Electronic Supplementary Material (ESI) for Catalysis Science & Technology.

Supporting Information

Heterometallic [Cu-O-M]$^{2+}$ Active Sites for Methane C-H Activation in Zeolites: Stability, Reactivity, Formation Mechanism and Relationship to Other Active Sites

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Dioxygen: triplet state:

Final energy = -83.03801974 Ry

O	-0.103631774	-0.148045181	0.000013708
O	0.862968774	0.610675997	-0.000013708

Water: singlet state:

Final energy = -44.0380161362 Ry

O	-0.000042774	-0.066169958	0.000026021
H	0.767266240	0.529078904	-0.000014055
H	-0.767223466	0.529058778	-0.000011966

H4MOR: bare zeolite with 4 aluminates and 4 protons

Final enthalpy = -6234.8778946579 Ry

CELL_PARAMETERS (angstrom)

13.771498018	0.046032246	0.060377045
-1.433825457	13.634765610	0.008031636
0.037612838	0.000070370	15.067271329

ATOMIC_POSITIONS (angstrom)

O	2.965088892	0.387957671	3.346026498
O	1.872154873	13.824435425	10.864171129
O	4.827998476	11.162629920	3.260329243
O	4.778028556	11.279041995	10.876440116
O	7.596337241	11.658907010	8.193129900
O	7.431273707	11.768961400	0.718431047
O	10.608861006	-0.024280805	7.150459186
O	9.218078610	13.462631083	14.712464039
O	7.866339266	2.589057398	7.087310773
O	7.767326077	2.583366706	14.751296849
O	5.039655359	2.023350867	3.720440319
O	5.147796352	2.070140651	11.263904770
O	12.337962817	10.952127192	0.537393376
O	12.535442896	10.755500479	8.057405126
O	1.906021062	7.783031703	0.387581376
O	2.048464740	7.881626925	7.964646846
O	1.491780211	5.229893934	3.495608715
O	1.423312729	5.015928159	11.180117833
O	-0.056511773	3.167740910	4.242877326
O	-0.012439460	2.878955287	11.820201061
O	10.966760104	5.745874678	4.266458429
O	10.832311518	5.696139686	11.808041825
O	11.074681663	8.617432032	0.334034078
O	10.873036516	8.664221208	7.857552024
O	9.444685337	13.147596089	4.574564491
O	9.425781880	13.210203211	12.077782298
O	7.464755981	2.799670599	4.436419569
O	7.536032081	2.876477457	12.108717291
O	5.256237591	1.884731393	15.234104694
O	5.133162861	1.820445176	7.818548451
O	2.929505238	0.556080317	0.671565196
O	2.871331837	0.458406373	8.210992014
O	4.900288021	11.187985216	0.568295546
O	5.083122632	10.920648131	8.225358204
O	7.460188335	11.816039244	3.372629304
O	7.509973356	11.822820320	10.812257724
O	0.306510033	2.767940614	6.870005247
O	0.353280743	2.822023167	14.462118736
O	10.652127713	6.212391426	6.876352279
O	10.778303855	6.203161066	14.423935760
O	11.015711798	8.333978110	3.681271441
O	11.004592132	8.307349819	11.352972698
O	12.306844929	10.650854535	3.192517015
O	12.314688650	10.572132162	10.721319418
O	1.923420187	7.784955519	3.049702777
O	1.879519874	7.517268258	10.573276599
O	1.237496130	5.130435041	7.761319464
O	1.359375370	5.206095480	15.138226669
O	2.891208064	12.303611559	1.850353022
O	2.864055863	12.054941367	9.147087157
O	9.679739382	1.711621664	5.344458595
O	9.660230499	1.670724757	13.085303838
O	0.519140255	9.601620847	1.702017261
O	0.665894085	9.585297100	9.453953514
O	11.898802126	4.028950345	6.067402010
O	11.974487506	4.018069896	13.527804375
O	3.534540775	1.162821331	5.776862811
O	3.640894333	1.150575315	13.271536982
O	6.194105059	11.623260475	5.903876714
O	6.303436892	11.738017027	13.382880555
O	9.615875302	12.380018620	2.014169603
O	9.681588153	12.490400293	9.518667103
O	7.083948210	1.739265459	2.069164626
O	7.268360313	2.111840379	9.649881510
O	11.765818672	9.956996624	5.664726741
O	11.715085448	10.053900493	13.220905452
O	1.495430992	6.975348399	5.511570842
O	1.379851520	6.878167723	13.058468830
O	1.048331836	3.226504920	1.857414729
O	0.896744885	3.078287817	9.397126799
O	11.558041490	6.494871011	1.845774267
O	11.335054953	6.549214032	9.391388819
O	2.595765481	2.924148596	4.022937045
O	2.624975891	2.726382917	11.395900148
O	9.817551905	10.859273219	14.884439670
O	10.019127913	11.087684272	7.268467450
O	9.773903991	10.590514877	3.989195562
O	9.793730651	10.640153862	11.469160755
O	2.933103668	3.095056192	14.983418513
O	2.832079894	3.031753306	7.562615747
O	7.124290801	0.038523079	0.029089054
O	5.745779100	13.468751803	7.867574764
O	13.232526378	7.096414984	14.903265460
O	13.070406973	7.255499786	7.485067263
O	5.489848826	13.819360525	4.236058559
O	7.114185963	0.264717007	11.575070049
O	13.279457883	7.007372909	3.811813978
O	-0.579398666	6.782520087	11.251240050
O	0.224262815	12.259056521	1.963265034
O	0.245389682	12.210000040	9.599007110
O	3.190790784	9.660048531	1.756253951
O	3.360013368	9.488225537	9.558448313
O	12.298936541	1.417936741	5.651697196
O	12.295240858	1.370942406	13.374222012
O	9.265613165	4.316843810	5.657828028
O	9.315466837	4.277293089	13.438380229
Si	6.769712381	1.549393081	0.503278035
Si	9.028769543	12.112692197	0.513105374
Si	9.132795037	12.222552383	7.991717484
Si	3.550079065	1.625486602	4.226218729
Si	3.665890936	1.528780740	11.693923803
Si	11.721361146	6.890508856	3.414672112
Si	11.604819291	6.844640737	10.955949106
Si	1.272058447	3.631476221	3.419102708
Si	1.236646939	3.422461208	10.934709387
Si	1.038141226	6.714936031	14.637847225
Si	11.306768560	10.094214522	7.217016362
Si	11.265720826	10.107946103	14.780028826
Si	6.100012002	11.961205329	7.465899391
Si	6.068217225	12.094910087	14.923647494
Si	3.625885034	1.627251727	7.339428195
Si	3.705902221	1.667280842	14.813998943
Si	6.626963653	1.646986781	3.636815198
Si	6.731171653	1.762747597	11.240747319
Si	9.137868552	11.995334613	3.521017615
Si	9.178198365	12.054762319	11.000244347
Si	1.108324890	6.732133657	3.978725188
Si	0.999077184	6.529900971	11.524738861
Si	11.239868802	9.870268349	4.130086546
Si	11.223550985	9.873002406	11.685818400
Si	11.657886994	7.097132739	0.347401293
Si	11.523040480	7.152023960	7.881386984
Si	1.399370053	3.604761823	0.320097378
Si	1.549480461	13.193719318	1.964764061
Si	1.625738237	13.062952919	9.446255188
Si	3.964302745	11.079496918	1.909840914
Si	4.046577670	10.985252465	9.486332696
Si	10.859620538	0.683740590	5.695208626
Si	10.866961259	0.626188161	13.312219818
Si	8.570122759	2.844234031	13.374884186
Si	-0.520580859	10.835968378	1.827570214
Si	-0.451081789	10.768699771	9.415176447
Si	1.887728642	8.715443252	1.727889178
Si	1.984812721	8.676187284	9.474196083
Si	13.005080081	2.884679006	5.730871662
Si	13.043882005	2.812531265	13.326209603
Si	10.694953762	5.070995243	5.719941516
Si	10.736771365	5.043644571	13.296015600
Si	1.322478168	3.541855052	7.884251952
Si	8.542748688	2.854060968	5.656935698
Al	0.892488398	6.661746937	7.091540938
Al	5.829347519	12.129393418	4.293739446
Al	5.932491465	12.194508242	11.761359959
Al	6.806373282	1.507034007	7.911003264
H	7.851275222	2.890451152	9.574741847
H	7.354380759	11.655626828	9.818558762
H	2.734017172	8.201646377	7.348244720
H	7.253151562	11.673110980	2.394577491

End final coordinates

M6W-H2MOR Optimized Structures

Co6W-H2MOR

Final enthalpy = -6659.0781636732 Ry

CELL_PARAMETERS (angstrom)

13.718605851	0.095247992	0.064198968
-1.379578802	13.513910599	0.021383868
0.042226345	0.015510221	15.040237297

ATOMIC_POSITIONS (angstrom)

O	3.378101418	0.255960301	3.465315140
O	1.947955654	13.909447840	10.961822968
O	4.894881832	11.134173649	3.426460580
O	4.996856965	11.378761105	10.795024077
O	7.603621651	11.730228395	8.288118005
O	7.689923371	11.897528318	0.702888730
O	10.605231508	0.116841514	7.237466645
O	9.505486254	13.670973449	14.744274559
O	7.864783932	2.813936358	7.119964916
O	7.966407111	2.601222730	14.743203701
O	5.198723816	2.167658847	3.760760396
O	5.256337665	2.220355100	11.318162764
O	12.629727446	10.935986739	0.574623394
O	12.472872080	10.931993060	8.147441387
O	2.054576150	7.796469290	0.429551122
O	2.198833469	7.697798277	8.284569086
O	1.694112031	5.130975839	3.619263994
O	1.748080416	5.278016093	10.913139611
O	0.044110531	3.172813460	4.359858720
O	0.150956800	3.350760925	11.820263948
O	11.134159374	5.767017884	4.336767651
O	10.908264174	5.836042586	11.845083012
O	11.164520368	8.729519771	0.472514734
O	10.931850911	8.721369923	7.871917317
O	9.436966194	13.113240620	4.683604313
O	9.622323101	13.234653152	12.134466190
O	7.586723781	2.956230408	4.449753402
O	7.608915213	3.037590518	12.124943607
O	5.409110851	2.081585078	15.278364300
O	5.275479230	2.157155461	7.892068501
O	3.129211359	0.684107566	0.823021169
O	3.002987773	0.751269920	8.301369950
O	5.274999740	11.039551821	0.776172600
O	5.102809505	10.947184939	8.139971189
O	7.584258926	11.788052097	3.330444838
O	7.632074520	11.908017813	10.926327164
O	0.398644138	2.676352159	6.985899429
O	0.509583421	2.924155777	14.442939531
O	10.756873571	6.278768508	6.947385574
O	10.845782038	6.369333168	14.479871853
O	11.194909342	8.359448327	3.823930734
O	11.167812039	8.410688068	11.306243157
O	12.444742438	10.677058722	3.231699128
O	12.468461117	10.711446923	10.800428897
O	2.156424664	7.649279277	3.096402021
O	1.932829627	7.936747324	10.926695891
O	1.165757650	5.135387322	7.681289361
O	1.386283720	5.264013940	15.405763672
O	3.075767612	12.111624688	1.713118763
O	2.990652297	12.183350599	9.207222419
O	9.765892186	1.875144706	5.448579356
O	9.840672140	1.894306598	13.003153665
O	0.811076520	9.600140112	1.906790362
O	0.789015283	9.715340169	9.314345327
O	11.914025422	4.004811979	6.182649068
O	12.033433305	4.189877565	13.629901454
O	3.816611853	1.208591861	5.856766801
O	3.761259702	1.279589110	13.360745138

O 6.390252576 11.520815662 5.902908590
O 6.386670610 11.641104773 13.441370035
O 9.781499540 12.536668978 2.091537136
O 9.777416373 12.468022040 9.566816793
O 7.246187113 1.863964548 2.091042199
O 7.400010508 1.942450562 9.733781033
O 11.838370561 10.103753754 5.727563189
O 11.885824764 10.054225737 13.265665840
O 1.819029047 6.900369651 5.598060317
O 1.566346558 6.647887806 13.162371089
O 1.087400354 3.156658636 1.946397269
O 1.219075069 3.123689020 9.431043054
O 11.742243114 6.583297472 1.929428788
O 11.576223921 6.634742513 9.404829401
O 2.662770795 2.756861691 4.056761360
O 2.768151775 2.944225716 11.581105534
O 10.102923190 11.070474888 14.919459830
O 9.959058858 11.065457268 7.292594936
O 9.899832394 10.608731295 3.955533182
O 9.923559606 10.677131885 11.550309122
O 3.049551803 3.214639586 15.103805495
O 2.960355124 3.240304595 7.383962679
O 7.109560909 0.072185101 0.129244429
O 5.761116700 13.516833121 7.612998476
O 13.319664041 7.257599098 14.903348368
O 13.180188598 7.436382260 7.362237563
O 5.720765955 13.825781587 4.259542750
O 7.130982591 0.429739360 11.929664877
O 13.457679527 7.007258419 3.954266055
O -0.404821474 6.770392569 11.373357211
O 0.438274367 12.254373399 2.067892572
O 0.357116941 12.335562414 9.572746090
O 3.490971361 9.496298418 1.857206276
O 3.454965609 9.584847650 9.612031305
O 12.362509161 1.426370561 5.701877819
O 12.483659143 1.598990853 13.174186381
O 9.302777943 4.495080336 5.703337068
O 9.371272804 4.448414543 13.489535436
Si 6.903711982 1.634520561 0.526294265
Si 9.274845878 12.295672113 0.551734367
Si 9.158709126 12.234360910 8.070445471
Si 3.769208379 1.598298075 4.289482020
Si 3.799877746 1.706149024 11.787688017
Si 11.907060754 6.929047190 3.510538641
Si 11.759415716 6.927779439 10.991228349
Si 1.373571109 3.550829708 3.499463559
Si 1.479418261 3.668184863 10.932335169
Si 1.161914325 6.715500251 14.723165377
Si 11.334877368 10.185868718 7.269841140
Si 11.473949867 10.195980797 14.827031698
Si 6.169568595 11.996061784 7.429519293
Si 6.256078663 12.067260043 14.971603280
Si 3.814359491 1.821699800 7.371544821
Si 3.859151650 1.809688156 14.891889656
Si 6.779855571 1.769373923 3.646407646
Si 6.861863453 1.861722689 11.237744806
Si 9.249399263 12.024047618 3.539357601
Si 9.304234792 12.088355358 11.074500963
Si 1.340647751 6.649807056 4.080958369
Si 1.201257140 6.651537554 11.585745545
Si 11.374703095 9.926289210 4.182179229
Si 11.382700897 9.953684441 11.726621745
Si 11.757464877 7.209477469 0.429026801
Si 11.688735193 7.250715566 7.891047698
Si 1.482803138 3.634463576 0.441287524
Si 1.829165544 13.090393443 2.025789118
Si 1.748164970 13.185088650 9.520695280
Si 4.188787190 10.956897902 1.990871658
Si 4.136500265 11.063534635 9.486865575
Si 10.889593565 0.774504387 5.775668740
Si 11.045583043 0.867469391 13.263071024
Si 8.672479374 2.987105802 13.334658988
Si -0.261897385 10.809840759 1.914031454
Si -0.325267850 10.879644826 9.425488068
Si 2.124371135 8.642265954 1.820342563
Si 2.065479003 8.739472792 9.512334054
Si 13.060914291 2.892056272 5.838581634
Si 13.162548759 3.074097620 13.291775466
Si 10.815213353 5.132515956 5.796343045
Si 10.793893544 5.204001659 13.347031229
Si 1.422618970 3.587490626 7.878842208
Si 8.613873858 2.986957635 5.712616047
Al 1.115546810 6.794796655 7.213493373
Al 5.998639105 12.124496600 4.321975092
Al 6.029472031 12.256755411 11.863736798
Al 6.927645325 1.651263865 8.094496634
H 7.421771122 11.741287717 9.949775127
H 7.413973530 11.705613509 2.335945827
O 6.943873134 6.124376963 5.388133919
Co 5.878679314 6.615602138 7.147798243
H 7.827407922 5.689878738 5.471708367
H 6.408518356 5.515806308 4.843555024
O 4.720183571 6.879615411 8.842570692
H 4.980357512 7.576702537 9.472232072
O 4.266911420 5.599982234 6.264636732
H 3.478299748 6.120900442 5.953232638
O 7.581124553 7.640265679 8.009466972
H 8.111057322 8.313875133 7.544927239
H 3.767247277 7.090858611 8.594430180
H 3.899760284 4.785581737 6.689738767
H 8.210720375 6.966813169 8.330026098
O 5.185158925 8.480567744 6.421875794
H 5.348138613 8.833484982 5.529331446
O 6.759608442 5.025824979 8.177960589
H 7.186222349 4.225743842 7.739979271
H 6.215543287 4.669636731 8.904116848
H 5.093793512 9.263648342 7.013519560
End final coordinates

Cr6W-H2MOR
Final enthalpy = -6745.3438292720 Ry
CELL_PARAMETERS (angstrom)
13.732955704 0.091718471 0.066350216
-1.384544265 13.508835370 0.032862771
0.044564192 0.028443134 15.036381409

ATOMIC_POSITIONS (angstrom)
O 3.265316309 0.281749036 3.531917681
O 1.915258442 13.847396906 11.055668381
O 4.917900666 11.040709191 3.478432816
O 4.969516067 11.359961947 10.867161592
O 7.605360116 11.856359421 8.320387563
O 7.676930975 11.964575190 0.752347198
O 10.631130189 0.211060907 7.234304994
O 9.500683484 13.738936524 14.790889882
O 8.102913995 2.768756740 7.205659109
O 7.932780521 2.706413161 14.770411163
O 5.147136428 2.155449824 3.791273454
O 5.196631619 2.210214294 11.344059328
O 12.602036037 10.967561359 0.584535983
O 12.480747713 10.939147480 8.154049766
O 2.032964182 7.765340929 0.457661340
O 2.155947561 7.763402327 8.228685737
O 1.692442870 5.186323063 3.524169414
O 1.794831737 5.265915594 10.959036111
O 0.033861274 3.290702793 4.387024165
O 0.101725845 3.408489751 11.823182050
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O 7.589814379 11.821654910 3.364989772
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O 0.385056058 2.726671147 7.001472159
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O 2.163746021 7.730109028 3.134534906
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O 11.894510667 4.024859290 6.220689278
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O 6.389238855 11.726134224 13.486595072
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Si 1.460488665 3.668810945 10.963418257
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Si 11.312743888 10.230307837 7.283733607
Si 11.449353931 10.250946680 14.822001536
Si 6.157095450 12.078656414 7.474892074
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Si 6.729362687 1.761181751 3.679556561
Si 6.806931702 1.894680967 11.244761287
Si 9.259963070 12.024939103 3.562838881
Si 9.289735212 12.120498884 11.089703380
Si 1.319607216 6.681806992 4.041271143
Si 1.209607727 6.654626397 11.569339495
Si 11.363549698 9.926781345 4.193353634
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Si 11.725041502 7.242671462 0.414957628
Si 11.649828527 7.288207190 7.864513377
Si 1.421250319 3.629278609 0.434544318

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Si 1.778646102 13.211478240 9.563245686
Si 4.185662663 10.968396605 2.041315849
Si 4.148957803 11.072846671 9.524483202
Si 10.934557745 0.801080420 5.746411846
Si 11.001555292 0.904695775 13.277152306
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Si -0.288545026 10.814433109 1.910420140
Si -0.321086385 10.934086664 9.417715762
Si 2.111596929 8.664654222 1.811793452
Si 2.061027358 8.769559233 9.495393320
Si 13.066412951 2.945543192 5.851225960
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Si 10.775813270 5.255228441 13.324105888
Si 1.394573755 3.634803377 7.913138480
Si 8.667061571 2.959077978 5.722105206
Al 1.054409225 6.825062190 7.204270563
Al 5.991915883 12.099428189 4.346895866
Al 6.023069397 12.273060448 11.884665441
Al 6.936933860 1.753796177 8.079498442
H 7.420713942 11.788551827 9.949532067
H 7.422654301 11.761805377 2.365541045
O 6.779535408 5.710787163 5.270073108
Cr 5.697834803 6.373873182 6.890671211
H 7.729581261 5.459726689 5.394931138
H 6.388512467 4.959581863 4.780915201
O 4.638161277 6.870064025 8.546562234
H 5.029687005 7.550950131 9.123272538
O 4.051180371 5.490480800 6.098984115
H 3.254139721 6.047095758 5.841185769
O 7.405224331 6.872944432 7.890652257
H 8.110360978 7.423850962 7.508181213
H 3.676248636 7.156157014 8.391512936
H 3.690747324 4.692849420 6.578718534
H 7.857438918 6.070261535 8.389939188
O 5.183163342 8.552869914 6.063840137
H 5.082723239 8.891096476 5.154817543
O 8.450639593 4.850904937 8.994435492
H 8.397373209 4.078553877 8.369230646
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H 5.126133985 9.343024238 6.638902446
End final coordinates

Cu6W-H2MOR
Final enthalpy = -6659.0781636732 Ry
CELL_PARAMETERS (angstrom)
13.718605851 0.095247992 0.064198968
-1.379578802 13.513910599 0.021383868
0.042226345 0.015510221 15.040237297

ATOMIC_POSITIONS (angstrom)
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O 1.947955654 13.909447840 10.961822968
O 4.894881832 11.134173649 3.426460580
O 4.996856965 11.378761105 10.795024077
O 7.603621651 11.730228395 8.288118005
O 7.689923371 11.897528318 0.702888730
O 10.605231508 0.116841514 7.237466645
O 9.505486254 13.670973449 14.744274559
O 7.864783932 2.813936358 7.119964916
O 7.966407111 2.601222730 14.743203701
O 5.198723816 2.167658847 3.760760396
O 5.256337665 2.220355100 11.318162764
O 12.629727446 10.935986739 0.574623394
O 12.472872080 10.931993060 8.147441387
O 2.054576150 7.796469290 0.429551122
O 2.198833469 7.697798277 8.284569086
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O 1.748080416 5.278016093 10.913139611
O 0.044110531 3.172813460 4.359858720
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O 11.134159374 5.767017884 4.336767651
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O 11.164520368 8.729519771 0.472514734
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O 0.398644138 2.676352159 6.985899429
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O 0.789015283 9.715340169 9.314345327
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O 11.838370561 10.103753754 5.727563189
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O 1.087400354 3.156658636 1.946397269
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O 6.943873134 6.124376963 5.388133919
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H 7.186222349 4.225743842 7.739979271
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H 5.093793512 9.263648342 7.013519560
End final coordinates

Fe6W-H2MOR
Final enthalpy = -6638.8211137294 Ry
CELL_PARAMETERS (angstrom)
13.730296290 0.088101370 0.066571907
-1.387829132 13.517868813 0.023414397
0.044795817 0.017968893 15.045241534

ATOMIC_POSITIONS (angstrom)
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O 1.939486542 13.894895513 10.984059026
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O 5.003281741 11.353722259 10.814690038
O 7.610776160 11.723825489 8.295906261
O 7.681915638 11.905930994 0.715147574
O 10.615946354 0.107787184 7.232455334
O 9.505936299 13.668423478 14.758433990
O 7.913212474 2.804615226 7.128688692
O 7.944927379 2.627890524 14.760204536
O 5.197809497 2.154954489 3.783624374
O 5.246900107 2.214888556 11.320412197
O 12.615933099 10.945755548 0.582472183

O 12.480413691 10.925751642 8.155845713
O 2.049919590 7.782389832 0.444409161
O 2.193150247 7.692168062 8.287491032
O 1.667737323 5.150952646 3.583040856
O 1.750704755 5.268910065 10.925826188
O 0.056317096 3.179352348 4.375043387
O 0.137879210 3.358454420 11.834521398
O 11.180251151 5.749477076 4.346750460
O 10.918064509 5.834391033 11.853862392
O 11.169045641 8.728124116 0.474446900
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O 7.588637638 2.946907360 4.465133591
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O 5.393919209 2.079007443 15.306769478
O 5.292546653 2.156345030 7.839057979
O 3.106217959 0.676943319 0.818745335
O 3.029979287 0.750425096 8.324071762
O 5.258876491 11.065169462 0.780514378
O 5.107891377 10.950237851 8.154294056
O 7.584396706 11.789301936 3.340137813
O 7.638418578 11.895717608 10.932870027
O 0.402505016 2.660124990 6.997755884
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O 9.821639003 1.880438110 13.032342810
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O 6.388130163 11.533952694 5.916785148
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O 9.786611954 12.517239648 2.095552784
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End final coordinates

Mn6W-H2MOR
Final enthalpy = -6783.6629213442 Ry
CELL_PARAMETERS (angstrom)
13.736870235 0.077011126 0.064334708
-1.399442205 13.521434011 0.026779858
0.042293347 0.021411405 15.051084174

ATOMIC_POSITIONS (angstrom)
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O 4.995649734 11.308790741 10.841877040
O 7.610213076 11.747624883 8.311659882
O 7.652179423 11.913450538 0.737239642
O 10.663304124 0.094809993 7.231992495
O 9.499266994 13.651512355 14.783443116
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O 7.925139414 2.669819999 14.800685702
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End final coordinates

Ni6W-H2MOR
Final enthalpy = -6682.7324499797 Ry
CELL_PARAMETERS (angstrom)
13.703617688 0.105214453 0.066713329
-1.368235431 13.514524869 0.020152863
0.044930757 0.014464542 15.034699170

ATOMIC_POSITIONS (angstrom)
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Si 1.770699314 13.181189470 9.538433239
Si 4.210410651 10.943775113 2.013754696
Si 4.160575996 11.060075364 9.497988016
Si 10.888748836 0.795190177 5.780834252
Si 11.043288937 0.878374688 13.265007607
Si 8.663338009 2.988314737 13.335147155
Si -0.241103663 10.812351783 1.916690535
Si -0.309222182 10.879355101 9.433075023
Si 2.139779057 8.639305484 1.830067635
Si 2.082174208 8.739824538 9.509975915
Si 13.043419696 2.923379540 5.845413189
Si 13.146937531 3.088639932 13.301613853
Si 10.790167475 5.149312333 5.797789018
Si 10.780547881 5.209155752 13.347708907
Si 1.419924286 3.591756515 7.894688588
Si 8.602517754 2.995832905 5.720123958
Al 1.112540246 6.792441455 7.217652428
Al 6.010854623 12.110597509 4.333665829
Al 6.042264020 12.246703698 11.877649554

Al 6.933823445 1.665346027 8.104946833
H 7.436212354 11.775140028 9.947657322
H 7.431248670 11.733045532 2.341617694
O 6.889510880 6.151936424 5.316828138
Ni 5.852384664 6.628347921 7.065667330
H 7.764383003 5.701183212 5.401278199
H 6.328416063 5.530923209 4.812042695
O 4.734690923 6.940347013 8.752471096
H 5.017994980 7.668879904 9.336111289
O 4.255642153 5.627808239 6.191460335
H 3.450586126 6.156133473 5.926118331
O 7.537481984 7.604757813 7.933926240
H 8.135828544 8.179002196 7.421001521
H 3.776517303 7.151915206 8.518396017
H 3.903842626 4.817353124 6.632905235
H 8.101269512 6.912433777 8.330351639
O 5.166074386 8.472550415 6.320191820
H 5.427552073 8.830017392 5.452592200
O 6.634895728 5.023708489 8.091889776
H 7.106704898 4.244668259 7.662123893
H 5.987583855 4.626306477 8.704838987
H 5.124670540 9.243874240 6.930276493
End final coordinates

Ti6W-H2MOR
Final enthalpy = -6680.9157047516 Ry
CELL_PARAMETERS (angstrom)
13.736322098 0.064718222 0.060259520
-1.411563918 13.524642982 0.031221606
0.037689384 0.025806440 15.061240474

ATOMIC_POSITIONS (angstrom)
O 3.306590159 0.311604345 3.429970001
O 1.847195134 13.929005705 10.976486574
O 4.873969761 11.095016150 3.439809253
O 4.954194457 11.361196051 10.822941418
O 7.583905632 11.636036020 8.293584266
O 7.666309274 11.893826017 0.692103551
O 10.595960149 0.034997555 7.227741897
O 9.513294581 13.634687502 14.750891068
O 7.932516243 2.795041778 7.116995356
O 7.908671751 2.655375864 14.769357737
O 5.210236898 2.136164019 3.805947484
O 5.230701221 2.187843110 11.331068631
O 12.610354346 10.900421544 0.581040792
O 12.445827561 10.875737632 8.154131459
O 2.037171312 7.756110596 0.453224849
O 2.171099925 7.694894738 8.312767446
O 1.572278316 5.153382703 3.591013541
O 1.729677657 5.289846527 10.926855987
O 0.071601084 3.090508436 4.369786919
O 0.135596327 3.367626790 11.837026307
O 11.214135227 5.727462341 4.341852053
O 10.933000700 5.846013457 11.875196274
O 11.168648957 8.686435544 0.462467748
O 10.920046032 8.651390136 7.878074539
O 9.439465419 13.077555614 4.682952531
O 9.533865041 13.241372932 12.127548231
O 7.620975572 2.909465719 4.446672261
O 7.584745094 3.028417666 12.143976941
O 5.367049687 2.051703941 15.303360674
O 5.291141396 2.104567652 7.762455196
O 3.086380879 0.634019426 0.780392531
O 2.992235246 0.773049465 8.309941445
O 5.236980391 11.083433946 0.783802652
O 5.059521585 10.970061708 8.157542717
O 7.564653063 11.767018038 3.338335929
O 7.597704064 11.851450823 10.936717418
O 0.421860505 2.653670390 7.002980279
O 0.468882405 2.890664887 14.454039633
O 10.809383333 6.208254506 6.959767616
O 10.837079693 6.329551602 14.520752107
O 11.142738291 8.316701411 3.813503282
O 11.178466190 8.413227167 11.295253020
O 12.425285393 10.621881667 3.237511981
O 12.428082497 10.747984728 10.817850615
O 2.176131444 7.661352551 3.119837038
O 1.967971869 7.933348135 10.948406629
O 1.140247826 5.130273347 7.693635343
O 1.343257569 5.240114478 15.400580115
O 3.060681150 12.151608513 1.773445945
O 2.994767259 12.260726644 9.231017022
O 9.807311039 1.827198493 5.438815608
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O 0.762565293 9.560573492 1.902150683
O 0.692802320 9.658027704 9.371896321
O 11.962583108 3.941913528 6.175629159
O 12.030417199 4.167808957 13.640363992
O 3.685896147 1.214015420 5.830527756
O 3.732775150 1.267004808 13.365624972
O 6.351758737 11.538438859 5.925822915
O 6.342170287 11.669183644 13.457006560
O 9.761549420 12.505593530 2.088550289
O 9.742567587 12.423024226 9.578576399
O 7.219722453 1.846474870 2.089725552
O 7.344028742 2.062775984 9.714801085
O 11.803752600 10.044949069 5.730211219
O 11.869020897 10.038379016 13.285239082
O 1.814273473 6.882702680 5.607863278
O 1.579184699 6.650557669 13.184721936
O 1.050327611 3.139932023 1.936703136
O 1.216206842 3.126987767 9.449735401
O 11.790662133 6.559400486 1.929556292
O 11.624638738 6.602399149 9.426963450
O 2.712224242 2.854168725 3.998197805
O 2.754566581 2.959874696 11.607268446
O 10.074134976 11.027461004 14.954670468
O 9.933602136 10.993181453 7.316625405
O 9.875841832 10.574313538 3.951476152
O 9.900933197 10.667410906 11.595328476
O 3.008132066 3.189642429 15.116618642
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O 5.816864260 13.527584277 7.700382293
O 13.317443941 7.226343475 14.885955643
O 13.199626212 7.418726628 7.364749259
O 5.696292647 13.796619797 4.251881814
O 7.164103343 0.422877771 11.845375573
O 13.468132810 7.097101274 3.965217604
O -0.400007840 6.822790816 11.408512959
O 0.413869516 12.216037411 2.087335210
O 0.348411375 12.309109459 9.536613779
O 3.442926641 9.522806890 1.825676129
O 3.365205586 9.646532107 9.598894465
O 12.395017542 1.349583297 5.746356865
O 12.448898841 1.585518811 13.135908088
O 9.363633323 4.447211881 5.664123172
O 9.368795713 4.436765505 13.475944324
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Si 9.134366761 12.170088297 8.081344275
Si 3.738344181 1.628495432 4.270720066
Si 3.765229833 1.700373710 11.795949817
Si 11.927073666 6.921854080 3.510641533
Si 11.783902651 6.927861975 11.009448058
Si 1.352354040 3.556532706 3.481580049
Si 1.466010488 3.678599196 10.949711335
Si 1.142208999 6.703852062 14.738805306
Si 11.313457268 10.120706425 7.276423358
Si 11.455692103 10.169778166 14.847967064
Si 6.152864711 11.999672753 7.457085435
Si 6.226840528 12.099043508 14.988074762
Si 3.791608719 1.819375691 7.343980360
Si 3.819930356 1.787192070 14.898643408
Si 6.785342475 1.737702599 3.653643637
Si 6.842882399 1.874136857 11.222225420
Si 9.234155284 11.993222919 3.537991000
Si 9.265973990 12.061936247 11.090377097
Si 1.316901556 6.678171627 4.089965824
Si 1.203857424 6.666903493 11.610242586
Si 11.343033347 9.879547624 4.181860054
Si 11.368305052 9.952452107 11.744652280
Si 11.770244653 7.170949673 0.422940079
Si 11.717586446 7.199098654 7.903980536
Si 1.444898518 3.601364984 0.427210871
Si 1.774571165 13.094673586 2.029885989
Si 1.707621673 13.207156585 9.526313056
Si 4.156911135 10.971340172 2.001637353
Si 4.093254819 11.094920961 9.505369062
Si 10.912988364 0.713481800 5.780721534
Si 11.020195605 0.842789626 13.266229789
Si 8.643966913 2.984309424 13.359803930
Si -0.299152931 10.781580881 1.923840351
Si -0.373851301 10.870381408 9.438428994
Si 2.098951216 8.632621970 1.825198019
Si 2.021047955 8.744941983 9.530515938
Si 13.100857030 2.815419464 5.850656680
Si 13.148994440 3.045567918 13.291702522
Si 10.874140637 5.080121645 5.791503737
Si 10.796128080 5.188521032 13.363012297
Si 1.425053407 3.587470219 7.896153724
Si 8.660865826 2.947845839 5.697762755
Al 1.110554847 6.789414631 7.224264627
Al 5.976462203 12.098289945 4.327569996
Al 6.000091449 12.254586241 11.864491655
Al 6.939771474 1.670501370 8.074830859
H 7.391392744 11.665811619 9.964795461
H 7.391626745 11.682776626 2.346561229
O 7.033679766 6.098238664 5.434881102
Ti 5.943741382 6.650499217 7.274337782
H 7.915399280 5.653171523 5.452300070
H 6.488191210 5.568963772 4.822895351
O 4.624296185 6.751155160 8.958276416
H 4.796680704 7.071564142 9.859056405
O 4.274604760 5.581977203 6.312122413
H 3.486238692 6.079748235 5.971860719
O 7.609911661 7.964305017 7.995854163
H 7.628844474 8.921412935 7.811188850
H 3.682271349 7.018768232 8.725329661
H 3.902941130 4.747536671 6.694305547
H 8.544532632 7.682810411 8.023900651
O 5.123376364 8.551452481 6.518093875
H 4.998859649 8.856022010 5.601271602
O 7.053238260 5.058002865 8.251121648
H 7.428365811 4.245047303 7.790996261
H 6.884800475 4.766981266 9.165182225
H 4.987222220 9.343983582 7.091726757
End final coordinates

V6W-H2MOR
Final enthalpy = -6711.2410182324 Ry
CELL_PARAMETERS (angstrom)
13.814294020 0.012869084 0.046789073
-1.471210340 13.600584570 0.021841730
0.023004097 0.013588721 15.113726332

ATOMIC_POSITIONS (angstrom)
O 3.168089446 0.478343200 3.350139832
O 1.838212968 14.031765715 10.926190264
O 4.902225924 11.091783553 3.408651862
O 4.944747090 11.378202854 10.834395680
O 7.572198639 11.747111007 8.280070026
O 7.617663821 11.884890465 0.683006662
O 10.762219104 -0.040557590 7.197519534
O 9.507118345 13.539979861 14.755924584
O 7.900789635 2.784878014 7.104496915
O 7.864310759 2.654420050 14.772501337
O 5.242786485 2.094683765 3.807490441
O 5.297165619 2.170534852 11.394570446
O 12.532663242 10.950818380 0.621691747
O 12.451449136 10.867448902 8.216443057
O 2.011536602 7.772242648 0.504280041
O 2.130897045 7.748159276 8.313979073
O 1.550834168 5.270413952 3.546242354
O 1.656456126 5.291559439 11.036602862
O 0.148457040 3.174677464 4.422150003
O 0.196414566 3.251374149 11.933910223
O 11.190042211 5.798145443 4.394575758
O 10.944574537 5.869262201 11.944814860
O 11.244398076 8.645327500 0.408130751
O 10.963405452 8.631781128 7.868847103
O 9.434947642 13.166691472 4.617750859
O 9.521541302 13.284147202 12.123147727
O 7.674034046 2.844472903 4.432255069
O 7.695826735 2.958612552 12.122347782
O 5.349815785 1.959018597 15.320245474
O 5.271677667 2.079178830 7.746881853
O 3.087489741 0.536205088 0.677848899
O 3.010220481 0.683188174 8.258235723
O 5.128109177 11.185287000 0.736383363

O 5.048416963 11.013691866 8.173462378
O 7.570919919 11.773037903 3.343576695
O 7.603177067 11.852504131 10.951566776
O 0.350448653 2.696646390 7.060651211
O 0.401489794 2.888714530 14.577948563
O 10.800255135 6.151784188 7.037012143
O 10.893766336 6.231158115 14.611250280
O 11.178892273 8.375543047 3.833712813
O 11.215434343 8.435039298 11.365077525
O 12.473116674 10.672332283 3.282747062
O 12.506436512 10.739816947 10.877198275
O 2.090965450 7.813508468 3.177927428
O 1.904892205 7.947497178 10.953669398
O 1.176986984 5.146942610 7.737668669
O 1.413727705 5.226106857 15.387121735
O 3.074009636 12.327991531 1.927573706
O 2.961030072 12.276397710 9.256581967
O 9.832505326 1.777556681 5.516013272
O 9.816260284 1.759519810 13.205716738
O 0.620378123 9.577339113 1.836837040
O 0.674362956 9.717830642 9.392978143
O 12.024405356 3.961114811 6.128214618
O 12.113446147 4.134672358 13.601003997
O 3.641883344 1.251094245 5.793975725
O 3.707191999 1.253197436 13.347946377
O 6.324031934 11.573652877 5.919734491
O 6.307496055 11.709829753 13.482438643
O 9.745704005 12.478017023 2.052918342
O 9.734398854 12.470924411 9.579388598
O 7.219910132 1.846778889 2.058160428
O 7.337389364 2.015588254 9.696414922
O 11.827797569 10.097822393 5.769855292
O 11.863748016 10.100051774 13.338763373
O 1.759613289 6.913448142 5.637720179
O 1.528025859 6.758897911 13.238180272
O 1.099316607 3.196413185 1.967760897
O 1.172267800 3.150263316 9.504144406
O 11.795250922 6.578546511 1.973442290
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O 5.752378486 13.576540375 7.650127440
O 13.370354611 7.109201503 14.993964165
O 13.218617454 7.322640423 7.405563779
O 5.676152125 13.816663620 4.181763211
O 7.219461570 0.365250464 11.821925078
O 13.481637195 7.100960285 4.003956510
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O 0.408436923 12.238358558 2.077461837
O 0.315198527 12.358495908 9.570999124
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O 3.352901565 9.661357179 9.624831869
O 12.448049938 1.379991132 5.670837470
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O 9.394793779 4.404509418 5.676702705
O 9.442350359 4.357605238 13.510674819
Si 6.892161830 1.618886054 0.490305135
Si 9.223229824 12.203474373 0.523581999
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Si 3.727537612 1.709049324 4.246208523
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Si 1.130546176 6.709541689 14.804202903
Si 11.328033359 10.124238257 7.316685220
Si 11.427500929 10.149712188 14.900725146
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Si 3.802095746 1.719535016 14.896793382
Si 6.815703433 1.693853790 3.627875258
Si 6.897692794 1.826318478 11.222816032
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Si 9.273476078 12.094282703 11.090780600
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Si 11.058884618 0.753191308 13.325935216
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Si -0.405911349 10.917399338 9.488218389
Si 2.005628441 8.715807376 1.832443583
Si 1.985922562 8.776006160 9.548411803
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Si 13.212403005 2.967377303 13.354519657
Si 10.889563100 5.074309408 5.815164612
Si 10.852650428 5.140754562 13.404067442
Si 1.395732146 3.593325150 7.948114190
Si 8.683156433 2.906745990 5.709000215
Al 1.071559161 6.802499556 7.260582907
Al 5.969378679 12.121690656 4.311823740
Al 5.994529849 12.273197116 11.873792376
Al 6.922724789 1.636217618 8.056794287
H 7.391387165 11.697210248 9.976615636
H 7.384387748 11.682213782 2.354897889
O 7.017534467 6.056934180 5.476134648
V 5.943024171 6.642134272 7.290663566
H 7.914806556 5.647092956 5.506074802
H 6.481352658 5.450204022 4.931115299
O 4.699207813 6.989224916 8.981243902
H 4.881639068 7.724701215 9.595037688
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H 3.444507115 6.153329821 6.075073132
O 7.763509179 7.664592523 7.972200237
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H 3.851205570 4.818656901 6.821462330
H 8.506972569 7.060224506 8.165620754
O 5.055247727 8.503719017 6.521682809
H 5.130945791 8.830229963 5.607161364
O 7.020270128 5.044581096 8.237913655
H 7.377306663 4.225536894 7.768822323
H 6.719296549 4.724441839 9.108169141
H 4.972054286 9.306402454 7.087878730
End final coordinates

Ag6W-H2MOR
Final enthalpy = -6852.2138057493 Ry
CELL_PARAMETERS (angstrom)
13.736568875 0.085104486 0.069168520
-1.391486846 13.519797856 0.028205590
0.047680948 0.023540285 15.040924161

ATOMIC_POSITIONS (angstrom)
O 3.259827983 0.285525760 3.534525817
O 1.896107627 13.865489702 11.054961040
O 4.910663895 11.050020935 3.481876430
O 4.969612983 11.345302789 10.875453158
O 7.607462461 11.852932835 8.324302350
O 7.673837669 11.969313666 0.750828673
O 10.646667061 0.192072184 7.244363030
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H 3.669035610 7.143274890 8.393317579
H 3.667971163 4.650189741 6.519591386
H 7.938595422 6.111465640 8.455146542
O 4.874534280 8.679520886 6.066565489
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O 8.479093434 4.836029318 9.034037408
H 8.402552828 4.070841002 8.405139246
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H 4.968904027 9.459330450 6.648571826
End final coordinates

Mo6W-H2MOR
Final enthalpy = -6860.8568034454 Ry
CELL_PARAMETERS (angstrom)
13.743088658 0.077769914 0.065586585
-1.399381003 13.513915571 0.030016672
0.043762645 0.025113150 15.039966476

ATOMIC_POSITIONS (angstrom)
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O 4.900362032 11.032321470 3.488544450
O 4.955648565 11.352584086 10.869654668
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O 7.667349750 11.963466802 0.746537971
O 10.644822142 0.185495285 7.239881520
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End final coordinates

Nb6W-H2MOR
Final enthalpy = -6831.3042615383 Ry
CELL_PARAMETERS (angstrom)
13.724020556 0.049084546 0.054558270
-1.425429598 13.514695390 0.036835608
0.031453382 0.031549959 15.053262444

ATOMIC_POSITIONS (angstrom)
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O 9.520079647 13.613798989 14.820714525
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O 0.163975244 3.377679233 11.942530658
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O 10.915929101 5.817703115 11.919162594
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O 6.255891124 11.560451770 13.543239964
O 9.740633252 12.453786070 2.146069887
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O 1.754566651 6.794910498 5.655329444
O 1.572428286 6.677203693 13.223607958
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O 1.196372318 3.098516295 9.540284971
O 11.749691854 6.526980736 1.981282755
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O 5.608292435 13.669628427 4.254873140
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O 13.441907496 7.157983636 3.980996651
O -0.386934917 6.720296278 11.418453796
O 0.438386904 12.129499010 2.193748306
O 0.279539161 12.328192513 9.499626682
O 3.356480735 9.566543515 1.823698650
O 3.382105158 9.601524444 9.613415443
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O 9.368112310 4.375623601 5.602263782
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Si 9.107749863 12.159376407 8.164795451
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Si 6.759156652 1.639918226 3.679611556
Si 6.846488839 1.779266389 11.265818676
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Si 9.233845761 11.990363000 11.165035950
Si 1.286379488 6.700223629 4.120378060
Si 1.219846547 6.631372792 11.642827235
Si 11.285461581 9.818291630 4.241536314
Si 11.383748853 9.917808582 11.795839870
Si 11.750841740 7.126805366 0.470103339
Si 11.652053085 7.136967079 7.933537362
Si 1.428308554 3.525268623 0.480770599
Si 1.745762362 13.083656378 2.172856398
Si 1.663121013 13.188769858 9.564341131
Si 4.134119551 10.949290931 2.156801000
Si 4.063900587 11.082091234 9.538594374
Si 10.934626573 0.666639560 5.821124062
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Al 5.970114981 12.171499331 11.944071274
Al 6.937378416 1.684974124 8.102143215
H 7.355515852 11.627326924 10.035088216
H 7.363467276 11.669684649 2.374727991
O 7.112073914 5.974948870 4.904949938
Nb 5.994360607 6.811119501 6.736023517
H 7.978955454 5.530829678 5.073407243
H 6.594535694 5.321647234 4.397999540
O 4.811363730 7.279622822 8.579079892
H 4.959617000 8.087158206 9.106794520
O 4.179492708 5.583781302 6.218283793
H 3.350903240 6.055264541 5.924553265
O 7.772587592 8.213936825 7.197986751
H 7.818471706 9.105720522 6.807860372
H 3.821513387 7.293903320 8.410433794
H 3.873391856 4.784273991 6.710637929
H 8.683489994 7.986055230 7.474850954
O 4.907772810 8.661398324 5.873170269
H 4.929142235 9.068815727 4.982168065
O 7.061837493 5.252164120 7.977552683
H 7.415441329 4.364241593 7.662794678
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H 4.827559017 9.411848520 6.496795924
End final coordinates

Pd6W-H2MOR
Final enthalpy = -6828.0130476694 Ry
CELL_PARAMETERS (angstrom)
13.718782756 0.091846963 0.069582720
-1.383076814 13.525423217 0.030202257
0.048063269 0.025872995 15.036117970

ATOMIC_POSITIONS (angstrom)
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O 1.913042787 13.878821938 11.056740284
O 4.910200060 11.073205233 3.484051884
O 4.977132390 11.377484135 10.877513120
O 7.629063798 11.863577310 8.325587686
O 7.681294571 11.965184640 0.760858004
O 10.651805699 0.203983641 7.240825082
O 9.499352412 13.740542856 14.796220403
O 8.096043672 2.791649152 7.225404777
O 7.951636202 2.699533324 14.791203586
O 5.146995577 2.159723408 3.804272349
O 5.198789349 2.216304222 11.358294712
O 12.597452890 10.977920450 0.585609652
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O 2.040008309 7.772277771 0.471299528
O 2.191087347 7.778104356 8.208535460
O 1.713004421 5.187784527 3.497712586
O 1.782621992 5.267360831 10.962451071
O 0.038075093 3.311475000 4.378742126
O 0.097462032 3.404835483 11.823450856
O 11.139252891 5.772324373 4.318249490
O 10.929287477 5.883561631 11.842612343
O 11.142065527 8.768320640 0.467854252
O 10.924062873 8.769490420 7.879607277
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O 7.502157153 2.904549755 4.597089741
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O 3.147633840 0.711778900 0.898294566
O 3.134585028 0.858530493 8.415835759
O 5.259517271 11.133804414 0.825708833
O 5.144733939 11.054491009 8.208299226
O 7.594393938 11.840764759 3.368392739
O 7.629978964 11.936867584 10.939757942
O 0.386418125 2.758649237 6.998022362
O 0.476693431 2.914124867 14.435455064
O 10.718523941 6.335701135 6.912817377
O 10.818162316 6.417991108 14.471579154
O 11.192141141 8.369292531 3.853618878
O 11.223997125 8.458411214 11.291088848
O 12.439226028 10.680110048 3.242334750
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O 1.976805736 7.917959666 10.865745437
O 1.164868995 5.196571436 7.777319818
O 1.328998928 5.271319702 15.347869537
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O 9.784448439 1.913716944 13.038573586
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O 11.818818370 10.146606646 5.740570381
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Si 1.226488204 6.669261163 11.568330953
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Si -0.299283007 10.927410244 9.422927139
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O 7.327267379 6.850065223 7.936817498
H 7.977302569 7.344540983 7.404475980
H 3.656197933 7.194658013 8.274509600
H 3.649608997 4.656753720 6.566159314
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O 4.585171747 8.862688053 5.947816753
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O 8.450036015 4.864519341 8.946202716
H 8.384749732 4.080205121 8.328160962
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End final coordinates

Rh6W-H2MOR
Final enthalpy = -6967.0668087545 Ry
CELL_PARAMETERS (angstrom)
13.709467738 0.102034048 0.071573807
-1.371865624 13.501122407 0.013210586
0.050287416 0.007267138 15.038009384

ATOMIC_POSITIONS (angstrom)
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O 5.005462794 11.338546438 10.821091165
O 7.618639492 11.794903999 8.294323683
O 7.686124834 11.928760844 0.724108227
O 10.642719294 0.167877182 7.263751364
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O 1.711316989 5.141411550 3.570674502
O 1.801480519 5.238728839 10.923790227
O 0.051920013 3.216976510 4.363868398
O 0.140474413 3.372249866 11.835978315
O 11.109486224 5.758081247 4.309718550
O 10.932045504 5.798387696 11.830186545
O 11.141314321 8.746318332 0.461511300
O 10.902786800 8.722371097 7.870456567
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O 5.284204874 2.237215930 7.913642766
O 3.162829975 0.706168817 0.872009697
O 3.058746042 0.754021661 8.345145998
O 5.276528392 11.052646221 0.796376867
O 5.145809937 10.947753955 8.158692660
O 7.583687398 11.773469538 3.335317002
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O 0.373309020 2.676544143 6.989971122
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O 6.410283110 11.619341731 13.458995136
O 9.780992998 12.552850901 2.109825801
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O 9.274805698 4.517845391 5.696580475
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Si 9.181594817 12.270409170 8.084758438
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Si 11.771184923 6.900965027 10.980361283
Si 1.385738791 3.560257880 3.496101581
Si 1.478019194 3.638394854 10.944421730
Si 1.149141775 6.696316647 14.712269865
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Si 6.262218533 12.067241880 14.981890769
Si 3.826347680 1.840659379 7.401534269
Si 3.877882028 1.811785559 14.910905446
Si 6.769588337 1.754269097 3.657298780
Si 6.845665891 1.830144564 11.250102649
Si 9.243787097 12.022873749 3.550072465
Si 9.316156134 12.068346554 11.082853665
Si 1.322088479 6.646308421 4.050798054
Si 1.227371672 6.616356212 11.566182395

Si 11.372159008 9.920975428 4.181229208
Si 11.399284207 9.933998033 11.724384997
Si 11.722469498 7.222119115 0.408623289
Si 11.682152346 7.258757629 7.889937756
Si 1.470140326 3.621884076 0.439803390
Si 1.831886188 13.087747509 2.056793275
Si 1.775205537 13.145427714 9.532733602
Si 4.192939505 10.941075372 2.010949944
Si 4.169083546 11.034638379 9.495476857
Si 10.890321349 0.795737359 5.782147087
Si 11.035911460 0.866909233 13.275732371
Si 8.661992204 2.977539752 13.332202081
Si -0.261056137 10.813725779 1.904936242
Si -0.296547476 10.844140409 9.411412794
Si 2.120764814 8.640724829 1.805021194
Si 2.100740958 8.710928985 9.495929393
Si 13.047119467 2.907530642 5.831681707
Si 13.146226204 3.073328063 13.308487530
Si 10.799141108 5.141516886 5.778067734
Si 10.784158776 5.193716945 13.339477434
Si 1.397563991 3.580769244 7.891578561
Si 8.603032688 2.998856459 5.727523823
Al 1.117167498 6.784404599 7.209537673
Al 6.001983629 12.096534274 4.331324697
Al 6.043539491 12.223718170 11.878757868
Al 6.928954832 1.666959497 8.106083351
H 7.436949071 11.753088860 9.947629308
H 7.417422310 11.705689730 2.337687395
O 6.981168322 6.168690158 5.346275255
Rh 5.934025920 6.638627710 7.115290497
H 7.841608071 5.684780021 5.452843522
H 6.385428275 5.552413351 4.870985205
O 4.756640825 6.978272180 8.775007100
H 5.033541727 7.751859667 9.304425613
O 4.202217793 5.465596813 5.966257958
H 3.414466055 6.033457341 5.761983580
O 7.816286693 7.731643896 8.423600026
H 8.587754064 8.176705885 8.019531921
H 3.801763679 7.180271777 8.491166375
H 3.826540568 4.690866623 6.446297277
H 8.195452890 6.968811218 8.896956612
O 5.234307323 8.455301254 6.251231377
H 5.646575201 8.723807211 5.408834360
O 6.564717531 4.943018959 8.144476554
H 7.132798182 4.248034772 7.678861628
H 5.799256812 4.423351608 8.471023142
H 5.261860112 9.252003803 6.830482976
End final coordinates

