11.225378
Si   -3.585657   11.808029    1.339407
Si   10.064869    3.898708    6.334444
Si    3.233711    7.821556   11.227762
Si   -1.425280    2.653582    1.429245
Si    5.341389    6.617824    6.327035
Si   -1.422095   10.444558   11.345104
Si   -5.164384    9.144081    1.449848
Si    8.520605    1.215467    6.349133
Si    1.642974    5.155565   11.218504
Si    3.839652   11.809675    1.432979
Si    3.736271    3.952910    6.286353
Si   -3.045926    7.854873   11.293304
Si    1.701826    2.686825    1.349821
Si    8.487988    6.608820    6.355047
Si    1.625511   10.572655   11.244400
Si    1.654002    2.646203   12.987104
Si    8.558475    6.639531    3.226277
Si    1.644305   10.625077    8.130796
Si    3.846063   11.790641   13.046539
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Si	3.845412	3.923000	3.196143
Si	-3.090206	7.890229	8.199763
Si	-5.200246	9.053422	13.044983
Si	8.507096	1.240987	3.205702
Si	1.630174	5.232113	8.078754
Si	-1.489116	2.653893	13.049628
Si	5.407092	6.578320	3.185736
Si	-1.445067	10.473557	8.128938
Si	-3.656203	11.753197	12.954264
Si	10.077848	3.928180	3.188590
Si	3.273331	7.882082	8.155614
Si	5.387037	9.078993	13.064959
Si	5.387020	1.120655	3.230203
Si	-1.487043	5.114228	8.174910
Al	5.331467	1.150064	6.310541
H	9.010035	5.118220	12.559611
H	6.732595	5.777626	13.334264
H	4.720078	4.654099	12.386792
H	7.271796	2.241694	9.853160
H	3.976896	0.734514	8.488038
H	3.795985	3.018882	10.970714
H	9.274886	3.344272	10.833984
C	8.128159	4.631439	12.144156
C	6.852605	5.000595	12.579849
C	5.720906	4.376728	12.052557
C	5.892090	3.385998	11.076990
C	7.164945	3.007773	10.619856
C	8.278382	3.636589	11.166596
N	4.810588	1.901922	9.636846
N	4.722560	2.770001	10.565725

TS PhNH=NOH^{+}/ZEO → PhN=NOH/H^{+}-ZEO

O	6.944654	9.507437	1.760494
O	7.007031	1.496926	6.322581
O	0.080978	5.481746	11.449836
O	2.222187	1.119062	1.534388
O	9.057362	5.057641	6.544715
O	2.142772	9.008749	11.328147
O	11.710604	1.102299	1.784351
O	4.831917	5.092564	6.561084
O	-1.954475	8.954840	11.598843
O	0.085780	2.268410	12.642413
O	6.940511	6.219396	2.910080
O	0.157175	10.139876	7.719231
O	4.959547	10.610329	12.587860
O	4.936270	2.741278	2.682731
O	-2.119669	6.535349	8.079399
O	-4.733454	10.551540	12.505514
O	9.019861	2.702614	2.855397
O	2.187943	6.730949	7.778218
O	4.921038	7.820468	2.215729

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O   -2.007272   11.713618    7.288403
O   -1.965367    3.933279   12.211802
O    4.686039    0.175842    2.009571
O   -2.221955    4.040888    7.137048
O    4.476660    8.017156   12.211136
O   11.411937    3.721987    2.201178
O    4.615725    7.678062    7.199503
O   -2.330025   11.584346   12.001449
O    8.965174    7.827333    2.214463
O    2.198849   11.796878    7.180110
O    2.125227    3.862975   12.055495
O    9.237652    0.150387    2.104911
O    2.405516    4.148677    7.108209
O   -4.324126    7.918832   12.232363
O    2.485033    3.691649    2.249261
O   -4.384516    7.630987    7.209285
O    2.494161   11.532638   12.142831
O    4.440839   10.357649    1.858839
O    4.382577    2.486888    6.898071
O   -2.407066    6.358991   11.376200
O   -4.232381   10.380891    1.866523
O    9.463379    2.447628    6.625353
O    2.525362    6.412188   11.642424
O    0.122810    2.697635    1.793102
O    6.952648    6.632011    6.646559
O    0.094503   10.616188   11.723201
O    2.534291    1.331163   12.631142
O    9.402602    5.307375    2.721467
O    2.676685    9.322105    7.871613
O   11.300550    1.361436   12.476232
O    4.450785    5.325700    2.777847
O   -2.259580    9.114740    7.657133
O    6.930091    8.849817   12.530112
O    6.949529    1.072925    2.915074
O    0.077454    5.160628    7.700082
O    5.237055    8.853341   14.584636
O    4.831753    0.863061    4.565889
O   -1.608968    4.472748    9.659328
O   -3.262446   11.557495   14.468675
O   10.566195    3.914455    4.672846
O    3.784293    7.699775    9.685552
O   12.019847    2.851243   14.573480
O    5.145316    7.009286    4.716134
O   -1.567714   10.740514    9.654196
O   -5.032057    8.878380   14.579869
O    8.963530    0.734008    4.659889
O    1.911971    4.802792    9.608948
O    3.571944   11.768851   14.537880
O    3.473757    3.752250    4.699688
O   -3.604813    8.035817    9.694977
O    1.808992    3.065165   14.533937
O    8.759506    6.978822    4.707019
O    1.737041   11.057838    9.661524
```

O	2.622132	1.498714	9.580358
Si	5.397771	9.136380	1.408220
Si	-1.468083	5.065285	11.173075
Si	-3.562681	11.743329	1.286643
Si	10.118576	3.860904	6.230838
Si	3.224978	7.805156	11.212173
Si	-1.438023	2.589967	1.392394
Si	5.384216	6.596852	6.267749
Si	-1.442469	10.459948	11.239268
Si	-5.178258	9.150169	1.408487
Si	8.561030	1.161623	6.189655
Si	1.648294	5.134202	11.183782
Si	3.821540	11.772408	1.374196
Si	3.780933	3.884362	6.281506
Si	-3.063545	7.823288	11.218992
Si	1.672498	2.634337	1.332080
Si	8.521207	6.565019	6.261178
Si	1.626421	10.547312	11.202546
Si	1.638426	2.627363	12.979067
Si	8.510207	6.584549	3.145925
Si	1.678142	10.578489	8.098141
Si	3.874049	11.772974	12.949911
Si	3.848461	3.862484	3.111952
Si	-3.089442	7.829716	8.158607
Si	-5.202984	9.060880	12.980294
Si	8.533026	1.171020	3.153356
Si	1.647547	5.224517	8.057307
Si	-1.468505	2.601667	12.988017
Si	5.375843	6.590599	3.159818
Si	-1.417583	10.445709	8.053883
Si	-3.665082	11.719525	12.912493
Si	10.088393	3.896694	3.119967
Si	3.307202	7.862775	8.133996
Si	5.398503	9.093866	12.992788
Si	5.346605	1.201641	3.091538
Si	-1.473840	5.055678	8.141015
Al	5.328425	1.115285	6.193198
H	9.259826	4.442000	9.484520
H	7.457267	6.075892	10.040297
H	5.127345	5.266496	10.439135
H	6.374350	1.238132	9.517479
H	2.429709	0.979571	8.768529
H	4.149157	2.163199	8.163320
H	8.727122	2.026263	9.232976
C	8.232363	4.099721	9.607913
C	7.224115	5.015571	9.936984
C	5.920662	4.575236	10.156344
C	5.627993	3.217846	9.959012
C	6.626743	2.295367	9.603763
C	7.937616	2.742039	9.458706
N	3.835436	2.077616	9.313480
N	4.313020	2.760212	10.227539

PhN=NOH/H^+-ZEO

O	6.943192	9.507381	1.761424
O	7.019054	1.501685	6.305614
O	0.080015	5.488386	11.448698
O	2.225761	1.121875	1.539335
O	9.062544	5.060094	6.539672
O	2.144937	9.011070	11.328595
O	11.709391	1.105902	1.783500
O	4.839097	5.102769	6.556372
O	-1.953875	8.955044	11.599205
O	0.086931	2.271483	12.644102
O	6.941738	6.220484	2.911307
O	0.159451	10.138626	7.713781
O	4.962974	10.612779	12.592079
O	4.942445	2.742854	2.664070
O	-2.119193	6.535209	8.073311
O	-4.732037	10.552383	12.505868
O	9.020612	2.705639	2.855683
O	2.196874	6.724907	7.770460
O	4.918937	7.823408	2.216940
O	-1.997687	11.700020	7.262050
O	-1.964099	3.934151	12.208599
O	4.690378	0.172799	1.997835
O	-2.216180	4.041730	7.133664
O	4.480010	8.020464	12.208074
O	11.412023	3.726707	2.197968
O	4.617721	7.685282	7.199958
O	-2.327956	11.582889	12.001356
O	8.964703	7.830009	2.215042
O	2.200662	11.794265	7.178811
O	2.123271	3.871983	12.064699
O	9.239279	0.151031	2.103450
O	2.413902	4.147060	7.108307
O	-4.322932	7.919237	12.234352
O	2.483343	3.692618	2.249158
O	-4.383484	7.635206	7.209790
O	2.495117	11.532273	12.143830
O	4.441425	10.358939	1.857152
O	4.397678	2.494762	6.842563
O	-2.408710	6.359582	11.375541
O	-4.235749	10.384578	1.868131
O	9.473735	2.447019	6.624902
O	2.524330	6.416523	11.642534
O	0.122059	2.700102	1.794912
O	6.958207	6.638424	6.647102
O	0.093931	10.614194	11.723815
O	2.533999	1.332837	12.638743
O	9.403231	5.309587	2.723593
O	2.673202	9.319589	7.870198
O	11.301177	1.363059	12.478724

O	4.453131	5.329739	2.776999
O	-2.256923	9.111553	7.651610
O	6.932533	8.852581	12.531077
O	6.955101	1.072979	2.915567
O	0.080609	5.158962	7.692429
O	5.237670	8.849024	14.583870
O	4.828448	0.869118	4.545624
O	-1.604987	4.476771	9.657161
O	-3.263661	11.556798	14.466158
O	10.570368	3.913305	4.671248
O	3.783444	7.701694	9.685058
O	-1.654436	2.855866	14.572155
O	5.146550	7.013063	4.715607
O	-1.565215	10.733433	9.649421
O	-5.031902	8.880020	14.580990
O	8.974674	0.733331	4.657177
O	1.906950	4.807855	9.610709
O	3.571041	11.768667	14.537574
O	3.486916	3.747654	4.685045
O	-3.601631	8.038563	9.694696
O	1.809163	3.066528	14.535480
O	8.760556	6.983286	4.706955
O	1.735124	11.056286	9.661678
O	2.625863	1.510950	9.605993
Si	5.397146	9.137225	1.405701
Si	-1.467857	5.067932	11.171963
Si	-3.564203	11.743273	1.281443
Si	10.124054	3.862855	6.229866
Si	3.226328	7.807188	11.212953
Si	-1.438461	2.593343	1.389918
Si	5.392969	6.612991	6.268003
Si	-1.442754	10.460341	11.236881
Si	-5.179452	9.152298	1.408235
Si	8.575864	1.161202	6.187606
Si	1.647806	5.137280	11.187089
Si	3.823105	11.773963	1.372131
Si	3.771865	3.926491	6.255365
Si	-3.063426	7.824323	11.219892
Si	1.670355	2.634181	1.330334
Si	8.527393	6.568091	6.261374
Si	1.625434	10.548480	11.204026
Si	1.640190	2.629650	12.978399
Si	8.511962	6.587341	3.146447
Si	1.677919	10.577890	8.099671
Si	3.875086	11.774256	12.949611
Si	3.855285	3.863382	3.092099
Si	-3.087965	7.830196	8.159313
Si	-5.200664	9.062691	12.980423
Si	8.539716	1.172616	3.152342
Si	1.646925	5.224440	8.062093
Si	-1.467005	2.604242	12.986225
Si	5.378718	6.595371	3.158571
Si	-1.415493	10.441180	8.051173

Si	-3.663931	11.721978	12.908188
Si	10.090647	3.899204	3.119297
Si	3.307522	7.863557	8.135277
Si	5.401277	9.095061	12.992012
Si	5.351902	1.202192	3.071375
Si	-1.471417	5.056822	8.139303
Al	5.360756	1.073117	6.160627
H	9.269374	4.440441	9.458011
H	7.463725	6.073237	10.005258
H	5.137259	5.268004	10.406284
H	6.387341	1.231828	9.547835
H	2.433767	0.980326	8.804263
H	4.199539	2.280479	7.873991
H	8.737268	2.021292	9.228457
C	8.244096	4.096063	9.593157
C	7.233701	5.010970	9.913481
C	5.928963	4.570261	10.134287
C	5.637055	3.209727	9.968379
C	6.640462	2.289091	9.628421
C	7.949584	2.736687	9.462159
N	3.854721	2.078615	9.304913
N	4.317492	2.746604	10.237440

TS PhN=NOH/H^+-ZEO → (PhN=N^+ + H_2O)/ZEO

O	6.962793	9.494982	1.801764
O	7.013325	1.603779	6.503776
O	0.174741	5.421369	11.652921
O	2.221245	1.134998	1.604958
O	9.069252	5.078856	6.644770
O	2.157600	9.008879	11.354409
O	11.791168	1.094820	1.775493
O	4.861916	5.111615	6.576777
O	-1.904609	9.017726	11.802240
O	0.113632	2.384008	12.732433
O	6.987626	6.218881	2.988738
O	0.175319	10.126348	7.797054
O	5.044210	10.642454	12.697073
O	4.959653	2.729176	2.757722
O	-2.085600	6.583975	8.123708
O	-4.650533	10.517409	12.632368
O	9.005854	2.743265	2.912873
O	2.182120	6.794409	7.837636
O	4.950566	7.800331	2.257269
O	-1.959249	11.765516	7.430511
O	-1.984720	3.947941	12.229227
O	4.665259	0.158295	2.153590
O	-2.212679	4.069629	7.251137
O	4.520216	8.069369	12.231835
O	11.437178	3.690305	2.321601
O	4.620184	7.698872	7.239947

O	-2.293364	11.639725	12.066478
O	8.997822	7.851814	2.331530
O	2.186947	11.805233	7.227838
O	2.262559	3.826887	12.053078
O	9.320318	0.182738	2.231810
O	2.409350	4.233609	7.135382
O	-4.270036	7.896944	12.286044
O	2.524279	3.708551	2.295047
O	-4.387879	7.648373	7.350313
O	2.577557	11.525710	12.175941
O	4.465296	10.347018	1.889606
O	4.324909	2.523817	6.985188
O	-2.234493	6.441342	11.489580
O	-4.232536	10.389922	1.875910
O	9.488179	2.467177	6.782953
O	2.595222	6.414909	11.701559
O	0.154706	2.761075	1.775849
O	6.964576	6.659562	6.743137
O	0.145225	10.669942	11.807752
O	2.496515	1.295657	12.642529
O	9.466180	5.336812	2.837155
O	2.717043	9.366360	7.953577
O	11.357316	1.375674	12.570901
O	4.499795	5.319694	2.873135
O	-2.259718	9.163451	7.656913
O	6.985912	8.849272	12.585172
O	6.973500	1.052905	2.932958
O	0.093708	5.218538	7.681836
O	5.268164	8.815236	14.628373
O	4.929218	0.891429	4.687847
O	-1.469748	4.571225	9.735023
O	-3.195164	11.652996	14.546177
O	10.554153	3.883215	4.783901
O	3.825738	7.704880	9.729379
O	-1.688925	2.942407	14.632884
O	5.199350	7.056984	4.770039
O	-1.563978	10.659786	9.747245
O	-5.002687	8.789113	14.654245
O	8.919801	0.828120	4.762027
O	1.869272	4.863926	9.653370
O	3.550274	11.769891	14.602440
O	3.480010	3.738602	4.754450
O	-3.448102	8.116436	9.795152
O	1.926452	3.072477	14.566717
O	8.779321	7.000502	4.819071
O	1.740877	11.092189	9.723955
O	3.542044	1.936916	9.222176
Si	5.418975	9.118386	1.449155
Si	-1.369999	5.099265	11.273511
Si	-3.551916	11.768211	1.361584
Si	10.127494	3.875479	6.350348
Si	3.262379	7.819058	11.253960
Si	-1.416531	2.616405	1.434782

Si	5.408499	6.625328	6.319653
Si	-1.396112	10.496852	11.342891
Si	-5.159084	9.132097	1.469254
Si	8.552713	1.221655	6.308801
Si	1.724193	5.128427	11.250277
Si	3.861331	11.778584	1.431830
Si	3.776028	3.927857	6.329886
Si	-2.957468	7.872827	11.333042
Si	1.715155	2.660756	1.364639
Si	8.536674	6.588614	6.375164
Si	1.666041	10.561074	11.257605
Si	1.694422	2.647505	13.015430
Si	8.550164	6.600916	3.254960
Si	1.688877	10.599259	8.165487
Si	3.926035	11.783188	13.027615
Si	3.877997	3.859317	3.176504
Si	-3.046254	7.880833	8.227745
Si	-5.147876	9.024393	13.059256
Si	8.545334	1.205804	3.228221
Si	1.647781	5.283404	8.098145
Si	-1.456220	2.657616	13.057609
Si	5.420896	6.594416	3.225261
Si	-1.392659	10.454706	8.135284
Si	-3.623985	11.733865	12.990839
Si	10.105747	3.899933	3.222249
Si	3.325609	7.896501	8.187574
Si	5.454462	9.105022	13.047811
Si	5.379215	1.197161	3.186747
Si	-1.428951	5.110641	8.196162
Al	5.348441	1.171408	6.332115
H	9.963402	5.582139	9.876911
H	7.961651	7.017737	10.008406
H	5.688727	5.953724	10.009085
H	7.546909	2.042800	10.008622
H	3.573594	0.953718	9.239722
H	3.860011	2.231685	8.095578