Ru6W-H2MOR
Final enthalpy = -6928.5756768870 Ry
CELL_PARAMETERS (angstrom)
13.701714993 0.102500698 0.065614719
-1.370760547 13.510870978 0.024694138
0.043664242 0.019377554 15.033944698

ATOMIC_POSITIONS (angstrom)
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O 1.928750049 13.883130733 11.001592470
O 4.924857304 11.075669825 3.461695445
O 5.009807186 11.361052376 10.818868123
O 7.606414954 11.787910372 8.310702385
O 7.696887705 11.938775270 0.732267125
O 10.617591206 0.154367439 7.251555130
O 9.518485335 13.703378810 14.760283106
O 7.873087847 2.833464755 7.138445320
O 7.995098374 2.598976042 14.756921246
O 5.180490970 2.138196325 3.736789088
O 5.242317193 2.190193691 11.303653830
O 12.624406264 10.929018870 0.590035477
O 12.456959679 10.922125866 8.166199517
O 2.046654589 7.783899703 0.444644888
O 2.196595553 7.713321214 8.274772740
O 1.735830632 5.134587024 3.616938483
O 1.793861070 5.272357264 10.924236964
O 0.047683380 3.222981639 4.379283544
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O 11.123341551 5.773934725 4.337725983
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O 11.140382412 8.736087578 0.481962018
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O 9.448309328 13.112727955 4.710233409
O 9.641054838 13.222306340 12.160559377
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O 5.427864200 2.127673794 15.280088075
O 5.291594470 2.224727928 7.917461543
O 3.179915663 0.694291730 0.873296121
O 3.041558399 0.781959989 8.340366164
O 5.293375093 11.048771135 0.810391526
O 5.117173427 10.968560866 8.158868261
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O 0.393062071 2.694443282 7.002054625
O 0.508281972 2.917917751 14.456258187
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O 10.815782071 6.379197067 14.478659365
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O 1.376971880 5.261500821 15.406796842
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O 0.831158308 9.602296159 1.920711488
O 0.805530618 9.724637608 9.327254235
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O 12.016616981 4.199269669 13.649753326
O 3.850499060 1.227920605 5.888781568
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O 6.409669436 11.632799154 13.463981353
O 9.795752893 12.560113347 2.113202648
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O 7.257107343 1.848670274 2.104410923
O 7.410989861 1.899240004 9.751744310
O 11.831447093 10.114200584 5.740548806
O 11.875542893 10.061502669 13.275996591
O 1.808772861 6.893851512 5.605214330
O 1.562309475 6.652706368 13.163495793
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O 3.509073496 9.482484305 1.848573996
O 3.473685864 9.581577156 9.606666956
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O 12.480807045 1.615329277 13.161286405
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Si 3.794479855 1.684699375 11.810236870
Si 11.899638781 6.931273782 3.509319671
Si 11.763144345 6.929597031 10.984473644
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Si 1.493144750 3.667847493 10.949022560
Si 1.154313248 6.713713515 14.723958518
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Si 11.463376480 10.206751075 14.835806758
Si 6.174040930 12.014786424 7.439773302
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Si 1.761358742 13.186351177 9.542072196
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Si 11.046313743 0.879449753 13.263142302
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Si -0.312970653 10.884451316 9.432189012
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Si 2.078548814 8.744064736 9.513977054
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Si 13.150806828 3.091619325 13.301547478
Si 10.788180129 5.143893325 5.795113128
Si 10.780293187 5.211795216 13.346651507
Si 1.422573396 3.599143869 7.896396916
Si 8.600815486 2.991497697 5.717201289
Al 1.104749279 6.801085425 7.220954720
Al 6.012230014 12.103186683 4.339300891
Al 6.041892900 12.242531328 11.885279236
Al 6.934934567 1.664078730 8.105823253
H 7.432397870 11.780674275 9.954460950
H 7.430648125 11.732379342 2.347327302
O 6.929239573 6.178600901 5.244437029
Ru 5.865729291 6.642119913 7.059320408
H 7.781796608 5.690784935 5.353474294
H 6.356232722 5.576732188 4.728048297
O 4.728673644 6.976708433 8.797132498
H 4.982386930 7.776430420 9.299332019
O 4.246280196 5.629819058 6.130212569
H 3.447101253 6.183736046 5.895325567
O 7.521907014 7.587222031 8.071763904
H 8.224960142 8.027395373 7.556350046
H 3.766442673 7.144300294 8.546169200
H 3.888714611 4.832209546 6.591054406
H 7.965577447 6.854411129 8.546676092
O 5.067917115 8.462220269 6.203263491
H 5.428048370 8.791624020 5.358426374
O 6.631051456 4.990083174 8.127450862
H 7.108920775 4.229218963 7.667311411
H 5.943726313 4.560747983 8.674302508
H 5.074452203 9.236750661 6.808551056
End final coordinates

Zr6W-H2MOR
Final enthalpy = -6804.3678543376 Ry
CELL_PARAMETERS (angstrom)
13.714026692 0.058374493 0.065845973
-1.415798661 13.528372986 0.031992025
0.043644579 0.027280652 15.055506648

ATOMIC_POSITIONS (angstrom)
O 3.192357707 0.260374652 3.473747413
O 1.794688887 13.857795774 10.996090492
O 4.839345581 10.994824209 3.466056299
O 4.924557263 11.302845856 10.807835547
O 7.560656122 11.640913860 8.289827476
O 7.642137117 11.913963992 0.672242881
O 10.596113423 0.033467598 7.235103073
O 9.519066983 13.652178659 14.759019415

O 7.935511428 2.832493228 7.140076690
O 7.923386995 2.649800190 14.774236497
O 5.130325981 2.060032891 3.734495239
O 5.185145713 2.119813570 11.305066552
O 12.566772745 10.851059732 0.551618957
O 12.416111713 10.769224378 8.149400604
O 2.000220783 7.723559605 0.412951918
O 2.091051257 7.640218767 8.283357752
O 1.581213769 5.141224202 3.569429322
O 1.773092369 5.260942415 10.905212513
O 0.020333913 3.125548363 4.351840015
O 0.116703508 3.400956238 11.822886648
O 11.239216353 5.657613424 4.311843515
O 10.940977364 5.805576840 11.834381357
O 11.081769143 8.661537567 0.454639170
O 10.795605906 8.610494109 7.806350262
O 9.390067104 13.009073819 4.698208036
O 9.508748860 13.175186547 12.155763722
O 7.516164811 2.822012602 4.480616029
O 7.523457825 2.974152142 12.155069495
O 5.363576743 2.072834971 15.257651156
O 5.279405253 2.119214188 7.765819186
O 3.111579244 0.629829699 0.819224692
O 2.993312254 0.778589595 8.333044057
O 5.226531292 11.104681745 0.818632113
O 5.042825871 11.003928140 8.128024951
O 7.525920435 11.732313391 3.307104537
O 7.560812525 11.827627382 10.931116317
O 0.407165918 2.599970833 6.969444667
O 0.451249364 2.850508457 14.434173487
O 10.696599978 6.179627898 6.881095446
O 10.777355242 6.315139998 14.469647362
O 11.095730427 8.257639926 3.830213062
O 11.162146127 8.377033512 11.238564932
O 12.381587930 10.559830575 3.205240389
O 12.390003685 10.733219286 10.814974179
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O 2.012888343 7.894189930 10.918207154
O 1.065579544 5.098718633 7.621618969
O 1.292065057 5.215757077 15.357543645
O 3.043114765 12.137715328 1.843847123
O 2.967413449 12.234983451 9.228710489
O 9.722601932 1.752127928 5.423719968
O 9.758814684 1.815327499 13.042943620
O 0.752993394 9.536401014 1.872096504
O 0.691292498 9.628295997 9.401989538
O 11.914973888 3.905953005 6.213303058
O 11.993309617 4.140854051 13.648455188
O 3.677623144 1.203559524 5.844694496
O 3.690996463 1.241004168 13.369966599
O 6.361642304 11.547238317 5.913528151
O 6.299040285 11.635713260 13.455640680
O 9.735934417 12.482747061 2.088716237
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O 11.755651269 10.026066032 5.705117927
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H 4.870366721 8.856731602 5.670971581
O 7.279774854 5.112367136 8.326732349
H 7.561809852 4.261444913 7.852074018
H 7.472961596 4.970973862 9.271412834
H 4.958619388 9.496556580 7.119549191
End final coordinates

M2O-H2MOR Optimized Structures

Cu-O-Co-H2MOR
Final enthalpy = -6649.1562081036 Ry
CELL_PARAMETERS (angstrom)
13.807763807 0.070042003 -0.004975905
-1.364908580 13.619791722 -0.023368551
0.001962879 0.006207408 15.017249477

ATOMIC_POSITIONS (angstrom)
O 3.130687404 0.510413665 3.288733918
O 2.275239924 13.784264299 10.724021837
O 5.241729243 11.062726782 3.304416272
O 4.947109501 11.304730160 10.785051478
O 7.917109388 11.589899796 7.622676348
O 7.691020317 11.834499190 0.570795899
O 10.818323976 0.080647151 6.952297983
O 9.465349005 13.488918635 14.500370686
O 8.189940798 2.580161219 6.998479108
O 8.127352861 2.652941033 14.620852538
O 5.193063595 2.180864411 3.603890337
O 5.371493611 2.136880592 11.155185991
O 12.599846740 11.009279862 0.464228059
O 12.961586356 10.692282791 7.938070656
O 2.223948338 7.683807946 0.432435684
O 2.113045207 7.991151392 7.852116395
O 1.755257741 5.337140827 3.402312188
O 1.703622438 5.008628335 11.195673372
O 0.100904544 3.357725141 4.172060453
O 0.200170551 2.888166280 11.740428889
O 11.046904665 5.949352398 4.169921767
O 11.225691403 5.764989709 11.683333582
O 11.393091226 8.657062402 0.153752394
O 11.101726560 8.784627034 7.707143915
O 10.161773243 13.356415938 4.365558855
O 9.599306267 13.191463432 11.872600237
O 7.615702499 2.883272612 4.413676219
O 7.755645459 2.935133810 11.987977177
O 5.558246075 2.136981547 14.960805359
O 5.398744853 1.867646505 7.728183410
O 3.567130601 0.469392096 0.652178981
O 3.120402088 0.524750977 8.137116344
O 5.138562938 11.319690809 0.632429166
O 5.463567799 10.922529280 8.206777476
O 7.941059169 12.058668644 3.690386288
O 7.667646177 11.727157826 10.752573259
O 0.584640715 2.965207380 6.764700604
O 0.531686681 2.736720916 14.387407183
O 10.686887014 6.330386604 6.801430306
O 11.086998930 6.204776891 14.300340358
O 11.377206193 8.498964576 3.491158230
O 11.394434143 8.390421624 11.280763769
O 12.861280859 10.694860585 3.112020069
O 12.586248731 10.719921808 10.580682049
O 2.006519097 7.946213745 3.085682275
O 2.250924640 7.487789559 10.475214472
O 1.518034729 5.240590090 7.781776002
O 1.572966045 5.155526117 14.924853163
O 3.142247619 12.162086328 2.179924379
O 3.153457132 12.037191538 8.915258536
O 9.860635162 1.693885062 5.091685411
O 9.926690552 1.748573241 12.873465692
O 0.936854033 9.754355601 1.456404052
O 0.974643708 9.618265241 9.612008282
O 12.215695577 4.364192152 5.967527028
O 12.206561625 3.980306437 13.400623780
O 3.781042316 1.261484788 5.709242563
O 3.902677716 1.126941197 13.164972111
O 6.005330401 11.577191865 5.705806547
O 6.323164522 11.801025648 13.316392464
O 9.872524338 12.542053344 1.893062633
O 9.718664266 12.555131155 9.299170789
O 7.273535835 2.007188831 1.974114156
O 7.511923260 2.135148510 9.535524618
O 12.173807662 10.000958353 5.538497971
O 11.904115185 10.260077204 13.071237348
O 1.727377312 7.002502717 5.508570076
O 1.612560990 6.964711738 12.971084443
O 1.258517464 3.295065350 1.810591389
O 1.119153101 3.143024877 9.330446785

O 11.872029974 6.575505263 1.758724542
O 11.547735749 6.674884578 9.269263891
O 2.747845317 3.020152886 4.020897703
O 2.822653017 2.667042970 11.309316255
O 10.029589030 10.894814836 14.814776445
O 10.489548570 11.266703038 7.112110870
O 10.262231220 10.788318096 3.830453442
O 10.038162377 10.645194820 11.184483405
O 3.101669499 3.004311289 14.919719216
O 3.093256676 3.109310180 7.534278744
O 7.305374524 0.151545153 0.061188773
O 7.423793585 -0.143747568 7.649294221
O 13.533102197 7.142797206 14.788682125
O 13.181293060 7.230620823 7.232053962
O 5.649586510 13.912903274 3.971098310
O 7.323970104 0.316961156 11.453755939
O -0.328431441 6.889819541 3.860855271
O -0.250725876 6.812530231 11.045146049
O 0.533226355 12.371771962 1.768527669
O 0.553555467 12.244704953 9.480724289
O 3.584829275 9.556985352 1.803007768
O 3.647789202 9.465820993 9.400070849
O 12.466161912 1.741645729 5.676161785
O 12.530662011 1.331021844 13.141621016
O 9.553697236 4.303098057 5.537671679
O 9.580848285 4.363441359 13.207308641
O 4.838111283 8.485412419 5.599641858
Si 7.057923560 1.714517917 0.406472323
Si 9.268346788 12.179649191 0.437276485
Si 9.398108067 12.285422875 7.709743772
Si 3.734471797 1.741316747 4.167592125
Si 3.917807045 1.520195848 11.589382755
Si 11.945332647 6.993592704 3.327164894
Si 11.948194358 6.931437950 10.813640100
Si 1.460105107 3.736283438 3.360872868
Si 1.463510194 3.434605737 10.879532499
Si 1.287796413 6.707247659 14.541227699
Si 11.684475548 10.170230098 7.076680565
Si 11.484447919 10.195393899 14.640443123
Si 6.341918973 11.946865834 7.292226963
Si 6.276505271 12.194608538 14.864470126
Si 3.876240572 1.702183499 7.279312827
Si 4.024842445 1.685094775 14.689346384
Si 6.781973736 1.812926035 3.514597612
Si 6.952274225 1.820370123 11.126173270
Si 9.514472197 12.183356695 3.447375322
Si 9.351265033 12.049127370 10.785958279
Si 1.281246858 6.783528570 3.951357846
Si 1.312631396 6.560494077 11.422387880
Si 11.670177249 10.013216581 3.991375282
Si 11.503156102 9.983442014 11.527468970
Si 11.978633459 7.145179059 0.244394585
Si 11.664022791 7.240224756 7.740337644
Si 1.614736216 3.561896340 0.250672850
Si 1.913139919 13.201054420 1.953440723
Si 1.947105889 13.064428617 9.299195087
Si 4.266417705 11.025576470 1.952347163
Si 4.296449495 10.961619257 9.365055759
Si 11.154326009 0.820359034 5.525595355
Si 11.069172963 0.635831069 13.129147124
Si 8.851262388 2.919724139 13.202342578
Si -0.173722169 10.916115888 1.719067091
Si -0.130852322 10.782226688 9.390562362
Si 2.180301055 8.736059440 1.677452116
Si 2.251082699 8.654146300 9.347150568
Si 13.247174639 3.151131258 5.635908761
Si 13.273759784 2.779312675 13.163891268
Si 10.874261395 5.226010106 5.619847611
Si 11.037916988 5.076768517 13.142389474
Si 1.587990978 3.649073328 7.845349335
Si 8.796554726 2.863705890 5.537490526
Al 1.026741334 6.744074727 7.139253714
Al 6.307438537 12.344558695 4.084812904
Al 6.075136175 12.233300547 11.683016423
Al 7.071295340 1.538995207 7.794960414
Cu1 3.283696771 8.041495300 6.275267332
Co2 5.187115258 9.980132028 4.915037870
H 8.115911759 2.898017693 9.462101275
H 7.412010289 11.234869066 9.941431561
End final coordinates

Cu-O-Cr-H2MOR
Final enthalpy = -6735.4625215183 Ry
CELL_PARAMETERS (angstrom)
13.813747855 0.062685057 0.005491316
-1.372746139 13.613766990 -0.011059174
0.013256371 0.020905483 15.022442383

ATOMIC_POSITIONS (angstrom)
O 3.117977646 0.518525857 3.296305275
O 2.277637424 13.788888555 10.750156702
O 5.160597282 11.052801740 3.391675613
O 4.951434503 11.344509915 10.810426701
O 7.917204419 11.573221001 7.617564904
O 7.700636084 11.809964229 0.577488943
O 10.836423690 0.067511270 6.966521741
O 9.474985449 13.497618489 14.526033540
O 8.220720242 2.568583352 7.029421215
O 8.139957279 2.665041096 14.644544859
O 5.212017678 2.152601654 3.623786916
O 5.380225155 2.145652856 11.163585903
O 12.613052295 11.010453157 0.451650816
O 12.977111593 10.726584810 7.934830072
O 2.222987236 7.680916132 0.427815300
O 2.161313300 8.039807230 7.836543839
O 1.714491610 5.326737390 3.340266108
O 1.714816631 5.012088757 11.201878953
O 0.114925148 3.314382672 4.161163382
O 0.193641573 2.901339862 11.722529199
O 11.053952807 5.920625895 4.164691181
O 11.215040593 5.770219559 11.691720229
O 11.416837986 8.653512283 0.161961903
O 11.155459393 8.772385489 7.725958996
O 10.134051973 13.346554005 4.384512729
O 9.599484709 13.199819867 11.895083287
O 7.637953685 2.854891863 4.445680629
O 7.760800556 2.964229788 12.014617504
O 5.576824428 2.137134787 14.995530056
O 5.416782463 1.870878774 7.708927691
O 3.560366723 0.466962744 0.658935449
O 3.131140384 0.550783475 8.150897419
O 5.153518872 11.328502008 0.719386994
O 5.455036518 10.906048483 8.239055724
O 7.929016794 12.005419132 3.715538543
O 7.664933166 11.720606813 10.821769479
O 0.611919578 3.026734966 6.761886652
O 0.552993489 2.751730034 14.362104401
O 10.756133466 6.327856559 6.802830947
O 11.101624074 6.221767150 14.311447022
O 11.360689978 8.479093386 3.519595199
O 11.396128424 8.389688752 11.272148917
O 12.844284948 10.668724384 3.102631894
O 12.578941403 10.720840664 10.573857351
O 1.976638694 7.937411959 3.081550715
O 2.232966721 7.482496183 10.455304616
O 1.573765113 5.276973099 7.842249263
O 1.593764644 5.161943986 14.931913453
O 3.107429631 12.154367936 2.212258383
O 3.158115978 12.056863255 8.928368032
O 9.923366159 1.734995974 5.129162303
O 9.930652503 1.759358186 12.886697196
O 0.933410397 9.758672331 1.442937527
O 0.960587904 9.619972334 9.600605140
O 12.206176269 4.309209029 5.950819792
O 12.224128401 3.997746720 13.409975851
O 3.761163586 1.272841686 5.712887307
O 3.940257043 1.127911641 13.180468556
O 5.958351659 11.584366488 5.765054782
O 6.283123590 11.785312321 13.367272768
O 9.860876889 12.525648480 1.915421871
O 9.695749760 12.538961925 9.325691580
O 7.290602068 2.000708288 2.000156818
O 7.521790799 2.145442093 9.564404968
O 12.183211672 10.008040301 5.546434456
O 11.926728721 10.251970983 13.072119340
O 1.753700363 6.928367944 5.491338065
O 1.644583118 6.968490224 12.973169399
O 1.254346761 3.256621762 1.790600589
O 1.148793308 3.140677272 9.331067222
O 11.889464350 6.575986241 1.765322326
O 11.598434894 6.655399301 9.278540451
O 2.768807669 3.039210602 3.993258460
O 2.823732162 2.668903815 11.340605986
O 10.056022066 10.906759018 14.822062713
O 10.486152113 11.239284592 7.146486015
O 10.259409517 10.777029776 3.852477997
O 10.039872231 10.644487587 11.217073095
O 3.121456208 3.014482200 14.914381594
O 3.118883826 3.133279168 7.537420197
O 7.328059562 0.148436540 0.083817183
O 7.441478505 -0.142452569 7.724721654
O 13.555427147 7.131094215 14.788421722
O 13.252573440 7.231320412 7.264279349
O 5.668667132 13.882085669 3.997201700
O 7.347904547 0.345817468 11.516338554
O -0.337648683 6.894755450 3.874226479
O -0.251935176 6.816372467 11.096857958
O 0.508043531 12.373454934 1.784344141
O 0.560163178 12.252349456 9.500665282
O 3.565691604 9.550210999 1.817703671
O 3.635052891 9.489807449 9.470539847
O 12.535048292 1.689599292 5.716274634
O 12.537210088 1.349414278 13.147897900
O 9.538085093 4.329584576 5.572977559
O 9.595918999 4.374918268 13.236992033
O 4.696435327 8.421439842 5.167923164
Si 7.068713070 1.709329456 0.432783125
Si 9.275509227 12.166920586 0.450587385
Si 9.398672051 12.266255486 7.733340184
Si 3.735418046 1.749506202 4.168375594
Si 3.928535395 1.528615417 11.607140767
Si 11.951670365 6.981430263 3.338838838
Si 11.961716009 6.926660133 10.828657289
Si 1.458116342 3.723429387 3.335590449
Si 1.473856669 3.439976665 10.882050379
Si 1.307867536 6.711517928 14.541690669
Si 11.704242336 10.167697298 7.089018623
Si 11.509347311 10.202322343 14.642743755
Si 6.342101488 11.950163490 7.349903787
Si 6.284994288 12.197362029 14.911284542
Si 3.885780074 1.720559762 7.279527927
Si 4.044814499 1.693545864 14.703871190
Si 6.802422196 1.792292298 3.540416364
Si 6.963675730 1.840613016 11.158844590
Si 9.502955887 12.164100291 3.469202892
Si 9.349356944 12.046552049 10.820982573
Si 1.276054300 6.761509218 3.956758831
Si 1.319148812 6.561812016 11.430060687
Si 11.665203092 9.995878864 4.003320913
Si 11.510334058 9.979117434 11.531827724
Si 11.993710423 7.137518599 0.249483608
Si 11.731208775 7.230082522 7.752257284
Si 1.618948517 3.550937735 0.237773031
Si 1.885501292 13.201961369 1.974452514
Si 1.947537079 13.080368321 9.320643517
Si 4.230229260 11.018137503 1.994049267
Si 4.287180226 10.978952131 9.404540181
Si 11.189203776 0.816497221 5.549191460
Si 11.078651088 0.651482119 13.140264861
Si 8.862026856 2.935317127 13.225863789
Si -0.184360288 10.911130641 1.710255728
Si -0.132276401 10.795370127 9.384824171
Si 2.161824543 8.722955159 1.680503685
Si 2.247683201 8.667456717 9.350308385
Si 13.276007486 3.125461199 5.643446303
Si 13.286094232 2.794440812 13.163483339
Si 10.890030583 5.213593674 5.623482951
Si 11.050154794 5.090482348 13.157193398
Si 1.617997309 3.684626785 7.857498384
Si 8.820732614 2.870069917 5.568782662
Al 1.098403415 6.757451466 7.121702717
Al 6.306196432 12.307663667 4.122911737
Al 6.071210706 12.252960519 11.738107819
Al 7.086396057 1.546087578 7.824394166
Cu1 3.352768979 8.227237209 6.338655580
Cr2 4.835556108 10.085800407 5.076848140
H 8.147769836 2.890602243 9.489760638
H 7.397149840 11.151848594 10.068805511
End final coordinates

Cu-O-Fe-H2MOR

Final enthalpy = -6628.9136872837 Ry

CELL_PARAMETERS (angstrom)

13.809355839 0.068618195 -0.002197456

-1.366471370 13.619198393 -0.020685945

0.004967632 0.009466802 15.017639365

ATOMIC_POSITIONS (angstrom)

O 3.132480949 0.506971646 3.289513403
O 2.279716981 13.785510293 10.726418959
O 5.238297857 11.058350957 3.303223114
O 4.954115449 11.305613845 10.780653198
O 7.920576834 11.597099780 7.642260773
O 7.685965934 11.835360805 0.576843896
O 10.823409218 0.083855588 6.956157466
O 9.465963259 13.490069770 14.507592055
O 8.188940577 2.583645795 6.998436258
O 8.131748397 2.654811872 14.622672829
O 5.195803352 2.177322966 3.605301353
O 5.374069109 2.141537272 11.158097973
O 12.598234286 11.003895151 0.470486474
O 12.958886329 10.694336651 7.947194172
O 2.222720853 7.684954692 0.435497824
O 2.111893223 7.989241579 7.855362748
O 1.761546380 5.339603228 3.403455820
O 1.704526910 5.010724251 11.198662955
O 0.104753798 3.363548251 4.175207143
O 0.203446602 2.889538558 11.745113348
O 11.047738163 5.950443414 4.173936996
O 11.230899026 5.764755674 11.689390338
O 11.391548075 8.654070074 0.156112379
O 11.096554886 8.786440697 7.711615965
O 10.161477994 13.353983440 4.371034030
O 9.603537599 13.189042129 11.881739680
O 7.617136731 2.882845889 4.411175118
O 7.759494416 2.937829058 11.990978362
O 5.562052127 2.141329351 14.958566791
O 5.398499022 1.872938874 7.729596006
O 3.566089171 0.471888378 0.651424819
O 3.121518439 0.523909496 8.136131512
O 5.132952178 11.319355324 0.623002243
O 5.457771067 10.922286968 8.198496440
O 7.943370120 12.053229170 3.690950529
O 7.674722512 11.729685816 10.750632111
O 0.580133316 2.961848390 6.768502576
O 0.533486416 2.740282000 14.393019507
O 10.682461850 6.328975222 6.806609582
O 11.091299517 6.204026219 14.305841652
O 11.380530236 8.499405838 3.495705393
O 11.397924736 8.390334790 11.288724108
O 12.865457450 10.695484305 3.117979543
O 12.589673241 10.719602332 10.588644164
O 2.004924063 7.947998539 3.090689283
O 2.253818469 7.494082247 10.484246141
O 1.511125763 5.240050831 7.784112305
O 1.575620910 5.159499467 14.927649316
O 3.143516813 12.163417991 2.177437014
O 3.152777275 12.036442951 8.915999906
O 9.860370370 1.693301047 5.095618969
O 9.930277345 1.748682931 12.874003847
O 0.938702648 9.757720870 1.458792844
O 0.976503634 9.620661988 9.617445872
O 12.216535513 4.364110785 5.972489951
O 12.211981910 3.981516039 13.406854930
O 3.782989923 1.258296748 5.709866805
O 3.903529968 1.130387159 13.165311541
O 6.021736162 11.590017172 5.716837960
O 6.339780872 11.806926547 13.312985737
O 9.874465573 12.540355368 1.897262643
O 9.732341938 12.559551969 9.306998203
O 7.271528303 2.007452282 1.973937214
O 7.511935798 2.145848812 9.538770095
O 12.176465118 10.001081773 5.545076395
O 11.902069826 10.263796874 13.077589188
O 1.718433984 7.001957613 5.512136852
O 1.613321963 6.967228322 12.975020217
O 1.262730756 3.297218623 1.813922521
O 1.116683950 3.143567225 9.333714581
O 11.870942121 6.573011191 1.760491502
O 11.543567511 6.676040543 9.276398583
O 2.749483833 3.017352904 4.025376159
O 2.824525675 2.667872801 11.307430547
O 10.027454717 10.894521126 14.822822774
O 10.488179520 11.267525310 7.116713183
O 10.265892746 10.788359056 3.833896172
O 10.040616850 10.643609864 11.186037875
O 3.104894641 3.009116484 14.918552806
O 3.089389576 3.107268000 7.534155637
O 7.304102027 0.151453245 0.058078888
O 7.427034512 -0.134557665 7.668939554
O 13.536839691 7.145756339 14.792493837
O 13.176501475 7.229970680 7.238389728
O 5.653463110 13.909720961 3.972508717
O 7.325320332 0.319919383 11.452295285
O -0.327714991 6.886316813 3.851487643
O -0.248574402 6.814427955 11.045035998
O 0.532469174 12.372806726 1.767006941
O 0.553673813 12.246693456 9.485899307
O 3.584792730 9.554460736 1.805296663
O 3.646481182 9.465199953 9.398986820
O 12.466908155 1.742144788 5.674225013
O 12.534248848 1.332502227 13.146916136
O 9.554729371 4.302588675 5.537040076
O 9.586284182 4.363718111 13.209127933
O 4.860093397 8.431308506 5.582230602
Si 7.057560417 1.714174418 0.406413872
Si 9.264488139 12.177695855 0.443796918
Si 9.404562393 12.290679922 7.719678012
Si 3.736543426 1.738440787 4.168018718
Si 3.920454515 1.522656012 11.589580794
Si 11.946448460 6.992693460 3.328526107
Si 11.951321842 6.931607966 10.819340218
Si 1.465111671 3.739428349 3.364281590
Si 1.464599073 3.436402967 10.881606035
Si 1.290125084 6.711001384 14.545190176
Si 11.684154576 10.171327257 7.082785541
Si 11.483338135 10.196795875 14.646950498
Si 6.348357030 11.959485780 7.308291089
Si 6.278736661 12.198075865 14.861306074
Si 3.876421458 1.702672723 7.279289928
Si 4.028000640 1.689925635 14.688789773
Si 6.784216957 1.810061977 3.514936273
Si 6.954476057 1.824564005 11.128859367
Si 9.516798466 12.181796953 3.451018110
Si 9.358468409 12.050589569 10.791485086
Si 1.280991873 6.783028798 3.956433890
Si 1.314587661 6.563044176 11.426115894
Si 11.673977029 10.013517665 3.996866655
Si 11.505444925 9.983560630 11.533566505
Si 11.979313412 7.143342842 0.247086315
Si 11.658877606 7.240673539 7.746127522
Si 1.615432052 3.562653163 0.253249473
Si 1.912451701 13.201020447 1.953948060
Si 1.947813852 13.065034992 9.302459418
Si 4.265365961 11.025011758 1.946964967
Si 4.294703060 10.959489008 9.364930512
Si 11.155604503 0.820854318 5.526526785
Si 11.073282676 0.636798702 13.133647256
Si 8.856188292 2.920822147 13.204335653
Si -0.174285866 10.917126443 1.720245883
Si -0.129554686 10.783458923 9.394997881
Si 2.177834623 8.735135793 1.682197558
Si 2.249525263 8.652410134 9.347483510
Si 13.248498326 3.151519277 5.638988046
Si 13.278500811 2.780260304 13.171045351
Si 10.875197850 5.225843156 5.623567375
Si 11.043370282 5.076774080 13.147958536
Si 1.584207732 3.648570930 7.847092020
Si 8.795829278 2.864842424 5.537312588
Al 1.023145649 6.746949036 7.141573875
Al 6.310930021 12.341760128 4.079964692
Al 6.081877557 12.235024141 11.679205839
Al 7.070983396 1.548641906 7.800891512
Cu1 3.297490115 8.029299879 6.279450139
Fe2 5.179482285 9.979489692 4.955379548
H 8.119037959 2.906500049 9.469577783
H 7.423626375 11.238738552 9.937313427

End final coordinates

Cu-O-Mn-H2MOR

Final enthalpy = -6773.7437737768 Ry

CELL_PARAMETERS (angstrom)

13.804781082 0.067474558 -0.003074153

-1.367144984 13.619505030 -0.023709642

0.004035106 0.006052666 15.023428066

ATOMIC_POSITIONS (angstrom)

O 3.135554412 0.510207959 3.289378069
O 2.274132009 13.785321861 10.726120646
O 5.236241655 11.065980054 3.292431060
O 4.959968124 11.304402921 10.770293600
O 7.917720298 11.594640481 7.642138982
O 7.680209395 11.829496596 0.570625614
O 10.820698915 0.078885034 6.957309473
O 9.461546898 13.484781479 14.508950060
O 8.184144964 2.585266923 6.999263413
O 8.126994611 2.652131183 14.628322990
O 5.191507497 2.186015439 3.606461668
O 5.369842075 2.139146389 11.161559947
O 12.596064359 11.002985146 0.465371945
O 12.960150992 10.682738764 7.946044585
O 2.223502794 7.687416755 0.433719969
O 2.100496611 7.992385884 7.860419167
O 1.753852981 5.338630584 3.391328800
O 1.704017319 5.009852742 11.199351104
O 0.100139580 3.359443968 4.173695337
O 0.201791076 2.887694821 11.745149150
O 11.043385695 5.949792008 4.175534677
O 11.222416232 5.762250951 11.687198992
O 11.385874518 8.653715498 0.150184663
O 11.093099137 8.780405771 7.709782725
O 10.146335594 13.353926428 4.367068664
O 9.599415290 13.189565443 11.880607956
O 7.615585588 2.890256803 4.412030959
O 7.755877590 2.934755670 11.996402696
O 5.556697012 2.133665500 14.965827408
O 5.395267933 1.871802349 7.727932859
O 3.554229414 0.474892613 0.648156045
O 3.121798014 0.523523074 8.136103873
O 5.125559064 11.319558092 0.611109311
O 5.444813000 10.923450083 8.184543032
O 7.929583465 12.040404393 3.692017426
O 7.672603418 11.728181055 10.751056224
O 0.579540913 2.964275583 6.770579650
O 0.532631281 2.739733498 14.393699869
O 10.677501058 6.325483506 6.809314670
O 11.085397704 6.203342550 14.302834297
O 11.368769945 8.496821811 3.496036354
O 11.394582734 8.389126392 11.288861550
O 12.857931238 10.689043761 3.115121782
O 12.578017841 10.724871546 10.587689893
O 2.008447614 7.948935682 3.093645744
O 2.252438115 7.494517886 10.490114901
O 1.510102086 5.241869409 7.792441399
O 1.575976120 5.157765908 14.940138978
O 3.140608023 12.169185955 2.168778017
O 3.148042374 12.039237022 8.916818582
O 9.852433782 1.689085736 5.098890144
O 9.924651830 1.743964327 12.881675094
O 0.941601332 9.760851153 1.458342465
O 0.974557792 9.623451531 9.631323738
O 12.212619086 4.363303510 5.970776729
O 12.205719558 3.979212669 13.406315279
O 3.781483936 1.262097166 5.709360587
O 3.901377199 1.126611920 13.168722355
O 6.022109029 11.591644716 5.716549785
O 6.337499169 11.809856373 13.310807417
O 9.858624719 12.538578270 1.895689999
O 9.731269942 12.557234504 9.307959630
O 7.268083240 2.011383350 1.974424882
O 7.508478746 2.150716463 9.543581416
O 12.169417397 10.001054880 5.543921420
O 11.897942691 10.262852025 13.078446753
O 1.708931939 6.987066340 5.510757782
O 1.608914814 6.961681524 12.981220036
O 1.258324593 3.287216112 1.811277804
O 1.119350068 3.137295933 9.335190886
O 11.845988542 6.572843995 1.757652338
O 11.537248334 6.674952747 9.276906322
O 2.743923980 3.020581665 4.021624641

O 2.822873018 2.669074253 11.314245934
O 10.024339182 10.890221296 14.827258577
O 10.487590246 11.262487221 7.120079580
O 10.258856510 10.787047715 3.834512049
O 10.033309440 10.640546166 11.192504025
O 3.102694181 3.009387386 14.921566162
O 3.086634007 3.108906867 7.535592749
O 7.303866928 0.151714407 0.063433986
O 7.431392829 -0.132049270 7.679606119
O 13.531240985 7.139407002 14.808870160
O 13.170384063 7.223450115 7.238157070
O 5.649224551 13.919690770 3.974964914
O 7.322339908 0.319360152 11.452966830
O -0.329885985 6.891792848 3.836497081
O -0.250889458 6.812055340 11.049913901
O 0.527075121 12.374152705 1.770246632
O 0.548898208 12.247573776 9.483559071
O 3.584769990 9.556242679 1.811283851
O 3.643300977 9.465619725 9.397963156
O 12.462113649 1.740750504 5.674707268
O 12.529487751 1.330178436 13.151642674
O 9.554231667 4.301679890 5.537659186
O 9.580766349 4.360667718 13.213108487
O 4.901899912 8.343903087 5.606193638
Si 7.054425020 1.715244437 0.407121174
Si 9.258226058 12.175688792 0.438377096
Si 9.403601011 12.287078790 7.720348242
Si 3.732440267 1.744751624 4.168407453
Si 3.916137362 1.521140258 11.593428173
Si 11.937299377 6.991342299 3.325012991
Si 11.945489521 6.929548208 10.819156723
Si 1.457737345 3.739153712 3.359695598
Si 1.463540330 3.435747585 10.882792066
Si 1.288331050 6.707505870 14.552456031
Si 11.682495562 10.164636702 7.083629388
Si 11.479933064 10.192673144 14.647651922
Si 6.346321276 11.963380457 7.307929764
Si 6.273676248 12.195691176 14.860549904
Si 3.872562494 1.704921109 7.279559376
Si 4.021727792 1.687757059 14.692036795
Si 6.779911616 1.819533728 3.516353479
Si 6.950376603 1.824037542 11.132449169
Si 9.504326823 12.177990596 3.449911281
Si 9.355976975 12.048633213 10.792640274
Si 1.279049477 6.781416742 3.956314445
Si 1.313086187 6.561888697 11.429523121
Si 11.666866596 10.009631222 3.996466935
Si 11.500159787 9.982059946 11.534826221
Si 11.970677050 7.142022896 0.245487981
Si 11.655828127 7.235735685 7.746760655
Si 1.613329193 3.562937464 0.253043406
Si 1.906465771 13.205431118 1.949526955
Si 1.942216315 13.066757975 9.301390280
Si 4.262119336 11.030435221 1.938662022
Si 4.289340848 10.959884784 9.359812773
Si 11.150043216 0.819858921 5.528987557
Si 11.069134836 0.633545112 13.138476858
Si 8.851740435 2.917262782 13.209772368
Si -0.175937285 10.916186370 1.719670019
Si -0.131969667 10.782856653 9.397918400
Si 2.177627582 8.734124681 1.683882040
Si 2.244905460 8.652323967 9.350762134
Si 13.244095078 3.150690430 5.639384340
Si 13.273214980 2.778255542 13.171146536
Si 10.872588416 5.226160859 5.624583366
Si 11.037010915 5.074728220 13.146336960
Si 1.582557472 3.651288247 7.850315693
Si 8.793316230 2.865849049 5.539326578
Al 1.022445396 6.746216088 7.139793731
Al 6.296497924 12.349507394 4.079936500
Al 6.080040037 12.235466001 11.676079748
Al 7.068128949 1.551587090 7.806298686
Cu1 3.332162485 7.979015276 6.318765713
Mn2 5.234322160 9.904742742 4.946517857
H 8.120415050 2.907710755 9.477135053
H 7.420837746 11.226625362 9.944883521
End final coordinates

Cu-O-Ni-H2MOR
Final enthalpy = -6672.7932858394 Ry

CELL_PARAMETERS (angstrom)
13.807017791 0.068543210 -0.004778136
-1.366311563 13.618168454 -0.025209091
0.002208729 0.004222170 15.017127617

ATOMIC_POSITIONS (angstrom)
O 3.132806299 0.510931940 3.286433749
O 2.272209851 13.782778162 10.720657427
O 5.253094442 11.059733566 3.265796873
O 4.926526918 11.307796728 10.797755450
O 7.917618271 11.576709518 7.620916442
O 7.682719969 11.825060619 0.570635448
O 10.816677824 0.075598652 6.954994530
O 9.460854056 13.482599430 14.500341879
O 8.191362490 2.573995299 7.002737168
O 8.123218030 2.653734008 14.623475684
O 5.195008436 2.180111889 3.607257809
O 5.371239565 2.137428193 11.152368356
O 12.599623630 11.005113247 0.458284664
O 12.963309522 10.689844088 7.931184311
O 2.223211745 7.684311288 0.432986727
O 2.118554364 7.978512151 7.855695661
O 1.748657772 5.336359020 3.406716038
O 1.701001061 5.006437028 11.197718928
O 0.101602743 3.349274326 4.170851757
O 0.196698854 2.884645160 11.734367191
O 11.050219860 5.941564351 4.168721572
O 11.218797754 5.763567716 11.681298962
O 11.392183860 8.655273176 0.151772339
O 11.099352040 8.782786775 7.706454342
O 10.156743134 13.350656671 4.364793985
O 9.587654389 13.184593512 11.872448946
O 7.616339113 2.879439746 4.417402765
O 7.753071472 2.934569558 11.988867020
O 5.555906974 2.129622616 14.969950615
O 5.403912906 1.862834374 7.722369415
O 3.548552648 0.473772031 0.647195723
O 3.121792918 0.523415330 8.136198464
O 5.120183885 11.318431975 0.594176674
O 5.475231079 10.918313734 8.230134448
O 7.930135131 12.058581197 3.688486156
O 7.661916377 11.716507339 10.740078322
O 0.591488171 2.965529907 6.760269906
O 0.532041570 2.738356126 14.381494964
O 10.685845605 6.327049753 6.799118597
O 11.089744286 6.200948552 14.299338467
O 11.364112108 8.495303115 3.491983118
O 11.390511429 8.386930142 11.275402128
O 12.849532775 10.691406804 3.106510997
O 12.582791240 10.713677646 10.573046719
O 2.012259976 7.944927573 3.086216931
O 2.249342985 7.485094441 10.480112848
O 1.528438172 5.239996967 7.770775460
O 1.575264943 5.155417939 14.927900230
O 3.140165026 12.163559454 2.163763427
O 3.152423676 12.032946412 8.909273181
O 9.864445311 1.694125538 5.093682022
O 9.922519529 1.745892112 12.878187667
O 0.937131671 9.757194331 1.462267620
O 0.970411921 9.609248230 9.606019132
O 12.216133941 4.357067418 5.967032398
O 12.207417555 3.980085751 13.395859672
O 3.775869691 1.260301783 5.708696974
O 3.905586087 1.128894508 13.163223773
O 6.009803109 11.560560752 5.704424822
O 6.348298881 11.805121950 13.303354297
O 9.863124535 12.535951085 1.892102993
O 9.715688731 12.549548100 9.297991214
O 7.274856183 2.001553485 1.978958494
O 7.512846661 2.126232271 9.533902803
O 12.169851585 9.998610321 5.534903747
O 11.900790621 10.255129849 13.066456982
O 1.730040112 7.005166726 5.507865859
O 1.610699341 6.962097054 12.973564012
O 1.258204075 3.297594335 1.808104337
O 1.120478739 3.148494006 9.326630885
O 11.873680227 6.574378491 1.758422667
O 11.553854604 6.669185210 9.265969687
O 2.751489649 3.022831527 4.017740047
O 2.820450456 2.665866569 11.309694463
O 10.025528455 10.888771855 14.813028425
O 10.489924923 11.264419672 7.111186276
O 10.250805166 10.783805205 3.829727593
O 10.035001235 10.641286866 11.183086978
O 3.103257056 3.007803083 14.916782590
O 3.099775645 3.107943111 7.535488572
O 7.308746899 0.150939712 0.060483311
O 7.427372841 -0.157575111 7.641624101
O 13.534531173 7.141163220 14.793282048
O 13.176616806 7.230228094 7.223707596
O 5.642960274 13.905944960 3.978451670
O 7.323823465 0.317101134 11.455629144
O -0.330255734 6.901564314 3.858932852
O -0.253678570 6.810263064 11.050865361
O 0.526750891 12.371764497 1.771621116
O 0.554831310 12.239813207 9.477760240
O 3.585201376 9.554819556 1.795847162
O 3.644015192 9.463558736 9.408250624
O 12.468680072 1.733625732 5.682125681
O 12.524982006 1.329226028 13.139080152
O 9.552064957 4.301185009 5.540243033
O 9.579327947 4.360786708 13.208818831
O 4.858001149 8.659901260 5.871368683
Si 7.058199163 1.712467800 0.410592980
Si 9.260135663 12.174058539 0.435975113
Si 9.392555265 12.277434326 7.708963490
Si 3.735525586 1.740947184 4.167607041
Si 3.918180672 1.520097082 11.586900523
Si 11.940085810 6.993235957 3.326572269
Si 11.945758838 6.927911567 10.812529343
Si 1.459071302 3.732998289 3.359996776
Si 1.462324940 3.433209676 10.877519571
Si 1.287743081 6.704851737 14.542433720
Si 11.683065636 10.168619675 7.074482508
Si 11.481118481 10.191334425 14.635727251
Si 6.338904802 11.926272303 7.283388980
Si 6.276937537 12.191411476 14.851036664
Si 3.880136995 1.698921406 7.278959716
Si 4.022385662 1.685013701 14.688162239
Si 6.783322012 1.806017432 3.520411429
Si 6.952191542 1.819175043 11.124791018
Si 9.502552897 12.180240840 3.447210225
Si 9.344484660 12.043110067 10.782959623
Si 1.276625649 6.784523605 3.948985111
Si 1.310355822 6.558211046 11.424959273
Si 11.659874764 10.011229327 3.989739324
Si 11.500220787 9.979966101 11.521921359
Si 11.978745840 7.144282951 0.243851018
Si 11.660549689 7.238672757 7.738209263
Si 1.614615120 3.562772356 0.247804035
Si 1.907198098 13.201859465 1.947662422
Si 1.948102852 13.060323263 9.295796285
Si 4.263643361 11.029017392 1.924892523
Si 4.294179751 10.958512212 9.370029111
Si 11.153807813 0.814814389 5.529414505
Si 11.063759545 0.631300264 13.130010442
Si 8.847684684 2.917763265 13.203931353
Si -0.179346241 10.916289457 1.717407334
Si -0.130049902 10.778011089 9.385076469
Si 2.178063272 8.736635305 1.675641620
Si 2.251842314 8.648265481 9.347576490
Si 13.248044736 3.143371550 5.636369932
Si 13.271087927 2.776148159 13.159237617
Si 10.875239830 5.220009959 5.620003932
Si 11.035931535 5.074041014 13.140424446
Si 1.594195159 3.648311745 7.841419359
Si 8.797114400 2.859630569 5.541846780
Al 1.022267910 6.745320262 7.145671957
Al 6.296565516 12.335358340 4.101451292
Al 6.075613413 12.230532766 11.672451239
Al 7.075209499 1.522156405 7.792516641
Cu1 3.293641384 7.983512904 6.243935792
Ni2 5.238761840 9.917664118 4.800413208
H 8.113551800 2.890857991 9.452581515
H 7.408778739 11.231591698 9.922963320
End final coordinates

Cu-O-Ti-H2MOR
Final enthalpy = -6671.0898937298 Ry
CELL_PARAMETERS (angstrom)

13.807592224 0.040524208 -0.005946906
-1.394001408 13.611527962 -0.015366810
0.000834208 0.014928479 15.006765785

ATOMIC_POSITIONS (angstrom)
O 3.143533501 0.564079513 3.283392229
O 2.177079737 13.838584138 10.694693919
O 4.940012429 11.106925860 3.591028289
O 5.207388157 11.332584971 10.464328614
O 7.811421484 11.515937896 7.881925178
O 7.766522162 11.638692265 0.218319071
O 10.699849297 -0.082248549 6.923011061
O 9.493234449 13.527811405 14.505820136
O 8.215467884 2.566128698 7.042207177
O 8.110188303 2.641141924 14.630664439
O 5.188168496 2.264240002 3.568876556
O 5.323670884 2.168917452 11.197063764
O 12.744962533 11.017389055 0.350201024
O 12.904284876 10.698088625 7.829408099
O 2.199806453 7.790058119 0.369766948
O 2.209198157 7.882917634 7.869105233
O 1.458277556 5.256742812 3.328427154
O 1.712504583 5.053006555 11.009884561
O 0.067895550 3.096253929 4.127074842
O 0.114109110 3.043222188 11.672454540
O 11.180735540 5.782416180 4.135083029
O 11.182942251 5.746302057 11.663180054
O 11.501559562 8.688200929 0.188494148
O 11.130714023 8.683080255 7.698708938
O 9.928278222 13.228100993 4.307719821
O 9.710402286 13.259576267 11.887785355
O 7.598147352 2.878482316 4.467164502
O 7.731469670 2.965909326 12.034869991
O 5.570941067 1.915254338 14.980429684
O 5.408040972 1.881785300 7.738581365
O 3.380416336 0.453866533 0.630110489
O 3.126089401 0.537037613 8.073415973
O 5.287336782 11.317887021 0.925818946
O 5.168375899 10.933604529 7.800677409
O 7.742617147 11.990337423 3.363833722
O 7.726903573 11.739429874 10.978925090
O 0.606469784 2.801676865 6.726611948
O 0.649607351 2.861740176 14.272425751
O 10.823895530 6.230209192 6.757676236
O 11.050403907 6.296715504 14.264895014
O 11.167879922 8.375408346 3.537587882
O 11.338937624 8.352829201 11.155090030
O 12.577990442 10.602270896 2.994345878
O 12.585899177 10.648550532 10.472178307
O 2.084580245 7.798805634 3.036495044
O 2.204691770 7.589157409 10.530305759
O 1.412861323 5.152529073 7.744424872
O 1.683181382 5.203943313 15.071799802
O 3.092426112 12.209828388 2.107464958
O 3.099668838 12.070273606 8.953266961
O 9.827796933 1.637447272 5.124905958
O 9.928640566 1.768690400 12.870156854
O 0.879471967 9.714808636 1.633897827
O 0.976034206 9.647721487 9.432576002
O 12.232316626 4.150245465 5.949996553
O 12.232431209 4.075811744 13.463134689
O 3.843768450 1.296029690 5.676154758
O 3.853208432 1.103052113 13.160405888
O 6.220831732 11.793865294 5.743846377
O 5.902718406 11.800083714 13.344693926
O 9.835899113 12.376179315 1.805603147
O 9.712305654 12.541121338 9.358461060
O 7.296281577 2.057003302 1.997196632
O 7.467665301 2.225536889 9.600129484
O 12.000293190 9.991537123 5.480425421
O 12.078397829 10.114144010 12.985539008
O 1.753778254 6.860390064 5.455245454
O 1.661348540 6.834871234 12.974397493
O 1.283079290 3.163724372 1.778166134
O 1.142767327 3.042456768 9.292066683
O 11.883025042 6.560852524 1.745928246
O 11.647161438 6.565157951 9.230962861
O 2.734466889 3.074592056 4.028191822
O 2.754973647 2.701505313 11.374466609
O 10.187630708 10.938742239 14.608645868
O 10.347281886 11.113972163 7.201437049
O 10.015785290 10.664379092 3.813358967
O 10.096037153 10.668190808 11.260311503
O 3.197439412 3.034689980 14.926373139
O 3.102742451 3.123832039 7.493500147
O 7.508837932 0.104152760 0.189830501
O 7.434683044 -0.111167529 7.903532243
O 13.549620480 7.054825781 14.750984043
O 13.277071086 7.246834630 7.217893896
O 5.559156934 13.927666893 3.960898097
O 7.284050906 0.351715603 11.484868763
O -0.345686851 7.111193223 3.832381649
O -0.271820003 6.835863642 11.129461678
O 0.455343357 12.334817884 1.966267020
O 0.493609027 12.264958471 9.405883918
O 3.533291778 9.586597403 1.845725424
O 3.636818963 9.488107954 9.407373991
O 12.445553013 1.513610495 5.694869426
O 12.558030963 1.442187028 13.180210770
O 9.580158399 4.259489381 5.535630125
O 9.584637284 4.373422113 13.252427485
O 4.963484162 8.614229003 5.498834127
Si 7.102962081 1.650542144 0.452387387
Si 9.312567588 12.106175781 0.298489635
Si 9.321095657 12.185124091 7.806526719
Si 3.741159838 1.806917910 4.145644530
Si 3.858317911 1.550940460 11.602079817
Si 11.933315139 6.960662256 3.322735400
Si 11.945566190 6.884123586 10.785606622
Si 1.382536610 3.642606383 3.332042924
Si 1.433527800 3.465140989 10.821089917
Si 1.322832709 6.701967765 14.554853458
Si 11.606799867 10.096639013 7.048435691
Si 11.623771320 10.188112192 14.545445197
Si 6.351898927 12.041637827 7.362021634
Si 6.249125947 12.133572008 14.882783260
Si 3.897603042 1.727421426 7.247337800
Si 4.000528068 1.635179967 14.692761954
Si 6.766695720 1.849954264 3.521913441
Si 6.907650460 1.862016613 11.180030198
Si 9.340449033 12.066642601 3.330101698
Si 9.404721640 12.071160798 10.874076379
Si 1.238288172 6.743603506 3.939465243
Si 1.307239822 6.565496363 11.412845607
Si 11.448836145 9.919242143 3.949437183
Si 11.545882535 9.924179920 11.467718673
Si 12.008358581 7.144198077 0.241640502
Si 11.762373558 7.163756218 7.710532712
Si 1.701843362 3.576753596 0.263957424
Si 1.819391940 13.206738379 1.981379277
Si 1.878122387 13.101967279 9.274376655
Si 4.202634478 11.040160221 2.085680578
Si 4.257567382 10.973844492 9.227908263
Si 11.074737854 0.680480372 5.511764309
Si 11.121387810 0.708388758 13.141880150
Si 8.850336113 2.933167629 13.229305809
Si -0.240128310 10.886641462 1.757706478
Si -0.158195076 10.788841304 9.270273089
Si 2.159121288 8.717942212 1.711837648
Si 2.244226695 8.651200030 9.311042456
Si 13.244744732 2.922230496 5.613821098
Si 13.295951068 2.888844472 13.145676502
Si 10.956562249 5.102046031 5.596141196
Si 11.024908661 5.120318781 13.155185667
Si 1.563355917 3.573637805 7.797611841
Si 8.797669877 2.838055139 5.567801084
Al 1.104034662 6.694942995 7.072838818
Al 6.225871975 12.359707408 4.039436873
Al 6.017071331 12.256798604 11.691392438
Al 7.078883892 1.587636657 7.880148340
Cu1 3.486666541 8.181518446 6.471735446
Ti2 4.786463390 10.309739702 5.516528346
H 8.079861477 2.983440585 9.563548966
H 7.450018984 11.127922935 10.260515184
End final coordinates