H	9.805175	3.119872	9.972054
C	8.989011	5.122672	9.970908
C	7.855671	5.934756	10.020207
C	6.594785	5.348776	10.028534
C	6.510625	3.950247	10.018817
C	7.652415	3.126523	10.040217
C	8.901059	3.727515	10.007430
N	5.025693	2.227028	9.932106
N	5.228100	3.398510	9.796130

$(PhN{=}N^{+} + H_2O)$/ZEO

O	-4.720090	10.780377	1.841652
O	2.158620	6.859678	6.861442
O	8.987210	2.813162	11.609166
O	0.095581	2.488276	1.682404

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O    0.124347   10.417676    6.743676
O    6.951898    6.484093   11.371668
O    4.904881   10.787837    1.810021
O   -2.111912    6.723426    6.796261
O    4.972093    2.790589   11.802865
O   11.695256    1.288602   12.793627
O   -1.959217    9.208090    2.948601
O    4.924436    5.249838    7.791675
O    6.955679    9.554921   12.874402
O    0.098945    5.621125    2.966041
O    6.911632    1.408831    8.190665
O    2.211295    1.246998   12.716322
O    2.143023    9.207213    2.893166
O    8.925850    5.327030    7.829375
O   -4.369388    8.190346    2.404259
O    2.471284    4.114732    7.496867
O    9.295117    0.229468   12.246258
O    2.158059    4.115371    2.236817
O    9.053671    0.169685    7.206207
O    9.009541    7.940781   12.281876
O    2.488275   11.800074    2.367608
O   -4.444758    7.915745    7.246758
O    2.520453    3.830822   12.136377
O   -2.307547   11.789107    2.396787
O    4.598082    7.865010    7.262869
O   11.420082    3.852838   12.096034
O    4.553180    8.203492    2.417698
O   11.243380    4.128055    7.201024
O    4.656830    0.199624   12.316756
O   -1.969679    4.076065    2.315436
O    4.806961    0.040349    7.333780
O    4.902378    7.977376   12.230517
O    6.927427    9.103375    1.841770
O   -0.034823    5.085376    6.861280
O    6.966763    1.084087   11.475126
O    2.533150    1.543970    1.884845
O    2.588787    9.467047    6.858947
O    9.349687    5.419866   11.754635
O   11.317095    1.554084    1.787619
O   -2.279663    9.345538    6.812534
O    4.600687    5.410771   11.887657
O    0.123294    2.899165   12.620321
O    0.089721   10.863727    2.825252
O    6.909020    6.998395    8.086661
O    4.518583   10.521953   12.646444
O   -2.329796    6.611677    2.781453
O    4.646375    2.639794    7.731898
O   -4.247496   10.483664   12.664357
O    2.519551    6.612766    2.797342
O    9.129540    2.720527    7.784837
O   -4.886119    8.911378   14.708272
O    1.938793    4.888452    4.775426
O    8.991032    0.906846    9.738512
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O	1.903081	3.110750	14.596175
O	1.855246	11.038220	4.808948
O	8.970923	7.154318	9.763689
O	10.245009	0.027973	14.666880
O	-3.404665	7.976192	4.824985
O	3.717173	4.025436	9.804180
O	3.580936	0.064046	14.699515
O	3.541367	8.025802	4.846766
O	10.386074	4.090691	9.695422
O	5.095600	8.907505	14.691393
O	-1.772540	4.977807	4.795627
O	4.872293	0.985116	9.813085
O	-1.659742	3.233786	14.593532
O	-1.648884	11.055238	4.851270
O	4.861880	7.028203	9.774469
O	-0.255791	2.464839	8.539210
Si	-5.180473	9.256267	1.506042
Si	8.557166	1.279992	11.258730
Si	1.666066	2.827942	1.417411
Si	1.689724	10.714340	6.388603
Si	8.549740	6.752808	11.281235
Si	10.662705	0.114722	1.471443
Si	-3.052445	7.984043	6.406781
Si	3.962119	4.003811	11.393479
Si	3.186911	0.119744	1.512510
Si	3.186583	8.005834	6.442296
Si	10.023659	4.024939	11.274560
Si	5.357940	9.253294	1.498230
Si	-1.537897	5.244402	6.387629
Si	5.366446	1.280774	11.331783
Si	-1.464134	2.844652	1.403766
Si	-1.449871	10.675058	6.419747
Si	5.345736	6.729063	11.300211
Si	-1.441960	2.803072	13.043086
Si	-1.458069	10.721849	3.271599
Si	5.313038	6.772811	8.211515
Si	5.378590	9.236311	13.129251
Si	-1.465352	5.316241	3.238507
Si	5.302919	1.270388	8.260763
Si	3.245727	0.053068	13.115356
Si	3.181523	8.001121	3.268956
Si	9.919873	4.079949	8.129145
Si	10.664134	0.068168	13.105019
Si	-3.004842	7.997568	3.254248
Si	3.908637	4.019089	8.175365
Si	1.688986	2.758448	13.034167
Si	1.649273	10.714316	3.234889
Si	8.503429	6.848795	8.225101
Si	-5.151373	9.226446	13.142364
Si	1.681929	5.294628	3.260716
Si	8.519019	1.296110	8.223152
Al	1.645061	5.240174	6.446593
H	-0.272967	10.310806	12.185433

H	-1.922042	8.483340	12.561918
H	-1.493180	6.202706	11.616505
H	2.176356	7.663598	9.796103
H	0.583485	2.746628	8.126753
H	-0.932382	2.929068	8.009222
H	1.771692	9.917905	10.822868
C	-0.095944	9.327371	11.748257
C	-1.025816	8.300118	11.969598
C	-0.812931	7.034835	11.436259
C	0.351373	6.850322	10.663857
C	1.296752	7.864975	10.407619
C	1.054233	9.111191	10.974598
N	0.888048	4.563483	9.814828
N	0.614404	5.593637	10.178362

TS PhNH=NOH$^+$/ZEO → (PhN=N$^+$ + H_2O)/ZEO

O	-4.729184	10.730092	1.727089
O	2.224157	6.790031	6.703864
O	8.956681	2.799673	11.509872
O	0.102754	2.387125	1.668774
O	0.093961	10.279090	6.632598
O	6.931119	6.344098	11.392623
O	4.929277	10.738500	1.693243
O	-2.035811	6.712483	6.667035
O	4.956982	2.781470	11.764766
O	11.725704	1.210948	12.722981
O	-1.941522	9.158089	2.919347
O	4.780220	5.211041	7.646604
O	6.939885	9.559776	12.750359
O	0.127601	5.535773	3.068081
O	6.911291	1.553433	7.986452
O	2.148124	1.178653	12.658568
O	2.107058	9.135516	2.887081
O	8.939963	5.185507	7.868183
O	-4.330763	8.143318	2.286685
O	2.354507	4.053824	7.525618
O	9.302501	0.232310	12.188564
O	2.142654	4.068959	2.128368
O	8.976646	0.066403	7.189742
O	8.961050	7.895636	12.191532
O	2.501916	11.708943	2.304715
O	-4.434529	7.760272	7.159883
O	2.488515	3.761577	12.072997
O	-2.313735	11.721425	2.312202
O	4.613261	7.843172	7.201261
O	11.375433	3.791373	12.115629
O	4.515718	8.161888	2.287143
O	11.294770	4.124881	7.166425
O	4.588920	0.183825	12.190543
O	-1.926889	4.039754	2.231117
O	-1.976879	11.828177	7.293200

O	4.914057	7.951511	12.110993
O	6.929930	9.036060	1.813181
O	-0.003713	5.025546	6.626677
O	6.944685	1.081470	11.547927
O	2.555133	1.493295	1.807171
O	2.586380	9.403735	6.746038
O	9.377665	5.396252	11.632395
O	11.308821	1.497665	1.789450
O	-2.373262	9.325796	6.711720
O	4.516032	5.396832	11.808772
O	0.093735	2.853700	12.528175
O	0.085571	10.829750	2.769728
O	6.897698	6.797752	7.850521
O	4.468251	10.462347	12.604210
O	-2.277414	6.573483	2.702523
O	4.532059	2.568251	7.600693
O	-4.256091	10.429341	12.599249
O	2.524938	6.551254	2.769595
O	9.287342	2.593725	7.737317
O	-4.955430	8.845259	14.615639
O	2.116199	4.728763	4.692569
O	8.833742	0.842918	9.690149
O	1.846651	3.043542	14.525619
O	1.839561	11.026732	4.753305
O	8.812307	7.133688	9.678381
O	10.238678	0.031478	14.611253
O	-3.441156	7.900432	4.731568
O	3.724708	3.923327	9.745541
O	3.596313	0.027511	14.608772
O	3.638302	7.993079	4.754339
O	10.501176	3.980812	9.664751
O	5.158060	8.831296	14.596751