Cu-O-V-H2MOR
Final enthalpy = -6701.3559681551 Ry
CELL_PARAMETERS (angstrom)
13.895129053 0.014614428 -0.005543745
-1.428266693 13.623374857 -0.016315789
0.001327915 0.014016940 15.091372443

ATOMIC_POSITIONS (angstrom)
O 3.212918558 0.581930626 3.221041645
O 2.191680240 13.870565765 10.731177131
O 5.197449445 11.040694630 3.356687597
O 4.990138419 11.309915566 10.798108306
O 7.847815631 11.524588328 7.656195193
O 7.719597619 11.716820616 0.461813813
O 10.853106167 -0.032997612 6.958155746
O 9.546026625 13.382302218 14.542233003
O 8.286318109 2.509131454 7.034208114
O 8.054998110 2.663855742 14.670350726
O 5.259789839 2.249257208 3.687452607
O 5.413965083 2.148515450 11.229833899
O 12.721607588 10.954255436 0.432188659
O 12.927787040 10.739899712 7.954448222
O 2.218215440 7.697245219 0.434343901
O 2.171092635 7.995013057 7.900703296
O 1.541744088 5.307609095 3.349601357
O 1.628540265 5.028715711 11.221925962
O 0.125481105 3.177386787 4.186426899
O 0.227872638 2.834482169 11.753279697
O 11.189088174 5.840577263 4.194632888
O 11.144149153 5.810455306 11.752833961
O 11.540499025 8.594624460 0.094523156
O 11.207643017 8.703748240 7.731045110
O 10.155238450 13.302326876 4.375166482
O 9.578431276 13.228521724 11.894311943
O 7.728836489 2.860778806 4.454457469
O 7.837052710 2.927419451 12.027194729
O 5.536663366 1.982841452 15.094507405
O 5.452092498 1.859718252 7.643194819
O 3.486694806 0.337890390 0.569810602
O 3.176233586 0.526069042 8.114337115
O 5.151605139 11.309289077 0.688681798
O 5.346935203 10.876281425 8.193343142
O 7.893533282 12.041052659 3.732697792
O 7.671464259 11.658744559 10.932375628
O 0.643080393 2.956711833 6.794319471
O 0.502171248 2.804854431 14.404617652
O 10.881660667 6.241820761 6.839789589
O 11.178062191 6.130787110 14.398786050
O 11.290951622 8.417512484 3.587301721
O 11.426208237 8.409079323 11.291457834
O 12.787530813 10.580101656 3.080567899
O 12.629868676 10.730219311 10.614529093
O 2.043541641 7.879421841 3.102575666
O 2.112724299 7.531740973 10.543915874
O 1.556707465 5.240004163 7.857554845
O 1.670814456 5.141762503 15.027441555
O 3.133790516 12.182228351 2.198300567
O 3.131743861 12.083438155 9.001567142
O 9.974755048 1.654506858 5.130476043
O 9.922538285 1.673859619 13.051051634
O 0.890744757 9.709325553 1.541425523
O 0.867311411 9.627111666 9.552521531
O 12.356175947 4.246713599 5.966151099
O 12.301921119 3.993048557 13.313666074
O 3.735900739 1.299746577 5.681598889
O 3.920952913 1.111143836 13.197127394
O 5.940348231 11.617359406 5.772227572
O 6.180398869 11.881885081 13.402221427
O 9.803242146 12.501655006 1.902998453
O 9.631323136 12.518842298 9.343211400
O 7.286447054 2.076661481 2.002701249
O 7.502791392 2.189328663 9.561892988
O 12.128799570 10.024575545 5.552742819
O 11.945969813 10.265959246 13.115194844
O 1.705228079 6.891026759 5.511098533
O 1.608206762 6.934400388 13.060516887
O 1.214451496 3.230217840 1.783943661
O 1.195636771 3.108947262 9.364382306
O 11.909568790 6.570564896 1.787306654
O 11.658278430 6.633515570 9.331673303
O 2.788933558 3.086007738 3.946381268
O 2.873873292 2.752021582 11.397560720
O 10.117428754 10.811292636 14.952884010
O 10.402684699 11.133078274 7.205163131

O 10.199229050 10.732495577 3.828469821
O 10.081043765 10.663967364 11.244676935
O 3.082972557 2.916564103 14.999185913
O 3.152622552 3.125979540 7.559396894
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O 7.453749621 -0.166421389 7.792970727
O 13.637973160 6.996578301 14.915458479
O 13.347806631 7.197162229 7.340662375
O 5.611525446 13.925345457 3.969920502
O 7.387350782 0.335134714 11.450929618
O -0.363683065 7.066366415 3.854015860
O -0.347716880 6.814956062 11.248423287
O 0.495685143 12.315730444 1.918760755
O 0.520290230 12.273095967 9.487557982
O 3.546523176 9.564614665 1.830733040
O 3.549206142 9.508184014 9.546503232
O 12.576849486 1.613988931 5.790676907
O 12.561278861 1.341240947 13.188913839
O 9.677294493 4.248559819 5.612304464
O 9.651293976 4.303363542 13.323465239
O 4.804334764 8.323243327 5.326587123
Si 7.071566170 1.688764574 0.453796200
Si 9.297304636 12.088805174 0.422252744
Si 9.337068077 12.199955055 7.758820001
Si 3.765883470 1.804576240 4.145178259
Si 3.937210097 1.562878785 11.636696913
Si 11.991614141 6.970825918 3.361100807
Si 11.963986607 6.922281508 10.891714848
Si 1.415541644 3.692703722 3.333275784
Si 1.482890546 3.441718036 10.916622942
Si 1.312895055 6.679361842 14.639570554
Si 11.676685502 10.131418532 7.108428162
Si 11.583009477 10.154821184 14.698799482
Si 6.286270402 11.941914307 7.378693767
Si 6.270728775 12.190322807 14.965639750
Si 3.909568310 1.715590945 7.252333767
Si 3.999730643 1.596721227 14.749302184
Si 6.834677705 1.844894663 3.551489624
Si 6.995955523 1.842702010 11.163638768
Si 9.471219791 12.143172040 3.462009785
Si 9.341996054 12.041864993 10.854213514
Si 1.231176296 6.771690920 3.979701407
Si 1.237897373 6.569664376 11.515638845
Si 11.606879832 9.952162580 4.010950571
Si 11.549254178 9.995478624 11.567459614
Si 12.076985467 7.070626328 0.256594930
Si 11.818454193 7.178498247 7.794968111
Si 1.615109742 3.530440064 0.239411621
Si 1.865928657 13.178971117 1.964193672
Si 1.905142895 13.107837597 9.320571758
Si 4.236937403 11.024770129 1.978940025
Si 4.245022678 10.972653938 9.424472821
Si 11.240589131 0.739074378 5.563879968
Si 11.123315179 0.605057766 13.199047416
Si 8.873502091 2.887415300 13.296229339
Si -0.226325002 10.873502159 1.760229449
Si -0.206081118 10.830714900 9.390234982
Si 2.157023582 8.705222611 1.717473944
Si 2.170285379 8.674365149 9.395059168
Si 13.378172826 3.015336470 5.673399001
Si 13.350330595 2.763751949 13.165644326
Si 11.026667750 5.136998636 5.654510262
Si 11.083451480 5.057400671 13.192836226
Si 1.640306300 3.650544515 7.880489701
Si 8.906238820 2.817772661 5.582922459
Al 1.099723660 6.735644259 7.150701195
Al 6.263954585 12.362355989 4.121718273
Al 6.048409778 12.268535566 11.747285678
Al 7.114107759 1.530059020 7.830527303
Cu1 3.469650242 8.134103540 6.513236372
V2 5.167516053 9.914296396 5.016637575
H 8.145141650 2.920156438 9.487856934
H 7.417000050 10.949255164 10.307077707
End final coordinates

Ag-O-Ag-H2MOR
Final enthalpy = -6984.4452435312 Ry
CELL_PARAMETERS (angstrom)
13.788797443 0.050591420 -0.009859513
-1.382283625 13.617092906 -0.023863664
-0.003364414 0.005144878 15.044347690

ATOMIC_POSITIONS (angstrom)
O 3.130271612 0.516953541 3.283332191
O 2.235361564 13.788650537 10.732284610
O 5.262402735 11.088047734 3.184322307
O 4.890281099 11.308910609 10.800368852
O 7.878165389 11.563981886 7.701122364
O 7.646892115 11.802513271 0.555240516
O 10.789968315 0.046885557 6.961841919
O 9.423290121 13.473868985 14.535557793
O 8.184183557 2.552682234 7.004483436
O 8.079927566 2.664794302 14.649934592
O 5.179962470 2.197094537 3.616641418
O 5.344496963 2.148758604 11.161238070
O 12.578847242 10.976588600 0.453832477
O 12.920620273 10.650386713 7.955629281
O 2.203544759 7.693817630 0.447506116
O 2.042760636 7.997018456 7.928162593
O 1.702989191 5.333373080 3.373813821
O 1.684342020 5.019131306 11.235798701
O 0.077486197 3.332801711 4.167615110
O 0.176588756 2.886763804 11.735424890
O 11.049192561 5.937242614 4.194549778
O 11.166990705 5.774961730 11.702598398
O 11.342116282 8.640510496 0.147327328
O 11.056823647 8.754675154 7.705835365
O 10.135858557 13.340877689 4.369807042
O 9.534696352 13.177754600 11.904114972
O 7.610463747 2.857774988 4.416796549
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O 5.526897898 2.109786203 14.996911097
O 5.396553588 1.862576073 7.713502449
O 3.493485022 0.488465269 0.633716596
O 3.111161274 0.537754856 8.145221807
O 5.064807310 11.320191002 0.517003897
O 5.416598170 10.898756954 8.220985064
O 7.886400111 12.077071619 3.702897970
O 7.624921871 11.725301864 10.727814760
O 0.606635580 2.992089054 6.756135089
O 0.520866611 2.755704945 14.383381403
O 10.650296547 6.290262471 6.824743886
O 11.054193753 6.185653941 14.327439392
O 11.310777243 8.487167337 3.511554614
O 11.356507387 8.393161625 11.273324610
O 12.780832604 10.690263204 3.109481044
O 12.513742528 10.744055084 10.595492458
O 2.052164455 7.936963441 3.105446039
O 2.226024622 7.513670672 10.557342532
O 1.545670510 5.270523646 7.778227324
O 1.546951703 5.163068035 14.989747217
O 3.127986992 12.191893820 2.126510724
O 3.106940758 12.032608873 8.922225498
O 9.856022474 1.673899936 5.103782256
O 9.879841085 1.731793958 12.917430005
O 0.909543954 9.744398971 1.510531416
O 0.926611193 9.637598983 9.687199338
O 12.198973837 4.337428345 5.980375028
O 12.178994785 3.981691068 13.388472029
O 3.747701842 1.281005261 5.711502374
O 3.877027976 1.141839442 13.175114897
O 6.006107740 11.587059995 5.735021448
O 6.345113431 11.832388542 13.294404420
O 9.821407249 12.518869790 1.898876095
O 9.706774177 12.550901555 9.328004208
O 7.250295009 1.988140058 1.981187607
O 7.485283134 2.156880454 9.543222000
O 12.121772899 9.999737839 5.546377566
O 11.862821825 10.236615803 13.090971523
O 1.711269144 6.960692634 5.509597677
O 1.560863639 6.960466882 13.028952764
O 1.235718066 3.266327511 1.801936618
O 1.103475461 3.188238802 9.332271175
O 11.797235203 6.567139028 1.770509654
O 11.526618052 6.657104298 9.281756511
O 2.727154044 3.029491495 4.011194483
O 2.799320815 2.675271855 11.310748211
O 9.994004706 10.884481883 14.837130461
O 10.446527998 11.241443739 7.147640455
O 10.189756927 10.772677456 3.849126557
O 9.977199610 10.634309268 11.223886022
O 3.085569839 3.025345523 14.928267168
O 3.101448929 3.124088324 7.560500721
O 7.314344615 0.150845884 0.051594092
O 7.413367888 -0.168556533 7.723120803
O 13.487913887 7.129747573 14.862911767
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O 7.294226743 0.320415896 11.433548243
O -0.326804210 6.955874900 3.824083461
O -0.277068418 6.819046388 11.082736668
O 0.503626794 12.365255951 1.790318435
O 0.511003081 12.261054994 9.479569330
O 3.566608821 9.575020475 1.782995645
O 3.600424814 9.462053713 9.415412733
O 12.455892204 1.711642041 5.721234295
O 12.485664323 1.329157527 13.155641988
O 9.539259410 4.280622736 5.535339294
O 9.548738956 4.351401004 13.228727361
O 5.448242871 7.834748871 5.663546771
Si 7.037476381 1.704204289 0.410858691
Si 9.224572611 12.159936746 0.438355292
Si 9.358163184 12.263348418 7.745552794
Si 3.716830675 1.753123239 4.164732443
Si 3.893434463 1.528659080 11.598093051
Si 11.912741667 6.995658189 3.333897667
Si 11.905895172 6.927197507 10.829139198
Si 1.429701345 3.730013843 3.348974323
Si 1.442656224 3.450242281 10.889110728
Si 1.255597742 6.710149614 14.602509256
Si 11.638942689 10.146915692 7.088745397
Si 11.444221450 10.176971650 14.661579055
Si 6.307448320 11.922360652 7.304001147
Si 6.246473165 12.190207343 14.848284990
Si 3.866902364 1.710035807 7.281918366
Si 3.989500302 1.690290402 14.704704115
Si 6.761591986 1.791481854 3.524131711
Si 6.925596638 1.827828597 11.131216225
Si 9.457381329 12.176522844 3.457261290
Si 9.305968518 12.041796220 10.806939819
Si 1.279563194 6.787115416 3.955777680
Si 1.280492147 6.565985732 11.478068070
Si 11.603473098 10.004965021 4.002515352
Si 11.450057394 9.982345284 11.546562055
Si 11.930806272 7.131551755 0.257207869
Si 11.625981889 7.214580197 7.749284515
Si 1.599221851 3.564116066 0.247869176
Si 1.877243884 13.209738824 1.941003983
Si 1.911170262 13.070507468 9.305612977
Si 4.248819354 11.052268408 1.884151622
Si 4.253492263 10.961217392 9.375994137
Si 11.142378492 0.792779818 5.543467660
Si 11.028466364 0.623207706 13.161607377
Si 8.811975500 2.912038235 13.231803784
Si -0.203133923 10.911171735 1.736685884
Si -0.174585569 10.798772223 9.417509413
Si 2.169153754 8.739211338 1.697848779
Si 2.191447486 8.665175946 9.417199463
Si 13.228602921 3.125209529 5.640598072
Si 13.237591831 2.772225659 13.160865174
Si 10.859459332 5.201728556 5.632867119
Si 11.000109202 5.071909189 13.157325933
Si 1.595087592 3.677179447 7.848531920
Si 8.787807148 2.839647236 5.541674285
Al 1.010709478 6.765825195 7.124483763
Al 6.235338148 12.306362350 4.118928552
Al 6.046811489 12.235548899 11.663441876
Al 7.067223097 1.516091837 7.812831028
Ag1 3.717313879 7.810997042 6.603403648
Ag2 5.425570761 9.503146984 4.618209884
H 8.064593084 2.937666778 9.461518559
H 7.389794715 11.288273017 9.877129228
End final coordinates

Cu-O-Ag-H2MOR
Final enthalpy = -6842.3158805069 Ry
CELL_PARAMETERS (angstrom)
13.801883896 0.061622025 -0.006325403
-1.372580992 13.615781256 -0.026099472
0.000486068 0.003050989 15.021863780

ATOMIC_POSITIONS (angstrom)
O 3.135859692 0.509679617 3.286283211
O 2.259994073 13.781722996 10.720424694
O 5.278743302 11.091774025 3.190030042
O 4.917420619 11.308069449 10.792966013
O 7.904524317 11.582492838 7.685389293
O 7.665915328 11.805558564 0.563131695
O 10.802289539 0.068308831 6.950148724
O 9.443115406 13.470288624 14.508998529
O 8.203013413 2.566256681 6.995929005
O 8.099968405 2.665606456 14.632956718
O 5.188409069 2.194085099 3.612998064
O 5.360802658 2.143920941 11.154865651
O 12.595990468 10.988467167 0.463034326
O 12.930697901 10.678435417 7.939665728
O 2.214435313 7.690812025 0.440251562
O 2.112952625 7.969337969 7.850051867
O 1.731083390 5.339961098 3.417055636
O 1.678531828 5.007680269 11.210388676
O 0.085951215 3.347271789 4.163616532
O 0.186656969 2.873251376 11.731762711
O 11.080681665 5.933765606 4.177352642
O 11.202087177 5.777213522 11.701353926
O 11.372865439 8.646948435 0.163222562
O 11.066052881 8.775116369 7.710186411
O 10.163559438 13.341528605 4.361503134
O 9.568750067 13.195110846 11.877011878
O 7.614511941 2.875787587 4.414171801
O 7.743109688 2.937868624 11.998948441
O 5.541322942 2.110671042 14.977189529
O 5.407983760 1.870865471 7.702375805
O 3.498692366 0.493589418 0.639619992
O 3.126423449 0.528890032 8.137502969
O 5.085245382 11.321120691 0.521566624
O 5.453678004 10.909551628 8.216054828
O 7.914073002 12.077643378 3.703158209
O 7.663026268 11.730866298 10.708432779
O 0.606274356 2.960593172 6.748112470
O 0.533540209 2.747240543 14.375885153
O 10.674510165 6.312678302 6.803123003
O 11.078240250 6.186097087 14.329702963
O 11.346591657 8.488885338 3.492467992
O 11.369376239 8.392408419 11.271566724
O 12.819061851 10.693337343 3.114668531
O 12.586251081 10.706843093 10.589736909
O 2.057193526 7.944083502 3.100458802
O 2.238188731 7.477561140 10.469785280
O 1.514111871 5.242537028 7.766719307
O 1.560844512 5.168641033 14.925637092
O 3.138400877 12.181873275 2.120362196
O 3.137726288 12.028267507 8.909118214
O 9.862674667 1.680633767 5.083182211
O 9.907256739 1.746375339 12.900506722
O 0.920595915 9.741413191 1.498874511
O 0.958961808 9.602856599 9.585421175
O 12.225843614 4.353171540 5.986312543
O 12.202069523 3.983426257 13.390400537
O 3.754404721 1.276888644 5.708762999
O 3.885563361 1.140886668 13.161793086
O 6.017251121 11.623799345 5.736956502
O 6.376347488 11.830574264 13.276513931
O 9.847279029 12.520750441 1.894616984
O 9.744682882 12.560035769 9.303555030
O 7.261924445 1.998730310 1.980684131
O 7.494584606 2.179444480 9.534284227
O 12.145037053 9.984227986 5.540144109
O 11.896475433 10.239231342 13.078663579
O 1.735324185 6.997557584 5.527678540
O 1.607897464 6.979143048 12.972511066
O 1.246090111 3.312941873 1.799623180
O 1.098872584 3.160516436 9.325263443
O 11.906679318 6.573080258 1.770115386
O 11.531635562 6.662245381 9.275221548
O 2.736392853 3.022773790 4.006242029
O 2.810977657 2.669722958 11.293684699
O 10.016668621 10.882010801 14.816194549
O 10.464090181 11.258033983 7.108200743
O 10.220254173 10.772695693 3.838209719
O 10.032325348 10.655978424 11.195597176
O 3.101620027 3.029753394 14.913703022
O 3.100701674 3.115901478 7.557550224
O 7.324084538 0.154027908 0.054931646
O 7.435511675 -0.146494250 7.745310949
O 13.520465591 7.151072844 14.777822562
O 13.151520782 7.241155067 7.237991527
O 5.621575215 13.899760437 3.979818198
O 7.320159713 0.326098663 11.416947762
O -0.311222006 6.953840576 3.882174726
O -0.264738167 6.824884917 11.052294630
O 0.516525438 12.365068949 1.785270371
O 0.545739096 12.237203209 9.471211923
O 3.581497220 9.573298999 1.777379223
O 3.636409724 9.459815389 9.395148338
O 12.461241918 1.727172581 5.690199022
O 12.509802787 1.330176259 13.155803601
O 9.565885018 4.285968504 5.523179771
O 9.569768121 4.361179167 13.219895659
O 4.976424963 7.920815750 5.769782702
Si 7.049287230 1.708317836 0.412679933
Si 9.242857558 12.161169255 0.438355627
Si 9.383734567 12.279715099 7.723395560
Si 3.727999865 1.746386492 4.162999522
Si 3.907674921 1.525172010 11.584951690
Si 11.954691693 6.999346225 3.336777864
Si 11.926779294 6.932027106 10.820785095
Si 1.444259461 3.735869358 3.354641504
Si 1.447308334 3.434428478 10.877661024
Si 1.280557052 6.719767027 14.542861665
Si 11.653307433 10.160043040 7.076748916
Si 11.470303744 10.180927514 14.647247153
Si 6.331808847 11.948895053 7.306434428
Si 6.270371573 12.189100780 14.830203871
Si 3.878573999 1.707441647 7.278051316
Si 4.003063952 1.691850677 14.689132003
Si 6.774088700 1.799632121 3.523244706
Si 6.943981575 1.833624505 11.120175802
Si 9.482414081 12.176620338 3.452276587
Si 9.343347450 12.055504445 10.783190828
Si 1.294437974 6.798525087 3.955284440
Si 1.296982354 6.562742018 11.429659611
Si 11.632504271 10.006522171 3.994463330
Si 11.490799281 9.982463052 11.532837989
Si 11.975373750 7.142316952 0.251972541
Si 11.631609265 7.234404937 7.748502676
Si 1.611262264 3.577362354 0.240247232
Si 1.893593541 13.205207334 1.938955892
Si 1.938649931 13.060543614 9.294771778
Si 4.271147754 11.049530725 1.889951916
Si 4.286357644 10.960382692 9.365170094
Si 11.150201644 0.803279789 5.525358391
Si 11.049045554 0.631234576 13.145507595
Si 8.833371452 2.920525850 13.217649809
Si -0.189164157 10.911358694 1.733236602
Si -0.143308904 10.777784625 9.385714615
Si 2.184697220 8.743671623 1.684866763
Si 2.244615571 8.649201774 9.349601076
Si 13.244562025 3.132533681 5.635213644
Si 13.259739485 2.773662191 13.159848704
Si 10.883258037 5.208765023 5.623332623
Si 11.024927984 5.075018277 13.155462022
Si 1.588828907 3.648967544 7.842767317
Si 8.800323659 2.849136656 5.530647023
Al 0.988558142 6.741661036 7.146567363
Al 6.262375052 12.312033430 4.106027406
Al 6.079339889 12.238707322 11.645892922
Al 7.080552870 1.536837248 7.805647466
Cu1 3.365833679 7.777662722 6.378941454
Ag2 5.262076900 9.612537405 4.778797615
H 8.079768279 2.955898901 9.457299920
H 7.427196356 11.299794595 9.854412350
End final coordinates

Cu-O-Mo-H2MOR
Final enthalpy = -6851.0428058549 Ry
CELL_PARAMETERS (angstrom)
13.807664574 0.061530958 0.001082696
-1.373275178 13.615449590 -0.020166401
0.008529772 0.010455869 15.024110461

ATOMIC_POSITIONS (angstrom)
O 3.125114865 0.522996584 3.292839306
O 2.269378860 13.788476703 10.732951576
O 5.168300669 11.072440881 3.352650322
O 4.926256574 11.341017886 10.815493454
O 7.914971964 11.573986088 7.565271649
O 7.691046838 11.807527654 0.570014851
O 10.841159992 0.075429222 6.966766871
O 9.459587368 13.484137600 14.513562405
O 8.217947130 2.573068035 7.028019529
O 8.123954623 2.661641215 14.642493189
O 5.210566129 2.165896047 3.628200069
O 5.370989378 2.146503475 11.155216818
O 12.615341264 11.001290169 0.441364976
O 12.971482981 10.716314962 7.919923962
O 2.218498982 7.680790904 0.444792331
O 2.163722212 8.010997903 7.847936130
O 1.701169057 5.331068461 3.296507641
O 1.705242860 5.007492971 11.196952910
O 0.114910514 3.323816806 4.150786090
O 0.179955455 2.892472599 11.709703076
O 11.052062773 5.925341551 4.158930148
O 11.203386424 5.761688583 11.676979038
O 11.398082013 8.655904756 0.144070812
O 11.140246062 8.775038677 7.719647565
O 10.130728223 13.353201942 4.372487295
O 9.574641748 13.189363539 11.879570694
O 7.637425949 2.865641419 4.443274889
O 7.749071040 2.958353075 12.009886542
O 5.564525499 2.122150020 14.999915254
O 5.413159506 1.867270847 7.704109521
O 3.532521238 0.481282620 0.650849981
O 3.126932836 0.547761844 8.143623570
O 5.142255332 11.322321069 0.673418573
O 5.473692930 10.913976252 8.255197100
O 7.921081192 12.010530749 3.726162612
O 7.646426557 11.703171780 10.803883919
O 0.622422838 3.030032035 6.747391119
O 0.549594021 2.744212755 14.348032577
O 10.746888015 6.330988458 6.794249843
O 11.095152829 6.215656349 14.291769856
O 11.339330408 8.482495532 3.503299212
O 11.388426464 8.386594498 11.264118390
O 12.829088280 10.672256624 3.094895924
O 12.568117550 10.718125299 10.559305068
O 2.000779246 7.943256179 3.106154851
O 2.233047865 7.491801113 10.482842763
O 1.557765096 5.272787558 7.863583951
O 1.574314756 5.153308268 14.950274456
O 3.112151773 12.172233013 2.171868501
O 3.161170013 12.056476186 8.909418583
O 9.917378643 1.736836892 5.127117982
O 9.912519425 1.746653737 12.890434126
O 0.937946540 9.761150902 1.465220587
O 0.954284675 9.609772891 9.594440902
O 12.207052404 4.317866815 5.944321734
O 12.214532582 3.990552305 13.393925011
O 3.751817210 1.283704525 5.709079600
O 3.933382679 1.121277328 13.173869068
O 5.929785575 11.577837444 5.749017105
O 6.294849249 11.802625413 13.347212991
O 9.844211770 12.530318960 1.909624306
O 9.674111587 12.530074176 9.307928941
O 7.286709260 2.009892512 2.000008956
O 7.512606474 2.145858030 9.556474115
O 12.170631091 9.997299841 5.533759472
O 11.907362088 10.254239207 13.061497351
O 1.732311851 6.869228881 5.489219186
O 1.629949550 6.952711856 12.989040454
O 1.257460704 3.231701381 1.781530114
O 1.146563452 3.125404174 9.325501258
O 11.845122382 6.573418303 1.751174348
O 11.588165593 6.655978612 9.268314716
O 2.769026218 3.050882138 3.985669933
O 2.816188286 2.667849518 11.342982715
O 10.046146089 10.899117115 14.822987467
O 10.485727282 11.243606651 7.130241088
O 10.246388286 10.779361889 3.848499993
O 10.027049099 10.636750698 11.197681121
O 3.116459537 3.016745138 14.897555184

O 3.122679717 3.136689381 7.543067166
O 7.327670899 0.151865893 0.094320535
O 7.437089141 -0.140568020 7.700025360
O 13.541324575 7.135144190 14.808337830
O 13.238775467 7.240832418 7.255384086
O 5.663087181 13.896814980 3.995297052
O 7.338648941 0.342461086 11.494772236
O -0.338622035 6.917531041 3.832533591
O -0.257220141 6.812476045 11.096154002
O 0.503435061 12.376611175 1.785423161
O 0.563410602 12.244079981 9.483179055
O 3.570894692 9.555000438 1.819774653
O 3.631633217 9.485620792 9.459689692
O 12.532322399 1.698512067 5.707439453
O 12.518480573 1.338141682 13.139160259
O 9.537191510 4.333786758 5.568496171
O 9.584674890 4.364512145 13.228150095
O 4.855232866 8.160495256 5.271985460
Si 7.063341584 1.713735015 0.433881231
Si 9.265353732 12.168265097 0.443206826
Si 9.392990798 12.268050086 7.710380796
Si 3.732671890 1.758898664 4.165071563
Si 3.921224224 1.525689920 11.600918461
Si 11.935465763 6.987272221 3.320612848
Si 11.950729395 6.922433765 10.819160626
Si 1.457076963 3.725967180 3.319458515
Si 1.465166154 3.433823041 10.876535443
Si 1.295242388 6.703390577 14.559619097
Si 11.695892104 10.164024539 7.075726084
Si 11.497467197 10.195036830 14.634038471
Si 6.335659728 11.950357976 7.333419003
Si 6.279214779 12.195018884 14.894382566
Si 3.881947047 1.720871618 7.277013550
Si 4.032118440 1.688956383 14.696875695
Si 6.799376472 1.803820786 3.540926763
Si 6.953493771 1.838933664 11.148335983
Si 9.493270030 12.167786067 3.465221880
Si 9.330045629 12.035948406 10.802896364
Si 1.271394196 6.755017129 3.950316699
Si 1.312165714 6.557027985 11.440173060
Si 11.651211065 9.995325422 3.992457233
Si 11.499253280 9.977163131 11.519219633
Si 11.976443931 7.141799055 0.240762968
Si 11.718273026 7.234522331 7.744040427
Si 1.616045390 3.549197744 0.231514380
Si 1.878903515 13.212308830 1.957901656
Si 1.947564559 13.077217473 9.302254970
Si 4.229092659 11.031243240 1.959533521
Si 4.282446366 10.975972219 9.399341655
Si 11.187446972 0.822725397 5.545988216
Si 11.060374063 0.637069044 13.136312963
Si 8.847260842 2.926595590 13.223296375
Si -0.185194930 10.912330093 1.712252534
Si -0.134510887 10.789224910 9.374510955
Si 2.164981106 8.723588301 1.697639488
Si 2.244368592 8.657708568 9.355684980
Si 13.274771999 3.133300429 5.630355029
Si 13.271630388 2.782404128 13.149261486
Si 10.888173281 5.218250126 5.616055277
Si 11.038510025 5.081168685 13.142519570
Si 1.617571435 3.680933034 7.856839891
Si 8.818468004 2.875555669 5.567678230
Al 1.084345831 6.744890562 7.119877220
Al 6.294764490 12.320629457 4.114906409
Al 6.060777695 12.254405716 11.718840337
Al 7.082511995 1.546965203 7.816857879
Cu1 3.450703356 8.079499693 6.436983534
Mo2 4.805195085 9.914351687 5.071772548
H 8.139727295 2.889857211 9.483733173
H 7.378837265 11.116609270 10.065068473
End final coordinates

Cu-O-Nb-H2MOR
Final enthalpy = -6821.5157982083 Ry
CELL_PARAMETERS (angstrom)
13.798265012 0.065485605 -0.010171691
-1.368116236 13.604924314 -0.010512358
-0.003881003 0.019673686 14.986166847

ATOMIC_POSITIONS (angstrom)
O 3.114346773 0.599075747 3.261035732
O 2.261492981 13.775621755 10.682614521
O 5.056412885 11.076773713 3.582457293
O 5.201688136 11.325671154 10.469877798
O 7.884252641 11.512843258 7.803476713
O 7.741226020 11.655086307 0.283823372
O 10.714608257 -0.042601054 6.880875886
O 9.417246742 13.552522116 14.471795060
O 8.254410504 2.509601761 7.033553809
O 8.152546422 2.641407159 14.611675538
O 5.164838151 2.297985099 3.563690155
O 5.296327652 2.185157500 11.159721023
O 12.701973135 11.047894379 0.377681253
O 12.988800197 10.656829573 7.828738126
O 2.232912055 7.747384181 0.403646646
O 2.150178147 7.947470440 7.828340776
O 1.458136807 5.282206476 3.282435258
O 1.733722282 5.006480150 11.073715898
O 0.046283896 3.146594933 4.111868015
O 0.078823122 3.010373488 11.641406019
O 11.097728967 5.832774916 4.122199530
O 11.190965542 5.778465455 11.650375930
O 11.490131847 8.703926035 0.167004669
O 11.128448352 8.723265408 7.696178688
O 10.051184213 13.305278577 4.280961496
O 9.701527059 13.257591056 11.870657907
O 7.579931934 2.879235961 4.480102906
O 7.686197839 2.997236394 12.031351328
O 5.586595675 1.989334868 14.916547224
O 5.437240568 1.872056533 7.670315374
O 3.508218283 0.397004797 0.636049034
O 3.154768635 0.551606738 8.073672672
O 5.237527183 11.340134672 0.913963470
O 5.252395699 10.903738435 7.812430139
O 7.822886110 12.065494639 3.451966550
O 7.723658421 11.755624963 10.951191835
O 0.633509572 2.908308298 6.701655918
O 0.627192242 2.840198373 14.238208044
O 10.762066032 6.279887786 6.750729957
O 11.052652401 6.304954768 14.252940825
O 11.174234148 8.423631089 3.515589861
O 11.388148753 8.386074467 11.157715519
O 12.671289503 10.605409982 3.017367693
O 12.583678614 10.712113727 10.458414314
O 2.016484745 7.845589007 3.062391134
O 2.247660973 7.520310393 10.473179792
O 1.466900910 5.200040606 7.823361543
O 1.689240470 5.182344401 14.996023067
O 3.083385047 12.151460359 2.245230757
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O 0.932748792 9.751311164 1.551841605
O 1.022060396 9.651857300 9.539169051
O 12.218456763 4.238564029 5.934524088
O 12.196328917 4.068879953 13.436785474
O 3.797008820 1.326368015 5.661671342
O 3.881931094 1.065415353 13.140157870
O 6.192323525 11.919585341 5.759457937
O 5.918453789 11.842990579 13.336444684
O 9.851926050 12.426646399 1.796718177
O 9.715003849 12.582478683 9.333935029
O 7.273400886 2.142530906 1.986572446
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O 1.743593310 6.822142790 5.461116615
O 1.669872873 6.880845351 12.951432486
O 1.250909615 3.173203201 1.758200347
O 1.142488111 3.045523888 9.282213584
O 11.891472181 6.588382980 1.745141471
O 11.614918314 6.595389227 9.222974864
O 2.713765380 3.103953660 4.004162500
O 2.712103117 2.613509452 11.364662285
O 10.150056766 10.963374829 14.597041731
O 10.453260844 11.183615160 7.196472269
O 10.100951317 10.736849514 3.815548544
O 10.086972051 10.672885430 11.206804535
O 3.165839585 2.978002954 14.906497596
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O 7.469971763 0.129846037 0.232666101
O 7.461116454 -0.125185244 8.018789412
O 13.555251541 7.086940580 14.737135041
O 13.236010176 7.234062949 7.196269084
O 5.551403589 13.940335552 3.884166241
O 7.259830603 0.379023847 11.457101701
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O -0.242286271 6.801142934 11.082108037
O 0.472994999 12.359447477 1.925773502
O 0.533687385 12.263242464 9.384176811
O 3.574130809 9.553400688 1.877289414
O 3.677586385 9.451896637 9.371385344
O 12.456101974 1.600618259 5.727247088
O 12.525792946 1.434878383 13.168184980
O 9.552874245 4.276220721 5.555985693
O 9.562339317 4.408806692 13.210465823
O 4.896123496 8.431697843 5.341064333
Si 7.105422201 1.692877627 0.450799955
Si 9.287472849 12.132602552 0.309171038
Si 9.378314183 12.220437773 7.771049468
Si 3.715782115 1.834102081 4.130134236
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Si 11.902294161 6.986806029 3.322194483
Si 11.958883114 6.908503266 10.769814562
Si 1.364103700 3.667025293 3.304937224
Si 1.420516625 3.431493980 10.823448560
Si 1.337646224 6.701358455 14.532247231
Si 11.667823841 10.114689714 7.047020270
Si 11.593539323 10.223004377 14.532911069
Si 6.407521464 12.063150515 7.376511444
Si 6.228675251 12.161738316 14.886040529
Si 3.908161057 1.742083464 7.231912358
Si 4.027792511 1.617722570 14.665870294
Si 6.742645488 1.884807080 3.502971335
Si 6.883182302 1.891186607 11.160927279
Si 9.415464238 12.135406737 3.342107470
Si 9.401923543 12.085476169 10.839300541
Si 1.211449531 6.743194931 3.940519086
Si 1.334679746 6.542444949 11.395886163
Si 11.509468785 9.951033231 3.950678039
Si 11.551860978 9.966041429 11.449618780
Si 12.013143402 7.165285166 0.236935989
Si 11.724764610 7.190074788 7.702076421
Si 1.687409549 3.553855043 0.240991948
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Si 1.930475208 13.077823056 9.249024974
Si 4.225087745 11.016974800 2.129646665
Si 4.285745073 10.945399846 9.215664782
Si 11.109902904 0.741451487 5.486909019
Si 11.076524136 0.726907467 13.105408937
Si 8.839962207 2.961992221 13.191623670
Si -0.203108790 10.898098126 1.744384096
Si -0.110617881 10.780917460 9.289784057
Si 2.179076429 8.721588535 1.715207934
Si 2.264625015 8.638877225 9.300936927
Si 13.240143468 3.014937194 5.607766306
Si 13.259285176 2.884079145 13.114659821
Si 10.910316737 5.150892777 5.589730292
Si 11.012690065 5.139152798 13.132751955
Si 1.594108139 3.615339907 7.812536210
Si 8.799663388 2.837731868 5.557057134
Al 1.082410732 6.697859663 7.088905284
Al 6.259320548 12.397308970 4.031069936
Al 6.015342468 12.278705587 11.675785247
Al 7.097782518 1.572124280 7.886859748
Cu1 3.357064503 8.135101553 6.317109286
Nb2 4.871469219 10.196878490 5.591837707
H 8.065644362 3.021242748 9.545307792
H 7.449340989 11.101781485 10.273140517
End final coordinates

Cu-O-Pd-H2MOR
Final enthalpy = -6818.0977970326 Ry
CELL_PARAMETERS (angstrom)
13.805859015 0.066076559 0.005419205
-1.368648307 13.624296766 -0.019577997
0.013193113 0.011520666 15.022988324

ATOMIC_POSITIONS (angstrom)
O 3.131999278 0.514204263 3.275040919

O 2.270754263 13.796837261 10.735590160
O 5.213573690 11.073223330 3.282932824
O 4.901984767 11.325191052 10.862208680
O 7.939623158 11.563632500 7.637573865
O 7.677494139 11.837070775 0.594641912
O 10.820916869 0.063692646 6.954811582
O 9.475271608 13.479704715 14.517668009
O 8.218256162 2.582289103 7.008266354
O 8.095592418 2.681622229 14.636940698
O 5.211141646 2.166075316 3.624542958
O 5.380060876 2.143877693 11.142451940
O 12.588556165 11.005181291 0.454035278
O 12.982356595 10.696941682 7.934987143
O 2.223515468 7.696649737 0.408675024
O 2.137902092 8.004281658 7.849491591
O 1.730651999 5.340189990 3.433448947
O 1.685077482 5.010548222 11.204092464
O 0.109243162 3.322511360 4.162307115
O 0.208691252 2.865725473 11.721845287
O 11.086291877 5.916899791 4.164778864
O 11.207379595 5.784275911 11.695348760
O 11.385582100 8.650276349 0.154592062
O 11.133096476 8.776109566 7.717997378
O 10.155433391 13.354747436 4.367191209
O 9.566752782 13.206723785 11.882179033
O 7.636722814 2.863788974 4.421157936
O 7.758346369 2.946308316 11.999940218
O 5.540840493 2.123849625 15.019664136
O 5.426051011 1.840549310 7.693174476
O 3.490900516 0.471518726 0.626160711
O 3.136951962 0.521893706 8.139337340
O 5.119476466 11.334874007 0.607964153
O 5.509830636 10.958202072 8.314214778
O 7.923487359 12.050851162 3.713504368
O 7.655146957 11.730374186 10.750573138
O 0.624226849 2.970872029 6.747355795
O 0.529937912 2.755556918 14.374112306
O 10.720581466 6.321989087 6.796764978
O 11.106230978 6.192062687 14.326784842
O 11.336305413 8.482205611 3.514197534
O 11.379171784 8.400127009 11.261495314
O 12.826869997 10.666812815 3.101817121
O 12.576679987 10.723156347 10.575665515
O 2.026691886 7.941248132 3.056643629
O 2.249170665 7.475561586 10.456524084
O 1.575266865 5.249369755 7.728425261
O 1.577867878 5.174027144 14.915527336
O 3.119736219 12.177795629 2.139490793
O 3.167430466 12.048824844 8.932491524
O 9.905638346 1.716853306 5.104616557
O 9.914209712 1.750478807 12.920140256
O 0.922317344 9.755157122 1.448995080
O 0.973113112 9.612988334 9.611212639
O 12.221265204 4.323516118 5.974515768
O 12.209245519 3.982332813 13.376153305
O 3.752172040 1.263132028 5.702465565
O 3.920913227 1.152401701 13.163456492
O 5.993228997 11.602681532 5.764192006
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O 12.175061344 9.991993955 5.541037520
O 11.897102954 10.253837988 13.071833178
O 1.764061138 7.066927322 5.491264831
O 1.641415244 6.982587819 12.959232179
O 1.244521815 3.322357373 1.795945606
O 1.131146726 3.173944816 9.313486956
O 11.923601594 6.588261145 1.767111989
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O 2.832271349 2.679812727 11.297182820
O 10.023059020 10.886680294 14.826786876
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O 3.646299103 9.482604903 9.440623203
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O 9.581336223 4.369568898 13.227252723
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Si 7.043961211 1.709450971 0.423581293
Si 9.256831843 12.168138341 0.451258809
Si 9.408588322 12.277427054 7.724235803
Si 3.738853330 1.739821779 4.158841543
Si 3.926765979 1.533106014 11.585359687
Si 11.953926010 6.997922422 3.338520359
Si 11.945629596 6.938259244 10.821196612
Si 1.458462239 3.733551866 3.352425544
Si 1.467240615 3.438044957 10.869479363
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Si 11.701161860 10.167331078 7.084037694
Si 11.480074108 10.193866468 14.642169090
Si 6.363254724 11.949053847 7.345969850
Si 6.288298566 12.209264408 14.870027571
Si 3.893922931 1.691503084 7.272478063
Si 4.012655935 1.693140167 14.695217179
Si 6.798412182 1.783707773 3.535629687
Si 6.962418323 1.831444934 11.131258858
Si 9.494216768 12.176311805 3.464525662
Si 9.337317148 12.059563600 10.795307269
Si 1.283393213 6.806524127 3.939239535
Si 1.312300125 6.567783447 11.420077746
Si 11.644499398 10.000278690 4.002196539
Si 11.493428583 9.990195844 11.525585700
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Si 11.692117618 7.231163806 7.741458205
Si 1.601746021 3.574604795 0.233181906
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Si 4.298149665 10.975675191 9.422070512
Si 11.174532468 0.808120667 5.536237472
Si 11.059797326 0.634237906 13.145354299
Si 8.841911712 2.929927924 13.226026932
Si -0.196702873 10.911603497 1.709863557
Si -0.123719083 10.785038640 9.386718950
Si 2.175169440 8.747117343 1.651411984
Si 2.261129502 8.660586295 9.347738232
Si 13.266759054 3.120495698 5.644994400
Si 13.273150319 2.776379753 13.156200565
Si 10.896395682 5.208528032 5.621198187
Si 11.038017177 5.081918914 13.150938342
Si 1.623660229 3.657766108 7.828522745
Si 8.818002942 2.865037091 5.544493937
Al 1.060502372 6.764453898 7.138234646
Al 6.283006243 12.304586113 4.117060801
Al 6.079323989 12.249615480 11.699230736
Al 7.101927937 1.538186860 7.804518643
Cu1 3.283011249 8.045435072 6.170524058
Pd2 4.997620926 9.856041366 4.995728602
H 8.151363174 2.895530739 9.472881710
H 7.398690237 11.224389280 9.947379485
End final coordinates

Cu-O-Rh-H2MOR
Final enthalpy = -6957.1874038025 Ry
CELL_PARAMETERS (angstrom)
13.811433778 0.071136644 0.010854742
-1.364171889 13.609207720 -0.007865639
0.019042561 0.024983453 15.005210584

ATOMIC_POSITIONS (angstrom)
O 3.116499726 0.525370959 3.294411343
O 2.291972742 13.787678178 10.745115083
O 5.226033225 11.042703369 3.375307120
O 4.940459033 11.344450585 10.828455745
O 7.935215007 11.571793189 7.615161831
O 7.697849146 11.803257376 0.591080950
O 10.830991825 0.078148550 6.958930644
O 9.477041358 13.502807395 14.522222566
O 8.243428569 2.563769652 7.032526067
O 8.149639383 2.684963963 14.643200342
O 5.209876897 2.165536617 3.630268825
O 5.380738146 2.155933768 11.159295678
O 12.618454651 11.019122385 0.458061468
O 12.990091666 10.727071442 7.927475647
O 2.232509111 7.683746828 0.424523196
O 2.178066571 8.063172555 7.790668273
O 1.706975715 5.328214067 3.348844769
O 1.713000713 5.014278218 11.184901963
O 0.110642290 3.312425095 4.153177130
O 0.191479827 2.903365047 11.705355708
O 11.039574601 5.926608390 4.157546172
O 11.226549234 5.790430736 11.697026826
O 11.422754398 8.658649380 0.172426990
O 11.158773934 8.780452635 7.731688705
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O 9.597124389 13.210903752 11.891762199
O 7.632296911 2.859501598 4.460618472
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O 5.432022913 1.875469974 7.696429716
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O 3.145844986 0.560212508 8.147375887
O 5.141301191 11.335993369 0.727008651
O 5.493043349 10.910564673 8.267571684
O 7.947598675 12.039199462 3.747395441
O 7.665939209 11.719844163 10.823315524
O 0.624701582 3.050139828 6.749298868
O 0.560377182 2.755834815 14.343198379
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O 11.114764803 6.224496499 14.320911682
O 11.359798243 8.485345704 3.511838806
O 11.401494026 8.406075122 11.255160353
O 12.850772329 10.669308263 3.106105472
O 12.594759982 10.734863764 10.567793185
O 1.953791857 7.936203131 3.074792603
O 2.239730198 7.472673652 10.401506568
O 1.594169821 5.284033798 7.843521293
O 1.609111914 5.168877624 14.889330178
O 3.115994827 12.136411836 2.250211960
O 3.175870342 12.056492605 8.924723274
O 9.940994580 1.754365578 5.116898561
O 9.933827157 1.779180678 12.882692101
O 0.940359328 9.759096759 1.438116477
O 0.980539514 9.624562998 9.582332536
O 12.203545939 4.320845909 5.943758024
O 12.223313523 4.002900784 13.403725258
O 3.760007525 1.279634501 5.711280608
O 3.936405631 1.130440136 13.172048053
O 5.967107231 11.631321842 5.782101584
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O 7.522962999 2.169661298 9.564997467
O 12.187492538 9.992321075 5.547702461
O 11.931659366 10.259777731 13.064315827
O 1.756709775 6.935621764 5.492360187
O 1.677504221 6.986033168 12.939191515
O 1.249485175 3.275405514 1.785111339
O 1.160478580 3.140900930 9.317724768
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O 11.593834030 6.658167813 9.275971821
O 2.767860389 3.044447004 3.990261618
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O 10.064236516 10.913249543 14.820300931
O 10.503297235 11.252373568 7.144386145
O 10.266419483 10.785269130 3.865927911
O 10.051119134 10.660397463 11.205734685
O 3.126278376 3.007617089 14.912357025
O 3.136301619 3.142440555 7.531604176
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O 13.572105493 7.154774149 14.746698256
O 13.252259681 7.239186780 7.269544746
O 5.676342981 13.885044949 3.992088651
O 7.347696382 0.357540737 11.501319033
O -0.348555435 6.891203016 3.920184141
O -0.241510350 6.824524099 11.077483363
O 0.520513495 12.372259666 1.788457901
O 0.575157296 12.255414379 9.482141626
O 3.576653109 9.539980935 1.827168364
O 3.657854419 9.488273242 9.449176257
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O 12.537756299 1.354774246 13.142340064
O 9.532390534 4.340884253 5.575507659
O 9.595764647 4.395618911 13.228658123
O 4.491527079 8.256326338 4.907985591
Si 7.069788380 1.723296618 0.443582206
Si 9.270719192 12.166799569 0.463801372
Si 9.409223378 12.273575828 7.730982037
Si 3.735009032 1.752829515 4.167360401
Si 3.931118889 1.532078011 11.599769238
Si 11.950106832 6.987753604 3.347215024
Si 11.967644454 6.940932292 10.822872890
Si 1.455553067 3.721918235 3.332986742
Si 1.476243636 3.440532560 10.870845535
Si 1.330039369 6.724018567 14.507060146
Si 11.711450336 10.171857122 7.088484373
Si 11.518101808 10.213322124 14.636334185
Si 6.360229921 11.960190974 7.366760110
Si 6.287062822 12.206767927 14.913911615
Si 3.900153120 1.726061790 7.274407413
Si 4.054709906 1.690873395 14.696193149
Si 6.799692737 1.800924830 3.546125713
Si 6.964644641 1.855041754 11.155542222
Si 9.516625949 12.178411180 3.483396791
Si 9.348846390 12.058187551 10.816908337
Si 1.262696445 6.761908608 3.948500771
Si 1.332212048 6.569162678 11.401278166
Si 11.669113970 9.999294155 4.004706413
Si 11.519828076 9.994636340 11.521528275
Si 12.012774398 7.147635187 0.254179799
Si 11.727350815 7.237585237 7.752863804
Si 1.620606175 3.555851037 0.231339441
Si 1.905764420 13.188185367 1.988404257
Si 1.966227961 13.079979786 9.314511017
Si 4.246167695 11.005897865 2.022499482
Si 4.304513534 10.982784759 9.408152109
Si 11.199675185 0.829507077 5.547828115
Si 11.074736957 0.663552480 13.135872927
Si 8.864927965 2.953705667 13.222168453
Si -0.175157725 10.912481739 1.710216549
Si -0.117021182 10.798629255 9.370455773
Si 2.170058172 8.727443908 1.677603295
Si 2.267907470 8.677431806 9.317102545
Si 13.277531949 3.138750021 5.645255545
Si 13.285803390 2.800598138 13.154462359
Si 10.884906775 5.221442603 5.619393462
Si 11.055227091 5.102652821 13.157604593
Si 1.635043185 3.688919646 7.849859258
Si 8.827815699 2.874062681 5.568462737
Al 1.094436213 6.756930238 7.136601796
Al 6.309680853 12.306358626 4.129966484
Al 6.069830210 12.261744872 11.736987930
Al 7.100661490 1.554923728 7.829769165
Cu1 3.266037463 8.157293547 6.189935236
Rh2 4.965226517 9.942546668 5.137021513
H 8.161641709 2.904038089 9.497068383
H 7.399713094 11.140922766 10.077434096
End final coordinates