O	-1.887663	4.896789	4.716919
O	4.977741	1.029669	9.728810
O	-1.637034	3.119324	14.561946
O	-1.669683	11.047588	4.785261
O	4.965488	6.930582	9.676003
O	0.654150	4.097157	9.437339
Si	-5.188780	9.198461	1.418356
Si	8.514192	1.258947	11.224692
Si	1.655345	2.755392	1.346780
Si	1.654032	10.638356	6.316451
Si	8.507936	6.695820	11.211830
Si	10.669543	0.063869	1.411533
Si	-3.059330	7.915130	6.308861
Si	3.921238	3.967299	11.353903
Si	3.190713	0.063963	1.418415
Si	3.231942	7.971253	6.335457
Si	10.038886	3.981416	11.219583
Si	5.374419	9.197372	1.402998
Si	-1.538991	5.197788	6.282679
Si	5.366009	1.276581	11.288722
Si	-1.450029	2.762758	1.373582

Si	-1.471840	10.612894	6.341068
Si	5.345222	6.666213	11.234054
Si	-1.450131	2.732453	13.002329
Si	-1.461878	10.681548	3.212413
Si	5.309722	6.702737	8.098430
Si	5.377913	9.195987	13.032498
Si	-1.463102	5.258294	3.195180
Si	5.330255	1.263377	8.157704
Si	3.216818	0.006928	13.032025
Si	3.189544	7.952790	3.197174
Si	10.006791	3.985396	8.108663
Si	10.656251	0.029264	13.048889
Si	-2.991741	7.942143	3.173665
Si	3.909033	3.948837	8.150911
Si	1.647229	2.698629	12.961483
Si	1.639749	10.660254	3.186733
Si	8.481003	6.719826	8.136765
Si	-5.181075	9.183669	13.048092
Si	1.727850	5.205996	3.212856
Si	8.497255	1.258272	8.152654
Al	1.649848	5.230818	6.270497
H	-0.164968	10.445826	12.821551
H	-1.823746	8.674413	13.398941
H	-1.710168	6.446658	12.272795
H	1.683133	7.796464	9.963575
H	1.618792	3.887668	8.238893
H	-0.384425	4.494202	10.137324
H	1.588946	10.000415	11.113394
C	-0.119602	9.473015	12.333753
C	-1.051580	8.481457	12.654212
C	-1.000067	7.236342	12.026274
C	0.001135	6.997257	11.074010
C	0.932061	7.994596	10.727768
C	0.865730	9.226316	11.366942
N	1.043040	5.334598	9.799942
N	0.046180	5.726681	10.479151

TS PhNH=NO/H^+-ZEO → PhN=NOH_rotated/H^+-ZEO

O	6.919874	9.563438	1.768464
O	7.052694	1.827389	6.447112
O	0.095815	5.469949	11.399804
O	2.169701	1.263866	1.780218
O	9.052208	5.111120	6.706139
O	2.155226	9.119869	11.478791
O	11.749413	1.216812	1.807424
O	4.664052	5.349600	6.490057
O	-1.974671	9.090007	11.717618
O	0.079115	2.442041	12.770016
O	6.939341	6.324402	2.959004
O	0.076364	10.148032	7.951624
O	4.934863	10.676830	12.657733

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O    4.922985    2.860144    2.725107
O   -2.035589    6.769511    7.952227
O   -4.699301   10.608856   12.671682
O    8.971762    2.829965    2.859835
O    2.243633    6.808964    7.772935
O    4.886401    7.898742    2.262354
O    4.961118    0.083578    7.398703
O   -2.003017    3.987860   12.187666
O    4.623224    0.266189    2.180273
O   -2.151043    4.217419    7.132456
O    4.514150    8.075717   12.235607
O   11.397667    3.818428    2.303176
O    4.644744    7.878034    7.287582
O   -2.294410   11.689577   12.216264
O    8.966476    7.969014    2.397596
O    8.869208    0.021481    7.226704
O    2.167660    3.954206   12.121828
O    9.278200    0.266764    2.228164
O    2.357958    4.214080    7.156131
O   -4.338952    7.989423   12.294001
O    2.493596    3.874348    2.262704
O    9.236864    7.709082    7.335090
O    2.482649   11.654648   12.231287
O    4.452773   10.463668    1.931712
O    4.501249    2.776416    6.975207
O   -2.311533    6.498618   11.632812
O   -4.295335   10.502902    1.937393
O    9.582056    2.500614    6.816241
O    2.496623    6.519295   11.729791
O    0.110196    2.904795    1.756134
O    6.918841    6.644328    6.785609
O    0.092149   10.722862   11.769641
O    2.459459    1.380798   12.587953
O    9.408899    5.429648    2.799873
O    2.610573    9.415584    7.885121
O   11.338538    1.427574   12.561796
O    4.448763    5.452003    3.017471
O   -2.434972    9.365125    7.751470
O    6.938277    8.930225   12.683957
O    6.938648    1.160542    2.955542
O    0.099143    5.282250    7.897173
O    5.145225    8.914937   14.644017
O    4.888998    1.071582    4.692408
O   -1.807960    4.747119    9.682208
O   -3.355148   11.830631   14.611968
O   10.464955    3.961652    4.756592
O    3.710116    7.827514    9.743620
O   11.920073    3.022692   14.621172
O    5.263358    7.293063    4.785713
O   -1.691979   10.903404    9.789442
O   -4.970024    8.871521   14.693225
O    8.930768    0.940792    4.753741
O    2.058179    4.923585    9.665401
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O	10.396120	0.015529	14.620622
O	3.385511	3.754981	4.740549
O	-3.507248	8.017962	9.789339
O	1.936423	3.066721	14.587412
O	8.714323	7.002280	4.842593
O	1.790081	11.130212	9.744733
O	2.931085	2.074501	9.625385
Si	5.362414	9.215651	1.456245
Si	-1.491125	5.175362	11.219031
Si	3.207835	0.051978	1.440405
Si	10.133783	3.943392	6.342711
Si	3.212113	7.905888	11.288670
Si	-1.461581	2.731486	1.427429
Si	5.379523	6.800154	6.327711
Si	-1.466222	10.595504	11.355652
Si	-5.184888	9.227275	1.500041
Si	8.565222	1.325627	6.303839
Si	1.686833	5.211385	11.228632
Si	10.676064	0.040666	1.452942
Si	3.723677	4.055005	6.283740
Si	-3.029301	7.915037	11.337639
Si	1.680549	2.767224	1.399153
Si	8.492958	6.610032	6.405491
Si	1.633046	10.652088	11.290168
Si	1.659285	2.709125	13.029581
Si	8.501087	6.682649	3.261997
Si	1.606022	10.649175	8.193171
Si	10.708336	0.014116	13.033110
Si	3.830256	3.970318	3.178440
Si	-3.100956	7.971134	8.211877
Si	-5.181785	9.115763	13.102886
Si	8.517720	1.302508	3.222556
Si	1.682722	5.330663	8.131948
Si	-1.493980	2.716942	13.052420
Si	5.393412	6.734601	3.259925
Si	-1.482442	10.609690	8.196972
Si	-3.683474	11.834244	13.031981
Si	10.052309	3.997241	3.189300
Si	3.294290	7.990663	8.179008
Si	5.383063	9.164901	13.063572
Si	5.343027	1.331138	3.183494
Si	-1.489691	5.261298	8.167616
Al	5.398152	1.336065	6.309108
H	9.157302	5.224470	11.693676
H	6.924179	6.179442	12.195726
H	4.873386	5.152651	11.209590
H	7.337959	2.375773	9.004320
H	2.965335	2.213623	8.642344
H	4.751417	2.962451	8.183620
H	9.379535	3.317755	10.097428
C	8.271314	4.798956	11.223959
C	7.010295	5.323022	11.526415
C	5.860942	4.761789	10.965222

C	6.007907	3.699685	10.063089
C	7.265146	3.195778	9.717650
C	8.398380	3.733911	10.325669
N	4.006610	2.611068	10.226596
N	4.873191	3.081017	9.440753

PhN=NOH_rotated/H^+-ZEO

O	6.915661	9.580037	1.769136
O	7.041486	1.690828	6.449368
O	0.074100	5.521478	11.461320
O	2.182127	1.268887	1.780190
O	9.014626	5.126037	6.713299
O	2.173105	9.145053	11.435365
O	11.741944	1.215990	1.802600
O	4.704173	5.330182	6.497785
O	-1.988836	9.090910	11.727468
O	0.067112	2.449521	12.773859
O	6.936513	6.326602	2.955826
O	0.079439	10.250906	7.860129
O	4.927025	10.696925	12.644817
O	4.914679	2.857963	2.761873
O	-2.036689	6.751140	8.020994
O	-4.710560	10.628564	12.639684
O	8.968122	2.843935	2.864312
O	2.216790	6.799500	7.776606
O	4.889318	7.903380	2.257980
O	4.851612	0.087021	7.421233
O	-2.014734	4.013271	12.220621
O	4.644691	0.278784	2.127200
O	-2.194084	4.218386	7.155862
O	4.512848	8.094235	12.235665
O	11.402955	3.816851	2.329024
O	4.606582	7.870803	7.273749
O	-2.304457	11.700605	12.192325
O	8.956770	7.978944	2.386107
O	8.980862	0.011742	7.217241
O	2.146848	3.984765	12.148852
O	9.265117	0.280219	2.208737
O	2.397866	4.204144	7.206441
O	-4.357477	8.003255	12.293811
O	2.488985	3.876434	2.272926
O	-4.411839	7.720402	7.314930
O	2.475780	11.674172	12.218634
O	4.442867	10.468821	1.946289
O	4.520894	2.746251	6.926346
O	-2.362335	6.498609	11.582938
O	-4.289756	10.513763	1.945314
O	9.528590	2.522398	6.803575
O	2.482296	6.546945	11.760060
O	0.109111	2.892846	1.788437
O	6.916440	6.704701	6.790774

O	0.089838	10.709395	11.798788
O	2.458288	1.407561	12.591183
O	9.410898	5.442666	2.783592
O	2.581642	9.399835	7.941454
O	11.319582	1.451788	12.584082
O	4.447192	5.451937	3.010332
O	-2.386746	9.340242	7.739233
O	6.928771	8.955607	12.687509
O	6.939542	1.173982	2.965558
O	0.092770	5.243527	7.855869
O	5.133795	8.944458	14.644623
O	4.868918	0.999606	4.666028
O	-1.754665	4.702849	9.702468
O	-3.376431	11.822866	14.592725
O	10.443247	3.996786	4.766233
O	3.717167	7.782997	9.745290
O	11.929242	3.041514	14.642315
O	5.250229	7.284269	4.782823
O	-1.649455	10.876539	9.786047
O	-4.970672	8.912264	14.687243
O	8.954482	0.937786	4.738753
O	2.003321	4.950314	9.697204
O	10.386959	0.001160	14.617435
O	3.364388	3.778411	4.753744
O	-3.538646	8.075431	9.782346
O	1.912747	3.077654	14.600104
O	8.710581	7.006387	4.833140
O	1.735633	11.167231	9.738636
O	2.916793	2.012244	9.624529
Si	5.357790	9.228158	1.459008
Si	-1.499271	5.184947	11.235384
Si	3.211488	0.055570	1.423131
Si	10.098388	3.961718	6.348886
Si	3.215222	7.912972	11.286529
Si	-1.460876	2.732948	1.445653
Si	5.374138	6.805033	6.328185
Si	-1.464120	10.590441	11.361519
Si	-5.188294	9.246456	1.497917
Si	8.582649	1.291928	6.293312
Si	1.660705	5.244765	11.263668
Si	10.668277	0.040867	1.448353
Si	3.731967	4.059759	6.292994
Si	-3.056258	7.932598	11.327104
Si	1.675532	2.768702	1.411146
Si	8.486802	6.633258	6.400398
Si	1.622198	10.669760	11.282773
Si	1.645487	2.726699	13.038859
Si	8.498157	6.691002	3.251565
Si	1.615862	10.676034	8.184172
Si	10.697252	0.027541	13.029752
Si	3.821818	3.975918	3.190856
Si	-3.091803	7.973094	8.218286
Si	-5.190822	9.141288	13.095764

Si	8.520819	1.312384	3.216404
Si	1.669102	5.318054	8.148056
Si	-1.501976	2.734798	13.071119
Si	5.390161	6.735775	3.254894
Si	-1.487283	10.621414	8.184260
Si	-3.693523	11.849714	13.010707
Si	10.047443	4.012559	3.194478
Si	3.273350	7.972167	8.191141
Si	5.374568	9.188133	13.063076
Si	5.340097	1.318446	3.171486
Si	-1.487801	5.237284	8.185340
Al	5.378657	1.259710	6.279977
H	9.108892	5.227211	11.654694
H	6.840107	6.101657	12.160120
H	4.829611	5.003073	11.160336
H	7.393020	2.334940	8.942903
H	3.033667	1.978881	8.640180
H	4.752361	2.844403	8.050875
H	9.399329	3.347696	10.039258
C	8.238717	4.774393	11.181085
C	6.959718	5.252873	11.486429
C	5.833765	4.653382	10.922385
C	6.012807	3.596933	10.019181
C	7.288391	3.145009	9.663760
C	8.402490	3.722683	10.272822
N	3.987777	2.587853	10.212045
N	4.893926	2.943153	9.414435

Interaction of BF_4/NO^+ with NH_3

$NO^+(NH_3)/BF_4^-$

O	5.834447	8.364629	5.466175
N	5.136948	8.003065	4.636880
N	6.128735	7.206479	3.159329
B	4.373877	4.780882	4.467421
F	5.403501	3.880903	4.702352
F	4.673868	6.003224	5.263039
F	4.406714	5.209696	3.079751
F	3.119924	4.326336	4.803921
H	7.046569	6.920102	3.504101
H	5.498788	6.391216	2.954010
H	6.187473	7.893573	2.407023

TS $NO^+(NH_3)/BF_4^- \rightarrow NONH_2/BF_3$-HF

O	5.977406	9.106347	4.241963
N	6.129551	7.992778	4.623318
N	6.199772	7.004503	3.459576

B	4.318543	4.768291	4.424764
F	5.623902	4.333924	4.191340
F	4.217652	5.596418	5.516949
F	4.090379	5.830620	3.166434
F	3.352489	3.833919	4.259278
H	6.727152	6.177402	3.772935
H	5.034007	6.487359	3.259442
H	6.575835	7.452061	2.613902

$NONH_2/BF_3$-HF

O	5.756719	8.797749	4.490066
N	6.374376	7.761204	4.564451
N	6.540942	7.127339	3.305743
B	4.261255	4.566367	4.912665
F	5.364586	3.816448	4.779873
F	4.352091	5.721522	5.587282
F	4.474710	5.527580	2.956762
F	3.064566	4.036953	4.662421
H	7.346461	6.498956	3.321339
H	5.238257	6.130796	3.093959
H	6.476149	7.765690	2.500840

$NONH_2$_rotated1/BF_3-HF

O	6.048303	7.844548	2.113082
N	6.364906	8.686767	2.987354
N	5.984750	8.398750	4.205875
B	4.480022	4.824699	5.041732
F	5.462097	3.942227	4.895550
F	4.738507	5.986546	5.676402
F	4.769415	5.871657	2.965749
F	3.219430	4.481217	4.807747
H	5.468500	7.538076	4.437453
H	5.286547	6.634333	2.561815
H	6.244442	9.073336	4.919304

TS $NONH_2$_rotated1/BF_3-HF → HN=NOH/BF_3-HF

O	5.737870	7.681304	2.188481
N	6.237592	8.587385	2.903949
N	6.091415	8.430438	4.190284
B	4.758922	5.131242	5.359310
F	5.860846	4.381140	5.309702
F	4.877014	6.390666	5.868874
F	4.749787	5.743648	3.345533
F	3.553218	4.569098	5.341755
H	5.595109	7.630250	4.614534
H	5.155079	6.544959	2.845436
H	6.509663	9.154537	4.766746

HN=NOH/BF_3-HF

O	5.107988	7.146120	1.925511
N	6.126190	7.765469	2.512020
N	6.390634	7.388821	3.684362
B	4.192250	4.773681	4.533328
F	5.030831	3.767271	4.178535
F	5.208952	5.919369	5.213800
F	3.695804	5.503582	3.431071
F	3.286190	4.544211	5.505083
H	5.764324	6.482302	4.528900
H	4.650398	6.478933	2.537280
H	7.177042	7.954374	4.024902

HN=NOH/BF_3-HF_rotated1

O	6.125674	8.112575	4.754527
N	7.262558	7.955754	3.676990
N	6.952170	7.221314	2.783068
B	4.367136	4.567118	4.364418
F	5.384718	3.741616	4.620705
F	4.956784	6.094705	5.740707
F	4.455756	5.371205	3.274678
F	3.165255	4.329320	4.886722
H	6.015629	6.765099	2.822782
H	5.429514	6.878216	5.360187
H	6.546352	8.718886	5.395461

TS HN=NOH/BF_3-HF_rotated1 → (N_2 + H_2O)/BF_3-HF

O	6.040549	8.050680	4.750584
N	6.953292	7.757391	3.400716
N	6.478907	6.930839	2.698747
B	4.318975	4.530787	4.380614
F	5.371161	3.747002	4.614251
F	4.924179	6.067314	5.698690
F	4.334913	5.290864	3.242747
F	3.130524	4.270776	4.913683
H	5.598999	6.416493	2.946668
H	5.417919	6.896966	5.382296
H	6.639122	8.641414	5.247430

(N_2 + H_2O)/BF_3-HF

O	6.022164	8.190536	5.273956
N	7.830623	7.873773	2.603119
N	6.939630	7.214773	2.673087
B	4.399830	4.649269	4.902250
F	5.516967	3.953010	4.687072
F	4.456339	5.727162	5.707539
F	4.576482	5.811599	3.006702

F	3.212533	4.145685	4.582784
H	5.405375	6.278434	2.908115
H	5.443523	7.502756	5.649090
H	6.570013	8.489884	6.018101

HN=NOH_rotated2/BF_3-HF

O	6.658607	7.891742	5.016262
N	6.931274	8.110976	3.603282
N	6.928026	7.020482	3.048277
B	4.318094	4.630823	4.285239
F	5.425329	3.969883	4.637010
F	4.679350	6.338790	5.632485