Cu-O-Ru-H2MOR
Final enthalpy = -6918.6821266773 Ry
CELL_PARAMETERS (angstrom)
13.809340172 0.065343924 0.003271141
-1.369716558 13.617035638 -0.010902826
0.010833899 0.020836913 15.012007395

ATOMIC_POSITIONS (angstrom)
O 3.111903078 0.522987726 3.295220191
O 2.274715995 13.791932966 10.743676016
O 5.190876706 11.070670474 3.368407555
O 4.931337507 11.348108492 10.818112658
O 7.914142698 11.576257573 7.583145194
O 7.694041735 11.813461881 0.584326314
O 10.832996776 0.070981276 6.956528609
O 9.470833137 13.493644218 14.509281988
O 8.225778570 2.567537549 7.023764917
O 8.134174655 2.669493050 14.630677571
O 5.209044956 2.157117121 3.621263711
O 5.374194473 2.150472924 11.155019092
O 12.608101260 11.007702127 0.456354060
O 12.973582370 10.720098248 7.933115826
O 2.225927167 7.687858557 0.436625139
O 2.148683152 8.058782768 7.819154079
O 1.716610967 5.330439669 3.349016825
O 1.711998579 5.018197990 11.201202639
O 0.109887921 3.321481762 4.154487997
O 0.192412918 2.901249015 11.710213890
O 11.046628822 5.931269577 4.160271213
O 11.209136796 5.784790430 11.689066485
O 11.405907180 8.653129755 0.163891129
O 11.143327859 8.777378658 7.720776645
O 10.156623150 13.362461484 4.376761732
O 9.591072604 13.204632180 11.880177896
O 7.634064772 2.864358519 4.442657945
O 7.757070623 2.967956236 12.001384324
O 5.571435653 2.142834439 14.976510599
O 5.419363771 1.878020098 7.705537124
O 3.556331029 0.476201135 0.660809336
O 3.133057740 0.556853273 8.148008103
O 5.143150569 11.336373814 0.712589270
O 5.473273874 10.911862013 8.259022653
O 7.939315472 12.029188993 3.737301834
O 7.651269074 11.721660433 10.811834543
O 0.621497042 3.040074290 6.747825901
O 0.552332351 2.758873577 14.349847187
O 10.736591966 6.335118286 6.795847171
O 11.101618991 6.215571040 14.311954950
O 11.361899592 8.489141081 3.511018805
O 11.395155657 8.401014437 11.253906136
O 12.848214535 10.679238774 3.105353443
O 12.570711419 10.740793963 10.570336367
O 1.984621216 7.940059171 3.089601486
O 2.231959606 7.486113203 10.437579453
O 1.578148004 5.286607951 7.836388623
O 1.589293220 5.172427745 14.922300497
O 3.107455290 12.164034136 2.211329391
O 3.158741748 12.060151610 8.921994083
O 9.918716612 1.733518337 5.117180367
O 9.926638722 1.762036944 12.878344305
O 0.940736487 9.765553041 1.451915803
O 0.962021428 9.628646266 9.606870979
O 12.207091281 4.327589731 5.948359632
O 12.218527842 3.999065425 13.392296672
O 3.760944655 1.279013897 5.711837966
O 3.925309276 1.133984200 13.169740305
O 5.934612964 11.591506592 5.756877659
O 6.285529922 11.805315426 13.359192273
O 9.857781747 12.533871787 1.913794447
O 9.677192126 12.539017057 9.312262432
O 7.285649231 2.019234287 1.995888835
O 7.518190006 2.145899218 9.554748150
O 12.182694639 10.006373620 5.544506309
O 11.913754167 10.254660307 13.065092123
O 1.756228213 6.933341286 5.496304115
O 1.650501483 6.983025449 12.963656261
O 1.254653069 3.267316506 1.788887975
O 1.143522434 3.155093926 9.320375123
O 11.903843257 6.580836654 1.767807355
O 11.589947741 6.657643002 9.269893738
O 2.767739986 3.042416644 3.992520073
O 2.821766607 2.674642302 11.323967442
O 10.045527825 10.904948370 14.818072227
O 10.488343464 11.248689278 7.137923920
O 10.262604140 10.787386367 3.851164639
O 10.027621828 10.647923785 11.206644333
O 3.119929443 3.025463648 14.902302288
O 3.124147680 3.140338520 7.537576649
O 7.324002508 0.153968223 0.096470878
O 7.435107278 -0.143017973 7.704654755
O 13.552047236 7.149357048 14.769990329
O 13.233654008 7.230886932 7.248860018
O 5.677421798 13.894419874 3.989710546
O 7.340362192 0.348970196 11.502087462
O -0.336487269 6.901745526 3.888642525
O -0.251718240 6.820325306 11.087413766
O 0.507930426 12.381672506 1.779866688
O 0.559009176 12.259072306 9.487352353
O 3.573083815 9.553897512 1.823692156
O 3.638359286 9.491980750 9.454399979
O 12.527445241 1.707170809 5.718954163
O 12.531674947 1.349289896 13.135650361
O 9.539429257 4.329692729 5.562173683
O 9.591047951 4.377608088 13.225156249
O 4.723901202 8.209289224 5.131755495
Si 7.064120527 1.716977774 0.430975583
Si 9.268969264 12.168773827 0.452088258
Si 9.391513428 12.270257969 7.717362823
Si 3.733888916 1.750859211 4.166968133
Si 3.922058282 1.531336169 11.595624174
Si 11.949944713 6.990554099 3.339647230
Si 11.956989303 6.934946488 10.818865139
Si 1.457670602 3.726127819 3.335185565
Si 1.471241340 3.447292827 10.872217625
Si 1.309746199 6.723567550 14.532020646
Si 11.699470494 10.170739964 7.084807090
Si 11.499270729 10.203043757 14.636595884
Si 6.334385137 11.948928584 7.342157041
Si 6.278482243 12.206579166 14.905335769
Si 3.888723387 1.725272878 7.277693041
Si 4.037775086 1.699999529 14.692026983
Si 6.800920847 1.800102957 3.535870657
Si 6.957041183 1.844526302 11.147825942
Si 9.509477466 12.178421766 3.471770245
Si 9.335530757 12.049356545 10.809215032
Si 1.274697467 6.765213391 3.955821931
Si 1.320797945 6.570770302 11.421545918
Si 11.666866137 10.004704463 4.000835612
Si 11.501459830 9.989708239 11.522086371
Si 11.995113418 7.142073217 0.250784689
Si 11.713889796 7.234570491 7.744387671
Si 1.619392695 3.560410968 0.235674260
Si 1.885484890 13.209661790 1.974084824
Si 1.948995204 13.083843255 9.312561221
Si 4.228167931 11.027480701 1.995176474
Si 4.286219146 10.983912030 9.402402238
Si 11.189340864 0.823073307 5.542235862
Si 11.072417327 0.650320407 13.127531641
Si 8.857353953 2.937727317 13.213184772
Si -0.179835758 10.917134197 1.713448999
Si -0.133178248 10.801647157 9.383975151
Si 2.168353006 8.730850821 1.688743107
Si 2.247321442 8.677903598 9.337898503
Si 13.271687177 3.139263446 5.637478205
Si 13.280642507 2.795432111 13.148925936
Si 10.884495835 5.221453904 5.617772181
Si 11.045289867 5.093487053 13.149146122
Si 1.622934257 3.693176254 7.849389924
Si 8.820600850 2.870903144 5.561352778
Al 1.083764624 6.764645841 7.130253916
Al 6.307399713 12.315726675 4.123048223
Al 6.060298358 12.260536140 11.729767684
Al 7.087702174 1.545467845 7.814713994
Cu1 3.315587289 8.155378512 6.264764570
Ru2 4.925833215 9.920870392 5.058674905
H 8.142778522 2.892008504 9.480480593
H 7.384092931 11.146393339 10.063374215
End final coordinates

Cu-O-Zr-H2MOR
Final enthalpy = -6794.5988006461 Ry
CELL_PARAMETERS (angstrom)
13.827731831 0.050945916 -0.004268922
-1.385661234 13.618472299 -0.013992133
0.002655646 0.016631554 15.013740551

ATOMIC_POSITIONS (angstrom)
O 3.154709429 0.527342866 3.299433286
O 2.209484138 13.834686645 10.709157521
O 5.026318533 11.076839013 3.552999056
O 5.227525679 11.340577481 10.457963052

O 7.831714671 11.576369619 7.883044301
O 7.766089510 11.719723166 0.253383156
O 10.747112470 -0.048154973 6.933395656
O 9.523113008 13.564871522 14.506814432
O 8.215541946 2.551893763 7.030635717
O 8.179844446 2.608469831 14.624022796
O 5.188671297 2.238485923 3.574874830
O 5.344141605 2.163804731 11.209738645
O 12.714809923 11.032011189 0.392625512
O 12.897469648 10.721128594 7.881391273
O 2.207994720 7.746747777 0.408229895
O 2.165885927 7.872261746 7.891583002
O 1.560251126 5.270047320 3.312966018
O 1.769447881 5.069320495 11.031684139
O 0.083789052 3.170966592 4.152371220
O 0.149939046 3.084720762 11.707524172
O 11.124025574 5.837891092 4.150866200
O 11.224992510 5.763848409 11.679712437
O 11.491143436 8.693499981 0.206052794
O 11.131573207 8.701087994 7.707986672
O 9.987639500 13.255298680 4.322906770
O 9.736036967 13.248473944 11.897723304
O 7.604361137 2.860828999 4.453566302
O 7.751072570 2.971739913 12.039516001
O 5.600284695 2.024345592 14.918222320
O 5.401628468 1.922455370 7.738220449
O 3.507555884 0.465226714 0.656334391
O 3.134929089 0.551585828 8.097717990
O 5.279021929 11.292046528 0.871222768
O 5.206535720 10.946615204 7.799780866
O 7.813953319 11.971257207 3.422745278
O 7.754708303 11.763623960 10.946521692
O 0.563389367 2.827389425 6.765144003
O 0.622108215 2.828831937 14.316262382
O 10.784835741 6.242876171 6.784426449
O 11.069315718 6.299662068 14.281653982
O 11.265923458 8.419329442 3.527399817
O 11.401980821 8.371809773 11.172805268
O 12.711081439 10.638793962 3.047414879
O 12.631295424 10.691638570 10.527613150
O 2.032077280 7.853365224 3.074916353
O 2.224597009 7.620383857 10.557438944
O 1.387313907 5.162424264 7.783728138
O 1.651862674 5.186669106 15.054499219
O 3.121425321 12.178053546 2.143115438
O 3.123729061 12.081661390 8.949761845
O 9.836840348 1.637284340 5.115954899
O 9.971682047 1.783726675 12.828102673
O 0.912960167 9.743719233 1.563634434
O 0.981204394 9.662872080 9.452079491
O 12.230655057 4.207161832 5.943325188
O 12.245784569 4.073022850 13.482386261
O 3.843649141 1.278978729 5.691526264
O 3.866648517 1.098299317 13.172197077
O 6.219347530 11.895193519 5.757653284
O 5.948726395 11.826754258 13.331378876
O 9.855119251 12.437524562 1.813158577
O 9.761502579 12.545833287 9.356515626
O 7.276119151 2.117899001 1.966209797
O 7.473288732 2.261234224 9.600746706
O 12.059295558 10.008094631 5.509324370
O 12.066205183 10.137754254 13.024808978
O 1.742134939 6.832367400 5.478007077
O 1.647566001 6.861659926 12.992577850
O 1.285977550 3.164636554 1.794529471
O 1.161119491 3.048848982 9.321811318
O 11.890118404 6.560894277 1.755451664
O 11.652529490 6.582525578 9.243407690
O 2.737275005 3.040906792 4.037530168
O 2.781912083 2.698264107 11.384660798
O 10.170404978 10.955144949 14.645296923
O 10.353547541 11.123713475 7.181766089
O 10.126436572 10.704660838 3.792845527
O 10.118212845 10.664810110 11.257652235
O 3.179082895 3.028429830 14.929909426
O 3.080596056 3.130882575 7.480780162
O 7.419827685 0.110369568 0.198750350
O 7.409680597 -0.088731248 7.971773593
O 13.562556944 7.084336551 14.779139987
O 13.251292998 7.243176736 7.195950267
O 5.594145808 13.921816406 3.859279893
O 7.317232395 0.359742458 11.465866943
O -0.351582221 7.003697256 3.855678428
O -0.248329616 6.812382116 11.107839828
O 0.494122425 12.361818837 1.886615225
O 0.512086236 12.278182793 9.415878399
O 3.557868151 9.560984584 1.857956742
O 3.645494023 9.495500676 9.380053921
O 12.455799570 1.571975075 5.672938849
O 12.591695184 1.442729327 13.143130771
O 9.574037941 4.258108413 5.537537417
O 9.606748167 4.384184875 13.245602926
O 4.993562650 8.396280862 5.505307999
Si 7.103012559 1.683360554 0.426870670
Si 9.322535545 12.153239279 0.311981652
Si 9.357469176 12.215107785 7.802306396
Si 3.745344088 1.777199856 4.156806474
Si 3.879680061 1.542997364 11.612680074
Si 11.947591931 6.962307009 3.331294699
Si 11.984645238 6.896520889 10.793104074
Si 1.410827257 3.658377564 3.341356765
Si 1.468405761 3.483282825 10.844824230
Si 1.311102274 6.699577475 14.571603256
Si 11.625478746 10.112777572 7.066836729
Si 11.607326111 10.201879316 14.583375407
Si 6.369107322 12.102882133 7.374049408
Si 6.246057767 12.161347212 14.878673258
Si 3.890669319 1.739289109 7.255104998
Si 4.034811566 1.663391509 14.691245065
Si 6.771272073 1.851770372 3.489294124
Si 6.929533232 1.870542144 11.180046493
Si 9.407099677 12.092632785 3.344630451
Si 9.437816347 12.072650228 10.868806573
Si 1.247447134 6.730166665 3.951422367
Si 1.331161106 6.578285954 11.423716867
Si 11.550159788 9.953726733 3.963742879
Si 11.577105797 9.944691481 11.493915930
Si 12.014433509 7.153933704 0.254358329
Si 11.745993203 7.174450920 7.718884265
Si 1.683728185 3.563217195 0.271594632
Si 1.874551464 13.203101054 1.981100069
Si 1.900399485 13.108662937 9.284926014
Si 4.236883167 11.017254742 2.069017131
Si 4.273462549 10.979363560 9.227144712
Si 11.103204800 0.709062881 5.511944243
Si 11.151284084 0.714989061 13.127399926
Si 8.888582739 2.935315851 13.215249914
Si -0.207471313 10.907838736 1.745731448
Si -0.152426679 10.805462512 9.302214986
Si 2.163991230 8.719645727 1.717809422
Si 2.244952991 8.660025673 9.314889036
Si 13.252547865 2.982691903 5.624468378
Si 13.319876506 2.896214199 13.160019859
Si 10.930887573 5.132546074 5.604905432
Si 11.050179868 5.128980373 13.165396251
Si 1.548964751 3.584459684 7.820792678
Si 8.799133351 2.831987732 5.558919254
Al 1.063662209 6.693004230 7.092889828
Al 6.275900932 12.371421662 4.026835378
Al 6.049540713 12.270927234 11.675016160
Al 7.067593048 1.613517083 7.894326131
Cu1 3.429956516 8.059004932 6.430095657
Zr2 4.767814754 10.210848018 5.557784075
H 8.080474583 3.023337209 9.563105122
H 7.473989714 11.211907994 10.182688241
End final coordinates

Pd-O-Pd-H2MOR
Final enthalpy = -6936.0025451773 Ry
CELL_PARAMETERS (angstrom)
13.776380564 0.041819278 -0.015046718
-1.389705609 13.621888447 -0.036097609
-0.008940648 -0.008895915 15.021878168

ATOMIC_POSITIONS (angstrom)
O 3.101804617 0.525620474 3.261062238
O 2.242866749 13.787535609 10.707755735
O 5.234003443 11.118242369 3.138156612
O 4.845270983 11.292407932 10.780105876
O 7.857509805 11.506772579 7.633192050
O 7.613988464 11.842760006 0.567304050
O 10.777656457 -0.008441763 6.923017939
O 9.434525458 13.419136738 14.496009734
O 8.231482717 2.495772853 6.977159459
O 8.004707184 2.701069683 14.637534404
O 5.189376616 2.162182731 3.600948039
O 5.353042739 2.150757139 11.105152517
O 12.540467256 10.943280504 0.441647473
O 12.919695464 10.612574407 7.957885050
O 2.199188458 7.701258602 0.438565648
O 1.936167257 8.085835668 7.903444337
O 1.686769260 5.344863475 3.405138623
O 1.643946165 4.997426317 11.218344387
O 0.085888207 3.306133916 4.158790687
O 0.184527908 2.831710997 11.706303719
O 11.125531724 5.892518333 4.177754934
O 11.102525241 5.819722638 11.706561896
O 11.311487444 8.608365689 0.157569299
O 11.080242424 8.699823752 7.688065381
O 10.176844875 13.318456380 4.340887472
O 9.451285422 13.189668212 11.852766710
O 7.630077599 2.822402874 4.395421438
O 7.727800972 2.902422590 11.976431496
O 5.475224455 2.086980150 15.074754812
O 5.424224755 1.828356826 7.652827729
O 3.398515979 0.493846203 0.598556306
O 3.120083526 0.544710690 8.133579202
O 5.039139757 11.365140866 0.468219714
O 5.392631509 10.860129472 8.201668947
O 7.889254726 12.095667822 3.722007878
O 7.574520507 11.707821027 10.664828279
O 0.664646032 3.028454189 6.727563757
O 0.480770451 2.751984330 14.362632065
O 10.639626526 6.242649443 6.803185519
O 11.046898732 6.122589031 14.354659959
O 11.293670290 8.455252983 3.518298382
O 11.330239100 8.412872269 11.163983466
O 12.737587872 10.674776360 3.099834150
O 12.451047685 10.804420386 10.588083270
O 2.117186955 7.939755586 3.095784697
O 2.189829579 7.478243479 10.490865693
O 1.605795142 5.288377905 7.800287347
O 1.514739064 5.164503831 14.941835691
O 3.105911993 12.233651674 2.072169472
O 3.087929087 12.028725449 8.881561326
O 9.922609893 1.673576731 5.068894917
O 9.839938188 1.709425876 12.976237364
O 0.879216333 9.719440666 1.531890198
O 0.895080972 9.664813654 9.771832351
O 12.180692893 4.264292400 5.983307927
O 12.156479424 3.966545269 13.298539270
O 3.711124676 1.289500415 5.690382089
O 3.917109199 1.157054730 13.149411425
O 5.953871055 11.478079026 5.688264747
O 6.375720410 11.776904628 13.241858483
O 9.816065524 12.479521949 1.893516079
O 9.656306027 12.532762091 9.286078836
O 7.281337598 1.860408370 1.990066437
O 7.510955944 2.086533062 9.507393821
O 12.120304789 9.976456169 5.540528904
O 11.796711521 10.188730761 13.064727650
O 1.808199098 7.003473601 5.522547756
O 1.623844683 6.962749979 12.986143648
O 1.219881557 3.303622069 1.790900848
O 1.115446043 3.174230887 9.305918923
O 11.927511036 6.570036354 1.777305499
O 11.564391977 6.599530557 9.254514942
O 2.751881260 3.049278753 3.966337485
O 2.808774995 2.673214443 11.288303815
O 9.934773262 10.822216136 14.828042428
O 10.436865317 11.187835944 7.151891216
O 10.156899012 10.737231060 3.862506615
O 9.919430484 10.636025874 11.205181287
O 3.052813772 3.028510599 14.883754160
O 3.148360052 3.133180837 7.567331082
O 7.305858963 0.173314687 -0.073288535
O 7.407423600 -0.226849298 7.646227962
O 13.471578926 7.146570479 14.738562269
O 13.131932735 7.113821058 7.146130649
O 5.568145768 13.867792042 4.056488009

O 7.260461367 0.292838655 11.431682958
O -0.273793554 7.038291061 3.887856570
O -0.299883498 6.821252585 11.128801121
O 0.473447610 12.347542571 1.782902419
O 0.497219274 12.280507863 9.459468388
O 3.548590672 9.613742756 1.735868980
O 3.559515007 9.453584830 9.385715090
O 12.512207903 1.650270018 5.754218202
O 12.450367138 1.304419268 13.117743958
O 9.532003042 4.267076826 5.482095497
O 9.520663199 4.340229541 13.214290793
O 5.143061223 8.087996703 5.635401833
Si 7.016065476 1.692778452 0.411319690
Si 9.204375521 12.139467772 0.437063627
Si 9.333378786 12.219425353 7.703329192
Si 3.712727516 1.752529651 4.142013891
Si 3.910454391 1.533063742 11.570133429
Si 11.966046375 6.992411924 3.347233285
Si 11.881933726 6.924118395 10.806574444
Si 1.429892411 3.737753466 3.343451544
Si 1.439630808 3.425220734 10.865808514
Si 1.257326816 6.715046985 14.546707973
Si 11.640898510 10.106058761 7.085263947
Si 11.390569100 10.128361614 14.639033535
Si 6.281376447 11.859802451 7.256053437
Si 6.235496347 12.195060316 14.778211549
Si 3.883063858 1.707636528 7.259634062
Si 3.954814993 1.687491558 14.688022705
Si 6.768512039 1.741808118 3.535935367
Si 6.928423153 1.801748518 11.095725450
Si 9.458635539 12.156393023 3.456437889
Si 9.249656924 12.037279525 10.766226043
Si 1.329976880 6.819281614 3.970580278
Si 1.269206578 6.549327046 11.455353253
Si 11.577128354 9.978199190 4.004584999
Si 11.397031153 9.988234972 11.509818683
Si 11.948999897 7.118369150 0.251882424
Si 11.636787367 7.154691835 7.716746692
Si 1.573739359 3.581306792 0.232763156
Si 1.828601320 13.224328993 1.905548775
Si 1.903843634 13.080298829 9.278669798
Si 4.222655300 11.094041452 1.830212773
Si 4.221625670 10.951807000 9.349797979
Si 11.180473668 0.761079289 5.529305995
Si 10.994897130 0.597423489 13.147434611
Si 8.776666266 2.905388753 13.231264887
Si -0.232994947 10.894375755 1.733264090
Si -0.198744069 10.822682647 9.434655472
Si 2.168155778 8.747663705 1.685170332
Si 2.133578066 8.686428049 9.419093218
Si 13.245988508 3.085952895 5.637345503
Si 13.207022757 2.744105127 13.115902126
Si 10.869534918 5.158203540 5.609101634
Si 10.971058886 5.060841994 13.137452692
Si 1.641987956 3.690905654 7.842581229
Si 8.817425876 2.805802311 5.510854798
Al 1.031026550 6.749124421 7.113085020
Al 6.233830314 12.290994354 4.107511018
Al 6.019850615 12.212394179 11.628093643
Al 7.088589736 1.465763058 7.759843835
Pd1 3.558139298 8.084450571 6.588592472
Pd2 5.184913272 9.612421911 4.591480332
H 8.115741205 2.847043635 9.418398621
H 7.345408252 11.260967767 9.818165616
End final coordinates

Rh-O-Rh-H2MOR
Final enthalpy = -7214.1696082748 Ry
CELL_PARAMETERS (angstrom)
13.792685059 0.054495531 -0.014069496
-1.378754823 13.619557064 -0.027759079
-0.007911389 0.000380841 15.024241440

ATOMIC_POSITIONS (angstrom)
O 3.114242494 0.512090925 3.285119328
O 2.259035923 13.780450177 10.724837596
O 5.255397181 11.083949387 3.215583365
O 4.885762147 11.304313564 10.789341471
O 7.880119982 11.547393009 7.579487484
O 7.647984114 11.820259594 0.569005526
O 10.803183459 0.044095643 6.940482494
O 9.438577810 13.444880543 14.489992474
O 8.202517419 2.546649051 6.996881855
O 8.089676588 2.665346338 14.627679013
O 5.190354872 2.162727676 3.600071262
O 5.355774652 2.146616378 11.143793136
O 12.567375561 10.984033455 0.444375913
O 12.942174105 10.644950139 7.948837297
O 2.220988356 7.694835223 0.432276254
O 2.023402454 8.031416347 7.898593678
O 1.750098032 5.345955161 3.444921632
O 1.688609567 5.008482482 11.217487571
O 0.093292565 3.348247381 4.169696096
O 0.192913842 2.872756322 11.735065774
O 11.064770586 5.919866893 4.168554272
O 11.178119192 5.783081697 11.694948073
O 11.358858969 8.633368454 0.154768668
O 11.075405756 8.751224442 7.692193230
O 10.160985385 13.341408285 4.350969174
O 9.540878989 13.184104586 11.854787490
O 7.607501681 2.859829781 4.416188572
O 7.739411407 2.925597237 11.987203721
O 5.532218156 2.121772330 14.991395806
O 5.405156762 1.854777340 7.711348919
O 3.516857665 0.484663066 0.637596511
O 3.114557912 0.535050844 8.141769117
O 5.073383754 11.341958248 0.554124473
O 5.432359275 10.893455504 8.216354607
O 7.920350030 12.052475274 3.728111981
O 7.609476420 11.708962453 10.730259886
O 0.607290485 2.977571231 6.754454952
O 0.515898538 2.746757565 14.388277952
O 10.651673535 6.295351397 6.796550408
O 11.064766704 6.168106631 14.327838658
O 11.347803214 8.477860691 3.507813034
O 11.366851535 8.394426304 11.226206433
O 12.822321033 10.674565758 3.096120109
O 12.509726402 10.760676453 10.584289277
O 2.029087234 7.952314079 3.081537213
O 2.233012872 7.490532352 10.503844538
O 1.551094094 5.261501668 7.755225041
O 1.550571192 5.164968422 14.941158295
O 3.114635196 12.180463597 2.147425684
O 3.107796168 12.027332529 8.903308439
O 9.865599573 1.671786711 5.082593884
O 9.891701308 1.725610951 12.901462241
O 0.920629780 9.755963888 1.459353245
O 0.937452234 9.647863800 9.707427603
O 12.204564459 4.334879505 5.976175303
O 12.187064415 3.972130711 13.368361054
O 3.762865388 1.264437456 5.708408416
O 3.891347330 1.145930088 13.163931269
O 5.922171760 11.549700122 5.699670809
O 6.329896801 11.797359368 13.292219611
O 9.829155472 12.518745965 1.889910097
O 9.659369578 12.524983942 9.287314276
O 7.276887183 1.977674944 1.978522323
O 7.504692915 2.123604224 9.530302426
O 12.156745687 9.996363999 5.536649763
O 11.843770274 10.222091844 13.068596098
O 1.756916287 7.054093816 5.522291986
O 1.604624724 6.969700690 12.986665536
O 1.254275121 3.321308837 1.813351911
O 1.103347729 3.183537363 9.321466108
O 11.896930274 6.570841158 1.768831507
O 11.538984185 6.637993999 9.258861590
O 2.746700012 3.022877866 4.016323927
O 2.808151313 2.663364906 11.287666908
O 9.976061250 10.855363498 14.826957023
O 10.469020642 11.238520647 7.125267855
O 10.231550269 10.770063518 3.830202278
O 9.969511377 10.627866960 11.192529559
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O 3.106343565 3.115908894 7.548957209
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O 13.501954044 7.139477158 14.776869365
O 13.143797987 7.187805476 7.197519882
O 5.631698929 13.889841283 3.980332042
O 7.289275508 0.311815063 11.446796078
O -0.309448029 6.930632789 3.890755818
O -0.268616880 6.811484259 11.067218744
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O 0.513328113 12.267172187 9.481144959
O 3.573566656 9.574285202 1.778916004
O 3.607524673 9.458919026 9.392526568
O 12.464796748 1.714052025 5.696822179
O 12.498042118 1.316095414 13.135989124
O 9.546215909 4.276370501 5.517687478
O 9.558815608 4.349453729 13.206561048
O 4.888846725 8.053782077 5.314454702
Si 7.049952633 1.711195187 0.408013196
Si 9.228916730 12.153837712 0.433764251
Si 9.355700627 12.250291144 7.694925632
Si 3.727435734 1.738336007 4.164023298
Si 3.906820214 1.525282679 11.585499934
Si 11.949703239 6.985976334 3.339309775
Si 11.917788181 6.921831416 10.804989823
Si 1.455648809 3.744652831 3.369541774
Si 1.449146883 3.438340838 10.876123822
Si 1.271971862 6.714784547 14.554162889
Si 11.662282191 10.143110418 7.075938723
Si 11.432776612 10.163800244 14.641077232
Si 6.297339165 11.912002008 7.272015289
Si 6.242761169 12.191969568 14.838508344
Si 3.877002911 1.703990369 7.276953566
Si 3.998494233 1.691563737 14.694515813
Si 6.778574241 1.783677330 3.518726299
Si 6.934570693 1.818728289 11.118662882
Si 9.485753686 12.168572563 3.450496034
Si 9.291535634 12.032648509 10.777030834
Si 1.301329337 6.810339999 3.967032284
Si 1.293602912 6.557585678 11.445996877
Si 11.640702222 9.999066063 3.991671116
Si 11.443999286 9.980317312 11.519459554
Si 11.965327019 7.130763547 0.249116120
Si 11.633667859 7.206007175 7.727960875
Si 1.606599739 3.576314702 0.250813587
Si 1.877049221 13.210847739 1.938404061
Si 1.916899791 13.071723331 9.297133425
Si 4.244245973 11.051315407 1.905153253
Si 4.253785472 10.960397101 9.362162145
Si 11.153470278 0.793267305 5.522813831
Si 11.038903089 0.612263608 13.131163743
Si 8.824649289 2.908891107 13.210695305
Si -0.196540934 10.914573397 1.713956763
Si -0.170146058 10.803469850 9.420129350
Si 2.173815186 8.748860588 1.674311264
Si 2.193897730 8.674538240 9.402565220
Si 13.238306530 3.126765653 5.631884372
Si 13.247258715 2.762259811 13.150334356
Si 10.866553093 5.195126566 5.614488248
Si 11.011616920 5.067311607 13.144010944
Si 1.601256394 3.667730790 7.837839560
Si 8.795764536 2.833933287 5.530344869
Al 1.011716461 6.755653768 7.127129838
Al 6.270936048 12.307932297 4.091624239
Al 6.034240422 12.229243185 11.667622999
Al 7.075039672 1.510173193 7.789181014
Rh1 3.480435502 8.092525694 6.413133700
Rh2 5.120614148 9.734569907 4.840376664
H 8.105436366 2.888273967 9.450175653
H 7.356969557 11.201760834 9.927680080
End final coordinates

Ru-O-Ru-H2MOR
Final enthalpy = -7137.1324145392 Ry
CELL_PARAMETERS (angstrom)
13.793841327 0.062828944 0.016195510
-1.370676814 13.614843944 -0.001938740
0.024795435 0.032047969 15.002588818

ATOMIC_POSITIONS (angstrom)
O 3.103751990 0.509089314 3.301214802
O 2.287764390 13.786210846 10.759788168
O 5.140112744 11.011373607 3.418370081
O 4.868738541 11.355320778 10.894742482
O 7.927027576 11.571040876 7.574111036
O 7.672478568 11.819857951 0.616175413
O 10.826393877 0.095193298 6.983809145

O	9.487573559	13.493696480	14.535197737
O	8.217084578	2.581438782	7.034623860
O	8.126336736	2.685655918	14.636559750
O	5.200259929	2.146948313	3.617342553
O	5.386096069	2.155897072	11.156400266
O	12.567068405	11.028067974	0.463480419
O	12.975012817	10.717118378	7.935391804
O	2.215522083	7.725662800	0.365273211
O	2.180409163	8.098670649	7.777041330
O	1.759210220	5.347051194	3.518829597
O	1.728261067	5.028898180	11.222595115
O	0.102907502	3.326475883	4.146083901
O	0.221061398	2.902104950	11.709800212
O	11.037441118	5.916715302	4.153201248
O	11.212930018	5.794732589	11.707525780
O	11.392010679	8.651423565	0.184437463
O	11.127494209	8.787908637	7.730868017
O	10.103817876	13.332472857	4.413865083
O	9.573440964	13.199938782	11.904112371
O	7.616769786	2.844484784	4.450923405
O	7.769539106	2.965560080	12.000406937
O	5.569411732	2.155652070	14.986744551
O	5.419487699	1.873516735	7.711881965
O	3.541330381	0.477489994	0.666003033
O	3.132171049	0.560427564	8.159493097
O	5.131357777	11.340771331	0.747195746
O	5.539521607	10.942878056	8.372986450
O	7.881245775	12.001752100	3.770540471
O	7.626587763	11.718635001	10.818855281
O	0.609480610	3.023954116	6.739982223
O	0.559286427	2.787097368	14.362355208
O	10.732402084	6.342722037	6.784363286
O	11.093170861	6.213734325	14.338034705
O	11.342968455	8.479095929	3.521505919
O	11.385925991	8.403101494	11.266332490
O	12.806155430	10.673365107	3.106787470
O	12.561012234	10.728728455	10.571975050
O	1.949632969	7.924227959	3.000126990
O	2.239502155	7.459400524	10.362033169
O	1.616381975	5.303045037	7.684654244
O	1.619812572	5.212892290	14.837152315
O	3.090358423	12.148047704	2.224776480
O	3.172758990	12.062076928	8.928191311
O	9.906428688	1.742501620	5.126162327
O	9.931855588	1.766235628	12.902623611
O	0.912884103	9.779688051	1.419849735
O	0.972605428	9.625149033	9.588031600
O	12.181499931	4.315403413	5.954687663
O	12.219485343	4.005560525	13.393749144
O	3.763049479	1.264779218	5.715402962
O	3.909332033	1.174057012	13.165534967
O	5.897289700	11.547883366	5.803508566
O	6.295695092	11.796001518	13.379150359
O	9.823836798	12.512824707	1.954269035
O	9.660897398	12.542447333	9.332742325
O	7.283720236	1.985932874	2.009284687
O	7.526516654	2.139125519	9.555344751
O	12.165567764	9.998272375	5.550775099
O	11.891935313	10.263960790	13.072202798
O	1.765307073	7.170362369	5.485450876
O	1.646635581	7.054576278	12.899576074
O	1.256824834	3.400478737	1.796362561
O	1.127669876	3.251648530	9.296271814
O	11.954744034	6.588185240	1.781434867
O	11.543296784	6.659498591	9.273043652
O	2.761386567	3.022079097	3.992320372
O	2.836317698	2.679201353	11.259654733
O	10.021465224	10.898740925	14.836451968
O	10.500657237	11.274627861	7.154522302
O	10.217823696	10.764147101	3.883362459
O	10.011264912	10.648695757	11.215214862
O	3.125618392	3.048604040	14.913918929
O	3.121738078	3.132693763	7.526014540
O	7.302915477	0.154033577	0.076947745
O	7.449624895	-0.141829164	7.686851055
O	13.542557043	7.165048174	14.722640813
O	13.218682536	7.243235894	7.280359974
O	5.644881815	13.865206222	4.020515057
O	7.343728590	0.345897863	11.504707075
O	-0.338640485	6.901739264	3.941672556
O	-0.246110865	6.822688205	11.021514948
O	0.488974454	12.387658934	1.788767649
O	0.571444879	12.254530100	9.498686645
O	3.556089802	9.550361862	1.791485990
O	3.656683278	9.497598227	9.460558231
O	12.515893908	1.691532872	5.700163835
O	12.534445223	1.354593624	13.141274167
O	9.513943422	4.338424782	5.559677960
O	9.589940144	4.382911404	13.232523874
O	5.264880486	8.004096499	5.657121345
Si	7.049217365	1.709729274	0.441685664
Si	9.247137990	12.159613363	0.485437742
Si	9.388698110	12.281071262	7.733930618
Si	3.731313678	1.733658150	4.169555780
Si	3.929929225	1.541517998	11.584346590
Si	11.943655485	6.987820083	3.355321757
Si	11.938628923	6.939631327	10.816114811
Si	1.465810582	3.752052459	3.367640137
Si	1.481609183	3.467297169	10.855417597
Si	1.317986729	6.763834748	14.462734115
Si	11.691439125	10.178814681	7.092621101
Si	11.480656825	10.213852754	14.644341002
Si	6.340512631	11.938319711	7.360505531
Si	6.273575962	12.212375558	14.920814218
Si	3.891682251	1.717746829	7.278767982
Si	4.036398672	1.718624222	14.694945952
Si	6.789742174	1.771805796	3.547713872
Si	6.967980253	1.842361656	11.148497656
Si	9.450751761	12.152542657	3.507376151
Si	9.311187825	12.049495852	10.825975575
Si	1.272725164	6.820931509	3.951081967
Si	1.322674861	6.584080379	11.376669652
Si	11.632588725	9.998927734	4.012362009
Si	11.485197736	9.993419897	11.529051865
Si	11.988064001	7.143175090	0.257770268
Si	11.686825367	7.242543921	7.752142378
Si	1.619244382	3.603387061	0.228764539
Si	1.877372948	13.198687072	1.985552286
Si	1.961614043	13.081265978	9.326628877
Si	4.221153964	11.011273914	2.030588856
Si	4.296309455	10.996590093	9.446699496
Si	11.165632071	0.819573805	5.552462955
Si	11.074821810	0.650333535	13.140695936
Si	8.858329948	2.941563291	13.221854736
Si	-0.204410831	10.929100531	1.706047471
Si	-0.125026746	10.801916662	9.376689746
Si	2.150642072	8.753591991	1.625513599
Si	2.268987594	8.695083859	9.317115803
Si	13.246945848	3.128559815	5.638733302
Si	13.283629133	2.801644746	13.160179097
Si	10.865742039	5.216765534	5.615768508
Si	11.042862329	5.099001114	13.164652709
Si	1.626761204	3.710003170	7.804934974
Si	8.802908772	2.874066204	5.567625217
Al	1.082875720	6.819170361	7.117536160
Al	6.237590279	12.268139454	4.167689859
Al	6.045672066	12.255839793	11.757015556
Al	7.089404297	1.539234327	7.814822316
Ru1	3.496832885	8.210137276	6.124587286
Ru2	5.013539410	9.752457456	5.133793324
H	8.132920340	2.899168204	9.470447356
H	7.352155118	11.180682470	10.043705591

End final coordinates

M-M-H2MOR Structures (after auto-reduction)

Cu-Co-H2MOR

Final enthalpy = -6607.4089232649 Ry

CELL_PARAMETERS (angstrom)

13.786920051	0.054593475	0.031073685
-1.378050967	13.597660702	0.002624278
0.040917968	0.038682755	15.008657847

ATOMIC_POSITIONS (angstrom)

O	3.080676810	0.518110884	3.299592879
O	2.323515794	13.754000683	10.776399437
O	4.985321204	11.012460047	3.511814865
O	4.857919654	11.384821450	10.931037596
O	7.939337092	11.528340940	7.569506824
O	7.672787798	11.777418821	0.614922192
O	10.866911576	0.059700697	6.994053769
O	9.501040324	13.484536252	14.578906936
O	8.286828031	2.524023559	7.078813015
O	8.130820421	2.723676174	14.688233761
O	5.229345289	2.086086778	3.649285684
O	5.388742276	2.174571363	11.154268486
O	12.557469956	11.014988542	0.433938255
O	13.042445036	10.694554629	7.929727838
O	2.225071956	7.702468959	0.363409413
O	2.204450116	8.166049814	7.791371337
O	1.755123235	5.343054754	3.416313483
O	1.736090349	4.996604036	11.224578934
O	0.148435787	3.305304043	4.143926865
O	0.202003085	2.885604821	11.677007705
O	11.067407167	5.820114054	4.130930928
O	11.189000353	5.788175458	11.700192950
O	11.390949718	8.638553314	0.196506895
O	11.222650224	8.741751817	7.737166556
O	10.064234959	13.279040995	4.420042793
O	9.549110150	13.180824865	11.939731603
O	7.642327531	2.780150403	4.507938973
O	7.757533421	2.986767210	12.053490206
O	5.580769922	2.132771052	15.063724563
O	5.469181643	1.840047207	7.658502022
O	3.490766503	0.470490876	0.657534887
O	3.174302902	0.559461698	8.167808452
O	5.142425683	11.375581268	0.841307284
O	5.535842151	10.887875595	8.412459476
O	7.863986123	11.875578512	3.785252078
O	7.608364221	11.699486597	10.875574276
O	0.657561855	3.069936426	6.737096292
O	0.577766880	2.781967110	14.334108419
O	10.822407481	6.322253515	6.756083073
O	11.118844082	6.221005200	14.336501473
O	11.319978625	8.407195884	3.591860962
O	11.386856212	8.385047300	11.214259210
O	12.779673274	10.583785119	3.077814807
O	12.518635398	10.738544609	10.547849226
O	1.922423116	7.949795195	3.000763583
O	2.236630434	7.422937313	10.352540254
O	1.714924983	5.318214037	7.739703248
O	1.618257224	5.199417496	14.862545848
O	3.000256241	12.111341437	2.220749034
O	3.176075366	12.027786108	8.922153195
O	9.993426488	1.765614743	5.159387125
O	9.913286343	1.761612651	12.947609749
O	0.917798940	9.789024519	1.372549450
O	0.978833197	9.627040935	9.666800204
O	12.159917555	4.207769029	5.958090446
O	12.235656460	4.015361305	13.393130348
O	3.742131937	1.247014842	5.714365567
O	3.983208723	1.151524131	13.182037074
O	5.834308554	11.596169233	5.899388589
O	6.245920207	11.768474391	13.424690722
O	9.810319486	12.436830592	1.975712261
O	9.632187816	12.522231088	9.362564489
O	7.313409110	1.957562953	2.049179319
O	7.531886304	2.177816044	9.596346643
O	12.195427083	9.995543320	5.556728594
O	11.898621999	10.215046125	13.056129576
O	1.839742656	7.115403776	5.444488812
O	1.696160995	7.016105138	12.904443852
O	1.275356015	3.326647826	1.778251578
O	1.187648845	3.218510059	9.288073735
O	11.966276311	6.577570817	1.783557764
O	11.623799560	6.607025934	9.255853382
O	2.809185875	3.045243885	3.972070163
O	2.819384322	2.631489374	11.313422214
O	10.035061358	10.886484319	14.817286082
O	10.531627861	11.221637535	7.219573767
O	10.215387495	10.703479211	3.918469697
O	9.991637177	10.625587939	11.235729765
O	3.147006521	3.046344454	14.885171097
O	3.179537275	3.131321630	7.525078483
O	7.351577433	0.168616699	0.078018897
O	7.498195163	-0.160893636	7.881737917
O	13.563677959	7.171574430	14.725907443
O	13.318539129	7.187220337	7.269280669
O	5.683732298	13.790506980	4.039711951
O	7.350714514	0.374162186	11.551043116

O -0.327273711 6.875728697 3.938811993
O -0.237615107 6.795931352 11.074740755
O 0.414095857 12.387174309 1.814683851
O 0.579927275 12.254837472 9.512818059
O 3.545226463 9.541380297 1.775095450
O 3.654816709 9.487629573 9.555974918
O 12.611507468 1.609258452 5.707610830
O 12.523284162 1.356042164 13.152061759
O 9.498000423 4.341672755 5.596056086
O 9.602764274 4.386631862 13.260527731
Si 7.061927697 1.708305733 0.480201467
Si 9.245619777 12.122508655 0.494146891
Si 9.403657233 12.234541262 7.760376451
Si 3.736471135 1.728019379 4.170592142
Si 3.952852804 1.527214369 11.603426049
Si 11.952985598 6.935107039 3.368308264
Si 11.953845414 6.911425163 10.808908482
Si 1.492214962 3.739192899 3.336549434
Si 1.490814280 3.437285078 10.855506043
Si 1.341707133 6.749432786 14.465493059
Si 11.744466801 10.149352353 7.108963611
Si 11.490622552 10.194296947 14.629555093
Si 6.351336070 11.924023044 7.443212082
Si 6.285681187 12.207569658 14.959299239
Si 3.926496167 1.709007785 7.271525126
Si 4.056969539 1.710312813 14.709417923
Si 6.821564976 1.718994593 3.585276972
Si 6.972246281 1.867436232 11.184280997
Si 9.433760411 12.076312202 3.527771577
Si 9.292473285 12.030649692 10.858520887
Si 1.288236214 6.799707280 3.944410153
Si 1.339199881 6.553418962 11.384588966
Si 11.629758999 9.937552602 4.031084971
Si 11.473315309 9.969058576 11.512475345
Si 11.995516911 7.133336646 0.261970507
Si 11.790002456 7.197400577 7.736212259
Si 1.619480900 3.576460291 0.212190482
Si 1.810618376 13.188391255 1.986263798
Si 1.979445122 13.063106771 9.340965320
Si 4.169148611 11.010385624 2.059014735
Si 4.296312212 10.978750118 9.495419274
Si 11.219789382 0.790393896 5.568326576
Si 11.066261591 0.651214604 13.170419999
Si 8.857376527 2.954548087 13.265659779
Si -0.227753419 10.906462757 1.676573335
Si -0.108868015 10.796620621 9.385135441
Si 2.137585739 8.744337559 1.609187551
Si 2.267551167 8.690515397 9.344219597
Si 13.288577460 3.082102668 5.650091178
Si 13.282427909 2.796843284 13.157003549
Si 10.889561541 5.165814460 5.614084839
Si 11.053136870 5.104020898 13.167261111
Si 1.689189599 3.724554581 7.811944498
Si 8.845015612 2.848245087 5.607470207
Al 1.214804281 6.823764890 7.095320955
Al 6.238141073 12.174869074 4.215639055
Al 6.034255064 12.267383724 11.807087290
Al 7.132089179 1.525228780 7.872508563
Cu1 3.096357049 8.675846734 6.056086640
Co2 4.206588319 10.639424368 5.300394990
H 8.176357909 2.905765486 9.515840698
H 7.332467117 11.108967904 10.141710369
End final coordinates

Cu-Cr-H2MOR
Final enthalpy = -6693.6366023761 Ry
CELL_PARAMETERS (angstrom)
13.792356203 0.056414317 0.014250503
-1.376825279 13.612394944 0.004446973
0.022656401 0.038961418 15.018804835

ATOMIC_POSITIONS (angstrom)
O 3.098669506 0.538088567 3.286459358
O 2.324949340 13.775578665 10.773263279
O 5.097862571 10.983794184 3.470177705
O 4.936730626 11.378075314 10.833335486
O 7.931730342 11.511932224 7.614881803
O 7.680717362 11.758569905 0.562744935
O 10.831893084 0.025975776 6.966592519
O 9.476780251 13.497425760 14.557503336
O 8.269797618 2.508974984 7.073481611
O 8.114198333 2.706406653 14.664509966
O 5.211439200 2.144832212 3.633656420
O 5.377171584 2.188643428 11.173153172
O 12.584240473 11.047380976 0.417789932
O 13.044021665 10.680225997 7.936282952
O 2.252873178 7.744599224 0.337165761
O 2.101107534 8.200384935 7.826155883
O 1.722000756 5.342856709 3.518144900
O 1.726224521 5.007775868 11.259766125
O 0.107777488 3.278215462 4.146993428
O 0.205128956 2.879485508 11.690598773
O 11.028565434 5.839634180 4.135438715
O 11.141769794 5.822751983 11.694422748
O 11.427888312 8.661447609 0.184348379
O 11.204023778 8.744814114 7.710421508
O 10.095389996 13.316583268 4.393760376
O 9.589357268 13.226794303 11.924384169
O 7.629394867 2.792725426 4.504942662
O 7.764441779 3.001017681 12.030170334
O 5.569392037 2.115773730 15.034360627
O 5.451679153 1.836980000 7.685769228
O 3.532877566 0.427450356 0.649221228
O 3.153042907 0.562350097 8.167059993
O 5.136940723 11.368877797 0.821849068
O 5.456943933 10.853926565 8.279021695
O 7.877129213 11.962398573 3.745593435
O 7.629203157 11.734937438 10.909789677
O 0.645094749 3.063955516 6.739558167
O 0.561969522 2.830431196 14.356290166
O 10.770400268 6.319822453 6.762780113
O 11.116753483 6.244660376 14.323646430
O 11.282733480 8.429627279 3.595847799
O 11.394421152 8.416423505 11.200458715
O 12.775606010 10.581753859 3.053189341
O 12.491046859 10.796064840 10.544356794
O 1.891446898 7.908885112 2.958482496
O 2.208838565 7.439988978 10.382982410
O 1.721753905 5.329483359 7.688390628
O 1.665234901 5.221070833 14.887729748
O 3.049808154 12.130127748 2.269762844
O 3.157199412 12.043475230 8.929995157
O 9.963657837 1.740759759 5.145171946
O 9.912697516 1.772804777 12.929638782
O 0.932401994 9.805472679 1.371287824
O 0.956301496 9.661065996 9.749302233
O 12.157094501 4.232249934 5.949925697
O 12.234253335 4.047156689 13.354928573
O 3.763950739 1.255065559 5.712781872
O 3.934487843 1.160842905 13.180284785
O 5.928273512 11.571406218 5.830919405
O 6.177750998 11.808558980 13.416519973
O 9.815976145 12.469121604 1.937411463
O 9.635901677 12.545372344 9.363652635
O 7.298295597 2.011788448 2.033561339
O 7.521788215 2.155944274 9.586366548
O 12.185148694 10.031051252 5.545479166
O 11.911122876 10.231305993 13.053688724
O 1.766035785 7.214041884 5.454038585
O 1.640317856 7.034059053 12.923498978
O 1.263746073 3.377114261 1.799996061
O 1.160510308 3.272230503 9.289132030
O 11.900445782 6.592100387 1.781124814
O 11.577349469 6.623651464 9.254069815
O 2.774346962 3.042329800 4.001883924
O 2.812701484 2.642760928 11.281738943
O 10.041627391 10.901669496 14.806670215
O 10.530864323 11.227431421 7.235028152
O 10.211556274 10.742547208 3.890849242
O 9.984434876 10.648108793 11.252604100
O 3.125625301 3.018694384 14.940438812
O 3.162152533 3.128369604 7.529625468
O 7.369887104 0.159481484 0.128331296
O 7.474385410 -0.186187758 7.808685112
O 13.569730230 7.150771506 14.795508042
O 13.277735042 7.149512300 7.259981183
O 5.633035580 13.835667304 4.001298630
O 7.331210106 0.385057238 11.556278353
O -0.368078411 6.889384885 3.927275374
O -0.269487279 6.778881703 11.077170928
O 0.451675007 12.385416896 1.839455705
O 0.559415026 12.283572152 9.515917712
O 3.552359707 9.538750633 1.829441914
O 3.624665104 9.490978390 9.552920289
O 12.573840981 1.623539414 5.742945226
O 12.523165472 1.384873151 13.180490743
O 9.494441729 4.321530795 5.600360349
O 9.595692025 4.395078008 13.277489502
Si 7.064190529 1.711165624 0.468916706
Si 9.250659069 12.132486469 0.459743888
Si 9.397030105 12.233852781 7.769025697
Si 3.732809850 1.746380697 4.173453382
Si 3.935028359 1.536078227 11.600219221
Si 11.911506166 6.953491993 3.364770733
Si 11.928497139 6.929171155 10.800585060
Si 1.461469739 3.746818637 3.372496469
Si 1.478114072 3.456199353 10.858083511
Si 1.340753861 6.762931094 14.492520181
Si 11.743900409 10.155320823 7.105336009
Si 11.502956030 10.217096725 14.626623046
Si 6.353025960 11.910571631 7.410128282
Si 6.261245945 12.216105978 14.957849197
Si 3.913263533 1.708862180 7.275710520
Si 4.037411243 1.691644934 14.716399040
Si 6.796662811 1.761486173 3.564022748
Si 6.959441981 1.878352372 11.181145775
Si 9.451855538 12.126273801 3.494324411
Si 9.311435064 12.063477103 10.865983846
Si 1.247711994 6.823376386 3.964589056
Si 1.309040071 6.562501345 11.402378800
Si 11.619541596 9.960588491 4.011610269
Si 11.472620261 9.997031304 11.512491213
Si 12.001108073 7.143678731 0.262298235
Si 11.754736357 7.194084272 7.728908982
Si 1.631776696 3.598571002 0.236053733
Si 1.846983618 13.191972649 2.002028533
Si 1.965232713 13.081036341 9.341153994
Si 4.190460383 11.010106876 2.063521186
Si 4.278803971 10.970343117 9.437365306
Si 11.203249508 0.783857889 5.560285808
Si 11.071649168 0.671302655 13.164595105
Si 8.853280172 2.960997459 13.253233853
Si -0.214499499 10.917659025 1.684890763
Si -0.124955353 10.821002937 9.411516895
Si 2.140528787 8.750654985 1.609595316
Si 2.220936433 8.706226096 9.368433336
Si 13.268843773 3.086363722 5.649261100
Si 13.283679014 2.824892628 13.153655227
Si 10.869895856 5.171309054 5.615125327
Si 11.038704955 5.125970200 13.157074571
Si 1.676792302 3.740285982 7.802934075
Si 8.831664391 2.836081926 5.604499110
Al 1.182208867 6.847527953 7.102880940
Al 6.251053362 12.255729440 4.169624895
Al 6.022445435 12.292017675 11.787828330
Al 7.113855934 1.504571316 7.859464027
Cu1 2.927014475 8.864196577 6.035092843
Cr2 4.823768892 10.052190874 5.197885089
H 8.156987377 2.891216117 9.493293419
H 7.366167227 11.055338517 10.255175680
End final coordinates