F	4.321604	5.359821	3.160408
F	3.151373	4.314080	4.852256
H	7.122803	7.210581	2.049805
H	5.449475	6.874192	5.375876
H	6.629597	8.800775	5.376430

TS HN=NOH_rotated2/BF_3-HF → (NNH^+ + H_2O)/BF_4

O	6.457806	7.680759	5.317426
N	6.738154	8.003279	3.628598
N	7.016322	6.958515	3.169511
B	4.466869	5.242472	3.916652
F	5.507552	4.408647	4.264671
F	4.487414	6.391075	5.041564
F	4.702392	5.933083	2.719617
F	3.213062	4.708039	4.005440
H	7.144915	6.944320	2.142760
H	5.490344	7.015841	5.219662
H	6.198275	8.569865	5.636899

(NNH^+ + H_2O)/BF_4

O	6.138692	7.285637	4.078758
N	5.630078	7.529045	2.279169
N	6.024590	6.641854	1.653668
B	4.200644	4.586313	4.339932
F	5.178617	3.622486	4.473560
F	4.639525	5.784695	5.196259
F	4.203849	5.117061	3.022168
F	2.962506	4.217951	4.793117
H	6.527160	5.780759	1.933658
H	5.433083	6.595074	4.555187
H	5.965918	8.170047	4.464603

$NONH_2$_rotated2/BF_3-HF

O	-1.502048	13.958939	4.623179
N	-0.821177	14.495292	5.536577
N	-0.188359	15.557375	5.142608
B	-2.223192	10.528869	4.554423
F	-1.119394	10.062223	5.199195
F	-2.583590	11.988992	5.495938
F	-2.011873	11.081908	3.322457
F	-3.375838	9.832068	4.726917
H	-2.105567	12.839430	5.107890
H	0.378572	16.029184	5.841722
H	-0.260283	15.885269	4.171486

TS $NONH_2$_rotated2/BF_3-HF → HN=NOH_rotated3/BF_3-HF

O	0.859610	5.830945	4.771129
N	0.512341	6.747881	5.664237
N	0.185283	7.716098	4.918017
B	3.599103	3.241058	4.474726
F	4.367918	4.071422	5.196138
F	1.818474	3.595125	5.502967
F	3.143766	3.664441	3.281818
F	3.646445	1.926449	4.726518
H	1.439595	4.459064	5.231343
H	-0.138514	8.575063	5.378703
H	0.523944	6.835697	3.974597

HN=NOH_rotated3/BF_3-HF

O	0.631881	5.402161	4.757484
N	0.219340	6.496457	5.555611
N	0.619683	7.557024	5.073720
B	3.504889	3.391972	4.571228
F	4.297936	4.091236	5.390354
F	1.799473	3.402879	5.812262
F	2.896133	4.055079	3.559069
F	3.628251	2.066396	4.491560
H	1.268746	4.158480	5.484685
H	0.270204	8.303340	5.699486
H	1.217075	5.752332	4.036323

ZEO(2Al_6ring)/Cu^{2+}(NO)

O	4.813239	10.664736	1.902329
O	-1.569481	6.899864	6.679543
O	4.777050	2.744932	11.615605
O	-4.801336	10.676977	1.904543
O	1.589231	6.909078	6.698384

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O     8.907639    2.739439   11.603050
O     0.016237    2.324177    1.913970
O     0.017262    9.911456    6.692790
O     6.834361    6.271797   11.979116
O     2.062789    1.172265   12.946505
O     2.052868    9.081994    2.966882
O     8.625284    4.929908    8.234466
O    11.629487    1.159779   12.912452
O    -2.026098    9.076401    2.978109
O     5.082927    4.938863    8.287105
O     6.833590    9.464231   12.699126
O     0.008731    5.499359    3.131186
O     6.858673    2.017951    8.253470
O     2.402746   11.679991    2.460899
O    -4.235568    7.367516    7.572540
O     2.393086    3.745635   12.336210
O    -4.396896    8.064772    2.311447
O     2.583863    4.478637    7.374121
O     9.210288    0.184691   12.317145
O     2.070660    3.924294    2.486840
O     8.453826    0.152982    7.254809
O     8.947816    7.858897   12.368933
O     4.426665    8.053637    2.325858
O    -2.531226    4.463081    7.395828
O     4.462071    0.181310   12.291602
O    -2.045758    3.924962    2.480275
O     5.258405    0.148348    7.257797
O     4.720716    7.852138   12.377207
O    -2.384444   11.673282    2.455394
O     4.279819    7.355111    7.541536
O    11.284607    3.740721   12.355271
O    11.227406    1.410064    1.970306
O    -2.520583    9.509931    6.994168
O     4.374450    5.332059   11.821996
O     6.849024    9.006749    2.074464
O     0.020031    4.787967    6.810158
O     6.840028    1.112564   11.764315
O     2.488765    1.421622    1.919292
O     2.561383    9.513589    6.993330
O     9.291820    5.321505   11.884538
O    -4.382326   10.423983   12.703559
O     2.414640    6.494053    2.787427
O     9.482701    2.470808    7.928214
O     0.004545    2.791201   12.753598
O     0.011236   10.727301    2.806576
O     6.856118    6.843470    7.831124
O     4.368721   10.412279   12.730532
O    -2.404647    6.488617    2.807040
O     4.246349    2.484813    7.887269
O     3.316700   11.792397   -0.001503
O    -3.522683    7.857338    4.817059
O     3.174556    3.946998    9.854116
O     8.466520    8.907750   14.730615
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O	1.906175	4.936827	4.902718
O	8.625897	0.773182	9.810958
O	1.713283	3.097811	0.009744
O	1.670675	10.944787	4.866816
O	8.447231	6.951635	9.956802
O	5.224800	8.886000	14.738215
O	-1.882245	4.919305	4.908349
O	5.062751	0.796396	9.799568
O	-1.707855	3.050639	0.015712
O	-1.648639	10.947533	4.864537
O	5.263090	7.009170	9.948653
O	-3.285503	11.749031	14.751222
O	3.522444	7.850370	4.816238
O	10.502829	4.002288	9.876942
O	-0.833293	9.216318	9.600745
Si	3.738382	11.834329	1.568009
Si	3.691017	3.938037	11.397257
Si	8.373386	9.164723	1.560346
Si	1.538070	5.263997	6.441521
Si	8.404093	1.214314	11.368367
Si	1.563760	2.693162	1.574542
Si	1.557023	10.611274	6.441249
Si	8.366619	6.597944	11.529021
Si	5.321285	9.154006	1.565490
Si	-1.500609	5.244777	6.444463
Si	5.278683	1.222384	11.362528
Si	-1.536683	2.680182	1.586312
Si	-1.519790	10.612504	6.435384
Si	5.308954	6.612439	11.512803
Si	-3.713207	11.829888	1.551735
Si	9.985894	3.944004	11.419731
Si	-3.709572	11.811483	13.185958
Si	3.121156	7.876875	3.272311
Si	9.929577	3.977987	8.351894
Si	12.136093	2.674467	13.214851
Si	-1.524299	10.583627	3.279212
Si	5.356630	6.559113	8.381581
Si	5.296408	9.154308	13.146955
Si	-1.575763	5.215011	3.330743
Si	5.353997	1.376742	8.300501
Si	1.549049	2.690574	13.215898
Si	1.547250	10.584833	3.281734
Si	8.352619	6.545801	8.378825
Si	8.374383	9.163415	13.138012
Si	1.596001	5.220191	3.326823
Si	8.359434	1.366856	8.313259
Si	3.717848	11.815016	13.193915
Si	-3.105426	7.879549	3.274857
Si	3.780206	3.978176	8.341774
Al	3.105765	7.946102	6.476279
Al	-3.090785	7.950553	6.471544
Cu	-0.005804	7.923815	7.322503
N	-0.295293	8.371030	9.044570

ZEO(2Al_6ring)/(Cu^+ + NO^+)

O	4.804959	10.670082	1.974670
O	-1.652128	6.859469	6.674589
O	4.779997	2.736330	11.670575
O	-4.786943	10.668443	1.989722
O	1.684780	6.896590	6.608942
O	8.904292	2.744552	11.682056
O	0.016491	2.312102	1.958688
O	0.015215	10.005109	6.630592
O	6.856462	6.290843	12.014879
O	2.084037	1.182461	12.856582
O	2.112240	9.099748	3.078469
O	8.774687	5.088461	8.158507
O	11.627591	1.172593	12.881348
O	-2.097667	9.087271	3.121248
O	5.081801	4.994716	8.324036
O	6.851793	9.440323	12.646269
O	0.019605	5.476859	3.176415
O	6.843199	1.976991	8.325757
O	2.358277	11.671039	2.381294
O	-4.265794	7.655592	7.691374
O	2.412803	3.777976	12.372645
O	-4.391222	8.038230	2.272234
O	2.596656	4.490728	7.396536