Cu-Cu-H2MOR
Final enthalpy = -6658.4871208241 Ry
CELL_PARAMETERS (angstrom)
13.783985866 0.056985222 0.034084118
-1.375413209 13.601955039 0.004248833
0.044189449 0.040773671 15.002721993

ATOMIC_POSITIONS (angstrom)
O 3.085918919 0.532148444 3.290253503
O 2.325107098 13.765023057 10.769466350
O 5.033267680 10.985889008 3.498829465
O 4.872499413 11.374196046 10.923533024
O 7.978470583 11.536404616 7.656563154
O 7.673496823 11.787444582 0.622588311
O 10.882869946 0.066612594 7.000827357
O 9.511515219 13.505123529 14.602571800
O 8.295190525 2.520050968 7.080352275
O 8.111300114 2.738836163 14.683985479

O 5.229232865 2.113220497 3.651032123
O 5.380949818 2.185206952 11.149684630
O 12.562091742 11.015296375 0.434155428
O 13.073961865 10.671560813 7.929264978
O 2.216545877 7.693133496 0.381386771
O 2.168557822 8.200937284 7.773555387
O 1.752233884 5.351471428 3.384387533
O 1.731000442 5.001593712 11.224560332
O 0.141570039 3.328534798 4.136439794
O 0.197675856 2.884024460 11.665349143
O 11.062614291 5.819058604 4.132402654
O 11.182203527 5.791168575 11.690180144
O 11.374725033 8.644362375 0.189034487
O 11.220063626 8.747293022 7.738645538
O 10.087026206 13.287499011 4.429201137
O 9.542147752 13.179952369 11.969203633
O 7.649726882 2.772514936 4.511159970
O 7.752618679 2.989521786 12.049575443
O 5.570111541 2.125514564 15.067833421
O 5.480299083 1.822649971 7.646773352
O 3.478151827 0.459166372 0.653214066
O 3.181543756 0.555321714 8.161545702
O 5.134336876 11.384484443 0.828759053
O 5.546909145 10.892278965 8.400638992
O 7.862711800 11.920939972 3.779261618
O 7.622188484 11.728317420 10.849071011
O 0.680484071 3.092927133 6.722992779
O 0.571918278 2.781676005 14.320392285
O 10.809347541 6.333348403 6.754332267
O 11.114281522 6.226517725 14.319195770
O 11.293522243 8.410765410 3.601830971
O 11.383367551 8.392774741 11.211973794
O 12.753812971 10.582626116 3.074892797
O 12.513909053 10.747552135 10.542683235
O 1.945835041 7.969201004 3.027692133
O 2.231776498 7.419502933 10.329717616
O 1.754057863 5.320407564 7.757344910
O 1.611840095 5.200779656 14.842335395
O 3.019944869 12.119351491 2.233196195
O 3.177382975 12.022336434 8.932809341
O 10.008677690 1.768872183 5.160764540
O 9.897776250 1.758406509 12.963375771
O 0.909599519 9.775869315 1.388815555
O 0.996843493 9.646400624 9.697064805
O 12.168585774 4.227147750 5.967694462
O 12.228696849 4.019177572 13.377789539
O 3.734888543 1.264762185 5.707246030
O 3.983057724 1.146744404 13.175686776
O 5.934091193 11.621351897 5.911779321
O 6.270242685 11.787384033 13.413827619
O 9.825346469 12.428097519 1.986845109
O 9.690767678 12.563821271 9.388489076
O 7.308958351 1.964024010 2.052632829
O 7.527130207 2.195121040 9.593710397
O 12.199527951 9.991324767 5.560166416
O 11.904198948 10.223087727 13.051485079
O 1.790562355 7.094626176 5.440431267
O 1.689329977 7.029712704 12.896846082
O 1.262971400 3.326951518 1.766676335
O 1.186568821 3.223119421 9.285062836
O 11.929702945 6.584670069 1.773857857
O 11.605823724 6.607868137 9.258487448
O 2.802680677 3.056008757 3.961671908
O 2.815917670 2.637556331 11.312940898
O 10.038063694 10.902784404 14.809557525
O 10.568230860 11.245412780 7.245490026
O 10.198530696 10.712644495 3.949302696
O 9.991293437 10.634812402 11.239082892
O 3.139592228 3.043249412 14.872652922
O 3.198143349 3.128993494 7.537853174
O 7.352788479 0.175761122 0.075482372
O 7.530962032 -0.159588284 7.920483378
O 13.558544862 7.183468515 14.728090935
O 13.310309256 7.174423872 7.285654235
O 5.658245064 13.796288504 4.032894148
O 7.334990248 0.376751099 11.535246697
O -0.337118594 6.889590296 3.894973276
O -0.239783221 6.804360593 11.064425565
O 0.427696504 12.375097553 1.832221858
O 0.577386884 12.267064918 9.505995744
O 3.549670037 9.547029693 1.769352035
O 3.670042639 9.480014195 9.529094814
O 12.620268490 1.625404506 5.716265643
O 12.514397981 1.362067648 13.144512143
O 9.501435059 4.335837536 5.605035616
O 9.594982085 4.391652101 13.253968664
Si 7.051907200 1.711020706 0.485811207
Si 9.247146231 12.130763161 0.507466897
Si 9.440501583 12.257522576 7.792671381
Si 3.737557947 1.741601022 4.163390206
Si 3.949210105 1.530707026 11.599549917
Si 11.927446654 6.941801346 3.357730397
Si 11.946752310 6.918739880 10.807810362
Si 1.486852370 3.743735672 3.321578174
Si 1.488328711 3.440874369 10.853525773
Si 1.338288034 6.755105653 14.459862915
Si 11.758852362 10.152331285 7.116086833
Si 11.490790039 10.205218681 14.623755216
Si 6.393458434 11.937039591 7.457819465
Si 6.290890200 12.219452359 14.953045061
Si 3.936125327 1.703036117 7.266314200
Si 4.049221385 1.704094652 14.704333890
Si 6.815726386 1.722379018 3.587408785
Si 6.964251144 1.874099729 11.177700862
Si 9.433533904 12.092298823 3.540184742
Si 9.306546762 12.048708529 10.866555399
Si 1.272277120 6.796382886 3.920639695
Si 1.335985870 6.559372575 11.377092268
Si 11.611050460 9.941667331 4.039969748
Si 11.471310472 9.976947791 11.510749030
Si 11.980243336 7.139970549 0.252643818
Si 11.776645538 7.199459970 7.741861987
Si 1.610210207 3.575415665 0.200966527
Si 1.822717602 13.185913986 1.993693836
Si 1.985237235 13.065205159 9.338405010
Si 4.186375959 11.012351219 2.071117250
Si 4.309821382 10.977007222 9.485169673
Si 11.234090464 0.795078036 5.573700855
Si 11.058848864 0.656562398 13.185273310
Si 8.847081200 2.959753422 13.265727323
Si -0.229998855 10.903485075 1.682206153
Si -0.099923896 10.803506379 9.389984427
Si 2.144247559 8.749938475 1.616692234
Si 2.269588235 8.703658566 9.341836417
Si 13.294219050 3.099001956 5.651755283
Si 13.274102370 2.799669080 13.147283190
Si 10.885828484 5.169253187 5.618773826
Si 11.045614966 5.105588318 13.154936838
Si 1.709052539 3.723634656 7.815460962
Si 8.851359303 2.840611288 5.609290775
Al 1.206688161 6.802611635 7.112873613
Al 6.230618960 12.189948049 4.225511444
Al 6.044196466 12.273644073 11.792600515
Al 7.143745877 1.519563735 7.875833682
Cu1 2.750254015 8.806711359 5.972116842
Cu2 4.519861248 10.311774854 5.312795488
H 8.160508986 2.932523630 9.515510481
H 7.352554656 11.174683408 10.083961003
End final coordinates

Cu-Fe-H2MOR
Final enthalpy = -6587.1456643566 Ry
CELL_PARAMETERS (angstrom)
13.798378313 0.056039406 0.021027058
-1.377770170 13.601465580 -0.003911402
0.030050643 0.030473310 15.019494012

ATOMIC_POSITIONS (angstrom)
O 3.107234201 0.522603846 3.293302608
O 2.312771371 13.766369982 10.768145896
O 5.084501364 10.986767713 3.439601182
O 4.909501367 11.354247104 10.874214704
O 7.942884171 11.530172812 7.628124280
O 7.679034615 11.782500513 0.597671286
O 10.848714124 0.051137231 6.987482479
O 9.483690452 13.491998243 14.576620046
O 8.264965878 2.536772252 7.064151654
O 8.124648922 2.707240260 14.682298775
O 5.223234409 2.131844250 3.646316139
O 5.385454580 2.170071185 11.161973044
O 12.584702249 11.026199427 0.430083523
O 13.047953102 10.679423535 7.929016458
O 2.221931104 7.704111470 0.371081505
O 2.138073153 8.155462728 7.821935674
O 1.735155175 5.336293214 3.447326366
O 1.720749230 4.997727740 11.218680942
O 0.128342325 3.292466741 4.149355956
O 0.195174497 2.884729116 11.696281301
O 11.064574155 5.840912141 4.135894876
O 11.194994318 5.780808090 11.696205328
O 11.408485088 8.652812455 0.177467485
O 11.215201799 8.740336869 7.730361943
O 10.085914798 13.295713332 4.408902558
O 9.562985015 13.183783031 11.941207087
O 7.641300011 2.809179668 4.490593950
O 7.759356630 2.975124590 12.047261628
O 5.573011228 2.126810771 15.059821204
O 5.456599442 1.841237004 7.676841999
O 3.509783374 0.455766882 0.651223929
O 3.164914715 0.549916616 8.164853058
O 5.140125285 11.343547073 0.767191336
O 5.494483641 10.876594332 8.328142030
O 7.872393421 11.941529323 3.746978887
O 7.632209981 11.710788538 10.853312330
O 0.641153555 3.050113969 6.746436160
O 0.567804368 2.777674133 14.350251241
O 10.795976844 6.318293372 6.768730589
O 11.107339072 6.227488735 14.323769175
O 11.312280330 8.424191237 3.573023965
O 11.392421176 8.389101967 11.230152597
O 12.780039913 10.602366803 3.076814837
O 12.515506081 10.751338900 10.545895692
O 1.948102769 7.929210590 3.007967786
O 2.233422799 7.440308595 10.395678061
O 1.692938021 5.297634762 7.751218794
O 1.620009999 5.188870984 14.892782753
O 3.064773566 12.133744762 2.214977329
O 3.167025929 12.029294760 8.936653783
O 9.973811682 1.756799316 5.154386494
O 9.915273344 1.760697873 12.940486331
O 0.911120765 9.770028885 1.402466140
O 0.971696974 9.642373550 9.706764209
O 12.171447376 4.229958215 5.952531154
O 12.231141276 4.011652275 13.400980260
O 3.753106647 1.249601424 5.713482664
O 3.969570696 1.148898258 13.186271088
O 5.921894507 11.563521482 5.850784909
O 6.267382537 11.788894888 13.397853492
O 9.830419550 12.452983182 1.955435331
O 9.674556223 12.537923711 9.365025079
O 7.305780095 1.972839320 2.041356026
O 7.530127877 2.167740960 9.586926720
O 12.185753244 10.003406672 5.550977746
O 11.907118309 10.234379423 13.058463422
O 1.789078887 7.129764070 5.460875023
O 1.674690140 6.993841831 12.930067180
O 1.265125937 3.326286461 1.789869192
O 1.173461046 3.196553968 9.300747883
O 11.928074830 6.580100470 1.768406707
O 11.614956950 6.616896708 9.263239397
O 2.790904980 3.039868681 3.987149663
O 2.819268415 2.644754254 11.322220420
O 10.042524981 10.893378645 14.821350588
O 10.530519054 11.222230538 7.220782421
O 10.209281075 10.722093013 3.903865660
O 9.997415205 10.626625463 11.235904002
O 3.132708232 3.026577923 14.912910359
O 3.163495706 3.120371330 7.529176056
O 7.344698300 0.163768698 0.090580773
O 7.486075717 -0.163037874 7.822138828
O 13.561117306 7.150013743 14.751040465
O 13.297843888 7.161089508 7.255837948
O 5.655011447 13.825762710 4.038131410
O 7.344582576 0.363270615 11.530314472
O -0.339143164 6.895848723 3.902394408
O -0.248226121 6.800544552 11.087624877
O 0.459836497 12.368715327 1.823561644
O 0.564201459 12.263855147 9.510374243
O 3.548324503 9.541173490 1.783903379
O 3.644355672 9.478673459 9.529188580

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O 12.525133359 1.355447732 13.167334220
O 9.506072206 4.338398641 5.590045307
O 9.597807189 4.384018032 13.259247621
Si 7.062012722 1.711061185 0.472528010
Si 9.252355072 12.135115996 0.479522405
Si 9.412519920 12.241029390 7.770306212
Si 3.740141285 1.736883237 4.173158171
Si 3.944920999 1.529956436 11.608279960
Si 11.942334386 6.948370953 3.351345515
Si 11.954513417 6.915927778 10.814733288
Si 1.475813864 3.733436967 3.350722715
Si 1.480304825 3.434173122 10.865617637
Si 1.328678260 6.734674068 14.492525340
Si 11.743422944 10.148278295 7.107570141
Si 11.501021470 10.205307138 14.632815610
Si 6.361704210 11.921554639 7.415528835
Si 6.283745077 12.203436858 14.939530201
Si 3.918245520 1.701683861 7.274467324
Si 4.048086135 1.697158920 14.717405172
Si 6.809540475 1.750521016 3.577762804
Si 6.968175918 1.859909894 11.176685310
Si 9.446856018 12.105365257 3.507205602
Si 9.315400353 12.038369442 10.854712849
Si 1.273694893 6.801709951 3.951264651
Si 1.327096949 6.552646856 11.402665164
Si 11.623900067 9.952485672 4.022601031
Si 11.480557360 9.975989032 11.516800669
Si 11.993951578 7.139639596 0.248588806
Si 11.776086032 7.193130893 7.738056277
Si 1.618925645 3.572630132 0.225570997
Si 1.849082632 13.185306895 1.984107628
Si 1.969414559 13.064041971 9.337638597
Si 4.201297402 11.006378246 2.022323409
Si 4.292094220 10.964971388 9.455835567
Si 11.207332768 0.792162725 5.567507936
Si 11.067426987 0.652425448 13.176173431
Si 8.855487961 2.948878154 13.262637105
Si -0.219647336 10.905809655 1.690984594
Si -0.118826632 10.801668008 9.396175700
Si 2.141736809 8.738061082 1.622768722
Si 2.244475903 8.689455727 9.362768215
Si 13.282939994 3.084918574 5.649499048
Si 13.283309125 2.796557358 13.164671605
Si 10.889182213 5.174912744 5.614947991
Si 11.049995755 5.100372890 13.163751480
Si 1.671782913 3.703968032 7.822900264
Si 8.837033486 2.854455085 5.597323638
Al 1.187400388 6.803607417 7.116351881
Al 6.245170883 12.227852522 4.178825207
Al 6.048094999 12.261031333 11.773532723
Al 7.121681778 1.524518511 7.857020079
Cu1 2.894509334 8.794556209 6.035071094
Fe2 4.701859417 10.129184527 5.198712992
H 8.165420342 2.904074337 9.509279703
H 7.363124715 11.106867936 10.128922084
End final coordinates

Cu-Mn-H2MOR
Final enthalpy = -6731.9753736141 Ry
CELL_PARAMETERS (angstrom)
13.790564672 0.060799143 0.014515220
-1.372316612 13.608268674 -0.006098014
0.023018709 0.027377489 15.021865647

ATOMIC_POSITIONS (angstrom)
O 3.106222525 0.529821354 3.287199899
O 2.317654411 13.768330114 10.760269267
O 5.106272142 10.999389809 3.424643263
O 4.914909527 11.357445858 10.855175410
O 7.952950379 11.524859357 7.629378590
O 7.685217724 11.774759280 0.571942540
O 10.847345275 0.044349569 6.978920033
O 9.484527327 13.499955955 14.570004690
O 8.264239989 2.532190413 7.070446968
O 8.107141112 2.708249388 14.674904363
O 5.214509996 2.145613663 3.633928857
O 5.369498334 2.181807971 11.163746456
O 12.587938105 11.034081972 0.419141320
O 13.057180783 10.662750362 7.931914914
O 2.237335467 7.719539212 0.363678100
O 2.094804084 8.166116885 7.835774804
O 1.733129732 5.341460981 3.469945325
O 1.719180519 4.997594623 11.226842833
O 0.113955901 3.299752199 4.148387446
O 0.190125445 2.880896503 11.693084305
O 11.050653130 5.847836420 4.137546940
O 11.165463401 5.797564715 11.688877349
O 11.406305540 8.663044540 0.173633164
O 11.200572287 8.747225749 7.716451466
O 10.091811853 13.311433252 4.392674029
O 9.567124216 13.201402566 11.935500080
O 7.630876483 2.804643541 4.495731502
O 7.748956827 2.982721383 12.040334020
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O 5.453311910 1.834134619 7.685957983
O 3.502644772 0.446909505 0.644133391
O 3.159031099 0.543148971 8.156788171
O 5.132619414 11.358434035 0.752349109
O 5.495300801 10.876249238 8.309628546
O 7.874853190 11.957001765 3.737303709
O 7.632753444 11.728320797 10.853110330
O 0.646738857 3.051895219 6.738305176
O 0.556268832 2.798599676 14.355870274
O 10.760381850 6.323967204 6.764777779
O 11.105109307 6.236845901 14.312622853
O 11.289690767 8.433905138 3.580815362
O 11.388150121 8.401006288 11.212239626
O 12.769557858 10.602318083 3.061616925
O 12.500774077 10.769666745 10.539647380
O 1.947251746 7.928996897 3.000472709
O 2.230011124 7.441321386 10.406136272
O 1.700539945 5.304309756 7.730098847
O 1.626694326 5.197576139 14.909576698
O 3.067295531 12.141316659 2.219211355
O 3.163447762 12.026218138 8.925954231
O 9.956191143 1.742152441 5.150116883
O 9.902311566 1.762514650 12.941857262
O 0.923590978 9.781185662 1.398570078
O 0.979249177 9.656142425 9.746982343
O 12.164660506 4.245501625 5.959278390
O 12.220835993 4.026411477 13.376920304
O 3.765491518 1.252177232 5.710303288
O 3.953442923 1.141893849 13.182446981
O 5.948038384 11.553901626 5.834389241
O 6.249047781 11.801202787 13.387217119
O 9.828698483 12.461622369 1.940835839
O 9.670505522 12.554010905 9.363202867
O 7.302164753 1.987955102 2.035468664
O 7.517951547 2.166509730 9.584836535
O 12.188192842 10.014760050 5.545499242
O 11.913958906 10.227701638 13.051026784
O 1.761087789 7.157608346 5.462458125
O 1.647694512 6.995472958 12.936414661
O 1.270753000 3.337667867 1.795821616
O 1.165161425 3.214500415 9.294517385
O 11.885208353 6.590287277 1.766944690
O 11.585548384 6.622209468 9.254471323
O 2.777035878 3.039670864 4.001108507
O 2.802261617 2.633880894 11.315564595
O 10.045346854 10.904795771 14.798874747
O 10.549564405 11.238642246 7.227501163
O 10.206074093 10.737005806 3.903645521
O 9.990527275 10.640154514 11.241858969
O 3.123766822 3.018928754 14.914915642
O 3.161812149 3.116572614 7.534425782
O 7.362175512 0.164271799 0.099876203
O 7.487659753 -0.172286223 7.806768694
O 13.554776460 7.155868976 14.785385933
O 13.267792559 7.146896138 7.247694669
O 5.641672157 13.835287241 4.020894094
O 7.323574136 0.369243210 11.527921632
O -0.348117182 6.902812337 3.883108489
O -0.257067129 6.790486624 11.073169954
O 0.459726523 12.375248870 1.833075668
O 0.561871179 12.270808591 9.506033055
O 3.558205735 9.549297342 1.796131846
O 3.646022941 9.474562234 9.517232109
O 12.571600435 1.636411893 5.721876514
O 12.514611874 1.368368177 13.167327219
O 9.502167987 4.328621458 5.584591278
O 9.586330441 4.386336260 13.261506261
Si 7.060814711 1.710585928 0.467896110
Si 9.256705479 12.141482333 0.462357456
Si 9.418838814 12.246491522 7.768801497
Si 3.736370494 1.742492328 4.170869442
Si 3.932946770 1.526577250 11.604822896
Si 11.918629446 6.959037503 3.348319998
Si 11.936039543 6.921447730 10.802850861
Si 1.468148895 3.740478125 3.359894350
Si 1.471563858 3.437196396 10.861305089
Si 1.326201086 6.740537396 14.504798296
Si 11.749241667 10.152024051 7.104416763
Si 11.500603480 10.208114868 14.623114419
Si 6.372030442 11.918205078 7.400640222
Si 6.278842711 12.206037505 14.930872753
Si 3.916614482 1.699172991 7.274456682
Si 4.035384618 1.686873397 14.714682010
Si 6.799897085 1.756928884 3.569341494
Si 6.952099324 1.867331684 11.174384706
Si 9.448770276 12.119729395 3.494763642
Si 9.315778718 12.053977459 10.853606526
Si 1.264167439 6.813036965 3.951536014
Si 1.316950995 6.551722904 11.406023866
Si 11.618424761 9.962203269 4.019328269
Si 11.474223885 9.984690936 11.511151275
Si 11.985504907 7.148140476 0.250007102
Si 11.747947710 7.195608045 7.729556133
Si 1.623384997 3.582432261 0.231023529
Si 1.851210120 13.191345840 1.981675931
Si 1.970108532 13.065878813 9.329596758
Si 4.209707924 11.019692104 2.020022172
Si 4.293212811 10.962622729 9.439467370
Si 11.201307032 0.791460896 5.561494384
Si 11.060164780 0.659824618 13.175141184
Si 8.842372192 2.951649218 13.258643024
Si -0.213303921 10.909921916 1.689448021
Si -0.114354856 10.804353763 9.407986237
Si 2.151653399 8.746343362 1.622356744
Si 2.237134728 8.692513223 9.374109412
Si 13.270318502 3.096705679 5.646538233
Si 13.272311626 2.809253788 13.156710398
Si 10.875840270 5.179081868 5.614407959
Si 11.034103271 5.109959525 13.154195421
Si 1.672362435 3.711739481 7.815828503
Si 8.829386479 2.846843426 5.599692004
Al 1.169111476 6.810425965 7.114866268
Al 6.247158935 12.243872618 4.170876738
Al 6.041249940 12.272665735 11.761742685
Al 7.118951982 1.514390308 7.857127763
Cu1 2.856404528 8.835693644 6.051882204
Mn2 4.791351785 9.996825998 5.182348183
H 8.138934330 2.914395617 9.498465102
H 7.370886767 11.119913861 10.130173506
End final coordinates

Cu-Ni-H2MOR
Final enthalpy = -6631.0716219536 Ry
CELL_PARAMETERS (angstrom)
13.764826194 0.050604124 0.033679478
-1.379802647 13.594565866 0.008462154
0.043767250 0.045401077 14.998908943

ATOMIC_POSITIONS (angstrom)
O 3.063756584 0.541522839 3.291796546
O 2.346815977 13.748702443 10.775495463
O 5.070418097 10.926090359 3.473997051
O 4.835409111 11.390595298 10.937260334
O 7.946145252 11.502314957 7.591720876
O 7.645966246 11.752812758 0.640077490
O 10.851486532 0.056041857 6.999188335
O 9.462877467 13.486354069 14.595307686
O 8.287935074 2.505400522 7.090652599
O 8.104531923 2.745355883 14.687801202
O 5.209940948 2.116857624 3.646431555
O 5.387148794 2.189880118 11.155525527
O 12.532377138 11.043186057 0.419826732
O 13.060983813 10.658209768 7.932139548
O 2.234715532 7.720566726 0.329359513
O 2.145238525 8.248724492 7.790616927

O 1.756575770 5.366396221 3.522093031
O 1.738763360 4.999557666 11.271619792
O 0.124914412 3.312024561 4.134390887
O 0.209290204 2.872280209 11.664927369
O 11.029830942 5.801101571 4.128222664
O 11.142437454 5.803007946 11.695129155
O 11.392901428 8.647083175 0.208467642
O 11.206541160 8.739013579 7.722811662
O 10.079892749 13.273908292 4.434676070
O 9.524766758 13.176888645 11.962212823
O 7.628846723 2.753207411 4.523217386
O 7.757048608 2.994890461 12.037796913
O 5.573283883 2.126164583 15.065193757
O 5.464733647 1.827287429 7.660144764
O 3.518456184 0.423752918 0.658219082
O 3.165417828 0.565084585 8.169922868
O 5.092237102 11.399645262 0.832791285
O 5.545852649 10.863914711 8.437721492
O 7.838382754 11.944661878 3.814100851
O 7.581209445 11.707517928 10.879789193
O 0.674883511 3.087474675 6.721361692
O 0.575686815 2.810252546 14.328706542
O 10.789633797 6.324927670 6.748403379
O 11.100813538 6.233741031 14.328186355
O 11.263763027 8.398244857 3.617107969
O 11.369962659 8.394923840 11.188187829
O 12.730812770 10.553620379 3.052990256
O 12.459920108 10.771806918 10.533671461
O 1.879036038 7.942422854 2.948002299
O 2.213933594 7.400720614 10.311794520
O 1.768421681 5.350037915 7.643487442
O 1.666407025 5.217227938 14.802252910
O 3.015707957 12.106779489 2.306292206
O 3.174315030 12.022633573 8.914979509
O 9.992838475 1.761712795 5.159255710
O 9.892515557 1.767812229 12.956816499
O 0.903986880 9.795365259 1.334452019
O 0.968952165 9.646012771 9.747548271
O 12.135172767 4.207595396 5.970145538
O 12.218429157 4.027321853 13.366959560
O 3.727498403 1.264149625 5.712898062
O 3.960640422 1.172291355 13.173234311
O 5.868436336 11.460269005 5.885095032
O 6.237391941 11.763675693 13.430167222
O 9.793040215 12.422667424 1.990217089
O 9.615219075 12.534008794 9.383600449
O 7.303241675 1.930217253 2.067191284
O 7.533680975 2.127908949 9.585294744
O 12.175881115 10.014235125 5.552151830
O 11.874933421 10.212541087 13.045113321
O 1.802264769 7.274400838 5.430250984
O 1.679167492 7.070401547 12.875563940
O 1.253879613 3.422404420 1.782697518
O 1.171107062 3.314611750 9.271477000
O 11.929243445 6.581263718 1.789885273
O 11.583474936 6.601241165 9.248328052
O 2.789696867 3.056696991 3.971005138
O 2.818885696 2.628427508 11.255838613
O 10.012070128 10.886989607 14.813802198
O 10.547111451 11.234330254 7.259257471
O 10.167919239 10.698054648 3.934234878
O 9.948087977 10.619318396 11.248260513
O 3.135800218 3.023630256 14.919415303
O 3.188589709 3.136999434 7.539332095
O 7.366481248 0.175318238 0.073299037
O 7.477780177 -0.199100468 7.768562256
O 13.551880088 7.153163219 14.734360841
O 13.293187925 7.161921905 7.271604952
O 5.596913694 13.772072247 4.075856073
O 7.334265831 0.378116660 11.571124851
O -0.353423051 6.883028623 3.948225436
O -0.252469948 6.777519521 11.062157717
O 0.424472555 12.374681182 1.840772036
O 0.576915087 12.265464414 9.517941920
O 3.531153211 9.537998879 1.775811240
O 3.642227142 9.484743852 9.569236606
O 12.602701105 1.609145870 5.729101875
O 12.500076211 1.362940391 13.167987709
O 9.470631989 4.330468782 5.606551931
O 9.583437511 4.396666557 13.270918126
Si 7.052790386 1.704967786 0.493172613
Si 9.217354095 12.109893872 0.512725105
Si 9.398117168 12.233365237 7.782368775
Si 3.720894809 1.743122231 4.170086815
Si 3.950995711 1.534288345 11.590239862
Si 11.905537838 6.931473494 3.375861888
Si 11.918876551 6.911510398 10.798256179
Si 1.477499228 3.770709302 3.355466172
Si 1.488269891 3.454222411 10.845121353
Si 1.352837151 6.767152288 14.434793911
Si 11.743647393 10.149553263 7.113609175
Si 11.473273104 10.207010746 14.619986235
Si 6.350934189 11.864250540 7.423347878
Si 6.270906226 12.211919026 14.962157808
Si 3.921239071 1.709225100 7.271660145
Si 4.051329856 1.696520888 14.712760293
Si 6.790718088 1.707498060 3.600114260
Si 6.967658273 1.867921574 11.181089873
Si 9.409857815 12.088299109 3.546506082
Si 9.264806211 12.033646755 10.874106488
Si 1.260907489 6.842659013 3.948988899
Si 1.326189097 6.557266140 11.373493777
Si 11.586717411 9.934509587 4.033287330
Si 11.438228094 9.975487143 11.503551575
Si 11.977201122 7.133081659 0.267180719
Si 11.763054652 7.190917356 7.730674848
Si 1.618817382 3.598181984 0.212121670
Si 1.824150452 13.172270928 2.015832462
Si 1.984100628 13.061676113 9.341706142
Si 4.168650446 10.997632730 2.079716020
Si 4.287576495 10.974310808 9.499252513
Si 11.216108773 0.785382194 5.576189269
Si 11.042543036 0.656097334 13.182657102
Si 8.839149041 2.964716930 13.266681620
Si -0.237932048 10.909174410 1.665499354
Si -0.112206847 10.807418789 9.401013894
Si 2.122788272 8.754502882 1.576051475
Si 2.241835029 8.710617373 9.358941666
Si 13.267348935 3.086091773 5.654271073
Si 13.262784949 2.802593966 13.149567010
Si 10.860346194 5.157197501 5.618201777
Si 11.030794534 5.113922915 13.160840513
Si 1.705485300 3.760495965 7.786108888
Si 8.835529626 2.830065369 5.615797024
Al 1.222280533 6.871418340 7.085752661
Al 6.191926472 12.172927410 4.235077974
Al 6.011794788 12.267290164 11.817492489
Al 7.124472137 1.487245769 7.849440444
Cu1 2.824324521 8.948966096 6.001494362
Ni2 4.836055020 9.955138140 5.165420318
H 8.157238672 2.871547738 9.479461219
H 7.302895987 11.104369819 10.156798153
End final coordinates

Cu-Ti-H2MOR
Final enthalpy = -6629.2046430894 Ry
CELL_PARAMETERS (angstrom)
13.787455544 0.058637711 0.020250357
-1.374080444 13.600420318 0.003759709
0.029171747 0.038841188 15.014912722

ATOMIC_POSITIONS (angstrom)
O 3.100981600 0.538651464 3.295071186
O 2.320903525 13.762123571 10.777435038
O 5.102948862 10.947029176 3.452850424
O 4.898863194 11.361718827 10.877240359
O 7.942255938 11.527793231 7.610479211
O 7.680451341 11.756699115 0.599686230
O 10.836800966 0.059529176 6.992654339
O 9.465260387 13.501893558 14.576386545
O 8.265725498 2.543270551 7.076502939
O 8.121101125 2.709003723 14.676990989
O 5.206791223 2.155524046 3.637524936
O 5.376640028 2.184352026 11.155082859
O 12.592829290 11.044999405 0.417922845
O 13.050986148 10.675736874 7.926693418
O 2.234190353 7.720977654 0.350257415
O 2.116589231 8.190766497 7.815247516
O 1.706380217 5.338235836 3.436691881
O 1.730136648 4.997720077 11.238719556
O 0.106863293 3.290058127 4.143155473
O 0.188169021 2.886912987 11.683910368
O 11.047092604 5.846857587 4.134485766
O 11.157225021 5.802630585 11.688564483
O 11.425418433 8.666349493 0.179484661
O 11.197758298 8.751820901 7.722923961
O 10.075162406 13.306376151 4.419883851
O 9.558985360 13.194597592 11.946956477
O 7.627790205 2.795789146 4.503959105
O 7.752585892 2.988459971 12.037901988
O 5.575269003 2.121716586 15.057754071
O 5.447159239 1.863049199 7.685804623
O 3.523050023 0.436129518 0.652500314
O 3.158301691 0.573530708 8.171624636
O 5.136497618 11.352179037 0.797661245
O 5.505094952 10.873739304 8.344579383
O 7.857615769 11.959340114 3.758748996
O 7.616850394 11.714032382 10.884856104
O 0.641880020 3.085885602 6.739086819
O 0.568086628 2.805694127 14.338138205
O 10.775213422 6.331827235 6.761791666
O 11.100606128 6.252373413 14.312376509
O 11.278031488 8.431922120 3.581179249
O 11.398228763 8.403546810 11.219245401
O 12.745578740 10.603462711 3.058308676
O 12.488250408 10.779240910 10.531325578
O 1.940708615 7.911126180 2.990447569
O 2.224675790 7.438226281 10.385616397
O 1.690795815 5.335022282 7.757037208
O 1.649755624 5.201647497 14.890973715
O 3.069982251 12.135727704 2.266395709
O 3.170776295 12.044075429 8.929975447
O 9.966505459 1.764160029 5.162678506
O 9.909073734 1.776660682 12.928344991
O 0.917925437 9.778352438 1.401190208
O 0.964407464 9.647046876 9.737066628
O 12.141784162 4.229543358 5.953205229
O 12.219216070 4.034638184 13.382461903
O 3.755566340 1.267545279 5.716682617
O 3.969083806 1.154346595 13.182139948
O 5.934740883 11.489392236 5.843430635
O 6.235773609 11.783621525 13.411930886
O 9.812168290 12.470006030 1.962892533
O 9.640885033 12.544841695 9.375447143
O 7.305423167 1.966999633 2.047982438
O 7.531110448 2.144459095 9.583523175
O 12.169386388 10.020178993 5.545253107
O 11.907572868 10.249754952 13.048356205
O 1.784757816 7.126823215 5.456699691
O 1.659088924 7.008961486 12.922022978
O 1.257471595 3.323190798 1.786750277
O 1.166275952 3.225914582 9.293525218
O 11.890983014 6.589431131 1.771401085
O 11.589932795 6.626038853 9.255524875
O 2.769124305 3.048476007 3.994433726
O 2.804693619 2.634127427 11.311148902
O 10.052021421 10.911910353 14.821181916
O 10.538401893 11.240026539 7.234963623
O 10.184765242 10.731126999 3.909031597
O 9.980320800 10.630188496 11.243845124
O 3.134153510 3.021239491 14.919792637
O 3.155967432 3.144511023 7.527621356
O 7.360972139 0.156960233 0.105238432
O 7.460252930 -0.163810135 7.740882854
O 13.558593194 7.142402776 14.771575662
O 13.280088707 7.172213441 7.253400192
O 5.604655501 13.822636531 4.049603834
O 7.325456069 0.372933444 11.547264240
O -0.350957253 6.918521727 3.894540502
O -0.254953401 6.777377293 11.078165113
O 0.466055503 12.368929737 1.846436582
O 0.566838530 12.268739682 9.507543560
O 3.549573172 9.533930606 1.798302024
O 3.632224829 9.485146991 9.542747077
O 12.582540649 1.629023310 5.735154409
O 12.513766056 1.373645421 13.172907770
O 9.483557515 4.349309460 5.584568994
O 9.584918013 4.398191139 13.266584358
Si 7.065206485 1.704093149 0.476451028
Si 9.249925229 12.135407067 0.483815183

Si 9.409182390 12.245965459 7.777871721
Si 3.726588668 1.754958093 4.177111070
Si 3.939345219 1.533206759 11.602733564
Si 11.921005850 6.960636175 3.353633276
Si 11.939439202 6.921587126 10.804532712
Si 1.455054311 3.739218797 3.348640781
Si 1.475312660 3.442949107 10.859275067
Si 1.336604684 6.743311804 14.487286842
Si 11.743604394 10.155442167 7.106726105
Si 11.510000609 10.223691803 14.623777468
Si 6.359920662 11.909545410 7.419329578
Si 6.282353360 12.202519148 14.950516318
Si 3.908040279 1.725353459 7.278437772
Si 4.048913962 1.694275311 14.715473042
Si 6.787273259 1.757972049 3.578929478
Si 6.957909513 1.868476371 11.175995558
Si 9.436683681 12.120599851 3.514951361
Si 9.300066728 12.044227193 10.868718339
Si 1.265406318 6.807079644 3.964601735
Si 1.323934376 6.553355945 11.395701279
Si 11.601976434 9.959063220 4.021086648
Si 11.472934512 9.988720780 11.509155066
Si 11.987969257 7.144242060 0.254030938
Si 11.761459739 7.203529055 7.731203464
Si 1.624536057 3.576290637 0.227134389
Si 1.852639443 13.187551527 2.005912279
Si 1.969350697 13.073415600 9.340141022
Si 4.187014715 11.001503182 2.036720541
Si 4.279548409 10.967312698 9.458427339
Si 11.202581803 0.802350874 5.576014630
Si 11.058458185 0.667604997 13.171894939
Si 8.847347554 2.961376520 13.255972300
Si -0.216669149 10.909198595 1.691630730
Si -0.115978361 10.805150643 9.398170397
Si 2.136247950 8.730207863 1.621869998
Si 2.231367426 8.693296701 9.355807368
Si 13.266773987 3.098370172 5.651076692
Si 13.270765688 2.817196214 13.154580834
Si 10.870072473 5.184699602 5.612995396
Si 11.033800179 5.121232662 13.158839029
Si 1.667915688 3.744612116 7.819187719
Si 8.829227607 2.860287034 5.605376419
Al 1.191290788 6.842487410 7.097787347
Al 6.232988328 12.248516581 4.184480302
Al 6.025905540 12.268908860 11.789242038
Al 7.108532066 1.528019867 7.847761280
Cu1 3.099945155 8.876708836 6.086375306
Ti2 5.008281120 9.862654504 5.139518421
H 8.167791058 2.878994310 9.492367626
H 7.355884174 11.046822150 10.216010600
End final coordinates

Cu-V-H2MOR
Final enthalpy = -6659.5090717798 Ry
CELL_PARAMETERS (angstrom)
13.875523820 0.027501375 -0.002566018
-1.414082025 13.701152982 -0.018328278
0.004589568 0.012275046 15.096282587

ATOMIC_POSITIONS (angstrom)
O 3.182967801 0.505816638 3.253839581
O 2.259506071 13.921983284 10.766233872
O 5.054960234 11.068700738 3.436160780
O 4.967944249 11.381498027 10.845947546
O 7.895618790 11.601528412 7.580699496
O 7.739318086 11.883893633 0.445809668
O 10.953061739 -0.037552611 7.014639198
O 9.670331411 13.484045218 14.597364184
O 8.272831186 2.505585557 7.065647928
O 8.043824043 2.678630152 14.677861549
O 5.278383032 2.116508235 3.705821920
O 5.445351998 2.147274025 11.261023858
O 12.663169388 11.005275300 0.437138824
O 13.012919829 10.719623423 8.000145007
O 2.216197098 7.829940121 0.315219873
O 2.076760372 8.233527301 7.862238564
O 1.726462158 5.341746444 3.665962660
O 1.705483052 5.074235067 11.350522973
O 0.170696194 3.211262797 4.182109918
O 0.311460937 2.853568955 11.764394636
O 11.117896597 5.877177543 4.182845805
O 11.101799763 5.900322673 11.765421369
O 11.476666984 8.640419201 0.077752168
O 11.254837918 8.717340803 7.670493709
O 10.097832667 13.340169259 4.405325465
O 9.623319231 13.294301393 11.948154218
O 7.735749699 2.753997521 4.472552966
O 7.886555975 2.911569341 12.020395396
O 5.516131276 2.036803142 15.116455178
O 5.447178873 1.825350574 7.645704160
O 3.439514906 0.424901276 0.585813293
O 3.174313339 0.515493357 8.161195590
O 5.223842936 11.378645280 0.795615736
O 5.420608004 10.929139534 8.273472134
O 7.879629606 11.978362425 3.737316053
O 7.663963434 11.733782229 11.009045311
O 0.615730726 3.048617656 6.807198949
O 0.497668949 2.908837309 14.442062694
O 10.859580022 6.240949880 6.820247778
O 11.171396155 6.149711725 14.409488918
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O 12.583199003 10.862793697 10.630962517
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O 2.123785328 7.512333573 10.442452802
O 1.749979879 5.338791604 7.621356388
O 1.711052175 5.260492445 14.914058043
O 3.087560983 12.240240119 2.102775633
O 3.151787150 12.128852244 9.005447042
O 10.032342542 1.683655109 5.219186646
O 9.942639936 1.661256313 13.117859797
O 0.892065554 9.803945107 1.506906468
O 0.912731972 9.728701344 9.751550039
O 12.259116918 4.195124971 5.900144023
O 12.319887926 4.060478680 13.241058189
O 3.699990571 1.267653408 5.704494807
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O 5.886351754 11.576692502 5.795773799
O 6.121486816 11.882758996 13.449671142
O 9.817343444 12.516958487 1.941315613
O 9.592322646 12.584575298 9.389656362
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O 11.933344692 10.302921434 13.121536400
O 1.675984326 7.326386733 5.477505959
O 1.517977576 7.114704460 12.993502902
O 1.233129609 3.511782779 1.797102873
O 1.164666005 3.380641535 9.341339527
O 11.840937088 6.642114463 1.788176414
O 11.562222755 6.668759222 9.313116917
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O 2.915038082 2.758540480 11.255776878
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O 10.480214967 11.188639683 7.314745963
O 10.228208730 10.767644233 3.876368381
O 10.053674595 10.713486271 11.277821552
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O 3.143997744 3.098644642 7.574747633
O 7.379925832 0.142932983 0.142176048
O 7.462186202 -0.203847461 7.736803157
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O 5.678069734 13.896294987 3.942015803
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O -0.346542092 6.770311093 11.126192948
O 0.454245222 12.413251213 1.846212799
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O 9.667835072 4.303926194 13.329553576
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Si 9.380820495 12.263215048 7.790724553
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Si 11.934913492 6.965276478 10.856311092
Si 1.483903953 3.759970581 3.389061647
Si 1.524891188 3.521996952 10.906968070
Si 1.293588849 6.794747241 14.568743768
Si 11.738746816 10.175524329 7.142016251
Si 11.541912520 10.201554791 14.696792901
Si 6.308480157 11.966848619 7.373435186
Si 6.263133363 12.272294953 14.990189258
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Si 3.973450967 1.674776854 14.766871406
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Si 7.021136526 1.816944752 11.192155117
Si 9.458421394 12.153448684 3.495031380
Si 9.336541688 12.112408655 10.907987568
Si 1.250366142 6.855250223 3.982535635
Si 1.237516604 6.619498211 11.467005518
Si 11.652722366 10.018899236 4.047958736
Si 11.537619977 10.062036575 11.569591730
Si 12.034507770 7.125543285 0.256198513
Si 11.806103726 7.170950678 7.772128475
Si 1.623307924 3.673475320 0.228995465
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Si 1.939742914 13.165027622 9.354109462
Si 4.200573316 11.081263907 1.993801179
Si 4.265961164 11.022700574 9.455700672
Si 11.281683644 0.725709687 5.599558873
Si 11.172242417 0.619133290 13.240408665
Si 8.892802742 2.884275476 13.315542287
Si -0.237660529 10.951656597 1.737817564
Si -0.167960239 10.899017665 9.458605370
Si 2.139842911 8.778441224 1.635283055
Si 2.175052415 8.761250892 9.399590299
Si 13.365806701 3.031434649 5.653380233
Si 13.374092846 2.828992178 13.162186993
Si 10.961544783 5.138585505 5.628898049
Si 11.076450640 5.100366351 13.181315208
Si 1.674397617 3.757827948 7.825367093
Si 8.899515997 2.802149077 5.613713916
Al 1.165728976 6.877945344 7.131165157
Al 6.249024242 12.302196350 4.149445871
Al 6.025124245 12.321991803 11.806041530
Al 7.108983087 1.487422148 7.831094292
Cu1 2.875719307 8.980960285 6.043176429
V2 4.825685131 9.992916366 5.108490441
H 8.164526131 2.837096517 9.484229196
H 7.416782567 10.991757054 10.418987188
End final coordinates

Cu-Ag-H2MOR
Final enthalpy = -6800.7175116409 Ry
CELL_PARAMETERS (angstrom)
13.783432901 0.063286828 0.043514368
-1.369045445 13.575690029 -0.013810717
0.054560906 0.022002955 14.993984090

ATOMIC_POSITIONS (angstrom)
O 3.104575603 0.539988330 3.272833179
O 2.417956644 13.700373255 10.713637465
O 4.977270587 11.065393654 3.445159668
O 4.837047234 11.368771350 10.919155440
O 8.008603629 11.528653569 7.591812624
O 7.671476849 11.765709376 0.599271879
O 10.933174760 0.084006594 7.019663161
O 9.553132506 13.464791196 14.621895433
O 8.333818495 2.485730577 7.069155732
O 8.031946831 2.782223312 14.686785520
O 5.249848081 2.127446366 3.665721400
O 5.408136385 2.181206299 11.139777918
O 12.553188990 11.017553727 0.435704215
O 13.109979360 10.627201848 7.923766775
O 2.208620141 7.695267750 0.375910824
O 2.206607724 8.142409911 7.772262489
O 1.791147544 5.346064110 3.342128493
O 1.753132219 4.954779072 11.220040334
O 0.167740383 3.343847613 4.124918971
O 0.209442815 2.848930841 11.649847409
O 11.136835024 5.747295459 4.128828739
O 11.163800510 5.796137903 11.685723550

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O 11.239901835 8.717872125 7.758673435
O 10.091606625 13.193389793 4.432923557
O 9.488405208 13.153467842 11.978888272
O 7.677842907 2.778240877 4.502411663
O 7.775193014 2.981910134 12.040270003
O 5.528690127 2.053234188 15.135066379
O 5.514917718 1.806106438 7.604717887
O 3.335269576 0.476851719 0.609809565
O 3.227432206 0.517574078 8.130401705
O 5.118610678 11.385765380 0.746833259
O 5.626068057 10.845187516 8.436753750
O 7.841152504 11.868473951 3.783879838
O 7.627371863 11.647965717 10.826443302
O 0.708976818 2.997272142 6.703558971
O 0.549160134 2.776877208 14.312958912
O 10.841557963 6.307857518 6.744905237
O 11.120887767 6.217562377 14.317106205
O 11.297889516 8.345389925 3.629273810
O 11.416524047 8.383346160 11.160924802
O 12.724613772 10.532885919 3.077519558
O 12.562377387 10.739442303 10.548470659
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O 2.249016751 7.367141776 10.316828753
O 1.738312636 5.267756642 7.699288555
O 1.612515106 5.183733472 14.848360852
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O 10.027912317 1.735324996 5.140610612
O 9.877476646 1.752687435 13.050182074
O 0.897434852 9.770405495 1.393828132
O 1.029543109 9.600030305 9.682432362
O 12.204123394 4.184239344 6.008229698
O 12.221023593 4.010758461 13.343344752
O 3.758086228 1.208237722 5.687995437
O 4.026211036 1.106065213 13.149665610
O 5.879535777 11.652896119 5.937650120
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O 9.824367242 12.335732573 1.992744841
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O 12.192261453 9.961739201 5.566165309
O 11.943186531 10.160081907 13.047742708
O 1.846994579 7.060096697 5.417457520
O 1.728207238 6.994838845 12.885370662
O 1.307450739 3.294645712 1.757743201
O 1.204394771 3.189854715 9.265825589
O 11.972845259 6.558504537 1.773596190
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O -0.224336637 6.754055320 11.083269253
O 0.375864749 12.360373162 1.875605130
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O 9.542189351 4.306409476 5.607156735
O 9.585678854 4.391028761 13.271679415
Si 7.028039655 1.707454621 0.499654259
Si 9.248913834 12.091136212 0.503591184
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Si 3.758112153 1.738964820 4.154879385
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Si 11.967832451 6.894162943 10.798922949
Si 1.517305668 3.738680003 3.307579418
Si 1.504461132 3.396729183 10.837109361
Si 1.350862915 6.734488487 14.445314954
Si 11.775520464 10.120939346 7.127942880
Si 11.506670840 10.170948064 14.614562289
Si 6.413890418 11.914285266 7.458623707
Si 6.313181509 12.192249604 14.898955517
Si 3.969132292 1.678651750 7.241407076
Si 4.023812566 1.671531919 14.678101439
Si 6.833148189 1.708127308 3.609081482
Si 6.993770143 1.873097905 11.157760861
Si 9.412165349 12.010220273 3.544558151
Si 9.301474840 12.020216086 10.866035367
Si 1.317362898 6.788163132 3.894397242
Si 1.356839326 6.513648869 11.374618671
Si 11.593374005 9.884608300 4.050545798
Si 11.509065895 9.959065755 11.500597581
Si 11.990917406 7.135985556 0.258670997
Si 11.806475935 7.173924118 7.734160685
Si 1.605653555 3.571711091 0.184468839
Si 1.775476388 13.175527485 1.946036644
Si 2.044888840 13.006255362 9.290565565
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Si 11.253296137 0.764244223 5.560381603
Si 11.041554990 0.646743517 13.219087436
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Si -0.061740004 10.762442676 9.373518333
Si 2.151550884 8.761989618 1.603097042
Si 2.301914177 8.654916348 9.337916702
Si 13.321856052 3.062655428 5.638661278
Si 13.265586496 2.787144550 13.134965263
Si 10.930909220 5.129151824 5.625024887
Si 11.036599617 5.101211815 13.148959761
Si 1.718119720 3.672674592 7.787252490
Si 8.882193031 2.815823708 5.597566188
Al 1.223686957 6.771214828 7.078474438
Al 6.201143647 12.126614033 4.231613209
Al 6.061554841 12.244527777 11.745384460
Al 7.175775211 1.505521299 7.875906603
Cu1 2.933321604 8.650056857 6.019994459
Ag2 3.656073805 11.205156622 5.561852453
H 8.164226728 2.966406132 9.493827868
H 7.370546397 11.094780746 10.055886135
End final coordinates

Cu-Mo-H2MOR
Final enthalpy = -6809.2018396312 Ry
CELL_PARAMETERS (angstrom)
13.786257626 0.063263941 0.017642137
-1.369388333 13.604979374 0.004409341
0.026348390 0.039271093 15.011539941

ATOMIC_POSITIONS (angstrom)
O 3.105570359 0.534176529 3.291455944
O 2.332409676 13.765930641 10.772196127
O 5.128018950 10.969090748 3.447149643
O 4.914168223 11.372491893 10.859085031
O 7.938907600 11.520634139 7.608958523
O 7.681013245 11.758995451 0.594459667
O 10.817981278 0.052865298 6.976170318
O 9.462949058 13.501989574 14.560830123
O 8.264273863 2.534411511 7.068591264
O 8.114525910 2.710405455 14.661340285
O 5.202345644 2.165661729 3.633320182
O 5.377338406 2.189050388 11.158764197
O 12.593820639 11.046929754 0.421625282
O 13.044291667 10.688300460 7.924724159
O 2.242890881 7.732210618 0.345549045
O 2.117090954 8.193024656 7.812742453
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O 1.730940664 5.002925661 11.249550274
O 0.097331408 3.281377407 4.143252149
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O 11.042040259 5.854154577 4.136215200
O 11.152172532 5.817298465 11.692061559
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O 11.103813495 6.251834927 14.318991096
O 11.274906204 8.441141474 3.580401456
O 11.397582791 8.414099807 11.215737732
O 12.759799215 10.604071579 3.059035319
O 12.494215855 10.786476608 10.534245047
O 1.935372522 7.903580479 2.978449949
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O 1.697742569 5.332998658 7.715349287
O 1.663050248 5.212664628 14.878443534
O 3.068312614 12.125654665 2.273192659
O 3.171795502 12.042328347 8.923452294
O 9.960980016 1.764104800 5.145808759
O 9.912434312 1.785485633 12.920102716
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O 0.967227754 9.651554875 9.729332763
O 12.147630902 4.243420974 5.957271741
O 12.219243404 4.042294019 13.369247559
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O 3.947556123 1.160441909 13.176198251
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O 1.653770811 7.028268053 12.914966069
O 1.252261890 3.360889297 1.793793336
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O 2.807694720 2.637689168 11.286134320
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O 10.534277080 11.245155861 7.226029773
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O 9.984955861 10.644471247 11.242036823
O 3.127300642 3.016019104 14.931720375
O 3.158288530 3.140101607 7.533617256
O 7.362266830 0.160236297 0.117072093
O 7.462258695 -0.171772796 7.757582039
O 13.561976560 7.147838725 14.772288498
O 13.271336959 7.177897620 7.261377006
O 5.612287195 13.841875111 4.026059966
O 7.329653907 0.380626544 11.545420641
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O -0.257392513 6.778175255 11.066967863
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O 3.563626754 9.528966600 1.816649433
O 3.636249633 9.485795566 9.542737406
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O 12.514615945 1.381322307 13.176479330
O 9.486084199 4.347863931 5.589252340
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Si 7.061930579 1.710517338 0.469017064
Si 9.249731234 12.139112182 0.477216009
Si 9.401299884 12.247201244 7.768192809
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Si 11.916437605 6.968952300 3.358093420
Si 11.933261930 6.930822093 10.802127541
Si 1.450054054 3.742947235 3.363195716

Si 1.474772403 3.450951403 10.855472270
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Si 11.508409187 10.225982115 14.624636079
Si 6.357702706 11.908581114 7.409946978
Si 6.277803160 12.210500061 14.949434634
Si 3.909643279 1.720826500 7.277363191
Si 4.043250543 1.692336551 14.711652988
Si 6.785186275 1.773412979 3.567428930
Si 6.959425096 1.875029292 11.171796800
Si 9.446942677 12.137307519 3.507682148
Si 9.306375775 12.058230533 10.861046302
Si 1.259220006 6.819818432 3.968510044
Si 1.320596231 6.559204173 11.392726783
Si 11.607023943 9.968560334 4.017506780
Si 11.474603192 9.998470876 11.509472286
Si 11.994252233 7.147289980 0.258893761
Si 11.749551721 7.212242811 7.732096979
Si 1.626973419 3.589534502 0.232339909
Si 1.861132363 13.184266712 2.005217406
Si 1.975090943 13.075085498 9.337070244
Si 4.198176813 11.000765547 2.047560459
Si 4.284981906 10.968439900 9.447784639
Si 11.196097584 0.803493241 5.567316103
Si 11.059286788 0.674120076 13.163570424
Si 8.847509336 2.967241785 13.246478939
Si -0.207988679 10.912641451 1.692483059
Si -0.114666634 10.811360133 9.398948463
Si 2.147683762 8.737565236 1.620001264
Si 2.234244776 8.698208518 9.353839505
Si 13.260961911 3.100287086 5.652460163
Si 13.271761423 2.824556531 13.152607522
Si 10.868131599 5.189572866 5.614730713
Si 11.031614258 5.127838947 13.156932942
Si 1.669529315 3.743445545 7.808642088
Si 8.826748602 2.860212282 5.598949688
Al 1.179713999 6.849113190 7.102662596
Al 6.238806713 12.265637484 4.178176642
Al 6.031002079 12.280149736 11.783668708
Al 7.110166854 1.519733676 7.845558267
Cu1 3.050768660 8.813212432 6.049827890
Mo2 5.036530786 9.772739633 5.158729210
H 8.158837824 2.888523952 9.485450224
H 7.362993886 11.060596463 10.214503968
End final coordinates

Cu-Nb-H2MOR
Final enthalpy = -6779.6199792216 Ry
CELL_PARAMETERS (angstrom)
13.788444602 0.059725140 0.019472944
-1.373071801 13.600367650 0.004378993
0.028357384 0.039455636 15.014063099

ATOMIC_POSITIONS (angstrom)
O 3.114923452 0.537203760 3.294777445
O 2.323133003 13.766697267 10.771257594
O 5.138600936 10.961087594 3.432290315
O 4.898359681 11.362111668 10.876463016
O 7.934592445 11.521983090 7.604357182
O 7.676797853 11.749781433 0.607124770
O 10.816597800 0.058063145 6.983139304
O 9.450242653 13.497743785 14.563894575
O 8.257168246 2.544801445 7.065944330
O 8.122954383 2.700607081 14.662401146
O 5.203610399 2.176757488 3.634912412
O 5.378761612 2.186595748 11.156870268
O 12.604284904 11.041038481 0.425418976
O 13.042981021 10.682110259 7.926790075
O 2.234898567 7.722018482 0.358548081
O 2.120681022 8.181116961 7.817344786
O 1.692807538 5.331919757 3.444898369
O 1.727361403 5.000546837 11.239380676
O 0.095207772 3.282516043 4.144328449
O 0.187700277 2.889963176 11.688118908
O 11.048820158 5.862135019 4.146255297
O 11.160762836 5.804557052 11.692951185
O 11.429272630 8.666360870 0.183978141
O 11.189132199 8.759708512 7.730559271
O 10.093394606 13.322164553 4.414919374
O 9.562569813 13.201277176 11.934179769
O 7.627055166 2.817776567 4.495812611
O 7.757080463 2.991134885 12.022593830
O 5.576994370 2.122696579 15.040352116
O 5.444689548 1.864401577 7.691750350
O 3.541204061 0.428378201 0.653669537
O 3.155388958 0.570921204 8.167216597
O 5.125950225 11.341443665 0.776283295
O 5.507059156 10.872908581 8.345663737
O 7.863047644 11.990938428 3.771324105
O 7.617448635 11.714127118 10.876378250
O 0.641226190 3.077023721 6.739669829
O 0.567335571 2.805894565 14.338932249
O 10.769970135 6.337973830 6.772636263
O 11.098512350 6.253148401 14.315066416
O 11.274545115 8.442994866 3.570763055
O 11.397645275 8.408341607 11.230153037
O 12.753660795 10.613120976 3.068018297
O 12.497156293 10.779449757 10.537947930
O 1.960778353 7.899241681 2.998014183
O 2.225605583 7.442619848 10.391708661
O 1.678732233 5.330263022 7.757820294
O 1.653081703 5.199800481 14.898080555
O 3.077893098 12.125152227 2.272845233
O 3.168776165 12.041476504 8.930442684
O 9.957825056 1.765782260 5.149486554
O 9.914116319 1.782693511 12.912979186
O 0.927740745 9.776324421 1.422043297
O 0.963785414 9.647828225 9.725292421
O 12.154111105 4.249974466 5.959414398
O 12.215830048 4.032405489 13.385465110
O 3.763021737 1.270099068 5.716986480
O 3.958375167 1.155174905 13.177251778
O 5.929376600 11.490196404 5.825967544
O 6.249373306 11.798663217 13.407828001
O 9.808439356 12.486096767 1.959517741
O 9.637485329 12.540458171 9.365671445
O 7.299500231 1.989069327 2.040115262
O 7.531737870 2.138203678 9.570790907
O 12.162511002 10.018706621 5.546483287
O 11.910267251 10.254249578 13.054765861
O 1.776097037 7.121122124 5.462350716
O 1.659069138 7.007075646 12.930455794
O 1.254361177 3.318028146 1.790645067
O 1.159791782 3.226610624 9.295904082
O 11.881712462 6.585579642 1.775618242
O 11.588094090 6.632877238 9.264003754
O 2.757768796 3.042941074 4.001210561
O 2.808412159 2.640209663 11.304954652
O 10.057149302 10.914024541 14.833013662
O 10.531626265 11.246450852 7.223461945
O 10.186575696 10.745551646 3.900928715
O 9.986017259 10.637548884 11.244414783
O 3.131175975 3.014566287 14.925170970
O 3.153106781 3.143878611 7.528289849
O 7.359057822 0.152850476 0.125246669
O 7.452020985 -0.169029708 7.707198700
O 13.558939786 7.137323677 14.780909428
O 13.273478895 7.186082016 7.260106558
O 5.602951830 13.843209865 4.043643853
O 7.325858788 0.374209834 11.537115217
O -0.350694957 6.938404457 3.886861250
O -0.254977250 6.785184480 11.086179238
O 0.476157907 12.371109420 1.845973804
O 0.566603236 12.271328799 9.509633267
O 3.563091278 9.526163223 1.811807160
O 3.634553144 9.485280101 9.539179854
O 12.564623871 1.642916202 5.754234173
O 12.514630784 1.371508473 13.177907253
O 9.492957883 4.350310593 5.590893970
O 9.581960400 4.401761457 13.266607292
Si 7.064897615 1.705980452 0.471076078
Si 9.244862915 12.136965792 0.484252709
Si 9.397636572 12.244886944 7.769415515
Si 3.728976916 1.758388552 4.178003625
Si 3.939744066 1.535951901 11.598421618
Si 11.918629548 6.970587639 3.354223279
Si 11.939786068 6.927975269 10.812845960
Si 1.445154172 3.732553923 3.353086849
Si 1.474128180 3.444863445 10.860930002
Si 1.337305001 6.742150461 14.496771567
Si 11.735229829 10.160527612 7.106865309
Si 11.515225678 10.226182482 14.631338566
Si 6.352130144 11.899824406 7.403221433
Si 6.281068978 12.201256418 14.950770535
Si 3.907461495 1.725165398 7.279689342
Si 4.048739246 1.690825259 14.711526923
Si 6.784861939 1.778003708 3.572500860
Si 6.959759074 1.869184622 11.164935885
Si 9.440508544 12.139637311 3.514468979
Si 9.300304499 12.046605600 10.861606526
Si 1.262933091 6.805481639 3.966520407
Si 1.323975979 6.556620852 11.402159690
Si 11.600455758 9.968005774 4.019619428
Si 11.476590687 9.994757503 11.515028330
Si 11.986870982 7.142624978 0.258975389
Si 11.754871770 7.212341835 7.740518625
Si 1.623889212 3.572627246 0.231773558
Si 1.867139870 13.182474998 2.008729685
Si 1.969740939 13.073535327 9.337840510
Si 4.199701967 10.996672592 2.036128424
Si 4.280876037 10.968237410 9.456640619
Si 11.193453506 0.808026704 5.574178408
Si 11.056888217 0.668632943 13.163646664
Si 8.848637138 2.962859245 13.243403772
Si -0.207072994 10.910296865 1.701296095
Si -0.117447998 10.808595232 9.396249252
Si 2.147034485 8.728248836 1.633537729
Si 2.233378194 8.694121455 9.357018756
Si 13.262283470 3.102798843 5.656001922
Si 13.269236631 2.816832740 13.156756645
Si 10.873730233 5.194114515 5.621792043
Si 11.032732292 5.121723752 13.159878216
Si 1.663410445 3.739312698 7.820528572
Si 8.827627423 2.866167710 5.598698567
Al 1.179485543 6.838245359 7.103030650
Al 6.229465992 12.267328299 4.182673253
Al 6.027041091 12.270975729 11.784092873
Al 7.105698021 1.520767112 7.833253788
Cu1 3.114380254 8.828876941 6.107379234
Nb2 5.130009738 9.683523297 5.111208695
H 8.153936116 2.884061674 9.472894745
H 7.354175161 11.060456331 10.194850539
End final coordinates

Cu-Pd-H2MOR
Final enthalpy = -6776.4331993244 Ry
CELL_PARAMETERS (angstrom)
13.777237453 0.052913077 0.027309528
-1.378777153 13.607933916 0.002639961
0.036908212 0.038378610 15.017093527

ATOMIC_POSITIONS (angstrom)
O 3.099130133 0.527615218 3.285945265
O 2.328547219 13.771891354 10.773500623
O 5.146655272 10.974503375 3.368890889
O 4.876966837 11.380892884 10.903470630
O 7.943487950 11.518898343 7.689141087
O 7.651988976 11.766458234 0.619930939
O 10.832399053 0.037416809 6.986913632
O 9.461176350 13.497307461 14.595603088
O 8.277335060 2.508283805 7.069263571
O 8.095787229 2.727899976 14.682424028
O 5.214755632 2.138524917 3.651546111
O 5.377302263 2.195603500 11.168481117
O 12.563865774 11.023830426 0.435049041
O 13.038547129 10.660629269 7.949881736
O 2.220171152 7.716139866 0.355900325
O 2.119223365 8.206367999 7.819439354
O 1.738044466 5.350749043 3.527861128
O 1.723135076 5.009887802 11.270613038
O 0.114807710 3.300969245 4.153299695
O 0.206600599 2.878594919 11.697700003
O 11.066105816 5.836881619 4.161676191
O 11.148202443 5.807897162 11.713132336
O 11.379754576 8.652837424 0.199527640
O 11.188582616 8.739044584 7.734844647
O 10.112074258 13.302856912 4.416329510
O 9.556216767 13.203594406 11.959965303
O 7.639288704 2.773077483 4.496984716
O 7.755428688 2.994133747 12.038773732

O 5.561515571 2.113189728 15.056046045
O 5.462225332 1.828212063 7.661806347
O 3.491269916 0.438951434 0.644911487
O 3.163999755 0.552760554 8.166963017
O 5.082561729 11.369042060 0.701906257
O 5.506060759 10.871243858 8.369924100
O 7.860113066 11.988356512 3.793479186
O 7.623037676 11.755621930 10.827041663
O 0.667607496 3.068264518 6.738021137
O 0.560592676 2.805187796 14.360728777
O 10.766788987 6.310213444 6.782463686
O 11.091557364 6.231182674 14.343261474
O 11.270021470 8.424508403 3.605981023
O 11.368103939 8.407157928 11.218819868
O 12.741005395 10.590555002 3.078668613
O 12.489055289 10.774104595 10.565683474
O 1.982073609 7.929970065 2.994345064
O 2.210052416 7.425370538 10.360045713
O 1.743557672 5.328536447 7.682762292
O 1.641378425 5.212132463 14.850691645
O 3.060119014 12.130663087 2.233895804
O 3.153978639 12.021399135 8.936314214
O 9.984460577 1.747584620 5.149986654
O 9.891962133 1.764076542 12.957780565
O 0.901651421 9.766052346 1.410968577
O 0.969985538 9.661023045 9.739458024
O 12.156884787 4.226350415 5.986928684
O 12.222671573 4.035054418 13.384999393
O 3.733529006 1.259748296 5.713483521
O 3.937967029 1.169207825 13.179369540
O 5.941604925 11.555560221 5.872457363
O 6.317823494 11.813607485 13.381463808
O 9.807339819 12.442713328 1.972406012
O 9.695676154 12.559307884 9.382594551
O 7.288520149 1.955249106 2.042614167
O 7.513231605 2.180090302 9.580053637
O 12.173934898 10.005173200 5.564256598
O 11.894860968 10.221637476 13.071657523
O 1.778817868 7.226989769 5.459155321
O 1.655654771 7.054120870 12.915279431
O 1.249694490 3.401848081 1.795763788
O 1.156721988 3.290551007 9.294469048
O 11.900894186 6.588030311 1.791845141
O 11.576116952 6.614615624 9.272773427
O 2.780784998 3.041981978 3.981417605
O 2.815469642 2.643725446 11.274230144
O 10.027242123 10.904398577 14.826153532
O 10.530870378 11.231078588 7.240742610
O 10.177937547 10.725532579 3.935523326
O 9.973610951 10.646814075 11.262051588
O 3.125779379 3.028820392 14.932339337
O 3.177808271 3.124230065 7.556357758
O 7.357808157 0.165959155 0.073627825
O 7.487535321 -0.185548270 7.844968950
O 13.539149968 7.154163411 14.769347786
O 13.269168897 7.158795175 7.279278069
O 5.610266316 13.802978783 4.041316912
O 7.326173572 0.381482294 11.520601924
O -0.335657684 6.938830988 3.899399333
O -0.263240685 6.795336869 11.079940517
O 0.454431617 12.365221992 1.840220948
O 0.559850825 12.279683370 9.517423492
O 3.551327378 9.553739451 1.756610044
O 3.644639412 9.481623005 9.545717211
O 12.587395574 1.618937396 5.755680698
O 12.500778649 1.370858667 13.190187054
O 9.494287654 4.322097728 5.591994327
O 9.582097646 4.388903300 13.274236787
Si 7.046444990 1.701148644 0.472569808
Si 9.223598841 12.129409035 0.498541520
Si 9.407926738 12.243800726 7.794174861
Si 3.731288426 1.738743809 4.169728388
Si 3.940807661 1.539613738 11.599298317
Si 11.915006050 6.959785980 3.372103783
Si 11.916882001 6.925622971 10.821571325
Si 1.466433972 3.751780209 3.367872853
Si 1.478395677 3.457313371 10.865735393
Si 1.327250645 6.760473481 14.477504858
Si 11.729904883 10.146896454 7.121186147
Si 11.481746417 10.210589529 14.644153060
Si 6.359962473 11.905268373 7.425189255
Si 6.283092225 12.215714524 14.926635786
Si 3.919858270 1.701891452 7.274004458
Si 4.033535867 1.695748648 14.717399761
Si 6.795349819 1.723208980 3.580816962
Si 6.959241187 1.880239019 11.171813402
Si 9.428576875 12.118441375 3.532174346
Si 9.308175380 12.064467705 10.867650841
Si 1.273268510 6.836798513 3.947297734
Si 1.312203103 6.565457547 11.402894385
Si 11.591398526 9.956198613 4.041069113
Si 11.454578516 9.989353617 11.530971322
Si 11.965291042 7.140687530 0.269634610
Si 11.740714758 7.190616144 7.750172908
Si 1.612916157 3.595632611 0.225918729
Si 1.847585113 13.180464536 1.993881914
Si 1.970971491 13.072647763 9.344872698
Si 4.213969033 11.016967003 2.010451268
Si 4.290775268 10.975938802 9.476717365
Si 11.212452103 0.781244686 5.574436332
Si 11.046348463 0.659459588 13.194131302
Si 8.835600931 2.957114771 13.267352956
Si -0.226991347 10.906025073 1.694879798
Si -0.122967769 10.817687018 9.413326562
Si 2.150649379 8.751909127 1.606272471
Si 2.236764776 8.712742288 9.379214381
Si 13.268693808 3.085209582 5.668224353
Si 13.265116952 2.807445415 13.171835079
Si 10.872961350 5.162903616 5.633469871
Si 11.027290084 5.112385185 13.175495127
Si 1.691587386 3.735790996 7.810297266
Si 8.837379715 2.829712376 5.598636081
Al 1.178133703 6.835250667 7.115646306
Al 6.204817496 12.198473923 4.203812197
Al 6.048717711 12.285760373 11.766249084
Al 7.124900800 1.500388876 7.857175275
Cu1 2.845218916 8.810797033 6.065225563
Pd2 4.949009512 9.704591381 5.188991181
H 8.114086683 2.942132838 9.481885545
H 7.366508872 11.213707590 10.048838823
End final coordinates

Cu-Rh-H2MOR
Final enthalpy = -6915.4564414378 Ry
CELL_PARAMETERS (angstrom)
13.774557525 0.054023720 0.034511711
-1.377363263 13.591950384 0.011934539
0.044679188 0.049334317 15.002125148

ATOMIC_POSITIONS (angstrom)
O 3.092151662 0.528280825 3.294935028
O 2.333870694 13.753143156 10.790285245
O 5.116278287 10.936166389 3.437191620
O 4.855505358 11.387544422 10.931948355
O 7.937219154 11.499288506 7.628352345
O 7.644782449 11.758151367 0.649334600
O 10.818836114 0.056999896 6.993166057
O 9.468760830 13.483116156 14.588072716
O 8.281000555 2.516927906 7.074688477
O 8.118235974 2.730280002 14.674609522
O 5.211743949 2.134463620 3.646756551
O 5.388117156 2.194339286 11.153692040
O 12.550498723 11.030800602 0.439382115
O 13.039371532 10.685567989 7.939977950
O 2.230287900 7.720902557 0.332717499
O 2.167190016 8.227830099 7.782962390
O 1.743122601 5.349203746 3.552734035
O 1.738551221 5.007012890 11.272791108
O 0.110488908 3.292783929 4.145836293
O 0.217570793 2.879206063 11.684800819
O 11.057596465 5.823008538 4.141984265
O 11.164734854 5.808472177 11.711946977
O 11.397571192 8.643510552 0.210718103
O 11.198633224 8.751196174 7.742453262
O 10.087462769 13.288109892 4.437991255
O 9.547904104 13.185681834 11.955062120
O 7.635125715 2.776905500 4.505470773
O 7.766140987 3.002081283 12.028979473
O 5.578553201 2.145539348 15.049069408
O 5.462961809 1.847601013 7.673539817
O 3.535574909 0.425721878 0.659007494
O 3.167115598 0.575003543 8.179274468
O 5.086251926 11.371031001 0.790417117
O 5.529850883 10.860751039 8.420059046
O 7.845256009 11.956604008 3.824714856
O 7.600264351 11.716499741 10.868262317
O 0.663199006 3.080478778 6.733117297
O 0.570210586 2.809962144 14.350589121
O 10.791452736 6.331330734 6.763222360
O 11.107388338 6.228869468 14.349880232
O 11.273975777 8.415981838 3.599211761
O 11.380069947 8.399330949 11.221702266
O 12.737501001 10.589123201 3.076929349
O 12.484681904 10.762792056 10.552305183
O 1.929013025 7.911096445 2.960777224
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O 9.908720047 1.774274849 12.940818904
O 0.901505937 9.774515941 1.382182900
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O 12.226457310 4.028953949 13.382048326
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O 6.280889746 11.779874242 13.417433942
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O 1.809252605 7.259460100 5.448480096
O 1.685775240 7.074475919 12.878633039
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O 1.163604451 3.307220515 9.281491914
O 11.958828874 6.586654472 1.798048038
O 11.583928071 6.616610302 9.263835581
O 2.774100823 3.035879621 3.983942776
O 2.823035901 2.641536686 11.260987379
O 10.021955485 10.890470990 14.844015541
O 10.531668042 11.238569438 7.238847514
O 10.173419254 10.713307711 3.934079500
O 9.964955249 10.627206060 11.251607322
O 3.134021309 3.029648582 14.934196842
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O 7.345809966 0.165884488 0.078655298
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Si 2.248415714 8.707968770 9.346200790
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Si 13.274180565 2.807467549 13.165770343
Si 10.871805008 5.171009493 5.625507354
Si 11.040291920 5.116417040 13.175120188
Si 1.691744251 3.758504522 7.795336077
Si 8.837419707 2.847960392 5.604054976
Al 1.207081821 6.870832954 7.093970856
Al 6.195184714 12.191504416 4.225297803
Al 6.031578281 12.272837529 11.804862498
Al 7.123329081 1.503699310 7.848220148
Cu1 2.994400763 8.826228726 6.027352550
Rh2 5.011597068 9.737024226 5.174384915
H 8.159039732 2.894215082 9.474984768
H 7.330087192 11.121782079 10.135431091
End final coordinates

Cu-Ru-H2MOR
Final enthalpy = -6876.9031377097 Ry
CELL_PARAMETERS (angstrom)
13.758677447 0.055342470 0.031883529
-1.374495830 13.600357913 0.008936294
0.041797090 0.045700303 14.997034806

ATOMIC_POSITIONS (angstrom)
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O 2.342997381 13.751003769 10.774008190
O 5.102651295 10.941282893 3.471586757
O 4.856642387 11.389194996 10.919822200
O 7.946042184 11.500238832 7.592295431
O 7.645825266 11.754741272 0.639488566
O 10.813468107 0.062259053 6.990166156
O 9.457157963 13.491265324 14.585943736
O 8.274733113 2.502738928 7.080855339
O 8.102075651 2.743323880 14.683501324
O 5.191189987 2.143170291 3.646723330
O 5.382739651 2.178596508 11.161334417
O 12.548885882 11.039687538 0.414252536
O 13.050916829 10.665746605 7.927773980
O 2.253966021 7.742464072 0.307507116
O 2.154316981 8.251877932 7.776920729
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O 0.096365112 3.298943741 4.129457582
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O 11.011652231 5.810943489 4.121890193
O 11.123763003 5.820746848 11.690231024
O 11.392509771 8.650608162 0.190764859
O 11.184672800 8.758237737 7.713782778
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O 3.532754497 0.404452132 0.661079417
O 3.157939343 0.569854876 8.167702593
O 5.090900755 11.400726591 0.840668861
O 5.542481405 10.854498231 8.417913468
O 7.843595269 11.984389362 3.826516707
O 7.590611444 11.718300922 10.891287737
O 0.676494406 3.112893029 6.711994944
O 0.578912346 2.834323704 14.314190416
O 10.771189782 6.343642020 6.739829979
O 11.109515452 6.234246185 14.327946788
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Si 7.046715185 1.704313170 0.485362090
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Si 11.476472838 10.215920323 14.616816432
Si 6.355456188 11.871768288 7.435411435
Si 6.266288687 12.213456442 14.963963244
Si 3.907864777 1.721750152 7.275023347
Si 4.040622254 1.688540937 14.714076442
Si 6.769995416 1.733694218 3.593563095
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Si -0.104346827 10.806555928 9.392524004
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Si 11.021207900 5.124317738 13.152934013
Si 1.698720169 3.782377276 7.787876163
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Al 6.195239402 12.218426729 4.227203906
Al 6.013549796 12.269827940 11.819447989
Al 7.113370971 1.490846647 7.849219623
Cu1 3.029672217 8.870075378 6.020534250
Ru2 5.033407853 9.763543809 5.169626327
H 8.184894525 2.836044821 9.492004924
H 7.318915776 11.080117204 10.197639122
End final coordinates

Cu-Zr-H2MOR
Final enthalpy = -6752.7046533044 Ry
CELL_PARAMETERS (angstrom)
13.797852332 0.064302230 0.013793700
-1.369509738 13.607502008 -0.000411230
0.022207054 0.033580403 15.023375466

ATOMIC_POSITIONS (angstrom)
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O 5.160361618 10.969412666 3.407421907
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O 7.689720066 11.759883755 0.576896723
O 10.822699379 0.053923605 6.977934009
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O 3.100792730 12.144432030 2.253279182
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Si 11.528089024 10.231971359 14.633236220
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Si 8.849081104 2.963839075 13.250160466
Si -0.199424371 10.911070374 1.709061570
Si -0.114855617 10.810832172 9.400829132
Si 2.153647972 8.726519007 1.646331152
Si 2.229284872 8.685638692 9.364330878
Si 13.265283961 3.106647593 5.653949656
Si 13.273185948 2.825236115 13.161568711
Si 10.877986303 5.199005359 5.622075055
Si 11.033715955 5.126144381 13.158581891
Si 1.648289650 3.721198234 7.831364466
Si 8.827589780 2.866721851 5.593317728
Al 1.157978856 6.816879774 7.111342207
Al 6.255847171 12.292347268 4.154179141
Al 6.046896873 12.276717661 11.757245400
Al 7.103112108 1.542136875 7.846191412
Cu1 3.092571310 8.809184607 6.110651847
Zr2 5.142039003 9.712645217 5.133889391
H 8.147314606 2.911177524 9.494610229
H 7.396983632 11.066115776 10.197385911
End final coordinates

RVV10-Geom-opts
Cu2O-H2MOR-RVV10-Opt
Final enthalpy = -6780.9741166052 Ry
CELL_PARAMETERS (angstrom)
13.789329673 0.108603680 -0.004664021
-1.324967665 13.593605559 -0.027146368
0.002329691 0.002014248 14.981806244

ATOMIC_POSITIONS (angstrom)
O 3.094687935 0.552945761 3.307835472
O 2.346637793 13.712915607 10.701270080
O 5.315998957 11.067224844 3.273924260
O 4.906902891 11.352287402 10.777095122
O 7.984427484 11.527428746 7.603625184
O 7.699979561 11.793498650 0.601061373
O 10.763042745 0.099974253 6.919383021
O 9.383098644 13.528681775 14.471470726
O 8.238810626 2.575983379 7.017657081
O 8.152659767 2.699540271 14.635287155
O 5.163290975 2.245520450 3.548760711
O 5.332521805 2.166520050 11.088936608
O 12.627460431 11.073535975 0.408262299
O 13.050177788 10.676354605 7.854479608
O 2.260316871 7.650855788 0.444737352
O 2.131314590 7.999193940 7.798031621
O 1.670208174 5.341492218 3.312591186
O 1.722647508 4.955012551 11.151421203
O 0.047164466 3.342685999 4.125086819
O 0.107948638 2.901751308 11.676806941
O 11.056685708 5.926134072 4.106770040
O 11.274522644 5.734463241 11.643948804
O 11.410080036 8.714706154 0.194946970
O 11.116832176 8.822376085 7.739366806
O 10.252906971 13.395580284 4.333757248
O 9.554747815 13.182401759 11.845702853
O 7.571423059 2.916979052 4.455092551
O 7.679255453 3.005344691 12.015276755
O 5.578317377 2.162516453 14.984564016
O 5.440339735 1.860933540 7.750476390
O 3.564588739 0.483864996 0.674485268
O 3.116975334 0.568965724 8.131768017
O 5.115543975 11.349530074 0.605332267
O 5.535934405 10.888503216 8.227461028
O 7.965700769 12.191877672 3.693143838
O 7.647627065 11.725322710 10.680169011
O 0.662485208 3.005134536 6.692053872
O 0.564354025 2.679061674 14.304935541
O 10.670454123 6.409631287 6.731751522
O 11.089152363 6.275857982 14.247985288
O 11.294545943 8.496885429 3.424257899
O 11.378209015 8.370868829 11.198114034
O 12.821108340 10.682265562 3.058695224
O 12.549718597 10.722886500 10.484178474
O 2.022129243 7.958845263 3.101397340
O 2.309760385 7.425790055 10.406096737
O 1.513617976 5.252979614 7.851708554
O 1.529130632 5.130587794 14.896784185
O 3.156675066 12.150943864 2.231961894
O 3.172119209 12.001957964 8.816147199
O 9.869352466 1.741232425 5.043985179
O 9.898530065 1.825182010 12.799260484
O 0.963384949 9.747167897 1.424988813
O 1.016035050 9.588582457 9.622768432
O 12.213887937 4.415666436 5.984875091
O 12.164183495 3.978583604 13.453225455
O 3.822315522 1.316510098 5.707838319
O 3.989180114 1.088761892 13.153247662
O 6.047459667 11.591919182 5.713951003
O 6.381848949 11.775176270 13.274596798
O 9.916088391 12.535973163 1.868827476
O 9.761725304 12.548811945 9.275091747
O 7.321855077 1.986526869 2.016199959
O 7.545984916 2.166407650 9.552970917
O 12.174422605 9.934521591 5.490652734
O 11.944238103 10.219100299 12.999466426
O 1.771353266 6.919161867 5.499935534
O 1.709165069 6.923968148 12.919981427
O 1.265974811 3.226977800 1.784033992
O 1.131121998 3.072999983 9.294121970
O 11.989095486 6.588745224 1.727826732
O 11.584838039 6.626283046 9.216518832
O 2.713061512 3.067426312 4.046349146
O 2.742240931 2.569370698 11.356592451
O 10.054335467 10.945575407 14.699221548
O 10.576617656 11.312993629 7.062839915
O 10.233634987 10.807558858 3.845646685
O 10.017041409 10.629075049 11.167208045
O 3.122427465 3.011547689 14.849085298
O 3.150422150 3.161060134 7.546131642
O 7.335822141 0.183568373 0.038253832
O 7.479687483 -0.145989670 7.719533326
O 13.550063862 7.228117352 14.657015382
O 13.177501652 7.279809829 7.173641822
O 5.601877688 13.917279375 4.040100947
O 7.300212150 0.368767824 11.494044030
O -0.336413638 6.964005075 3.924141831
O -0.202308526 6.807696508 11.015907635
O 0.548298112 12.365988267 1.795819360
O 0.582712193 12.220920335 9.443518679
O 3.616614768 9.550247886 1.804392609
O 3.692535528 9.442061953 9.376301135
O 12.458763462 1.785542131 5.746428448
O 12.486530386 1.328687296 13.111445799
O 9.539711281 4.340349679 5.533117479
O 9.549829803 4.437359520 13.184677611
O 4.868747282 8.392111451 5.571614734
Si 7.088333618 1.737037461 0.439223315
Si 9.267415096 12.190821509 0.422964373
Si 9.442396866 12.277298048 7.681130191
Si 3.721274821 1.793588400 4.164195770
Si 3.916969187 1.483942992 11.575732367
Si 11.944140456 7.014912908 3.300432414
Si 11.973980414 6.913311736 10.766078577
Si 1.419499770 3.725590644 3.325772979
Si 1.429961918 3.381332873 10.854864198
Si 1.324903352 6.693237359 14.485663682
Si 11.730725066 10.170421162 7.037936154
Si 11.509940665 10.228319940 14.570649494
Si 6.405805016 11.918633782 7.297359529
Si 6.302673495 12.179079373 14.824343418
Si 3.915048524 1.736712887 7.286245128
Si 4.056428250 1.684941107 14.672473932
Si 6.753324191 1.839594611 3.540568715
Si 6.924125548 1.869046982 11.129403052

Si 9.543213615 12.231704893 3.436498462
Si 9.337984657 12.037134189 10.750100905
Si 1.274493592 6.784105409 3.937450281
Si 1.365987275 6.519178561 11.375120913
Si 11.633826206 10.000623217 3.951130679
Si 11.496692946 9.965815093 11.459035114
Si 12.014068046 7.202510309 0.220336822
Si 11.662623563 7.266164952 7.709393344
Si 1.618032929 3.531638895 0.224064685
Si 1.932967380 13.196714375 1.979593746
Si 1.982837943 13.039284991 9.256645248
Si 4.296908215 11.027114280 1.961829746
Si 4.320069695 10.953682361 9.339647051
Si 11.154028492 0.860217617 5.513296648
Si 10.999986124 0.672335705 13.091781048
Si 8.823455405 2.986732199 13.190527428
Si -0.156799072 10.908632564 1.692170829
Si -0.091642184 10.749293836 9.341783450
Si 2.209903749 8.730057437 1.673899299
Si 2.294589811 8.630637687 9.316051145
Si 13.238572113 3.195309578 5.627069261
Si 13.227153958 2.783568886 13.132173024
Si 10.866011863 5.260375889 5.588407112
Si 11.032693200 5.105468963 13.126987768
Si 1.620153993 3.654661695 7.838881933
Si 8.794622374 2.890002126 5.538567537
Al 1.033183718 6.725829469 7.131437073
Al 6.314743936 12.361594662 4.098408012
Al 6.080804916 12.245942399 11.657613049
Al 7.116973305 1.539524978 7.819211171
Cu1 3.318341132 7.966624396 6.235525652
Cu2 5.257274315 9.948767377 4.900117236
H 8.168868698 2.914630809 9.479980728
H 7.388551047 11.197352280 9.890186442
End final coordinates

Cu6W-H2MOR-RVV10-Opt
Final enthalpy = -6790.8990536249 Ry
CELL_PARAMETERS (angstrom)
13.737256174 0.127521898 0.082590042
-1.349449846 13.481896132 0.030101978
0.062519672 0.027314727 15.023970894

ATOMIC_POSITIONS (angstrom)
O 3.303730337 0.252113008 3.558319329
O 2.006483934 13.794147043 11.072899163
O 4.925508575 11.071394789 3.477616281
O 5.018971408 11.364973251 10.848423414
O 7.665088873 11.850813904 8.307457296
O 7.725506604 11.966819363 0.739342940
O 10.612061671 0.280621240 7.234187033
O 9.541160391 13.786726661 14.796975818
O 8.148321844 2.757638817 7.216323874
O 7.970805910 2.719180191 14.774497542
O 5.132979143 2.188933413 3.766375973
O 5.202580624 2.246854457 11.324720129
O 12.650713323 11.013183815 0.570104000
O 12.546788146 10.989084656 8.137182144
O 2.063690384 7.741911385 0.456219559
O 2.189319107 7.739638188 8.213888289
O 1.747189183 5.165161904 3.478511554
O 1.848300021 5.245236253 10.914619953
O 0.003928299 3.354505235 4.380938056
O 0.092214728 3.462784998 11.807698737
O 11.212096230 5.735352023 4.314623179
O 10.954429054 5.882953633 11.816216884
O 11.171321172 8.811152639 0.521210571
O 10.955904593 8.807164504 7.916500750
O 9.542007855 13.074110624 4.737624248
O 9.612639851 13.232320432 12.207641814
O 7.480898607 2.964587660 4.598476843
O 7.556834956 3.116685861 12.145597246
O 5.415467200 2.199961329 15.354911099
O 5.383177767 2.385401743 7.715804339
O 3.121993646 0.767688463 0.930190422
O 3.189245123 0.914652688 8.451357529
O 5.315189851 11.098445752 0.825636700
O 5.197966547 10.955882641 8.183684193
O 7.614417404 11.826576828 3.358030910
O 7.669373145 11.920806770 10.928246481
O 0.411326822 2.709822901 6.976972044
O 0.486254319 2.897193940 14.413864273
O 10.728494438 6.392229971 6.886990863
O 10.842072007 6.489956855 14.436934195
O 11.211275069 8.344033703 3.848406426
O 11.293210969 8.460963051 11.245452450
O 12.455593532 10.670921231 3.224666894
O 12.538732401 10.823361388 10.807885862
O 2.200050096 7.725596826 3.141319372
O 1.982063621 7.910122855 10.882980921
O 1.100260771 5.172393916 7.767633259
O 1.274068402 5.261416671 15.390015373
O 3.114807898 12.149691482 1.795924020
O 3.045623981 12.156305129 9.210483059
O 9.818846409 1.926291364 5.263775304
O 9.803465094 1.972447673 12.989781223
O 0.810527380 9.594437675 1.854988826
O 0.841383761 9.751629374 9.333547265
O 11.888237387 4.053596091 6.280021469
O 12.018154696 4.263497218 13.691850348
O 3.777673408 1.244385254 5.914847091
O 3.830736488 1.267345909 13.437584021
O 6.449112165 11.590986711 5.940763051
O 6.446220525 11.709554743 13.465938602
O 9.836032249 12.548113340 2.124419982
O 9.824647819 12.582225484 9.596954878
O 7.258497544 1.954963746 2.160960632
O 7.368965661 2.054811135 9.751790762
O 11.863827717 10.123877922 5.733262276
O 11.933639077 10.072594229 13.256459349
O 1.810946403 6.797373146 5.580647684
O 1.598908748 6.645489826 13.145348919
O 1.042362262 3.120509194 1.947058265
O 1.229187312 3.093868160 9.447503923
O 11.760136945 6.605416674 1.903031728
O 11.645851973 6.648322456 9.358779063
O 2.590763355 2.769547862 4.109374643
O 2.667941536 2.838983779 11.677594588
O 10.150085303 11.172000796 14.868281697
O 10.036776274 11.201457347 7.299555065
O 9.904166675 10.576156076 3.952702888
O 9.984912235 10.703809463 11.517735348
O 3.025087890 3.269714844 15.080588043
O 2.962575410 3.330142789 7.402156340
O 7.095841383 0.170451083 0.167321344
O 5.711255406 13.554793636 7.676899995
O 13.337543296 7.369194675 14.854278000
O 13.170728333 7.508571203 7.282335952
O 5.681102917 13.801345000 4.272028948
O 7.126125624 0.485563094 11.919904036
O 13.504425363 7.049179354 3.903781097
O -0.348874930 6.712402454 11.316561570
O 0.450827459 12.244148207 2.084892442
O 0.413940175 12.395015259 9.490581192
O 3.501892695 9.521725401 1.804334709
O 3.521082047 9.556258894 9.588466135
O 12.408256169 1.510110883 5.655672537
O 12.454703836 1.684974609 13.112922630
O 9.304361863 4.537018723 5.665615862
O 9.359642400 4.546657556 13.452208057
Si 6.898260642 1.733070263 0.590170731
Si 9.312719610 12.364140476 0.578878280
Si 9.219539699 12.358236665 8.085027798
Si 3.711146492 1.616892116 4.340419682
Si 3.783219568 1.666776519 11.854742511
Si 11.942378519 6.931632592 3.491383595
Si 11.832574395 6.949824528 10.946491215
Si 1.346737224 3.590566207 3.480565672
Si 1.472502945 3.652507216 10.952644112
Si 1.151072670 6.726572558 14.698332672
Si 11.373766876 10.258965835 7.282216844
Si 11.513001958 10.272448550 14.812422549
Si 6.209010443 12.054242746 7.469126651
Si 6.307675862 12.142848620 14.996083634
Si 3.886147399 1.943720309 7.392662498
Si 3.876078042 1.874390005 14.946844510
Si 6.725467602 1.798997113 3.698020932
Si 6.818829244 1.924688257 11.252858902
Si 9.291397266 12.019379869 3.568281955
Si 9.343781106 12.124962300 11.088359776
Si 1.365169583 6.651672851 4.031839529
Si 1.259814990 6.624581242 11.556332928
Si 11.392421777 9.918134382 4.190853310
Si 11.459820858 10.002651291 11.700979578
Si 11.755564762 7.283874444 0.419679116
Si 11.686386684 7.321291175 7.862592192
Si 1.418321227 3.623499203 0.436907376
Si 1.834905609 13.094402491 2.100422434
Si 1.841104164 13.190480560 9.564582297
Si 4.216073415 10.966738025 2.026248824
Si 4.202129247 11.042844772 9.506897467
Si 10.933111595 0.848499437 5.733840382
Si 11.019655310 0.953866788 13.269473530
Si 8.650756489 3.082028739 13.341808039
Si -0.263686137 10.807931410 1.896586443
Si -0.272031520 10.928041624 9.400239067
Si 2.140990574 8.652102851 1.808550333
Si 2.108640382 8.748101733 9.486230096
Si 13.069172640 2.990254463 5.864595863
Si 13.142009480 3.152332434 13.293547154
Si 10.818500598 5.185546063 5.795513982
Si 10.798314917 5.290264744 13.333075832
Si 1.406805555 3.620973539 7.909050273
Si 8.674083946 2.996240258 5.722022129
Al 1.076764025 6.804248790 7.193471182
Al 6.017899187 12.109285442 4.349290759
Al 6.068081943 12.274957379 11.874579605
Al 6.968604318 1.757864550 8.087948539
H 7.464511653 11.771920451 9.946060479
H 7.443416257 11.746495992 2.363552179
O 6.764000354 5.756530482 5.311817061
Cu 5.690841710 6.389882613 6.879631181
H 7.715973556 5.522588437 5.463432746
H 6.373070344 4.953585752 4.903828364
O 4.645779215 6.759671462 8.519656983
H 5.083984451 7.443784968 9.062341897
O 4.129404080 5.457677861 6.061932293
H 3.333215708 6.031172633 5.830380655
O 7.323108894 6.887008270 7.927163899
H 8.020683332 7.391698640 7.468801907
H 3.705205687 7.102804215 8.338458307
H 3.764902917 4.699815448 6.604725940
H 7.779137271 6.072787037 8.393943103
O 5.265435317 8.548555818 6.141551125
H 5.158213579 8.899063207 5.237396518
O 8.444453545 4.857360917 9.008547077
H 8.415350728 4.079281585 8.389205249
H 8.132406906 4.504610775 9.864451214
H 5.216010540 9.328828370 6.735240663
End final coordinates

H4MOR-RVV10-Opt
Final enthalpy = -6311.4128791493 Ry
CELL_PARAMETERS (angstrom)
13.786368369 0.053299508 0.060617963
-1.428161988 13.632901788 0.006189965
0.037873910 -0.001930360 15.079201743

ATOMIC_POSITIONS (angstrom)
O 2.962358434 0.387046362 3.370834595
O 1.884544509 13.807766682 10.889683447
O 4.839039278 11.166862804 3.258334999
O 4.760955210 11.301848551 10.895381944
O 7.628929524 11.627256086 8.177895771
O 7.447672318 11.759077738 0.719287811
O 10.602402349 0.002226633 7.169627302
O 9.214008087 13.486007521 14.734868566
O 7.892984598 2.588055704 7.116672567
O 7.788374380 2.597887905 14.785372272
O 5.041577383 2.036861838 3.705147135
O 5.127565918 2.098626830 11.246814779
O 12.356258711 10.990877017 0.523607691
O 12.574100427 10.772293071 8.035222486
O 1.917394002 7.764544649 0.391247190
O 2.062942006 7.883434412 7.954082263
O 1.481365157 5.227152646 3.431450654
O 1.411883066 5.001524467 11.148978780
O -0.077652877 3.178131629 4.215112589
O -0.075202529 2.900332293 11.794424713
O 10.989017124 5.721841266 4.244604119

O 10.880203034 5.662821530 11.798452783
O 11.092964194 8.646351864 0.356201104
O 10.878755176 8.692488330 7.882789350
O 9.459818394 13.149223559 4.584860635
O 9.434596275 13.206724236 12.087848293
O 7.452130968 2.822539715 4.473524589
O 7.504846656 2.905818393 12.143003431
O 5.275141239 1.895834323 15.299232636
O 5.157851908 1.804015204 7.860830833
O 2.919014102 0.589061472 0.692634456
O 2.856391616 0.492942687 8.240216011
O 4.913442735 11.180730829 0.559187552
O 5.106943295 10.912039243 8.248427167
O 7.471563969 11.801235779 3.386694087
O 7.507101719 11.828455120 10.816537695
O 0.353578476 2.767035587 6.835214335
O 0.390588156 2.788393711 14.432737224
O 10.684622178 6.256036208 6.852022033
O 10.774642767 6.253212658 14.401557376
O 11.011157313 8.320689012 3.649270515
O 10.990426376 8.290062864 11.370209020
O 12.313575844 10.650538037 3.180452713
O 12.294456102 10.561562987 10.695521994
O 1.928594241 7.798574449 3.064475973
O 1.908741776 7.501761499 10.571697878
O 1.214406179 5.134412203 7.804298372
O 1.326675872 5.192123941 15.164032658
O 2.925110357 12.342465911 1.839750135
O 2.872522763 12.069958431 9.121167115
O 9.690917194 1.728053292 5.335588171
O 9.641031669 1.670626599 13.072791296
O 0.496062808 9.574119354 1.680824788
O 0.654457497 9.558884274 9.463876784
O 11.933293659 4.049372976 6.092556853
O 12.004984541 4.046235553 13.598863164
O 3.579536714 1.166495306 5.794607220
O 3.706993171 1.129637862 13.300662738
O 6.191010739 11.608003092 5.907367978
O 6.324961642 11.741806091 13.385519517
O 9.637361510 12.369947771 2.020294534
O 9.704133670 12.467794498 9.524806192
O 7.131454034 1.740186977 2.098582990
O 7.291629940 2.120747634 9.676138608
O 11.798971237 9.911773936 5.654779457
O 11.747450472 10.046259705 13.220937209
O 1.500404363 6.913561913 5.510026184
O 1.411297764 6.844540404 13.060856391
O 1.080212987 3.174223518 1.840615258
O 0.924578352 3.026336222 9.388229540
O 11.592281287 6.479921950 1.818360831
O 11.361184855 6.548876195 9.386965737
O 2.583780343 2.926069808 4.055083763
O 2.577041069 2.692463792 11.468834680
O 9.838382815 10.882626468 14.868152094
O 10.066821639 11.128205492 7.226890201
O 9.786938624 10.583685191 4.011683474
O 9.785355837 10.628390962 11.500929800
O 2.961665713 3.113580217 14.966345149
O 2.869844021 3.063467745 7.558924333
O 7.139346135 0.044408444 0.038653870
O 5.784083538 13.459576720 7.895164582
O 13.246740473 7.125166090 14.869494089
O 13.099971290 7.310852108 7.492698131
O 5.497757951 13.827027603 4.270235781
O 7.089719952 0.284680187 11.616243598
O 13.291540728 7.024973985 3.814631717
O -0.566761766 6.814849083 11.258292802
O 0.251088498 12.244708430 1.971241018
O 0.254045718 12.197208016 9.613623390
O 3.173684568 9.681304023 1.753001113
O 3.359856335 9.497289252 9.566884152
O 12.314551728 1.428738126 5.660567504
O 12.284232541 1.388528889 13.382676344
O 9.284782542 4.331291733 5.685923042
O 9.332909637 4.285628475 13.444347784
Si 6.797032909 1.557499434 0.531067023
Si 9.043008541 12.123196563 0.513010889
Si 9.156381398 12.225952651 7.987096766
Si 3.557897040 1.632558664 4.240591268
Si 3.666018897 1.521024126 11.721203002
Si 11.736253990 6.879049793 3.393956476
Si 11.627245586 6.841549390 10.957680756
Si 1.270437355 3.620764350 3.400168729
Si 1.215443095 3.400909395 10.933569021
Si 1.041440474 6.704776144 14.640474751
Si 11.336754272 10.104771129 7.204781189
Si 11.288653759 10.126776797 14.781413464
Si 6.122851773 11.946939280 7.473824463
Si 6.086691539 12.091556876 14.932157676
Si 3.649444073 1.639530989 7.360670768
Si 3.732923012 1.674899978 14.840122157
Si 6.635595615 1.659491315 3.659351740
Si 6.715593271 1.785876628 11.261011758
Si 9.155242526 11.990211057 3.532200276
Si 9.184860864 12.046582612 11.010439128
Si 1.109693818 6.720106145 3.967949166
Si 1.012974738 6.520518144 11.521072591
Si 11.254423606 9.852480360 4.120296517
Si 11.224252855 9.861076738 11.690675124
Si 11.674247128 7.119926792 0.328265816
Si 11.545946148 7.181112396 7.884159897
Si 1.413275378 3.587580502 0.302401190
Si 1.561450928 13.205700454 1.974225341
Si 1.627933897 13.068497754 9.456423152
Si 3.973255182 11.089997808 1.903290914
Si 4.048421774 10.995713217 9.493386888
Si 10.868992560 0.696585455 5.703874587
Si 10.857611292 0.634367623 13.320921772
Si 8.567022646 2.859291892 13.390871486
Si -0.519340786 10.833717966 1.817900088
Si -0.452619972 10.758271226 9.411679360
Si 1.885504046 8.711726171 1.725773253
Si 1.992291031 8.669133850 9.474821253
Si 13.030481443 2.896641062 5.723932777
Si 13.050930047 2.823493221 13.331687956
Si 10.720225824 5.083819776 5.721286729
Si 10.756892963 5.055112530 13.307458212
Si 1.343131500 3.540023851 7.883296822
Si 8.553798110 2.868985630 5.677873741
Al 0.893225759 6.658880068 7.098761867
Al 5.833754285 12.132118131 4.301863257
Al 5.927357466 12.209946603 11.772702273
Al 6.835864835 1.501423713 7.939594631
H 7.867937035 2.905194888 9.599334548
H 7.348941137 11.621580089 9.836042534
H 2.773621092 8.177882369 7.353225142
H 7.257263616 11.617679960 2.419919691
End final coordinates

O2-RVV10-Opt
Final energy = -83.7783780825 Ry
ATOMIC_POSITIONS (angstrom)
O -0.105803382 -0.149728755 -0.000009630
O 0.865140382 0.612359571 0.000009630
End final coordinates

Water-RVV10-Opt
Final energy = -44.4243654013 Ry
ATOMIC_POSITIONS (angstrom)
O -0.000042774 -0.066169958 0.000026021
H 0.767266240 0.529078904 -0.000014055
H -0.767223466 0.529058778 -0.000011966
End final coordinates

Cu-OH-H3MOR: PBE-D3
Final enthalpy = -6489.5611852962 Ry
CELL_PARAMETERS (angstrom)
13.745788595 0.076684246 0.059391295
-1.400890836 13.620520841 0.016973050
0.037516039 0.009875688 15.014164254