O	9.204368	0.178058	12.332462
O	2.077229	3.949840	2.425228
O	8.486130	0.174973	7.272474
O	8.986585	7.858333	12.423980
O	4.408603	8.039041	2.249704
O	-2.435366	4.389541	7.428609
O	4.498502	0.165117	12.333864
O	-2.042972	3.939308	2.448072
O	5.182534	0.149858	7.300670
O	4.726812	7.838164	12.433412
O	-2.340157	11.652565	2.376070
O	4.312280	7.443440	7.583445
O	11.297601	3.757535	12.362529
O	11.208440	1.417913	1.947817
O	-2.546784	9.540796	6.857606
O	4.414741	5.327930	11.818930
O	6.847963	9.005313	2.094159
O	0.056658	4.819103	6.761995
O	6.848343	1.100505	11.698351
O	2.497317	1.418716	1.958024
O	2.582910	9.548504	6.857429
O	9.305179	5.327466	11.884378
O	-4.382288	10.430701	12.633184
O	2.406807	6.510959	2.835755
O	9.405272	2.549116	7.881391
O	0.016181	2.786597	12.701067
O	0.007090	10.630987	2.814802

O	6.877901	6.882271	7.865734
O	4.403140	10.425408	12.653317
O	-2.382975	6.495062	2.850037
O	4.274924	2.527391	7.886434
O	3.388595	11.739455	14.744034
O	-3.665941	7.765236	4.828899
O	3.198625	3.929819	9.877912
O	8.455762	9.009606	14.738400
O	1.962313	4.846381	4.888495
O	8.727941	0.838556	9.818433
O	1.681125	3.014273	0.000740
O	1.665643	11.089257	4.836402
O	8.471709	7.016131	10.004370
O	5.268989	9.002198	14.731811
O	-1.893932	4.853880	4.911510
O	4.963133	0.810899	9.823247
O	-1.645006	3.031939	0.004985
O	-1.661289	11.086160	4.841871
O	5.313515	7.055585	9.986386
O	-3.390057	11.732870	14.743865
O	3.689575	7.815808	4.806467
O	10.458761	3.965041	9.887855
O	-4.309818	10.047355	9.267063
Si	3.739350	11.826715	1.560534
Si	3.708268	3.938778	11.421822
Si	8.372133	9.176477	1.583449
Si	1.586032	5.262977	6.410961
Si	8.425717	1.220687	11.375081
Si	1.558846	2.676508	1.582468
Si	1.562967	10.669258	6.397201
Si	8.386789	6.611302	11.577010
Si	5.323221	9.176982	1.573706
Si	-1.481653	5.226050	6.435529
Si	5.273000	1.218010	11.377876
Si	-1.526877	2.675891	1.584738
Si	-1.508628	10.674114	6.395771
Si	5.328094	6.625120	11.541879
Si	-3.724769	11.823741	1.565168
Si	9.985373	3.934930	11.442872
Si	-3.718132	11.812943	13.162655
Si	3.174101	7.870685	3.297372
Si	9.968086	3.999595	8.339321
Si	-1.517879	2.676049	13.197229
Si	-1.532573	10.592381	3.289696
Si	5.362833	6.613448	8.414291
Si	5.312878	9.176393	13.130548
Si	-1.569294	5.196994	3.348710
Si	5.324572	1.380738	8.332737
Si	1.552502	2.684733	13.189653
Si	1.553189	10.599432	3.286618
Si	8.372584	6.643010	8.420391
Si	-5.291685	9.184502	13.138564
Si	1.614681	5.205162	3.336201

Si	8.368683	1.384139	8.324641
Si	3.739291	11.807731	13.165525
Si	-3.153566	7.850276	3.309248
Si	3.793057	4.008598	8.361946
Al	3.164374	7.964124	6.442343
Al	-3.089803	7.932211	6.433086
Cu	0.030954	7.962566	6.719621
N	-3.541890	9.232137	9.136638

ZEO(2Al_8ring)/Cu^{2+}(NO)

O	4.790712	10.654554	1.950108
O	-2.032022	6.916016	6.920895
O	4.803083	2.753607	11.654238
O	-4.850312	10.710598	1.910103
O	2.318902	6.615942	6.519823
O	8.844699	2.678744	11.732606
O	0.014000	2.417568	1.961944
O	-0.147655	10.224126	6.806324
O	6.757081	6.624664	11.426866
O	2.011210	1.243056	12.825104
O	2.003999	9.064609	2.982637
O	8.692120	5.184365	7.948663
O	11.464377	1.244640	12.945990
O	-2.037832	9.091344	3.091685
O	4.771685	5.269285	7.957448
O	6.786080	9.436070	12.797705
O	0.022294	5.570742	2.968271
O	6.854954	1.532038	8.118359
O	2.417468	11.681939	2.578168
O	9.120083	7.755692	7.333630
O	2.447678	3.832017	12.323570
O	-4.424509	8.118132	2.424096
O	2.390738	4.138534	7.415497
O	9.099484	0.117386	12.437699
O	2.111157	4.022962	2.394706
O	1.979709	11.714370	7.423903
O	8.910571	7.884126	12.375074
O	4.399588	8.035769	2.378992
O	-2.233755	4.306758	7.476826
O	4.399952	0.186567	12.311613
O	-2.057978	3.892523	2.744897
O	4.724960	0.131511	7.295178
O	4.633309	7.913064	12.382555
O	-2.398205	11.649307	2.378471
O	4.502443	7.864275	7.349067
O	11.225391	3.970187	12.223573
O	11.255525	1.419178	2.012670
O	-2.672395	9.472960	6.812616
O	4.507467	5.355088	11.864117
O	6.823931	8.994034	2.070381
O	0.099025	5.352468	7.055448

O	6.782613	1.055020	11.741633
O	2.461644	1.468530	1.980321
O	2.255923	9.180221	6.953240
O	8.947137	5.307706	11.885925
O	-4.478132	10.464763	12.737721
O	2.492143	6.472774	3.236440
O	9.348593	2.384894	7.896753
O	0.020137	3.000322	12.645497
O	-0.009103	10.754784	2.882675
O	6.782712	7.002120	8.241557
O	4.352172	10.463762	12.819671
O	-2.439154	6.492404	2.881155
O	4.491664	2.651546	7.923394
O	3.263829	11.792700	0.088784
O	-3.542069	7.828006	4.903034
O	3.309871	4.061505	9.857917
O	8.509380	8.874165	0.007526
O	1.574298	4.624273	4.923566
O	8.676914	0.747190	9.894015
O	1.699821	3.060095	14.742741
O	1.667423	10.844810	4.951903
O	8.878191	7.047109	9.860793
O	5.136023	8.837518	0.018130
O	-1.611728	5.122064	5.015062
O	4.927524	0.827920	9.819690
O	-1.778364	3.266580	0.178291
O	-1.773541	11.064416	4.862966
O	4.664798	7.106027	9.864524
O	3.419925	0.012086	14.738951
O	3.656285	8.220983	4.885972
O	10.368331	4.061005	9.940572
O	1.012046	5.545928	10.104150
Si	10.566604	0.011174	1.641954
Si	-3.196146	7.976662	6.485407
Si	3.779765	3.985005	11.423411
Si	8.358255	9.181838	1.596778
Si	1.595710	5.177986	6.450275
Si	8.361716	1.133456	11.431577
Si	1.552732	2.742261	1.563534
Si	1.431604	10.502794	6.519604
Si	8.364477	6.741898	11.367681
Si	5.283177	9.146805	1.600216
Si	-1.474839	5.406492	6.602833
Si	5.223994	1.206082	11.370883
Si	-1.565040	2.759794	1.685952
Si	-1.666947	10.678627	6.435674
Si	5.148103	6.759672	11.379070
Si	3.067975	0.034484	1.555657
Si	3.185927	7.975013	6.418182
Si	9.743125	3.977850	11.478518
Si	3.035681	0.026783	13.166166
Si	3.126509	7.948685	3.370692
Si	-1.561723	10.630590	3.312550

Si	5.195071	6.799367	8.350560
Si	5.231205	9.176329	13.207403
Si	-1.521229	5.265237	3.406721
Si	5.268589	1.280135	8.292414
Si	1.527145	2.769208	13.151389
Si	1.526554	10.581073	3.357128
Si	8.374205	6.707664	8.326709
Si	8.341302	9.170864	13.189978
Si	1.546143	5.174643	3.382206
Si	8.433335	1.159901	8.325707
Si	10.494696	0.015525	13.273968
Si	-3.109266	7.891909	3.338671
Si	3.761376	4.037522	8.284376
Al	9.898783	3.973425	8.170763
Al	-1.577407	2.802891	13.305169
Cu	-1.501275	4.309809	10.528293
N	0.053846	4.924989	10.148758

TS $Cu^{2+}(NO) \rightarrow (Cu^{+} + NO^{+})$

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O	2.027235	1.183003	1.892829
O	8.463323	4.817570	6.739858
O	2.079775	9.075763	11.610226
O	11.670368	1.173962	1.920703
O	5.056223	4.975706	6.741902
O	-2.023252	9.059098	11.986407
O	0.016440	2.375526	12.954731
O	6.839700	6.316892	2.960754
O	0.031260	9.962472	8.233751
O	4.817641	10.653126	12.928597
O	4.788219	2.776886	2.974309
O	-1.742664	6.874700	8.299800
O	-4.769681	10.647910	12.696526
O	8.921792	2.753131	3.118166
O	1.691455	6.940022	8.262255
O	4.766121	7.924399	2.470997