ATOMIC_POSITIONS (angstrom)
O 3.294338036 0.354671262 3.342407381
O 2.201225776 13.883548612 10.834748360
O 5.125002642 11.304382523 3.137278753
O 5.014487608 11.409126351 10.808684984
O 7.923457823 11.803856212 8.074367870
O 7.700164223 11.953261320 0.675909460
O 10.861379566 0.199552085 7.093233819
O 9.438289475 13.704558041 14.636609505
O 8.111363289 2.775901341 7.028511366
O 8.095131307 2.707691423 14.662920049
O 5.228691410 2.165641556 3.667848513
O 5.326834094 2.265829685 11.181541243
O 12.637595281 11.077748858 0.427368634
O 12.932061271 10.823860760 7.938310443
O 2.132040042 8.017093527 0.209903739
O 2.124687985 8.245415552 7.729979848
O 1.872725057 5.341730435 3.757588566
O 1.701483959 5.140676653 11.192906381
O 0.113259248 3.362120329 4.091122001
O 0.167010026 3.039815753 11.659393120
O 11.156864257 5.947539714 4.138491919
O 11.102728807 5.846059708 11.651397032
O 11.258261744 8.811207190 0.245828581
O 11.110147092 8.860162608 7.706683969
O 9.723451271 13.298081222 4.541951075
O 9.717033312 13.336996311 12.023340474
O 7.635817835 2.945859518 4.388935327
O 7.708258844 3.044742259 12.041322218
O 5.534823179 2.141683574 15.046268882
O 5.384455077 1.954337969 7.704862089
O 3.239941963 0.823975489 0.707972934
O 3.117508212 0.627896262 8.191616625
O 5.202590278 11.266630403 0.450726858
O 5.410710823 11.076286997 8.185074168
O 7.730718462 11.979180471 3.322993294
O 7.751476509 12.046442778 10.693293089
O 0.569289778 2.992758080 6.707683957
O 0.638807713 3.020602975 14.309375527
O 10.753198182 6.417638925 6.733629830
O 10.979703087 6.415692527 14.245412354
O 11.366197696 8.534400723 3.564614597
O 11.258539217 8.462693393 11.235944395
O 12.563844594 10.896776921 3.091831219
O 12.454928342 10.782918252 10.556602737
O 2.208656243 7.809654548 2.847049087
O 2.193178468 7.536901981 10.270444157
O 1.609379061 5.343123668 7.480686373
O 1.621461887 5.453428213 14.829408743
O 3.168588809 12.377237399 1.659417210
O 3.131673621 12.160967857 9.033390143
O 9.875149330 1.866550307 5.252301479
O 9.907793322 1.863238263 12.886062856
O 0.828796841 9.764999658 1.713844696
O 0.967960824 9.749349968 9.592536791
O 12.093961960 4.259267074 5.966401269
O 12.193409432 4.207928677 13.439016560
O 3.726312635 1.266437060 5.725382898
O 3.815711903 1.351188701 13.193883303
O 6.469673592 11.755925824 5.827559436
O 6.625584096 11.939745418 13.263172420
O 9.881632425 12.577258451 1.973095721
O 9.961174095 12.676213550 9.456211393
O 7.273318805 1.914060305 2.010545909
O 7.464970002 2.291565574 9.574043638
O 12.089761568 10.151470842 5.555932905
O 11.943275098 10.237529316 13.077111079
O 1.690786667 7.439437329 5.386362152
O 1.585562343 7.209628591 12.816243307
O 1.270192310 3.668743995 1.759522475
O 1.078589372 3.409732765 9.237851885
O 11.788802267 6.674044966 1.712595834
O 11.489089009 6.731228634 9.233201555
O 2.732606355 2.896065872 3.862954426
O 2.772894766 2.771271433 11.198992915
O 10.098516792 11.114832549 14.765642073
O 10.410824925 11.343594433 7.196828081
O 10.047644900 10.751121095 3.918711101
O 9.970341679 10.766558599 11.364665707
O 3.194337097 3.335409142 14.894651036
O 3.081216533 3.175344976 7.481654996
O 7.291328362 0.179180884 -0.003925105
O 7.470370884 -0.000085783 7.768607436
O 13.431488040 7.344223530 14.703168456
O 13.215877208 7.322093136 7.265068532
O 5.717855992 13.946857076 4.163479793
O 7.268012727 0.436747445 11.476820839
O -0.207698849 6.968761738 3.598495051
O -0.301158735 6.896356076 10.969671525

O 0.509762926 12.430169858 1.798038385
O 0.506724897 12.359589716 9.522933667
O 3.507869672 9.743984683 1.686035329
O 3.644279926 9.600395475 9.441079175
O 12.503546351 1.646782922 5.553335192
O 12.531582163 1.562110165 13.282932727
O 9.465019682 4.476014526 5.504795290
O 9.538298344 4.458692852 13.278619196
Si 7.015763858 1.717234692 0.436209598
Si 9.288527809 12.328731007 0.472014290
Si 9.445202120 12.415245560 7.918183951
Si 3.763080677 1.681460381 4.162680171
Si 3.866848534 1.658021008 11.599746289
Si 11.963207983 7.049566519 3.282763070
Si 11.839591496 7.007746025 10.784918359
Si 1.501611602 3.803258134 3.362108483
Si 1.436768486 3.588749130 10.800761709
Si 1.265133970 6.971872576 14.386776999
Si 11.635959745 10.278955493 7.114634796
Si 11.508547063 10.305364371 14.637057114
Si 6.401755276 12.103032410 7.388156177
Si 6.344998988 12.252903536 14.804134175
Si 3.863728079 1.764219300 7.277515801
Si 3.964828123 1.907291366 14.717081304
Si 6.818056098 1.793473216 3.575552283
Si 6.907376240 1.941236193 11.156941324
Si 9.403398066 12.163784311 3.473151911
Si 9.421641514 12.218972064 10.917602142
Si 1.383305958 6.878586181 3.873691826
Si 1.275866131 6.693820046 11.308559548
Si 11.533393441 10.071205568 4.032756434
Si 11.426312654 10.037614585 11.552157414
Si 11.861713646 7.298739630 0.219406473
Si 11.684519037 7.317919449 7.721336496
Si 1.653795421 3.869478684 0.195466954
Si 1.871742005 13.306677859 1.883730023
Si 1.915505122 13.170936951 9.396198149
Si 4.266320223 11.179734086 1.792216894
Si 4.318536455 11.091762723 9.399168210
Si 11.082645440 0.877944961 5.621903227
Si 11.100164458 0.820876849 13.199425338
Si 8.810694091 3.013444234 13.246039865
Si -0.222558560 10.997639741 1.731512761
Si -0.150579503 10.894093566 9.361710130
Si 2.173035106 8.854843624 1.602841584
Si 2.251995375 8.811396101 9.270968693
Si 13.197180705 3.118998936 5.607785219
Si 13.266132144 3.011161551 13.200056727
Si 10.868419661 5.268454681 5.590754028
Si 10.961923997 5.225620228 13.146826284
Si 1.588742861 3.764724751 7.721497982
Si 8.747177668 3.015232477 5.574842657
Al 1.144449680 6.912451730 7.023400891
Al 6.072871472 12.259353170 4.228332771
Al 6.169392537 12.358616036 11.651336199
Al 7.060629315 1.663477279 7.830655851
Cu 2.348856153 9.202326073 6.002370002
H 7.618813747 11.851967894 9.702745012
H 7.997283033 3.105789066 9.497840395
O 2.877515542 10.843132096 5.597165392
H 2.210750337 11.553564005 5.671186346
H 7.524294371 11.837596190 2.344719163
End final coordinates

Cu3O3-H2MOR: PBE-D3
End of BFGS Geometry Optimization

Final enthalpy = -6996.3200059199 Ry
Begin final coordinates
new unit-cell volume = 19019.93730 a.u.^3 (2818.46388 Ang^3)
density = 1.83836 g/cm^3

CELL_PARAMETERS (angstrom)
13.793143464 0.052521559 0.048169081
-1.380365581 13.594690302 0.008876745
0.059447758 0.047820408 15.025170485

ATOMIC_POSITIONS (angstrom)
O 3.050211460 0.451772927 3.391092579
O 2.278524520 13.741462208 10.876691761
O 5.124642035 11.003107259 3.233401026
O 5.123393400 11.268004525 10.802674629
O 7.905650561 11.932024052 8.047600674
O 7.541484264 11.786301609 0.681820512
O 10.999239941 0.187935991 7.048711646
O 9.340663677 13.510428368 14.631464543
O 8.224692974 2.557537783 7.065107060
O 8.245269164 2.597359799 14.721571175
O 5.248408874 1.919685805 3.646160548
O 5.367493514 2.171879533 11.208708671
O 12.395138058 11.062778483 0.631737624
O 12.786511346 10.725216208 8.137541767
O 2.170309108 7.820343504 0.354842554
O 2.236983274 7.897459789 7.804890546
O 1.997639568 5.383574924 3.430796761
O 1.676750317 5.009207322 11.273498379
O 0.299513692 3.445600950 4.230662490
O 0.200556661 2.866557973 11.820620171
O 10.914487286 6.007907338 4.239635029
O 11.227885776 5.752693998 11.759287107
O 11.282360336 8.663225146 0.325856314
O 11.014476035 8.748193828 7.691827719
O 10.008450502 13.152226868 4.505035073
O 9.851872478 13.232047656 12.047976804
O 7.613604133 2.708021877 4.467821130
O 7.756520095 2.949978220 12.122302993
O 5.644681239 2.241910472 15.010396541
O 5.356082005 2.107598642 7.740029837
O 3.482693020 0.731133154 0.764885729
O 3.223133388 0.552848917 8.256177039
O 4.979936640 11.236662800 0.524809312
O 5.478393566 10.926305833 8.213343976
O 7.896774064 11.698910383 3.741353781
O 7.847580046 11.935742230 10.786868946
O 0.401593662 2.888095426 6.859802325
O 0.649497658 2.875087055 14.453867961
O 10.712625267 6.223465002 6.895579001
O 11.086792143 6.280864432 14.370045796
O 11.708410844 8.477894543 3.627106572
O 11.373896680 8.377891879 11.422146864
O 12.953580593 10.780988490 3.244457511
O 12.766250345 10.593488668 10.793745077
O 1.617103919 7.995243956 2.966008473
O 2.246268912 7.456788659 10.435927601
O 1.388945423 5.212706158 7.692094196
O 1.585957228 5.319831545 14.996044584
O 3.045745675 12.222983491 2.070253010
O 3.211668073 12.022934960 9.062999890
O 9.908153461 1.681356505 5.169885462
O 9.994158893 1.779957979 12.870516830
O 0.891778841 9.926840851 1.323377850
O 1.021647127 9.574116230 9.421203832
O 12.127091954 4.253909420 5.872254844
O 12.271621602 4.071236317 13.540355273
O 3.764286388 1.224077422 5.789435217
O 3.922254344 1.239395594 13.242445247
O 6.179413161 11.684167435 5.960067586
O 6.449438316 11.787742276 13.326510223
O 9.755981090 12.463667657 1.985698572
O 9.970918696 12.664150625 9.447083916
O 7.302922973 1.824870566 2.019213628
O 7.481507248 2.296183120 9.632051703
O 12.174388179 10.122974177 5.666566325
O 11.917716743 10.237888287 13.236508591
O 1.657404828 7.085304870 5.479799126
O 1.587333127 7.040725380 12.951287559
O 1.406873377 3.362114478 1.843840448
O 1.026612255 3.201952877 9.382491292
O 11.844267706 6.547484426 1.832161935
O 11.495282014 6.720078752 9.349513087
O 2.917621945 3.025392548 4.033226590
O 2.801937429 2.653744365 11.283927730
O 9.939147562 10.914972101 14.862788202
O 10.331187025 11.218446675 7.226470446
O 10.319934220 10.646354394 3.810900048
O 10.162515465 10.703067596 11.277094395
O 3.232837812 3.256373661 14.869798958
O 2.947220608 3.086901248 7.534661765
O 7.172099913 0.098167712 -0.012348876
O 7.220377946 -0.009483739 7.943871297
O 13.513589890 7.265606948 14.853290276
O 13.157977337 7.289251739 7.328255923
O 5.758992561 13.675697813 4.033175123
O 7.329482304 0.359252857 11.466630773
O -0.333366458 6.477148761 3.906028730
O -0.255451517 6.832798967 11.021872814
O 0.429422468 12.506210700 1.685188521
O 0.602614769 12.200580514 9.527830105
O 3.463326077 9.564335714 1.941638065
O 3.686514259 9.441793615 9.482213679
O 12.551927205 1.658019128 5.407622896
O 12.562989095 1.415088650 13.472797167
O 9.468289022 4.290377303 5.545076047
O 9.624576595 4.369395699 13.321415200
O 4.090797522 7.659090250 4.487323633
O 6.354585067 9.167667664 4.888771504
O 4.846755916 8.325658367 6.985945636
Si 7.051242693 1.649650840 0.443347044
Si 9.121312754 12.134364494 0.536668284
Si 9.489602620 12.413209450 7.898233171
Si 3.765429630 1.656403995 4.231386990
Si 3.917307430 1.549299515 11.648458189
Si 11.974644963 6.903766036 3.414305226
Si 11.923291489 6.937843853 10.891738261
Si 1.647949253 3.788580971 3.394561405
Si 1.431154859 3.440192388 10.924954586
Si 1.279003245 6.841208919 14.530537015
Si 11.590652507 10.181957572 7.180098007
Si 11.411187431 10.231131818 14.781531027
Si 6.356737013 12.165625584 7.505772128
Si 6.243385972 12.167089435 14.866818693
Si 3.851144348 1.753497135 7.333538919
Si 4.089117496 1.876385992 14.733611911
Si 6.843428239 1.588752036 3.566690196
Si 6.952881427 1.875317867 11.210452004
Si 9.441787076 11.987911655 3.523329238
Si 9.539136598 12.145592929 10.923858493
Si 1.264713402 6.739900078 3.923561291
Si 1.300367399 6.576317533 11.417191458
Si 11.779849036 10.023052394 4.090483676
Si 11.572174543 9.962062231 11.680037641
Si 11.909203006 7.164446551 3.334586357
Si 11.627420439 7.226047246 7.799871112
Si 1.676479999 3.685584454 0.278316699
Si 1.816330960 13.288963562 1.978542808
Si 1.991184878 13.041989503 9.428090524
Si 4.156690894 11.072659516 1.903805183
Si 4.343346990 10.924170800 9.458364374
Si 11.202017492 0.781873518 5.521231834
Si 11.129117563 0.695443919 13.275741023
Si 8.907326081 2.920079178 13.286582890
Si -0.241568887 11.034062909 1.716418387
Si -0.097440641 10.743146415 9.429560669
Si 2.021541878 8.812654377 1.634148219
Si 2.314405373 8.602345404 9.286426831
Si 13.245926426 3.105682250 5.612719315
Si 13.321091205 2.846634436 13.340602595
Si 10.809235442 5.184147017 5.643122197
Si 11.064129721 5.116423920 13.245497648
Si 1.450677847 3.629222659 7.859758618
Si 8.793243294 2.810342921 5.583207386
Al 1.000986176 6.772285782 7.124430768
Al 6.282020832 12.037686217 4.187943234
Al 6.208269436 12.256841732 11.700324721
Al 7.002102746 1.708752157 7.913360757
Cu1 3.368892268 7.794101814 6.136760097
Cu1 5.696897848 9.777728724 6.440066322
Cu2 4.865426067 9.119403778 3.860942056
H 8.136709798 3.016649499 9.592197737
H 7.672980882 11.799307541 9.810022960
End final coordinates

Adducts with methane: PBE-D3
Cu-O-Co-H2MOR-methane-adduct
Final enthalpy = -6672.3765759835 Ry
CELL_PARAMETERS (angstrom)
13.805446430 0.050682715 -0.013566032
-1.383769987 13.624082572 -0.037628835

-0.007300434 -0.010449264 15.021760751

ATOMIC_POSITIONS (angstrom)
O 3.157958277 0.548007542 3.256365318
O 2.229654640 13.786568526 10.692947709
O 5.228825304 11.099351571 3.276697300
O 4.915709943 11.286452948 10.764193978
O 7.897243102 11.517038402 7.560914482
O 7.689288420 11.793753665 0.527143878
O 10.808965656 0.012276069 6.923398034
O 9.447861964 13.450530872 14.471161395
O 8.252069480 2.527660496 7.011943219
O 8.075217817 2.654408279 14.624486699
O 5.199079280 2.238278953 3.613767688
O 5.351095229 2.131889123 11.124502307
O 12.623624783 11.003195660 0.407799925
O 12.964095235 10.633923966 7.886657230
O 2.222027554 7.705246043 0.416419029
O 2.066719517 7.994759803 7.844188680
O 1.630265916 5.331058125 3.382746258
O 1.672670729 4.998455158 11.181789204
O 0.085912010 3.258322574 4.138673339
O 0.169772978 2.868343991 11.697285360
O 11.065102703 5.906383559 4.148608662
O 11.161567656 5.764989542 11.667156593
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O 11.078708814 8.741499207 7.690121228
O 10.205784400 13.360736805 4.324615661
O 9.530421422 13.191372000 11.830990244
O 7.624418881 2.882988666 4.449390427
O 7.727375949 2.920295556 11.991457473
O 5.527321507 2.056597788 15.014052953
O 5.437903288 1.835480561 7.670862308
O 3.485024953 0.437994734 0.608073278
O 3.141945159 0.530852527 8.115650253
O 5.123223855 11.321551368 0.606755339
O 5.427089748 10.897174752 8.181089802
O 7.926056114 12.137760571 3.682577186
O 7.621742565 11.673132542 10.765494205
O 0.655169283 2.964657978 6.722995899
O 0.516529396 2.750269670 14.342399544
O 10.682965371 6.284337295 6.782521770
O 11.073541464 6.182696342 14.284098220
O 11.253179004 8.468486209 3.478326292
O 11.372927779 8.386962801 11.222766795
O 12.776123075 10.635901094 3.059198646
O 12.538119359 10.732694270 10.522452830
O 2.019697157 7.922660276 3.074355833
O 2.208099152 7.482067039 10.467727728
O 1.544648128 5.239159327 7.783632070
O 1.592503262 5.146681532 14.926649966
O 3.124536499 12.185209082 2.130910746
O 3.132928379 12.037477380 8.893267830
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O 0.919872778 9.750656565 1.478849716
O 0.945250792 9.626161117 9.627182116
O 12.295290007 4.378002018 5.944880464
O 12.186919086 3.969961565 13.346913465
O 3.757462908 1.293175621 5.685026596
O 3.919465796 1.104855465 13.149787377
O 5.964636247 11.608349988 5.687320080
O 6.275248791 11.829791643 13.301470050
O 9.858057941 12.526045382 1.864196051
O 9.651259809 12.523415693 9.272186797
O 7.282902090 2.051826243 1.994607162
O 7.507728037 2.139777770 9.531093742
O 12.125740147 9.952720405 5.502886537
O 11.892894063 10.241383094 13.026923244
O 1.692523132 6.981809791 5.496816426
O 1.597654336 6.948086803 12.967846641
O 1.243971311 3.278662225 1.775982513
O 1.144153377 3.123307595 9.307938202
O 11.848762481 6.574950698 1.737626555
O 11.535846639 6.630018123 9.252300733
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O 10.031801237 10.864570160 14.792139055
O 10.481970001 11.224122067 7.117745194
O 10.199908335 10.786259449 3.829948678
O 10.005471417 10.634667507 11.170531664
O 3.086519354 2.973296318 14.898668141
O 3.147267652 3.123607683 7.547961452
O 7.360043806 0.153006699 0.123592199
O 7.468323065 -0.178059575 7.707282177
O 13.527796011 7.089349199 14.792238833
O 13.162984328 7.191703199 7.215149321
O 5.596138749 13.934620119 3.953218971
O 7.298748379 0.306247006 11.425156905
O -0.363555777 7.005881704 3.838581770
O -0.286996693 6.797588789 11.069188547
O 0.498025691 12.362053944 1.827150398
O 0.525722793 12.252579465 9.417728405
O 3.568218295 9.571592061 1.807302915
O 3.607375593 9.456862731 9.385624686
O 12.440257589 1.739354634 5.756382036
O 12.494115114 1.318502807 13.115864198
O 9.630056391 4.224482858 5.533674413
O 9.555986670 4.341184728 13.209829081
O 4.756194354 8.538291737 5.569771031
Si 7.056721107 1.713347143 0.436804543
Si 9.263579155 12.158355453 0.405368558
Si 9.364015215 12.231293058 7.680744367
Si 3.734689906 1.782717972 4.146134366
Si 3.903841027 1.512311092 11.578501208
Si 11.905111356 6.996705487 3.304833154
Si 11.915172468 6.911156316 10.797422927
Si 1.422685203 3.718781529 3.329625900
Si 1.450278365 3.421794087 10.864235205
Si 1.285995243 6.693708805 14.540946294
Si 11.665931760 10.122012654 7.050119485
Si 11.488062706 10.173424487 14.600587629
Si 6.325774591 11.920743260 7.283344134
Si 6.259889499 12.183015589 14.858483271
Si 3.902575501 1.705993449 7.257850107
Si 3.996242826 1.641350815 14.684699543
Si 6.779784694 1.839656078 3.529578467
Si 6.932845068 1.814302286 11.111629228
Si 9.500943283 12.200907313 3.425537766
Si 9.299434282 12.026503289 10.763407901
Si 1.235928221 6.796850852 3.939033204
Si 1.282585989 6.548829765 11.421376113
Si 11.592630462 9.979263822 3.965153571
Si 11.478968476 9.977888237 11.483922653
Si 11.978602221 7.134669911 0.222590428
Si 11.648284346 7.200635243 7.726156861
Si 1.613829101 3.563236950 0.221746055
Si 1.877009331 13.206973434 1.930447515
Si 1.925251330 13.068929918 9.261423814
Si 4.247967701 11.043637864 1.928982667
Si 4.263334716 10.948514305 9.342885636
Si 11.166093545 0.781696301 5.521140245
Si 11.037632017 0.611772385 13.118784237
Si 8.815856148 2.902791492 13.211916336
Si -0.201702803 10.906811050 1.715302477
Si -0.154358581 10.786357525 9.356224663
Si 2.171288732 8.738014457 1.678314809
Si 2.208649490 8.649812748 9.341637632
Si 13.272899872 3.114364310 5.626891532
Si 13.247040901 2.761754514 13.119105485
Si 10.917594212 5.186798726 5.602527546
Si 11.007566406 5.061174187 13.122305833
Si 1.630144276 3.647151482 7.833190032
Si 8.832544329 2.811408496 5.541231830
Al 1.008576566 6.724381127 7.132367583
Al 6.284087007 12.380469450 4.070910382
Al 6.029781848 12.232409097 11.662175800
Al 7.106878630 1.506794392 7.796587546
Cu1 3.234425480 8.043300803 6.272979661
Co2 5.162393011 10.013645350 4.880910221
H 8.119452617 2.896388527 9.460708319
H 7.359759427 11.053750791 10.051408981
C 6.912142989 6.140886391 7.066979136
H 6.860978305 5.301484558 6.363769334
H 7.959058230 6.438483506 7.199445473
H 6.489471091 5.832321100 8.031019313
H 6.336080010 6.985304778 6.669038802
End final coordinates

Cu-O-Cr-H2MOR-methane-adduct

Final enthalpy = -6758.6823676913 Ry
CELL_PARAMETERS (angstrom)
13.817593883 0.055273517 0.001137847
-1.380404381 13.613568759 -0.015310522
0.008561982 0.015740211 15.023671420

ATOMIC_POSITIONS (angstrom)
O 3.126650264 0.525216375 3.290640626
O 2.266688162 13.786779599 10.742898343
O 5.149719678 11.073349923 3.378975554
O 4.942922528 11.335074293 10.803853380
O 7.906697140 11.557430648 7.599078989
O 7.694529776 11.799675418 0.564977683
O 10.842075856 0.052020391 6.962819435
O 9.470517197 13.482390399 14.518343835
O 8.238256336 2.543485847 7.025893342
O 8.130820882 2.661964009 14.645248067
O 5.219107881 2.161364182 3.633259301
O 5.380276349 2.144218720 11.158427441
O 12.613250962 11.010771997 0.440419166
O 12.969614256 10.711387105 7.923507737
O 2.218776457 7.695567558 0.416517410
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O 1.696291047 5.325133405 3.332768501
O 1.706474866 5.007444657 11.198039753
O 0.123464093 3.289678299 4.151166648
O 0.187560328 2.894447326 11.714654910
O 11.051566353 5.903080288 4.152495353
O 11.203424841 5.762411320 11.684817854
O 11.419682770 8.650927776 0.153602907
O 11.155102822 8.754485408 7.717991468
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O 9.587980043 13.193245926 11.885315446
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O 7.759101245 2.957866448 12.013927472
O 5.568876354 2.119462523 15.009644301
O 5.429573669 1.867770801 7.685946584
O 3.530174114 0.475394149 0.649183567
O 3.143331300 0.550250249 8.147433642
O 5.145348289 11.324074210 0.702089851
O 5.441986383 10.893125277 8.227382034
O 7.926649081 12.013274258 3.715886251
O 7.653857292 11.705444045 10.823332918
O 0.624927795 3.013336663 6.753676126
O 0.551997958 2.753957799 14.354823103
O 10.760822578 6.309558848 6.792836890
O 11.098654876 6.214468516 14.304046458
O 11.346689356 8.462718599 3.513868574
O 11.392163287 8.382765142 11.259110846
O 12.833894678 10.648324642 3.090437076
O 12.573524510 10.716507243 10.564633672
O 1.962262777 7.933538368 3.070325501
O 2.219304866 7.483756959 10.451889674
O 1.570911070 5.267912466 7.839039879
O 1.594158065 5.163855509 14.927626560
O 3.101299791 12.166684575 2.186759910
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O 9.918474457 1.699098805 5.112707932
O 9.922802615 1.747246273 12.892904696
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O 0.948321756 9.619765428 9.597251050
O 12.239930690 4.315488359 5.935689179
O 12.230302892 3.997349138 13.396251109
O 3.753922710 1.277055229 5.708370632
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O 5.942128416 11.591844595 5.759088527
O 6.270591907 11.797340106 13.358991809
O 9.855211185 12.514240120 1.906029447
O 9.681741192 12.524308920 9.316716765
O 7.294524992 2.014199709 2.002427909
O 7.518412859 2.152238413 9.561381781
O 12.171012089 9.995520501 5.536614781
O 11.918851059 10.243136059 13.063567232
O 1.744229014 6.926693388 5.485340256
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O 1.262101436 3.252686545 1.780291855
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O 11.889748223 6.567312880 1.754273009
O 11.592242947 6.641066467 9.269640147
O 2.780414159 3.049771611 3.981026122

O 2.823510218 2.668269689 11.340606311
O 10.048358196 10.891874776 14.816385159
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O 10.247788241 10.760655072 3.842229379
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O 3.122751449 3.019543436 14.898196212
O 3.131665035 3.132909064 7.541915810
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O 13.553244839 7.124352761 14.778159939
O 13.252811491 7.216899861 7.259753820
O 5.672167173 13.894280273 3.996684887
O 7.347417902 0.342058926 11.500478775
O -0.349523482 6.900132336 3.872123844
O -0.264833339 6.807093618 11.098190321
O 0.493043073 12.376811423 1.798372413
O 0.551839474 12.253541507 9.485697052
O 3.557475820 9.556825370 1.820746794
O 3.624229676 9.483387263 9.462905380
O 12.530079633 1.689703396 5.717590919
O 12.530698528 1.343893561 13.143630915
O 9.571302142 4.296025388 5.572060528
O 9.594396357 4.362285108 13.238538127
O 4.632644524 8.448380551 5.111834856
Si 7.070429076 1.710086893 0.438276281
Si 9.269655666 12.156681553 0.440744149
Si 9.387731525 12.249420236 7.723920572
Si 3.739513715 1.755458213 4.165212575
Si 3.928918806 1.527003247 11.603002402
Si 11.944589924 6.969131977 3.328558835
Si 11.953218326 6.916142733 10.819918888
Si 1.460643042 3.718822152 3.326151892
Si 1.470839679 3.433632841 10.877176178
Si 1.302741162 6.712884441 14.536188966
Si 11.695584053 10.151711931 7.080302362
Si 11.504634379 10.194521875 14.634821546
Si 6.331263613 11.941928231 7.346425957
Si 6.274925023 12.193692641 14.905785631
Si 3.894689567 1.719823293 7.274140701
Si 4.036691984 1.690093836 14.700156268
Si 6.808608173 1.802985592 3.542768358
Si 6.963089386 1.838652140 11.152787973
Si 9.501670787 12.155250121 3.462010191
Si 9.337339409 12.036881989 10.814153740
Si 1.263197610 6.760775535 3.950083052
Si 1.309076860 6.557904749 11.426551021
Si 11.654407199 9.979968405 3.993565561
Si 11.504707525 9.972495508 11.521710192
Si 11.996617721 7.134857031 0.240103386
Si 11.731185338 7.214030226 7.744235904
Si 1.625057003 3.556704030 0.228578951
Si 1.871883885 13.208062312 1.964067048
Si 1.943215653 13.077343000 9.311887626
Si 4.222385041 11.026734011 1.980180043
Si 4.279115255 10.970034463 9.397281127
Si 11.195865286 0.799923083 5.544243207
Si 11.074356642 0.641001797 13.138529872
Si 8.856492304 2.925393372 13.227712961
Si -0.194385763 10.913398964 1.708775102
Si -0.143254326 10.796457005 9.377029234
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Si 2.234446228 8.665602516 9.342367866
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Si 13.285853508 2.786336055 13.154162041
Si 10.908313292 5.197667110 5.613790060
Si 11.046506017 5.081975702 13.151092833
Si 1.625775416 3.675443344 7.852138943
Si 8.835170287 2.847866911 5.565763367
Al 1.092735393 6.746923504 7.119151297
Al 6.301706516 12.316529937 4.119171089
Al 6.057774563 12.251515809 11.728060244
Al 7.095065045 1.536968506 7.825927330
Cu1 3.314420042 8.237012911 6.306318842
Cr2 4.799008904 10.112450944 5.063365319
H 8.135794367 2.904603158 9.489883965
H 7.389439994 11.113042951 10.088146670
C 6.894829470 6.226555832 7.011991823
H 6.925982805 5.363997343 6.337868488
H 7.907008349 6.631319988 7.128797676
H 6.504001925 5.912175623 7.987149125
H 6.237813291 6.990928863 6.580741095
End final coordinates

Cu-O-Cu-H2MOR-methane-adduct
Final enthalpy = -6672.3765759835 Ry
CELL_PARAMETERS (angstrom)
13.805446430 0.050682715 -0.013566032
-1.383769987 13.624082572 -0.037628835
-0.007300434 -0.010449264 15.021760751

ATOMIC_POSITIONS (angstrom)
O 3.157958277 0.548007542 3.256365318
O 2.229654640 13.786568526 10.692947709
O 5.228825304 11.099351571 3.276697300
O 4.915709943 11.286452948 10.764193978
O 7.897243102 11.517038402 7.560914482
O 7.689288420 11.793753665 0.527143878
O 10.808965656 0.012276069 6.923398034
O 9.447861964 13.450530872 14.471161395
O 8.252069480 2.527660496 7.011943219
O 8.075217817 2.654408279 14.624486699
O 5.199079280 2.238278953 3.613767688
O 5.351095229 2.131889123 11.124502307
O 12.623624783 11.003195660 0.407799925
O 12.964095235 10.633923966 7.886657230
O 2.222027554 7.705246043 0.416419029
O 2.066719517 7.994759803 7.844188680
O 1.630265916 5.331058125 3.382746258
O 1.672670729 4.998455158 11.181789204
O 0.085912010 3.258322574 4.138673339
O 0.169772978 2.868343991 11.697285360
O 11.065102703 5.906383559 4.148608662
O 11.161567656 5.764989542 11.667156593
O 11.415292166 8.652601963 0.112236970
O 11.078708814 8.741499207 7.690121228
O 10.205784400 13.360736805 4.324615661
O 9.530421422 13.191372000 11.830990244
O 7.624418881 2.882988666 4.449390427
O 7.727375949 2.920295556 11.991457473
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Si 11.488062706 10.173424487 14.600587629
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Si 9.299434282 12.026503289 10.763407901
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Si 1.630144276 3.647151482 7.833190032
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Al 6.284087007 12.380469450 4.070910382
Al 6.029781848 12.232409097 11.662175800
Al 7.106878630 1.506794392 7.796587546
Cu1 3.234425480 8.043300803 6.272979661
Co2 5.162393011 10.013645350 4.880910221
H 8.119452617 2.896388527 9.460708319
H 7.359759427 11.053750791 10.051408981

C 6.912142989 6.140886391 7.066979136
H 6.860978305 5.301484558 6.363769334
H 7.959058230 6.438483506 7.199445473
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H 6.336080010 6.985304778 6.669038802
End final coordinates

Cu-O-Fe-H2MOR-methane-adduct
Final enthalpy = -6652.1349818330 Ry
CELL_PARAMETERS (angstrom)
13.807958833 0.043226215 -0.019046104
-1.391379875 13.624553575 -0.029149664
-0.013299265 -0.001666787 15.026550077

ATOMIC_POSITIONS (angstrom)
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O 2.209282030 13.798940065 10.696553180
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O 4.917301074 11.292665075 10.772272156
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O 7.701321381 11.772937602 0.505576474
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O 5.338381289 2.145857795 11.116151806
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Cu1 3.286598992 8.030838294 6.259778313
Fe2 5.144020193 10.001788218 4.950120214
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End final coordinates

Cu-O-Mn-H2MOR-methane-adduct
Final enthalpy = -6796.9652482409 Ry
CELL_PARAMETERS (angstrom)
13.811943229 0.038263164 -0.014702354
-1.396598396 13.615934446 -0.035287329
-0.008540384 -0.007967288 15.032144927

ATOMIC_POSITIONS (angstrom)
O 3.165398283 0.601423994 3.221359051
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O 7.870696146 11.514922240 7.621912960
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O 7.865815855 12.141077526 3.647020311
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O     7.302485955   0.326990555  11.403920671
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O    -0.319243080   6.792929256  11.093534598
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O    12.424992624   1.710186538   5.744791723
O    12.479090007   1.342877053  13.123830108
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O     9.542664864   4.343629916  13.236175729
O     4.905869737   8.342024290   5.570303494
Si    7.050279803   1.702059033   0.449904012
Si    9.269893387  12.140524076   0.395260783
Si    9.341712131  12.227515735   7.710910839
Si    3.729909078   1.827372652   4.130902896
Si    3.890642802   1.525448278  11.572190766
Si   11.915800707   6.999067246   3.293326295
Si   11.894116356   6.903346724  10.794745148
Si    1.395940264   3.716906977   3.310036132
Si    1.431143376   3.424778391  10.852153521
Si    1.288915906   6.697225682  14.533382934
Si   11.636555648  10.120936726   7.038568276
Si   11.519566628  10.180226826  14.588954138
Si    6.309583616  11.930199572   7.314529708
Si    6.263248133  12.177231554  14.868692948
Si    3.902135298   1.719195579   7.240788206
Si    3.971880751   1.618852774  14.685648182
Si    6.775074025   1.865327298   3.541267691
Si    6.923791684   1.834918806  11.105186760
Si    9.448108952  12.172978575   3.419862462
Si    9.298228231  12.032853740  10.788185809
Si    1.225529742   6.812904291   3.932495470
Si    1.257998215   6.550047292  11.417064959
Si   11.519294095   9.954484142   3.952137079
Si   11.481258811   9.969683914  11.476800230
Si   11.990614773   7.133349457   0.207604171
Si   11.673757916   7.200136370   7.720188717
Si    1.616793648   3.570017498   0.206696580
Si    1.853162726  13.212180267   1.929132256
Si    1.909806046  13.068829395   9.255349039
Si    4.234584291  11.063956527   1.928905360
Si    4.249434209  10.945660180   9.352216581
Si   11.146791628   0.756940821   5.521811997
Si   11.029288312   0.627323694  13.141609042
Si    8.793523407   2.910501539  13.227642197
Si   -0.230270578  10.896539149   1.731583854
Si   -0.170995451  10.782372970   9.324449010
Si    2.158957912   8.736289935   1.676337823
Si    2.202920170   8.640744320   9.321780717
Si   13.289302755   3.065374923   5.617454994
Si   13.237334001   2.782409192  13.111528554
Si   10.972760663   5.162247281   5.589396527
Si   10.988297724   5.073653112  13.126159091
Si    1.613703300   3.629775862   7.819847618
Si    8.849078278   2.809777318   5.531625819
Al    1.026270555   6.733119428   7.114756709
Al    6.235668725  12.396139654   4.084527059
Al    6.022035625  12.248886178  11.664384331
Al    7.108029446   1.526453547   7.793709705
Cu1   3.339499225   7.957080905   6.281229960
Mn2   5.223822694   9.913945829   4.926111602
H     8.071808958   2.959857038   9.455153834
H     7.375860260  11.016708391  10.111998938
C     7.006949005   5.929400621   7.302021170
H     6.857138022   5.129199750   6.569735047
H     8.078517794   6.134249715   7.399039398
H     6.594106048   5.617714811   8.269739247
H     6.488101872   6.830773979   6.957815227
End final coordinates

   Cu-O-Ni-H2MOR-methane-adduct
   Final enthalpy          =   -6696.0129550911 Ry
CELL_PARAMETERS (angstrom)
  13.793784197   0.062998219  -0.020623402
  -1.370440557  13.618808314  -0.037031235
  -0.014992104  -0.010569579  15.017798991

ATOMIC_POSITIONS (angstrom)
O     3.165966138   0.602574692   3.206852214
O     2.235473422  13.778634989  10.661973650
O     5.278306818  11.118174724   3.281144103
O     4.922889559  11.300173563  10.753269238
O     7.897382750  11.486162518   7.589644259
O     7.720010282  11.738742797   0.497542990
O    10.733149363  -0.001308445   6.893486504
O     9.426738831  13.455098853  14.455851407
O     8.262497032   2.541236216   6.998526605
O     8.032633308   2.665224030  14.609974168
O     5.186717088   2.311311677   3.604546057
O     5.328831677   2.139660973  11.099089817
O    12.691132186  11.002171525   0.384515374
O    12.974129073  10.626581775   7.846427032
O     2.245255822   7.707134841   0.410917172
O     2.099503208   7.974955050   7.838933214
O     1.470110927   5.313147718   3.404465502
O     1.660795729   4.984020381  11.161341213
O     0.051596945   3.150917644   4.124228720
O     0.129589727   2.874030968  11.669854783
O    11.119578439   5.913575771   4.144062663
O    11.126966578   5.798814121  11.676205279
O    11.463727927   8.665742157   0.081757804
O    11.072968939   8.750324503   7.683830918
O    10.221564180  13.391583674   4.308820253
O     9.522969172  13.221919140  11.819939960
O     7.616902186   2.936536318   4.442726032
O     7.701769630   2.946708556  11.976403732
O     5.512098709   1.989851277  15.026927922
O     5.453409642   1.834278627   7.618109440
O     3.476274454   0.353874463   0.566237384
O     3.165037280   0.513164656   8.073845844
O     5.135384467  11.326161315   0.616798535
O     5.427091006  10.884632824   8.168999942
O     7.914871044  12.231561190   3.659556134
O     7.624692413  11.694517407  10.763604852
O     0.685402912   2.939762994   6.696677470
O     0.519880303   2.771482283  14.306368347
O    10.704973973   6.289999319   6.774436803
O    11.058506149   6.188303114  14.302200859
O    11.165585756   8.482130041   3.461194722
O    11.365152955   8.410506206  11.217019274
O    12.722742728  10.627532430   3.033377727
O    12.536711134  10.735824383  10.479630667
O     2.094697820   7.861149978   3.073757365
O     2.200894460   7.465638914  10.455485495
O     1.542451099   5.218981163   7.770284994
O     1.656312466   5.135606210  14.921615950
O     3.156567975  12.183158405   2.176743215
O     3.130845137  12.009054719   8.878149205
O     9.850462786   1.654062050   5.033109182
O     9.856162798   1.746291170  12.898568645
O     0.943041572   9.713994626   1.544865597
O     0.964627779   9.621440201   9.603373634
O    12.313766125   4.374952203   5.938178746
O    12.155351776   3.987893308  13.334277786
O     3.736309152   1.322205021   5.651938704
O     3.920779142   1.085822695  13.127011349
O     5.994520141  11.633672456   5.685952734
O     6.254674660  11.844008340  13.300135653
O     9.866257006  12.541600507   1.847914231
O     9.651730372  12.544357535   9.263603469
O     7.282259729   2.065246197   2.001668682
O     7.494582317   2.156772347   9.517479803
O    12.089367639   9.949476083   5.477934145
O    11.933600979  10.269342611  12.999771235
O     1.694304725   6.974463813   5.500383191
O     1.626377369   6.931186058  12.957871584
O     1.205357011   3.278570829   1.758666631
O     1.131634394   3.104499414   9.290104055
O    11.883746917   6.607042789   1.739573123
O    11.520576469   6.643329042   9.255830954
O     2.722699725   3.099445686   3.959275406
O     2.765788629   2.637192504  11.334604375
O    10.083100108  10.885768793  14.774098879
O    10.486414335  11.239121715   7.114667729
O    10.153801451  10.814769213   3.830627953
O    10.014337243  10.667154355  11.172108224
O     3.077909533   2.912931578  14.920734190
O     3.161532724   3.115730211   7.562948173
O     7.419611096   0.148359203   0.166818616
O     7.478405302  -0.177688034   7.725937095
O    13.539360007   7.053672949  14.765177672
O    13.171077897   7.214431508   7.245115533
O     5.567602883  13.984898507   3.996536488
O     7.289057976   0.330548703  11.424800830
O    -0.362629934   7.163905881   3.847845634
O    -0.293499455   6.790184956  11.088730547
O     0.528890174  12.327098378   1.893672666
O     0.530073885  12.247331186   9.382179382
O     3.599487172   9.568067202   1.823095463
O     3.627527319   9.440287241   9.400084254
O    12.410018255   1.730640076   5.822868403
O    12.467505074   1.341107277  13.117500813
O     9.640802526   4.252371048   5.516020335
O     9.522410578   4.364404795  13.213829026
O     4.726527645   8.577823135   5.547542197
Si    7.061439582   1.701905660   0.448605501
Si    9.283308531  12.154817088   0.389207423
Si    9.352793333  12.227319300   7.678595726
Si    3.723571969   1.829344455   4.118564329
Si    3.888867270   1.503602691  11.558641679
Si   11.900558340   7.047067868   3.301519536
Si   11.897946800   6.929427325  10.801340416
Si    1.361061120   3.694431892   3.320549802
Si    1.425798566   3.407712947  10.847896101
Si    1.318394253   6.676926632  14.532611370
Si   11.658422725  10.125805462   7.031025454
Si   11.534738730  10.189699118  14.574862811
Si    6.335117650  11.914969180   7.288966431
Si    6.275985508  12.170123605  14.862997821
Si    3.912681912   1.704990627   7.228630665
Si    3.984660881   1.584412576  14.674802585
Si    6.762594952   1.887902275   3.536128202
Si    6.914526985   1.833574880  11.097479575
Si    9.491312425  12.244146722   3.410351370
Si    9.300434801  12.053010215  10.757570101
Si    1.214621270   6.812000139   3.944232045
Si    1.281049130   6.534719824  11.416652053
Si   11.537070842   9.988589154   3.947276016
Si   11.487241180  10.001755194  11.466046731
Si   12.003646774   7.141048300   0.214496380
Si   11.648681048   7.213277726   7.731304037
Si    1.625725882   3.550503328   0.214931127
Si    1.901225052  13.187273092   1.937173791
Si    1.934736654  13.056176175   9.231949379
Si    4.280078542  11.041650501   1.952578678
Si    4.271933872  10.938013227   9.337297070
Si   11.135890881   0.791298166   5.517466905
Si   11.009987215   0.637543341  13.114222020
Si    8.783164218   2.924401354  13.204680661
Si   -0.177214531  10.879534449   1.739431629
Si   -0.139990454  10.775988740   9.325259761
Si    2.213301037   8.715860878   1.695112577
Si    2.226832229   8.638544079   9.336529546
Si   13.261425362   3.085254454   5.626777382
Si   13.217638352   2.784912303  13.097028714
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Si 10.976359354 5.082103394 13.125915180
Si 1.636954373 3.628259736 7.822106935
Si 8.831076546 2.844872102 5.526089506
Al 1.018456397 6.714691488 7.141526423
Al 6.272975994 12.432796166 4.082870850
Al 6.028353598 12.249205087 11.659041984
Al 7.120493308 1.511199100 7.779954303
Cu1 3.242799461 8.011684829 6.252639500
Ni2 5.296693639 10.005178231 4.867260476
H 8.084303253 2.930676854 9.445946902
H 7.367462776 11.080219293 10.043624448
C 6.816454792 6.124063056 7.101651914
H 6.655363475 5.330891828 6.362964490
H 7.892510417 6.282037432 7.236637604
H 6.357270142 5.832794485 8.053928720
H 6.354475057 7.051250658 6.742243518
End final coordinates

Cu-O-Ti-H2MOR-methane-adduct
Final enthalpy = -6694.3118684694 Ry
CELL_PARAMETERS (angstrom)
13.797219337 0.031839923 -0.005851243
-1.401561879 13.609961070 -0.014861434
0.000943116 0.015520121 15.005726224

ATOMIC_POSITIONS (angstrom)
O 3.153499001 0.578462859 3.265586593
O 2.132575805 13.860458773 10.688140643
O 4.912485186 11.135786942 3.584905731
O 5.207131568 11.324321256 10.455740426
O 7.786172419 11.508146350 7.884203757
O 7.775732401 11.629982052 0.184448734
O 10.668771684 -0.091169010 6.912023142
O 9.505148199 13.525850607 14.500391665
O 8.236017629 2.576780118 7.026626838
O 8.072062068 2.656126142 14.616428560
O 5.184202330 2.294648592 3.554598209
O 5.317023943 2.174892869 11.173749065
O 12.774493906 10.998886302 0.330618917
O 12.868996962 10.715081120 7.799765830
O 2.188604008 7.821206632 0.342371827
O 2.230909036 7.858226312 7.862743790
O 1.396778331 5.247849712 3.331648630
O 1.689827246 5.074153911 10.967229926
O 0.060487885 3.054840364 4.112107939
O 0.112048540 3.057718294 11.652082453
O 11.245012586 5.770551052 4.130230190
O 11.156924374 5.742700885 11.644030444
O 11.501697807 8.684935016 0.173803185
O 11.115926598 8.678373410 7.679879172
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O 3.315272287 0.458128122 0.604689366
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O 5.138951938 10.959835126 7.786697175
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O 0.634267701 2.774171764 6.706938763
O 0.653206222 2.891573188 14.250436681
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O 1.384570345 5.144936678 7.722757323
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Si 1.569574176 3.569746922 7.781264990
Si 8.810922279 2.842528573 5.549212515
Al 1.108054425 6.694665965 7.051607367
Al 6.204227204 12.380955342 4.031015674
Al 6.003130909 12.265106824 11.678796365
Al 7.094319338 1.605187275 7.864049167
Cu1 3.528614023 8.171634799 6.497777508
Ti2 4.765698031 10.332751973 5.511867091
H 8.046245444 3.033585216 9.543889453
H 7.437757653 11.119662339 10.269412407
C 6.795113873 5.997195497 7.273809324
H 6.586722752 5.178831564 6.575765605
H 7.879202058 6.090883552 7.407273386
H 6.314441964 5.786139959 8.237252536
H 6.397209595 6.930582276 6.858421704
End final coordinates

Cu-O-V-H2MOR-methane-adduct
Final enthalpy = -6724.5816074857 Ry
CELL_PARAMETERS (angstrom)
13.908105047 -0.019080110 -0.008292717
-1.462921604 13.643941926 -0.025605126
-0.001509922 0.003653195 15.105895813

ATOMIC_POSITIONS (angstrom)
O 3.243716662 0.580208262 3.209254285
O 2.142560964 13.900912616 10.731640903
O 5.185697292 11.077682497 3.303076323
O 5.000974403 11.271990209 10.783384790
O 7.809807701 11.520763230 7.648452582
O 7.697560977 11.740861922 0.453805443
O 10.885110765 -0.079102831 6.968102358
O 9.561563604 13.349168350 14.544059707
O 8.293380494 2.464592778 7.026349769
O 8.048637840 2.612204302 14.671194997
O 5.288164936 2.235532078 3.732792776
O 5.423315621 2.138894974 11.234170473
O 12.684386449 10.955569353 0.446381004
O 12.885982747 10.730242271 7.969471517
O 2.199552722 7.726956275 0.412522811
O 2.153583731 8.000763513 7.891758917
O 1.540122920 5.307223409 3.371568830
O 1.607718676 5.037015324 11.253996076
O 0.161056447 3.138271382 4.182813415
O 0.244031701 2.816677845 11.764165532
O 11.153332153 5.828768664 4.187808595
O 11.110131787 5.784376532 11.757380564
O 11.535658241 8.582341740 0.074959212
O 11.196143158 8.671179059 7.711200050
O 10.162980436 13.285127395 4.376295390
O 9.582716777 13.205108951 11.894713962
O 7.769978358 2.844836447 4.442256594
O 7.862380768 2.877506452 12.021929688
O 5.525337984 1.969540308 15.114517071
O 5.453925947 1.842548927 7.605200806
O 3.448085906 0.365988463 0.552335634
O 3.189561018 0.502709218 8.120008681
O 5.131870564 11.277032062 0.633722079
O 5.298181992 10.865250613 8.166371110
O 7.892397667 12.027872482 3.740752371
O 7.665150300 11.638869286 10.943759937
O 0.645761059 2.956110326 6.798363170
O 0.494682423 2.820020105 14.415841568
O 10.894699574 6.199330235 6.837987840
O 11.171801412 6.100887621 14.397609122
O 11.294263743 8.406933015 3.590038164
O 11.419273020 8.387073952 11.331394612
O 12.796622324 10.565091255 3.088622415
O 12.628422063 10.701070089 10.633053888
O 1.995767893 7.886771549 3.080471858
O 2.065897011 7.532864850 10.535029206
O 1.577668586 5.242208029 7.832162765
O 1.663564368 5.159091583 15.025717859
O 3.133829195 12.231181617 2.122859469