O	5.141250	0.055142	7.616492
O	-2.042138	3.947698	12.336554
O	4.499567	0.222385	2.290248
O	11.085850	4.483521	7.371552
O	4.446513	8.069455	12.323197
O	11.306074	3.753086	2.485442
O	4.085961	7.417013	7.245146
O	-2.327130	11.691977	12.365485
O	8.913353	7.856861	2.326404
O	8.553074	0.037849	7.398005
O	2.083264	3.950622	12.281832
O	9.250647	0.184006	2.476930
O	2.478994	4.590259	7.261141
O	-4.439834	8.009739	12.382708

O	2.368693	3.784077	2.434707
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O	2.404318	11.629267	12.363150
O	4.393270	10.426942	1.963523
O	4.150605	2.540423	6.889387
O	-2.425623	6.456549	11.815997
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O	2.464498	6.475907	11.755519
O	0.009565	2.868092	1.902309
O	6.706983	6.971120	7.000024
O	0.037112	10.700349	11.883735
O	2.461196	1.420779	12.697493
O	9.265767	5.341450	2.811981
O	2.587174	9.446718	7.931933
O	11.257114	1.399174	12.744981
O	4.405965	5.368419	2.787548
O	-2.495494	9.368807	7.827823
O	6.845397	8.992033	12.724958
O	6.858710	1.174484	2.800418
O	-0.032865	4.927694	7.880731
O	5.133168	8.758612	14.768697
O	5.109553	0.839506	4.788430
O	-1.815216	4.715500	9.854055
O	-3.477007	11.791099	14.725221
O	10.347231	4.095850	4.916968
O	3.647588	7.870649	9.811579
O	11.831526	3.025973	0.007624
O	5.031439	6.891628	4.870189
O	-1.807193	10.796448	9.965571
O	-5.084421	8.970792	14.739959
O	8.489162	0.832110	4.905829
O	1.839820	4.768646	9.796824
O	10.179637	0.059209	0.016641
O	3.356895	4.079414	4.840276
O	-3.439145	8.074332	9.950135
O	1.866373	3.037417	14.742884
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O	1.786383	11.093536	9.883322
O	4.662914	2.991468	9.549758
Si	5.299844	9.153441	1.570529
Si	-1.559437	5.165865	11.395937
Si	-3.749374	11.835049	1.553794
Si	9.866532	3.959912	6.459413
Si	3.156492	7.885075	11.369057
Si	-1.558169	2.698789	1.572384
Si	5.254395	6.651474	6.451446
Si	-1.532481	10.544475	11.536162
Si	-5.264928	9.184595	1.568315
Si	8.384333	1.321240	6.445370
Si	1.584690	5.181296	11.359001
Si	10.585262	0.009040	1.586627
Si	3.702070	3.995196	6.407091

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Si   -3.075203    7.904080   11.513712
Si    1.570498    2.702028    1.539799
Si    1.578799   10.611601   11.423998
Si    1.592820    2.695551   13.182168
Si    8.412777    6.644062    3.283734
Si    1.517822   10.596037    8.355255
Si   10.591419    0.004767   13.217805
Si    3.743388    3.977208    3.258038
Si   -3.005059    7.927460    8.382019
Si   -5.277565    9.163742   13.148037
Si    8.375977    1.241384    3.329915
Si    1.480137    5.319629    8.300344
Si   12.115625    2.685425   13.215226
Si    5.286767    6.628195    3.281272
Si   -1.504078   10.520655    8.388187
Si   -3.745737   11.837455   13.135088
Si    9.952541    3.986588    3.338354
Si    2.996693    7.927935    8.316466
Si    5.307354    9.126108   13.198163
Si    5.301542    1.245958    3.256815
Si   -1.558867    5.264724    8.341170
Al    8.337444    6.648649    6.495900
Al    5.262192    1.268418    6.429400
Cu    6.699777    3.930197    7.343106
 N    5.654564    2.921601    8.998124
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ZEO(2Al_8ring)/(Cu^{+} + NO^{+})

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 O    2.467526    6.569210    6.435437
 O    8.750877    2.870233   11.386966
 O    0.144334    2.359241    2.221045
 O   -0.085714   10.212183    6.844244
 O    6.817370    6.369876   11.705020
 O    1.971859    1.265059   12.787789
 O    2.078732    9.085145    2.944691
 O    9.024731    5.165519    8.209790
 O   11.801939    1.065146   13.218321
 O   -1.930909    9.060476    3.180150
 O    4.637922    5.259236    8.135582
 O    6.768971    9.530881   12.787472
 O    0.052799    5.591845    2.909094
 O    6.934481    1.611322    7.938174
 O    2.490051   11.713885    2.657920
 O    9.154288    7.719633    7.303593
 O    2.471644    3.850909   12.398879
 O   -4.337276    8.225882    2.401187
 O    2.399644    4.067286    7.311451
 O    9.316253    0.435183   12.405656
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O	4.471097	8.004710	2.382299
O	-2.084642	4.228727	7.380032
O	4.386712	0.266746	12.238337
O	-1.992344	3.843262	2.868608
O	4.795940	0.108381	7.332762
O	4.709042	7.902577	12.323795
O	-2.361571	11.576939	2.345615
O	4.603317	7.823720	7.319354
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O	4.367220	5.426797	11.578586
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O	0.186926	5.462294	6.986883
O	6.840446	1.126344	11.878447
O	2.627414	1.541895	1.923872
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O	2.525106	6.502330	3.256520
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O	0.053608	10.767150	2.872645
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O	-2.433388	6.475712	2.811420
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O	-3.502651	7.756226	4.886842
O	3.141914	3.829854	9.836128
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O	1.595880	4.609555	4.854940
O	8.552215	0.699655	9.881248
O	1.503388	2.989898	14.737157
O	1.699101	10.791730	4.972132
O	8.521867	7.247642	9.824191
O	5.209405	8.742196	14.765891
O	-1.563353	5.264519	4.998099
O	5.157372	0.919913	9.814256
O	-1.476571	3.257417	0.352730
O	-1.674391	11.106451	4.868010
O	5.179325	7.255896	9.812960
O	3.460622	0.046958	14.682698
O	3.717422	8.282076	4.874479
O	10.879503	3.902278	10.099515
O	7.205691	4.071067	6.351877
Si	10.598907	0.013187	1.659565
Si	-3.147362	7.955091	6.465744
Si	3.711667	3.973897	11.362202
Si	-5.278013	9.248477	1.568772

Si	1.654839	5.174650	6.382127
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Si	1.591345	2.743355	1.583874
Si	1.497378	10.480452	6.548761
Si	8.362807	6.752564	11.371185
Si	5.331812	9.112468	1.570739
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Si	5.305842	1.291204	11.391000
Si	-1.420120	2.705982	1.847909
Si	-1.598073	10.674353	6.437171
Si	5.271884	6.741004	11.355190
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Si	3.271189	7.966483	6.403859
Si	9.931507	3.983461	11.484896
Si	3.039740	0.071718	13.114521
Si	3.187032	7.966429	3.364687
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Si	5.230007	9.164876	13.200935
Si	-1.480262	5.287867	3.390202
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Si	1.487926	2.785428	13.126957
Si	1.583625	10.581346	3.368100
Si	8.416047	6.683952	8.304594
Si	8.328648	9.231752	13.159488
Si	1.578109	5.198276	3.328212
Si	8.472868	1.172027	8.321092
Si	10.579220	0.039092	13.355224
Si	-3.051042	7.886692	3.324263
Si	3.676918	3.959863	8.299267
Al	10.272724	3.901723	8.414829
Al	-1.564531	2.738624	13.503540
Cu	-1.067675	3.563350	10.971549
N	8.332017	4.136385	6.384782