O 3.119880664 12.101197338 9.037137603
O 9.975032356 1.580122989 5.132073950
O 9.919838593 1.601176223 13.074666478
O 0.849634060 9.720750939 1.515419934
O 0.827284522 9.623955656 9.531306558
O 12.417968504 4.256728112 5.912517322
O 12.330092814 3.987272440 13.290692609
O 3.690670818 1.300144992 5.679987895
O 3.910581131 1.130119806 13.200332271
O 5.924085169 11.592007928 5.742558890
O 6.181731671 11.900281332 13.390977066
O 9.786187540 12.498947219 1.900183161
O 9.609423737 12.490626454 9.341340604
O 7.279452126 2.061829626 2.000647844
O 7.491046976 2.162847854 9.546230049
O 12.114746483 10.021567238 5.556408709
O 11.920691465 10.273565852 13.133695175
O 1.659641617 6.924040782 5.504637633
O 1.550990411 6.959777314 13.062542479
O 1.222285628 3.255035281 1.771910299
O 1.181265850 3.138827971 9.372163360
O 11.863760943 6.559316471 1.776548574
O 11.600098602 6.629134893 9.342900303
O 2.823800862 3.094805234 3.910766042
O 2.889668730 2.776867657 11.385411613
O 10.083477736 10.774610389 14.983038905
O 10.360767403 11.091827756 7.210290930
O 10.199297424 10.719265090 3.812164630
O 10.073418397 10.639282014 11.243529019
O 3.083039263 2.939874939 14.995185520
O 3.151251046 3.106385207 7.587551017
O 7.426201657 0.104885889 0.221108415
O 7.439762203 -0.204593074 7.770649912
O 13.625601020 6.961351894 14.948802766
O 13.345227753 7.152798884 7.385911556
O 5.608833628 13.931886177 3.967374998
O 7.375477396 0.296589531 11.417671216
O -0.397279448 7.044511675 3.833751557
O -0.389711086 6.799817696 11.234731802
O 0.485608355 12.328486609 1.910252059
O 0.499857602 12.273282078 9.494153361
O 3.502266054 9.592861707 1.835118539
O 3.508349310 9.512505121 9.552369899
O 12.570503343 1.609008806 5.802238619
O 12.566252871 1.325599135 13.200290275
O 9.734049066 4.176914102 5.628069850
O 9.671254722 4.237073233 13.343342609
O 4.680605643 8.349121493 5.210101362
Si 7.060892224 1.667770768 0.453833794
Si 9.282638968 12.081451407 0.419773169
Si 9.307202027 12.174724877 7.757635912
Si 3.778686159 1.802200325 4.144679974
Si 3.937066645 1.574653225 11.638073557
Si 11.966064488 6.949746547 3.350938760
Si 11.931464866 6.899116451 10.900843227
Si 1.433612562 3.691696422 3.326757287
Si 1.483606779 3.452928860 10.925478243
Si 1.284519856 6.693399057 14.644864986
Si 11.650049002 10.111064869 7.109693953
Si 11.556571439 10.138940487 14.715779031
Si 6.246945522 11.923253663 7.354279467
Si 6.245172544 12.184780801 14.959030739
Si 3.902210119 1.700107286 7.250799057
Si 3.985882244 1.608559000 14.753859166
Si 6.857328867 1.828993594 3.557921256
Si 7.001010024 1.812321833 11.152176489
Si 9.468912353 12.132068652 3.460195388
Si 9.334833737 12.018446883 10.856394640
Si 1.199914973 6.777036669 3.970504801
Si 1.196272351 6.577706620 11.518206919
Si 11.606745420 9.942334370 4.010503418
Si 11.540143069 9.977858166 11.586038784
Si 12.061034055 7.055786587 0.248379382
Si 11.806170570 7.148812143 7.803583705
Si 1.616303288 3.558341629 0.226607523
Si 1.843930300 13.209845869 1.932881553
Si 1.879814292 13.117043047 9.328258531
Si 4.214207177 11.047296560 1.933813216
Si 4.222859699 10.965628318 9.419994760
Si 11.260618380 0.696509128 5.573197394
Si 11.145893023 0.558818709 13.212414164
Si 8.882405082 2.827521389 13.304597888
Si -0.251907494 10.894477326 1.757494156
Si -0.237648985 10.836964720 9.396444745
Si 2.119904977 8.723678567 1.703255736
Si 2.135098608 8.675555394 9.386198234
Si 13.406089770 2.987899221 5.662429734
Si 13.364656914 2.741687132 13.166934483
Si 11.052501696 5.106406273 5.643913432
Si 11.084031834 5.023341746 13.194536438
Si 1.642486246 3.652775289 7.883767655
Si 8.932854235 2.766385475 5.583343880
Al 1.080854414 6.736958985 7.152352068
Al 6.260785051 12.368714136 4.107788418
Al 6.035344017 12.257473307 11.731404384
Al 7.109330079 1.492726161 7.813741440
Cu1 3.410243116 8.156000004 6.464970905
V2 5.141348376 9.918188757 4.931223631
H 8.115842402 2.907818740 9.459823309
H 7.403703581 10.919187941 10.333959015
C 6.867902282 6.168985925 7.121729540
H 6.792593908 5.343849371 6.404233887
H 7.920073043 6.453825175 7.240694934
H 6.456100206 5.852327426 8.088008174
H 6.292996228 7.023461730 6.744843803
End final coordinates

Cu-O-Ag-H2MOR-methane-adduct
Final enthalpy = -6865.5387650495 Ry
CELL_PARAMETERS (angstrom)
13.801609146 0.028376461 -0.004955632
-1.405466785 13.632444982 -0.034248132
0.001903557 -0.005789397 15.025718342

ATOMIC_POSITIONS (angstrom)
O 3.195471180 0.586143852 3.195047887
O 2.138710265 13.858917336 10.671566509
O 5.194337720 11.192123639 3.182450159
O 4.929603655 11.327690157 10.719132977
O 7.782638834 11.589867523 7.865098970
O 7.698999752 11.780370281 0.472972492
O 10.727760251 -0.053273707 6.903562822
O 9.493496987 13.447205886 14.481079255
O 8.299780550 2.476292933 6.961990537
O 7.929772778 2.690043317 14.610054309
O 5.222736756 2.285122396 3.619547826
O 5.356637185 2.140385034 11.096707352
O 12.656644147 10.975266466 0.405559224
O 12.773753552 10.737139257 7.888279435
O 2.190644175 7.795121009 0.385154425
O 2.122503290 7.968935692 7.814433649
O 1.500418715 5.316593683 3.408734603
O 1.611445996 5.045001700 11.109922375
O 0.085340483 3.148656698 4.122360834
O 0.176580627 2.879984532 11.658221441
O 11.216685083 5.850673289 4.167675306
O 10.988466077 5.879443709 11.710493581
O 11.416693448 8.637355835 0.167875285
O 11.050503078 8.692777612 7.712060980
O 10.169387248 13.272850286 4.334862059
O 9.522948858 13.304435759 11.826083031
O 7.681323212 2.881698707 4.391870291
O 7.743142378 2.936378021 11.963102418
O 5.443271386 1.939915504 15.120023137
O 5.461348970 1.922216550 7.556712572
O 3.249467116 0.454356524 0.526622271
O 3.190101459 0.565582515 8.078163931
O 5.122213574 11.308701640 0.493201330
O 5.284231760 10.886383176 8.098202222
O 7.848708434 12.193854734 3.578991995
O 7.668188469 11.786862992 10.651332393
O 0.693865550 2.894513736 6.698729507
O 0.488489113 2.897600319 14.305373188
O 10.750093494 6.218622609 6.790862352
O 11.061799502 6.164694768 14.363856733
O 11.191900932 8.417006658 3.491016882
O 11.311467187 8.447885914 11.127976458
O 12.620991050 10.648854353 3.064121573
O 12.558163245 10.764947884 10.556696015
O 2.145780678 7.866278636 3.055973596
O 2.058484292 7.542873118 10.433415797
O 1.491723189 5.220856726 7.734174851
O 1.638473849 5.226304422 14.984081841
O 3.133235392 12.292871609 1.948688483
O 3.068045730 12.060789654 8.931122332
O 9.920939253 1.619428226 5.016949217
O 9.844037299 1.736425775 13.017298633
O 0.847933782 9.705940120 1.635311832
O 0.861541869 9.661552625 9.426340838
O 12.313505444 4.252919168 5.969937578
O 12.169714766 4.049843029 13.227789153
O 3.713652989 1.323266446 5.640969993
O 3.905835462 1.155641649 13.120827164
O 6.098149217 11.633374773 5.713988554
O 6.364694132 11.837783484 13.219275332
O 9.869331247 12.469387935 1.851626424
O 9.775987813 12.543240503 9.283682829
O 7.287405466 1.924572301 1.992042258
O 7.492485418 2.188928148 9.494041062
O 11.997915507 9.944557012 5.507078416
O 11.951178578 10.155196990 13.044624493
O 1.763079392 6.973957205 5.496875922
O 1.649882348 6.949929231 12.950896023
O 1.212620962 3.298963829 1.747964133
O 1.159200349 3.114533931 9.278309221
O 11.984191480 6.568862983 1.768213723
O 11.582047227 6.589508895 9.265890560
O 2.759729122 3.097592319 3.920357026
O 2.826297952 2.752078475 11.313375420
O 10.069370907 10.858755510 14.761438188
O 10.260841706 11.108721506 7.093457937
O 10.043574262 10.704897748 3.817328600
O 10.029825737 10.739502800 11.274759082
O 3.070440649 3.018774999 14.867924505
O 3.166451006 3.162880238 7.521721124
O 7.386848205 0.133422198 0.027019308
O 7.363044068 -0.177444912 7.764782615
O 13.527970503 7.099004243 14.717874421
O 13.181599159 7.231514563 7.222140152
O 5.538196026 13.951670324 4.067279528
O 7.318504702 0.327364206 11.376801686
O -0.306233955 7.191942308 3.877700226
O -0.380657243 6.811656055 11.215554650
O 0.475516458 12.332461599 1.927218563
O 0.468408269 12.314108318 9.350468256
O 3.525871759 9.657508300 1.778229402
O 3.540112522 9.489908969 9.433428524
O 12.479018553 1.604592429 5.785265464
O 12.475525729 1.396282089 13.146195742
O 9.657520181 4.218660148 5.498667202
O 9.514828582 4.354706117 13.284891802
O 4.971868211 7.956473541 5.699817941
Si 7.002917867 1.653251622 0.430767532
Si 9.277412952 12.135248456 0.382631819
Si 9.299005635 12.220344087 7.742486998
Si 3.745675797 1.816987114 4.102983751
Si 3.893223642 1.563997238 11.551127484
Si 11.970446706 7.006723883 3.332126451
Si 11.843514171 6.941263426 10.824680559
Si 1.387927992 3.696606908 3.311167975
Si 1.448046818 3.454793139 10.829123577
Si 1.303921247 6.746158140 14.524363630
Si 11.532364687 10.103576809 7.051971136
Si 11.520406211 10.147838604 14.613382912
Si 6.246802038 11.942058663 7.307512376
Si 6.291232034 12.175109038 14.780187018
Si 3.917131910 1.746442973 7.203443965
Si 3.917921754 1.641525449 14.671536717
Si 6.787495595 1.817180229 3.540592993
Si 6.942995225 1.833906762 11.079650472
Si 9.429047949 12.161672405 3.396701891
Si 9.338130208 12.110391741 10.783016522
Si 1.269515387 6.821479723 3.935264879
Si 1.215538167 6.578760950 11.427063873
Si 11.464648895 9.947258017 3.967909101
Si 11.481686416 10.011269930 11.501027669
Si 12.002146512 7.124664998 0.243837270
Si 11.666723084 7.173691418 7.741936740
Si 1.602374505 3.627259320 0.207288880
Si 1.816747877 13.239217465 1.879358651

Si 1.878913161 13.120612210 9.242091111
Si 4.244635893 11.122372988 1.837980566
Si 4.214206393 10.974825314 9.336931764
Si 11.164433142 0.705579707 5.513119406
Si 11.037136242 0.659233957 13.154994787
Si 8.762396525 2.922202920 13.245355134
Si -0.253982121 10.899011794 1.770085277
Si -0.229860117 10.856632488 9.297730924
Si 2.167854995 8.766521441 1.693814743
Si 2.150133941 8.691580909 9.300157766
Si 13.289841270 2.992179296 5.629905936
Si 13.229296017 2.831552072 13.084438159
Si 10.982318562 5.125720374 5.606532850
Si 10.944841044 5.108324446 13.142541813
Si 1.632715091 3.632372499 7.801268803
Si 8.875317378 2.793122312 5.495716732
Al 1.008866802 6.730942508 7.113090457
Al 6.223397977 12.376817361 4.095838876
Al 6.082168363 12.254467763 11.585525414
Al 7.108041166 1.524061489 7.764049064
Cu1 3.379283270 7.799912673 6.350789672
Ag2 5.217660161 9.656475635 4.711547246
H 8.033094494 2.997676327 9.418352747
H 7.482427661 11.518653606 9.708069367
C 7.048070310 5.783770921 7.677748615
H 6.724036446 5.066643369 6.915105008
H 8.142607977 5.777639488 7.742503354
H 6.608028051 5.511438365 8.645100739
H 6.705033948 6.786821088 7.395529542
End final coordinates

Cu-O-Mo-H2MOR-methane-adduct
Final enthalpy = -6874.2631307057 Ry
CELL_PARAMETERS (angstrom)
13.819673438 0.045295416 -0.002364200
-1.390263873 13.591441107 -0.029913170
0.004859519 -0.000703465 15.016638838

ATOMIC_POSITIONS (angstrom)
O 3.155541198 0.586521381 3.248318511
O 2.270415108 13.760980458 10.702549483
O 5.128867746 11.098633360 3.335019534
O 4.909993495 11.288882232 10.797545361
O 7.905259371 11.508253491 7.519482343
O 7.681543034 11.752375385 0.539680189
O 10.839918056 0.047913219 6.951504982
O 9.447053475 13.435268603 14.505465503
O 8.295617090 2.503908264 7.028838047
O 8.065179592 2.655387544 14.636180214
O 5.236509400 2.231765994 3.649917768
O 5.364004107 2.172836746 11.100691298
O 12.624563604 11.009302765 0.397191427
O 12.985898900 10.693246532 7.869335230
O 2.217970430 7.687134639 0.420532711
O 2.170634158 7.993664477 7.806827001
O 1.609023208 5.324712694 3.230645315
O 1.660740031 4.974124837 11.190267271
O 0.129498257 3.247492884 4.112098184
O 0.155912542 2.838580601 11.665785033
O 11.081914780 5.850614975 4.109934320
O 11.152890430 5.744604122 11.653112768
O 11.431383239 8.644733562 0.125282989
O 11.159505742 8.742938608 7.719723849
O 10.168704036 13.290050999 4.361197223
O 9.515171384 13.147314055 11.866857254
O 7.673606612 2.884238128 4.471264262
O 7.738199143 2.947643794 12.003248159
O 5.522628663 2.065410071 15.092387317
O 5.457950601 1.853074723 7.633729460
O 3.410929351 0.478190407 0.590204105
O 3.167844002 0.550298979 8.124957265
O 5.133176471 11.282453974 0.652156052
O 5.457096472 10.846211223 8.231621983
O 7.895167694 12.038408720 3.719584876
O 7.615103922 11.630860280 10.816274724
O 0.687090696 3.010186100 6.705623400
O 0.523938205 2.739177849 14.307734990
O 10.804404531 6.317245367 6.745177782
O 11.107377553 6.187220865 14.275568852
O 11.278164803 8.423068287 3.487621641
O 11.373104882 8.359376161 11.222526736
O 12.752572725 10.611009723 3.047175146
O 12.557980975 10.690287816 10.509841933
O 1.980741166 7.925871530 3.080957195
O 2.188705671 7.443493244 10.425465936
O 1.565554626 5.258064056 7.861830185
O 1.561477862 5.143828001 14.917626588
O 3.101672223 12.207301802 2.099078592
O 3.158490327 12.021431610 8.886086424
O 9.950014815 1.689735670 5.081089249
O 9.877319053 1.717740993 12.917257442
O 0.891151317 9.740012706 1.452884617
O 0.930352801 9.579164539 9.555686315
O 12.300592684 4.316459810 5.916685613
O 12.206839864 3.965699729 13.331041643
O 3.732203849 1.315162496 5.683485010
O 4.004877442 1.114483144 13.145429122
O 5.902631756 11.556876746 5.737544237
O 6.255458990 11.823576989 13.325376858
O 9.826780060 12.482472009 1.899201379
O 9.612644301 12.509401632 9.293391739
O 7.317665557 2.030431923 2.031964332
O 7.518492376 2.165858657 9.530858293
O 12.125847385 9.956777412 5.502673126
O 11.897806398 10.230443752 13.018622028
O 1.746450683 6.812238164 5.457423823
O 1.659363058 6.939558747 12.952961450
O 1.276213024 3.201615958 1.738284400
O 1.160491650 3.095163323 9.300058003
O 11.919911602 6.559322719 1.724877204
O 11.610462465 6.609482029 9.242770184
O 2.793381837 3.108211813 3.947884419
O 2.799490210 2.646070631 11.349989264
O 10.044729840 10.851847214 14.799954458
O 10.485739756 11.208335954 7.144505093
O 10.177796598 10.716858464 3.833545180
O 10.016590690 10.605210136 11.156813465
O 3.102011367 3.012344213 14.815970656
O 3.169314916 3.145409937 7.557266017
O 7.344963798 0.148987588 0.160620033
O 7.455678851 -0.179145162 7.741758058
O 13.557391704 7.118546498 14.731156791
O 13.277633365 7.233238625 7.250995869
O 5.627793181 13.903694529 4.027299985
O 7.308767575 0.341417228 11.433161771
O -0.362183624 6.965452457 3.866889394
O -0.291755307 6.786437603 11.126562558
O 0.470913460 12.350169089 1.849667082
O 0.561520372 12.222255405 9.452163617
O 3.526051996 9.572333155 1.818735551
O 3.607869191 9.449247312 9.454004320
O 12.548105197 1.680032637 5.731532402
O 12.495146101 1.310445261 13.114556122
O 9.624300850 4.274408237 5.594584812
O 9.573346975 4.339638384 13.247367066
O 4.831737004 8.158667776 5.199969827
Si 7.050738526 1.709383256 0.477163402
Si 9.254738275 12.122795038 0.430198774
Si 9.368982495 12.221765302 7.694745753
Si 3.748743883 1.810812360 4.145462344
Si 3.933872964 1.525663184 11.575902695
Si 11.941629028 6.956718790 3.300981254
Si 11.936476424 6.888470960 10.801182376
Si 1.448748129 3.710640909 3.274285347
Si 1.449218297 3.399945848 10.857765092
Si 1.301823436 6.695658302 14.519178770
Si 11.693709960 10.131471854 7.056140216
Si 11.504924148 10.171086218 14.595976035
Si 6.325078527 11.893693993 7.327658980
Si 6.262560739 12.163694207 14.882905193
Si 3.912867999 1.727137777 7.253472438
Si 4.007398325 1.669291949 14.675638691
Si 6.816608770 1.836491616 3.570171518
Si 6.945280645 1.849997413 11.112286401
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Si 1.245055314 6.744580290 3.928244601
Si 1.288460422 6.530062477 11.419126639
Si 11.589256243 9.939906136 3.967016610
Si 11.491597491 9.950256456 11.475169952
Si 12.009967615 7.129908809 0.211566708
Si 11.754446957 7.209299994 7.726601346
Si 1.608936467 3.547139290 0.187832102
Si 1.835985728 13.216455538 1.926638193
Si 1.949667365 13.050048924 9.271841368
Si 4.200476628 11.042262494 1.934307362
Si 4.269389908 10.932046421 9.378006304
Si 11.217749039 0.787325998 5.536476257
Si 11.036314031 0.613600967 13.135683920
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Si -0.145464416 10.771365824 9.335726672
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Si 2.221942605 8.627749731 9.320019841
Si 13.327716052 3.092565534 5.608377042
Si 13.258104457 2.748628518 13.105653933
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Si 11.024658746 5.057913957 13.121329309
Si 1.649506625 3.667416965 7.843152077
Si 8.878025986 2.834129410 5.569187605
Al 1.098368813 6.718041135 7.090357384
Al 6.266044142 12.327449249 4.115561142
Al 6.023669810 12.237586993 11.688650593
Al 7.119143829 1.515035237 7.802739684
Cu1 3.461007344 8.057000380 6.405239336
Mo2 4.771013900 9.915699083 5.036550281
H 8.147337576 2.907430747 9.449783274
H 7.357927832 10.933081434 10.179086058
C 6.913689490 6.097415132 7.174591002
H 6.835097754 5.271052265 6.459618921
H 7.965092667 6.389125080 7.278462097
H 6.515443842 5.779593352 8.145363421
H 6.331492824 6.947370184 6.801302643
End final coordinates

Cu-O-Nb-H2MOR-methane-adduct
Final enthalpy = -6844.7364082337 Ry
CELL_PARAMETERS (angstrom)
13.808252686 0.049255984 -0.012798476
-1.385324889 13.609471515 -0.011664165
-0.006727656 0.018258231 14.993339083

ATOMIC_POSITIONS (angstrom)
O 3.125617533 0.585261225 3.263692420
O 2.231099755 13.798735184 10.682753818
O 5.032412470 11.091387796 3.573866592
O 5.190531847 11.334251518 10.457831938
O 7.845783089 11.523499936 7.799633004
O 7.733266370 11.669148156 0.246830659
O 10.734789233 -0.059149201 6.884325641
O 9.438552358 13.547154434 14.461928870
O 8.259773737 2.499158552 7.020886811
O 8.164753294 2.620985556 14.601654890
O 5.172009905 2.291186602 3.563317840
O 5.305043010 2.186475559 11.169808042
O 12.694858836 11.046851563 0.358191230
O 12.935234312 10.668184673 7.834033407
O 2.226499820 7.767411714 0.380756898
O 2.144524859 7.950223577 7.820013396
O 1.477029065 5.282378412 3.292288410
O 1.738545236 5.030869175 11.042991981
O 0.058428812 3.139227829 4.099215802
O 0.094236699 3.037221084 11.641706894
O 11.087796659 5.816154096 4.105324879
O 11.183882299 5.776746184 11.644965790
O 11.486056786 8.697634099 0.173858599
O 11.116050334 8.696205362 7.677597857
O 10.044102999 13.273250665 4.281849027
O 9.712586360 13.254109146 11.855686530
O 7.592006411 2.873729342 4.465030969
O 7.704916926 2.992713677 12.025649835
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O 5.433627571 1.891255801 7.668103213
O 3.503452803 0.433725740 0.635240649
O 3.148956870 0.565403001 8.076186523
O 5.241318595 11.320213039 0.904685476
O 5.216873992 10.922569493 7.799760858
O 7.813222700 12.030192739 3.453827018
O 7.712797339 11.753793156 10.958942684
O 0.628041794 2.885648184 6.694057938

O 0.639783969 2.850108439 14.236181358
O 10.773199390 6.249882332 6.739412660
O 11.055794673 6.300995524 14.250599462
O 11.190128118 8.407226698 3.502797376
O 11.385817778 8.378619038 11.125102661
O 12.673482003 10.599825805 3.002753708
O 12.586662050 10.711023033 10.473407289
O 1.982049228 7.850212521 3.039253323
O 2.220166339 7.554438062 10.472225596
O 1.451324688 5.196439986 7.788244882
O 1.678602964 5.200550690 15.000502993
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O 9.934352522 1.795378818 12.778049650
O 0.916555015 9.761204115 1.524082679
O 0.991127075 9.667491098 9.500455770
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O 12.222655784 4.079376870 13.429886652
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O 7.261757355 2.168962862 1.963747773
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O 12.033154067 10.153571946 12.973330126
O 1.748412302 6.842315230 5.451860911
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O 1.266083348 3.186502524 1.749521560
O 1.134521478 3.058038134 9.272148613
O 11.906782594 6.574977777 1.734100372
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O 13.555680021 7.089206751 14.728575341
O 13.240195765 7.228733942 7.179047243
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O 0.462856615 12.370183237 1.901938006
O 0.503666493 12.283172846 9.377962123
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O 3.648396062 9.472689341 9.365866905
O 12.451828223 1.590039724 5.701866215
O 12.544953155 1.441474213 13.154987710
O 9.586073178 4.232481612 5.536268103
O 9.581433674 4.393593429 13.219732162
O 4.872234815 8.458977586 5.310954499
Si 7.105952539 1.692814492 0.434513163
Si 9.282240311 12.133628172 0.295229745
Si 9.351372479 12.202644946 7.764983470
Si 3.723526597 1.825187035 4.128461176
Si 3.857955182 1.527782251 11.579715222
Si 11.906296370 6.965109602 3.312727324
Si 11.958003930 6.897019223 10.756637522
Si 1.377225715 3.668137419 3.299885206
Si 1.426760491 3.453543127 10.808632458
Si 1.326832403 6.715238801 14.524872744
Si 11.634802821 10.099459030 7.036094478
Si 11.579884507 10.210813970 14.533887485
Si 6.373781486 12.081898332 7.371212509
Si 6.209161107 12.163445963 14.881783948
Si 3.906389566 1.748479993 7.227779977
Si 4.025289897 1.640194255 14.659706132
Si 6.750812727 1.887131920 3.482212955
Si 6.892363999 1.893913474 11.154862803
Si 9.404351198 12.113524747 3.332946435
Si 9.393871221 12.072795313 10.838389924
Si 1.205505024 6.744532575 3.935962511
Si 1.323179537 6.557299534 11.387119130
Si 11.510764765 9.938382578 3.933371718
Si 11.543806811 9.953518475 11.444012179
Si 12.018311780 7.161240432 0.228907742
Si 11.730344336 7.170106478 7.687841033
Si 1.697346638 3.573217400 0.232880275
Si 1.851049895 13.202595598 1.986393040
Si 1.902872442 13.096540736 9.251113854
Si 4.213497944 11.022098972 2.114440948
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Si 11.114820269 0.713060208 5.480094203
Si 11.103000085 0.718178857 13.094511030
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Si -0.143214994 10.801053767 9.283523502
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Si 2.239266192 8.656833641 9.286310692
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Si 13.281493156 2.889550402 13.109604787
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Si 8.810463183 2.808287270 5.543219275
Al 1.076477946 6.705400642 7.075298677
Al 6.252089373 12.399508544 4.017292046
Al 5.998276571 12.286133186 11.669515082
Al 7.093390345 1.583573406 7.883061455
Cu1 3.344525070 8.149560349 6.300294641
Nb2 4.845634582 10.221450191 5.579553829
H 8.035622852 3.060448349 9.535983702
H 7.431557125 11.096564528 10.285944642
C 6.889660911 6.052990862 7.246700702
H 6.791159698 5.220795038 6.541437569
H 7.945622446 6.335341581 7.326623582
H 6.504779934 5.749818975 8.228058355
H 6.309286731 6.903601271 6.871865382
End final coordinates

Cu-O-Pd-H2MOR-methane-adduct
Final enthalpy = -6841.3177281180 Ry
CELL_PARAMETERS (angstrom)
13.808256237 0.049015168 -0.003796070
-1.385703312 13.639772435 -0.028786205
0.003244735 0.000376318 15.034469166

ATOMIC_POSITIONS (angstrom)
O 3.133566500 0.533603842 3.247364760
O 2.220573603 13.825623848 10.709582444
O 5.186568469 11.105223368 3.279382391
O 4.869593824 11.322991387 10.865616239
O 7.917593027 11.560744870 7.625321471
O 7.680058701 11.848978826 0.561045038
O 10.832495243 0.032240573 6.954995448
O 9.493193341 13.475962524 14.521368228
O 8.238270398 2.571466092 7.003481001
O 8.056081448 2.677790009 14.638075577
O 5.212742128 2.179208397 3.629358813
O 5.373517553 2.129402504 11.140441257
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O 12.965334941 10.660004221 7.914536279
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O 1.681613665 5.342818084 3.446258778
O 1.663048161 5.022599210 11.191367225
O 0.109639381 3.274929519 4.145194558
O 0.209845277 2.858183564 11.705612151
O 11.107599728 5.894475781 4.145318494
O 11.151821865 5.800861794 11.684864520
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O 11.106252498 8.748170388 7.687779645
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O 7.640551318 2.866656162 4.424475537
O 7.754490603 2.924711133 11.996197194
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O 3.448908676 0.463024564 0.594845832
O 3.147603608 0.512911317 8.115097578
O 5.126137490 11.342327371 0.602558221
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O 7.899527742 12.054967552 3.702180017
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O 0.641829290 2.936441290 6.731848324
O 0.507099001 2.778095469 14.361705066
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O 11.095503232 6.172664753 14.320299340
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O 11.364566552 8.409000706 11.227989032
O 12.790178014 10.655452566 3.081687310
O 12.553871074 10.735674167 10.554965276
O 2.039996173 7.935832381 3.047280948
O 2.216660746 7.493545534 10.464287373
O 1.570510300 5.235788366 7.691344542
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O 0.902899755 9.757575287 1.465685336
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O 7.273273829 1.993161060 1.989907073
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O 11.911759827 6.589716418 1.745122884
O 11.558659607 6.647905381 9.257558420
O 2.773549169 3.052883460 3.956212891
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O 10.010194142 10.665164415 11.200243136
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O 7.333283759 0.313599367 11.428349275
O -0.331748999 7.005106879 3.862848439
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O 0.483344548 12.372609285 1.799671274
O 0.533783753 12.261371384 9.449573359
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O 3.622843601 9.488904295 9.429196101
O 12.484581449 1.688286797 5.706566241
O 12.503676483 1.333814690 13.122765037
O 9.608492175 4.263354248 5.513616888
O 9.570621109 4.347145638 13.234148503
O 4.797861384 8.812007413 6.486964419
Si 7.030418637 1.709247334 0.425179752
Si 9.261179117 12.171267565 0.432965620
Si 9.389450777 12.266416942 7.721279651
Si 3.733494256 1.755002597 4.140631329
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Si 11.944143951 6.997478114 3.316358625
Si 11.916472906 6.936100785 10.808142789
Si 1.445438607 3.733582763 3.338794475
Si 1.462694908 3.447632087 10.856471106
Si 1.289300763 6.731774685 14.525933994
Si 11.675367556 10.145103680 7.068704343
Si 11.468172539 10.181119050 14.626845087
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Si 6.272826012 12.216543459 14.869101954
Si 3.896689580 1.688181520 7.250085516
Si 3.980607790 1.676770247 14.689631292

Si 6.797068989 1.793193378 3.535539248
Si 6.955879869 1.819090330 11.118304450
Si 9.471419740 12.163794263 3.452965448
Si 9.307212754 12.058513414 10.792297181
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Si 1.284037155 6.576042032 11.421902944
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Si 11.477600977 9.995848127 11.508711736
Si 11.984956192 7.142961998 0.222007221
Si 11.679971639 7.210219953 7.727799701
Si 1.594940603 3.592814428 0.216214562
Si 1.855666379 13.227102190 1.915447070
Si 1.927638095 13.085564269 9.287271084
Si 4.238592677 11.070784900 1.918565314
Si 4.272114157 10.983570329 9.419915969
Si 11.169822317 0.772281952 5.531662806
Si 11.051095949 0.618840029 13.153673005
Si 8.822675651 2.911903940 13.235662326
Si -0.216475257 10.917000434 1.709900374
Si -0.147660482 10.796588706 9.373192847
Si 2.166984177 8.760159144 1.649913736
Si 2.234948870 8.670130042 9.347367746
Si 13.279844760 3.087276281 5.627977223
Si 13.263453668 2.773048290 13.125593350
Si 10.928913142 5.180933692 5.600131193
Si 11.017336822 5.075859206 13.133165255
Si 1.628935085 3.646329682 7.811810507
Si 8.833451599 2.834543169 5.535190469
Al 1.047420026 6.758133189 7.133140990
Al 6.263579705 12.329418013 4.111923698
Al 6.054240769 12.252799506 11.686652912
Al 7.108583100 1.537051364 7.791954088
Cu1 3.242132896 8.079274527 6.168633743
Pd2 4.945875098 9.900223916 4.997601925
H 8.112583692 2.923646236 9.464277834
H 7.371068110 11.209029168 9.938630419
C 6.940388453 6.082930120 7.113604395
H 6.854790819 5.280307045 6.372774228
H 7.992812756 6.370346331 7.216763351
H 6.552935427 5.731764043 8.077529743
H 6.356939577 6.953321623 6.789606300
End final coordinates

Cu-O-Rh-H2MOR-methane-adduct
Final enthalpy = -6980.4077726082 Ry
CELL_PARAMETERS (angstrom)
13.814331180 0.069158007 0.005757228
-1.366364585 13.599312344 -0.012363006
0.013549734 0.019460677 15.002118280

ATOMIC_POSITIONS (angstrom)
O 3.130925993 0.542828406 3.285749155
O 2.290363823 13.771172599 10.737493925
O 5.224340609 11.050285547 3.359716535
O 4.952407082 11.315437323 10.816074273
O 7.932894424 11.548227913 7.586278276
O 7.695028911 11.771524101 0.590725283
O 10.830160632 0.069284149 6.945249256
O 9.455620415 13.478685033 14.507723900
O 8.281447581 2.533191039 7.042364385
O 8.145847583 2.679410163 14.648159466
O 5.220206119 2.191014213 3.643981966
O 5.369042867 2.162754176 11.151044291
O 12.611005562 11.044131023 0.444682275
O 13.003347593 10.714603131 7.902973357
O 2.237625068 7.686125358 0.406702919
O 2.185595285 8.052003670 7.776253134
O 1.675669109 5.325119863 3.328187999
O 1.697899226 4.993792894 11.176359059
O 0.116410475 3.273048320 4.129515824
O 0.161600846 2.886236567 11.677624235
O 11.020195426 5.902491825 4.121436256
O 11.214248317 5.777126936 11.678242747
O 11.454382248 8.667007686 0.166240017
O 11.167462626 8.773806615 7.723975885
O 10.198360776 13.346105407 4.372298931
O 9.583994894 13.196808661 11.878215784
O 7.644233024 2.867308993 4.479147885
O 7.746056666 2.967733005 12.025557347
O 5.584924390 2.124508976 14.987354292
O 5.450563916 1.879554888 7.660894395
O 3.566985742 0.448472996 0.657119812
O 3.164616121 0.561116573 8.143019281
O 5.128184606 11.323941667 0.709938016
O 5.485509226 10.883313614 8.248690532
O 7.951807081 12.044743295 3.760690858
O 7.665070776 11.694731561 10.819264132
O 0.648738989 3.061733121 6.724407875
O 0.568423970 2.758814769 14.308660383
O 10.775805820 6.345723627 6.759215896
O 11.114920668 6.232292295 14.293160230
O 11.339209702 8.467166669 3.496096021
O 11.407129995 8.394510794 11.248678769
O 12.851135018 10.633091300 3.083593835
O 12.595997715 10.718056266 10.543643670
O 1.900932999 7.937010658 3.049780986
O 2.231635259 7.454510132 10.388471395
O 1.606800526 5.282524773 7.848089507
O 1.620730663 5.163025765 14.881550585
O 3.104781355 12.129760975 2.237502299
O 3.179950853 12.039362459 8.919227095
O 9.946683318 1.731060814 5.095152233
O 9.924701301 1.772818656 12.883364524
O 0.940315644 9.771570570 1.393949147
O 0.984045846 9.614139648 9.569476269
O 12.239676646 4.336119289 5.910793777
O 12.223525915 4.002512294 13.389648706
O 3.746516737 1.290948475 5.702668335
O 3.953661691 1.114003255 13.166334199
O 5.946705519 11.643624227 5.776929621
O 6.281915749 11.820892873 13.359191366
O 9.858596902 12.517764550 1.913985747
O 9.686524866 12.541400230 9.308330396
O 7.293281563 2.054266701 2.021232961
O 7.508143798 2.193216708 9.561556495
O 12.183317022 9.977690855 5.528518555
O 11.930119084 10.265799036 13.045394156
O 1.746763028 6.929889904 5.476208037
O 1.667417756 6.975521481 12.920786372
O 1.253761184 3.262078215 1.763042606
O 1.163997935 3.124824437 9.302161615
O 11.948734825 6.577762051 1.751791834
O 11.584273399 6.645545116 9.258335308
O 2.777372208 3.062344206 3.968039265
O 2.801435143 2.650622007 11.346675340
O 10.055817756 10.894036790 14.803153376
O 10.509682372 11.242938710 7.138392333
O 10.262563924 10.771717643 3.847890255
O 10.051164090 10.646013710 11.184617644
O 3.134358352 3.002504937 14.889622696
O 3.154287252 3.145788295 7.537334145
O 7.354688636 0.160604188 0.148084500
O 7.459199898 -0.145700688 7.804029061
O 13.578057885 7.138727886 14.730211707
O 13.263253401 7.231507391 7.269651511
O 5.673097239 13.889104934 3.990420751
O 7.338363787 0.355207790 11.466130686
O -0.376349363 6.876048460 3.934101921
O -0.251621825 6.809642695 11.059326012
O 0.503679670 12.375185788 1.814363379
O 0.576350347 12.246370793 9.467119005
O 3.565857281 9.534659685 1.833303932
O 3.657174548 9.466892617 9.442809848
O 12.547124393 1.705575175 5.746373767
O 12.525908261 1.348749946 13.143990836
O 9.564938775 4.315589708 5.585023393
O 9.592150848 4.387307788 13.229156436
O 4.446518621 8.285649890 4.864914308
Si 7.078364199 1.724698559 0.461517859
Si 9.265301088 12.149003277 0.455409076
Si 9.402911128 12.256408561 7.715191257
Si 3.740868363 1.770676824 4.160922723
Si 3.926483742 1.525300469 11.597440328
Si 11.936290350 6.972694652 3.327395172
Si 11.959681705 6.926945371 10.806189270
Si 1.452203661 3.714480845 3.310961071
Si 1.460360031 3.420011058 10.860213195
Si 1.332163555 6.713993880 14.491018011
Si 11.717252504 10.162706503 7.072158647
Si 11.519477259 10.214187510 14.618585411
Si 6.355177057 11.945172108 7.364867573
Si 6.282035845 12.191445524 14.913467765
Si 3.911960793 1.728617880 7.264953923
Si 4.055634789 1.677607337 14.689695890
Si 6.807163239 1.818233236 3.557693293
Si 6.953794716 1.858657639 11.148055513
Si 9.519119316 12.170856495 3.475687591
Si 9.344137150 12.043449368 10.801963949
Si 1.236293023 6.757225785 3.936646404
Si 1.320802579 6.551022511 11.385237322
Si 11.662312776 9.979946590 3.985546050
Si 11.521484618 9.985169078 11.503859967
Si 12.024770131 7.148277904 0.236146388
Si 11.734756434 7.231017188 7.738295872
Si 1.632442384 3.552560486 0.212360520
Si 1.896639193 13.184772075 1.983174877
Si 1.971634867 13.066496609 9.304066945
Si 4.238079314 11.002093856 2.012364317
Si 4.305971912 10.959468635 9.398181132
Si 11.212172561 0.820630963 5.538654142
Si 11.063704682 0.654886608 13.130735786
Si 8.857457141 2.946833146 13.226004415
Si -0.181127077 10.912418263 1.698690784
Si -0.113834784 10.787708500 9.355242833
Si 2.157674697 8.728975516 1.659396279
Si 2.266668551 8.659862403 9.305228305
Si 13.294739650 3.133293151 5.625216104
Si 13.277278601 2.793407534 13.133406486
Si 10.903676383 5.214074413 5.595065289
Si 11.049792766 5.096690689 13.143288212
Si 1.648909755 3.687350810 7.842235207
Si 8.850948669 2.855524782 5.574870510
Al 1.099948784 6.747093741 7.127788155
Al 6.307778239 12.309858864 4.123693125
Al 6.068551837 12.252764967 11.721948369
Al 7.113525526 1.546353835 7.833689750
Cu1 3.256909427 8.157317174 6.172470142
Rh2 4.932675324 9.964919929 5.127338675
H 8.141136957 2.931419896 9.485950051
H 7.404641950 11.068858565 10.111020946
C 6.870443915 6.227668819 7.036338463
H 6.855936549 5.378879903 6.344616364
H 7.900222781 6.584273013 7.152054270
H 6.470964940 5.914481491 8.008026677
H 6.249053680 7.033535444 6.627337488
End final coordinates

Cu-O-Ru-H2MOR-methane-adduct
Final enthalpy = -6941.9023106983 Ry
CELL_PARAMETERS (angstrom)
13.817316730 0.054757312 0.001174593
-1.380843176 13.603132927 -0.017820998
0.008604928 0.012972424 15.006350271

ATOMIC_POSITIONS (angstrom)
O 3.126276728 0.553120063 3.279871023
O 2.277986059 13.773045531 10.730466143
O 5.176323106 11.083160179 3.351245064
O 4.921118533 11.311487756 10.809895130
O 7.909165677 11.523006978 7.547204639
O 7.681308138 11.771856703 0.577999210
O 10.836665902 0.044007391 6.940504279
O 9.451179033 13.452376671 14.496721133
O 8.285751603 2.514311077 7.035614140
O 8.113398314 2.671985450 14.638320310
O 5.224296225 2.184213328 3.642027574
O 5.372112156 2.163348782 11.132300490
O 12.606404096 11.014568450 0.432097691
O 12.983292751 10.702832910 7.903847432
O 2.226344617 7.699404564 0.409990558
O 2.142519675 8.069644744 7.784797158
O 1.651594508 5.326669974 3.301954480
O 1.679826617 4.991783935 11.189666303
O 0.124603897 3.259669064 4.124727792
O 0.169451403 2.861559087 11.675000504
O 11.038092220 5.890590188 4.122794557
O 11.181556554 5.773609629 11.672092715
O 11.427746678 8.647094721 0.154559897
O 11.163403012 8.751535507 7.723302382
O 10.194103114 13.333783086 4.364083914

O 9.553207731 13.186285969 11.860336759
O 7.650112018 2.863730494 4.474997411
O 7.750253360 2.953676236 12.005751972
O 5.561236440 2.109571978 15.023476462
O 5.451554228 1.865656919 7.655423505
O 3.498921440 0.477615681 0.636838576
O 3.158783428 0.564397051 8.141173358
O 5.120471253 11.318116963 0.690823822
O 5.461566858 10.869390366 8.243790460
O 7.938400122 12.047400888 3.747562733
O 7.631076435 11.672876586 10.820733984
O 0.663986715 3.063768726 6.717758242
O 0.550951953 2.758820335 14.311251228
O 10.772709455 6.318290377 6.764265925
O 11.115489880 6.202025279 14.295129054
O 11.321824207 8.454148693 3.492108320
O 11.394164695 8.389025278 11.225619248
O 12.818194543 10.632290744 3.079200576
O 12.561898737 10.733210122 10.542988773
O 1.940543453 7.931817048 3.063886520
O 2.202017862 7.452639897 10.393062381
O 1.605395558 5.291287251 7.852657393
O 1.588083395 5.169364275 14.896582324
O 3.092479977 12.174005748 2.180243872
O 3.161865256 12.045650122 8.905392735
O 9.950169833 1.709010135 5.090442873
O 9.908138774 1.745002411 12.896801836
O 0.921524163 9.768271118 1.426608022
O 0.943893723 9.616823721 9.598101298
O 12.256633971 4.324113531 5.904414370
O 12.221129118 3.986829121 13.356116702
O 3.734572305 1.301597898 5.700299588
O 3.964149322 1.125179751 13.158871362
O 5.916969299 11.577005965 5.745631117
O 6.264315601 11.815087880 13.349252968
O 9.844326930 12.509553292 1.906697302
O 9.638928322 12.517317197 9.294896300
O 7.303667031 2.035152717 2.022754738
O 7.519209477 2.152159307 9.544390436
O 12.165288719 9.962143915 5.524603928
O 11.898578823 10.245243878 13.040908252
O 1.762699819 6.898763826 5.473032807
O 1.663119193 6.975403763 12.931742186
O 1.265532641 3.247545678 1.754352032
O 1.161824693 3.129505731 9.298938458
O 11.946011402 6.567041640 1.748725357
O 11.599385419 6.625077624 9.253034431
O 2.787455412 3.079301929 3.960179490
O 2.807239531 2.654897859 11.335791625
O 10.036108262 10.869540334 14.808834933
O 10.489550907 11.215337209 7.135303826
O 10.238962250 10.758114880 3.846604423
O 10.019087852 10.629339403 11.178797287
O 3.123798082 3.026036216 14.858161822
O 3.162424169 3.152700733 7.546719391
O 7.349703824 0.155548485 0.140984784
O 7.449671909 -0.173328608 7.733468645
O 13.565521236 7.141151095 14.728803751
O 13.257471815 7.209350827 7.245653760
O 5.662698926 13.891227441 4.005616397
O 7.325021178 0.341191218 11.464098121
O -0.368861829 6.912694749 3.920827460
O -0.274334533 6.803997574 11.094373275
O 0.479676070 12.374456858 1.816266349
O 0.559674729 12.251321723 9.464248941
O 3.548197299 9.556042821 1.835073954
O 3.617966135 9.472248025 9.447817491
O 12.551396544 1.692865873 5.750182092
O 12.514427244 1.332316875 13.130814891
O 9.580744929 4.293639950 5.579947374
O 9.588302068 4.362570040 13.230040517
O 4.692110395 8.214695957 5.078137735
Si 7.068433496 1.717561520 0.462793493
Si 9.254979607 12.136953058 0.447573646
Si 9.378037573 12.230988423 7.698237658
Si 3.739413682 1.779391627 4.158089189
Si 3.930502045 1.528880423 11.587576715
Si 11.941571707 6.967748317 3.323715865
Si 11.946596089 6.915020208 10.804397146
Si 1.453455908 3.714295339 3.300127226
Si 1.458854296 3.418374903 10.857925477
Si 1.314490309 6.720566231 14.499328332
Si 11.703533570 10.142515052 7.069807211
Si 11.497681143 10.188095283 14.615727052
Si 6.329062402 11.909039080 7.335399488
Si 6.266205900 12.186360882 14.901538478
Si 3.909634086 1.731710840 7.264648857
Si 4.033357113 1.688940349 14.683752731
Si 6.810868080 1.812320731 3.559652983
Si 6.953815983 1.844846621 11.131854022
Si 9.509033729 12.161958817 3.468520383
Si 9.309290560 12.024824755 10.792418924
Si 1.243753446 6.757245564 3.941105249
Si 1.302752986 6.549357058 11.398904654
Si 11.639833872 9.966690832 3.984184914
Si 11.495223694 9.977858147 11.495760718
Si 12.017776617 7.136316132 0.232721210
Si 11.736349652 7.210631763 7.732076804
Si 1.624095602 3.562417851 0.203488004
Si 1.858684041 13.210287830 1.961626209
Si 1.953919915 13.072141318 9.295260004
Si 4.208481907 11.030003299 1.981449947
Si 4.277587334 10.957461451 9.389862232
Si 11.219428485 0.803459711 5.537663757
Si 11.055685094 0.632239871 13.126145247
Si 8.844691061 2.927448970 13.222427764
Si -0.204515063 10.911283721 1.704389686
Si -0.142292473 10.797511857 9.362874693
Si 2.146832473 8.731462775 1.671183122
Si 2.226166569 8.664156526 9.314915396
Si 13.307773608 3.117292340 5.619221312
Si 13.274063663 2.773107589 13.120554700
Si 10.916190774 5.196809744 5.593309286
Si 11.041383222 5.079240247 13.133943259
Si 1.654190578 3.696804057 7.842266268
Si 8.858376040 2.839142274 5.569819126
Al 1.096827665 6.750694403 7.113180513
Al 6.300678382 12.315104747 4.120794407
Al 6.038923732 12.244893108 11.714295521
Al 7.113426213 1.519501672 7.811700056
Cu1 3.315508640 8.149640119 6.243032595
Ru2 4.895740311 9.926657518 5.030343955
H 8.150510330 2.891530148 9.462112988
H 7.371202998 11.014813883 10.142339211
C 6.890064992 6.192868312 7.060567969
H 6.864237334 5.353334664 6.357576889
H 7.923669965 6.539051969 7.173276601
H 6.493903735 5.871177604 8.031091205
H 6.274256605 7.008277701 6.665122759
End final coordinates

Cu-O-Zr-H2MOR-methane-adduct
Final enthalpy = -6817.8209462393 Ry
CELL_PARAMETERS (angstrom)
13.816672096 0.026776249 -0.011828930
-1.408406185 13.617810460 -0.022343649
-0.005569044 0.006669328 15.015412987

ATOMIC_POSITIONS (angstrom)
O 3.191621065 0.531260023 3.290994150
O 2.120988807 13.863941017 10.689986798
O 4.963016206 11.120169233 3.533746410
O 5.199650778 11.320270552 10.449718629
O 7.780768565 11.552936042 7.857503647
O 7.780492767 11.674142302 0.190219584
O 10.726811142 -0.078645226 6.929688072
O 9.518928488 13.531847237 14.477470656
O 8.237913898 2.556198340 7.032515044
O 8.128576176 2.610959433 14.616224450
O 5.175498940 2.303490148 3.550874869
O 5.315445551 2.163671941 11.203502014
O 12.767114058 10.992821963 0.345682276
O 12.832093780 10.713470162 7.828618205
O 2.188753796 7.796751761 0.361925336
O 2.164840923 7.822127176 7.887948884
O 1.467681445 5.243753404 3.309628489
O 1.711230351 5.086670184 10.949135244
O 0.058533115 3.098434468 4.117198610
O 0.122119454 3.089613934 11.669228960
O 11.192933285 5.786858834 4.128456890
O 11.188819992 5.734109906 11.645173662
O 11.503424337 8.678699550 0.187021116
O 11.093830203 8.666865688 7.664800087
O 9.947638129 13.192218621 4.318115496
O 9.708724653 13.257054413 11.859347007
O 7.586208379 2.873139753 4.472790637
O 7.720957104 2.964172811 12.040270220
O 5.571331081 1.910630552 14.956795029
O 5.411958407 1.932759335 7.730325711
O 3.384027983 0.476746241 0.630526680
O 3.144839794 0.556997123 8.072819689
O 5.300506197 11.286282604 0.861770337
O 5.153286727 10.972120136 7.778149529
O 7.744129506 12.000479325 3.369364108
O 7.727700855 11.736900568 10.953357132
O 0.593160797 2.760848070 6.723589221
O 0.644120115 2.864440335 14.268042806
O 10.786707503 6.200513017 6.753806337
O 11.043577045 6.291913161 14.245673241
O 11.194627738 8.370242604 3.502993536
O 11.334405239 8.347875174 11.144055381
O 12.588506230 10.618608723 2.992377985
O 12.598593303 10.645348782 10.484689297
O 2.109083204 7.782343292 3.035381508
O 2.184504152 7.651055394 10.558444960
O 1.324160168 5.125319305 7.750027245
O 1.668383947 5.202273527 15.088762601
O 3.113653586 12.216319393 2.029809871
O 3.090766276 12.101070438 8.968859691
O 9.780752410 1.557796804 5.095281016
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O 0.935584757 9.650507021 9.367984669
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O 12.244041235 4.079928392 13.458297209
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O 3.828299876 1.108722119 13.160587093
O 6.169752374 11.924117441 5.736980361
O 5.917806271 11.860722119 13.317433525
O 9.826690594 12.420304284 1.792379179
O 9.721649718 12.510536191 9.335949057
O 7.284033444 2.141516361 1.970795137
O 7.449479230 2.288784715 9.597944784
O 11.972167246 9.994474252 5.460252457
O 12.067805812 10.094215564 12.991484022
O 1.724293187 6.814047781 5.455030106
O 1.652965088 6.806993509 12.974301517
O 1.278769685 3.149758926 1.766701235
O 1.158746634 3.010819009 9.292835089
O 11.883830267 6.533808793 1.723616024
O 11.642490687 6.567678360 9.215703835
O 2.711870047 3.042529245 4.024235156
O 2.763978854 2.742135189 11.382763613
O 10.197648395 10.934999191 14.631295005
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O 10.010614581 10.641944176 3.743196232
O 10.098044466 10.662647936 11.258571515
O 3.193552516 3.041925325 14.928115682
O 3.087536150 3.141763159 7.469838516
O 7.501772193 0.106601823 0.243346527
O 7.424874941 -0.073551404 7.974831374
O 13.543708825 7.038066051 14.736992362
O 13.237799295 7.239181516 7.169965498
O 5.515602206 13.949194036 3.847639476
O 7.288434277 0.357863432 11.421638839
O -0.333956244 7.108105207 3.793095308
O -0.282721612 6.851360147 11.125793638
O 0.471182968 12.335169600 1.953462099
O 0.475058693 12.272861258 9.370231587
O 3.535598550 9.586172696 1.829167128
O 3.601853960 9.505039340 9.347535377
O 12.402720313 1.543518772 5.660060591
O 12.563920235 1.451952700 13.137030248
O 9.635526901 4.192039859 5.493592038
O 9.596780462 4.352095978 13.237993062
O 4.961632593 8.441145688 5.494111922
Si 7.105471045 1.666772561 0.442425343
Si 9.329949499 12.130496615 0.279429302
Si 9.305981511 12.183682964 7.785659827
Si 3.747818116 1.801134238 4.141507701

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Si 11.948753364 6.949329583 3.297196514
Si 11.944727619 6.880854713 10.771399238
Si 1.376018474 3.631209318 3.319800253
Si 1.441532769 3.490452831 10.808001244
Si 1.309254577 6.695451372 14.555903642
Si 11.562354865 10.087090594 7.024115405
Si 11.625875066 10.170407569 14.554452238
Si 6.330841572 12.114816433 7.357299906
Si 6.252554926 12.150261046 14.866847779
Si 3.903311402 1.752495897 7.241613934
Si 3.994366804 1.641432944 14.690618729
Si 6.752021057 1.885066485 3.487181457
Si 6.900848097 1.873834153 11.167297650
Si 9.342738116 12.064471800 3.311548104
Si 9.408332643 12.060764925 10.855272232
Si 1.243727103 6.727445580 3.925268147
Si 1.299064273 6.585197679 11.403949947
Si 11.449886967 9.915939640 3.920140514
Si 11.547356755 9.916595444 11.468274612
Si 12.009586174 7.133666425 0.224624054
Si 11.731780922 7.151379148 7.687556642
Si 1.700057219 3.581679848 0.258054077
Si 1.832992095 13.209597594 1.959918668
Si 1.854193637 13.123116220 9.264780386
Si 4.216209258 11.041775386 2.028842293
Si 4.235092403 10.988575935 9.216648619
Si 11.067183726 0.659671222 5.499069160
Si 11.135337103 0.704614461 13.114841714
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Si -0.193559768 10.801439969 9.251800533
Si 2.160673316 8.712160029 1.714274306
Si 2.209790066 8.656229583 9.287616435
Si 13.248250019 2.921453251 5.600088650
Si 13.306448846 2.896176144 13.128677789
Si 10.974044559 5.088426583 5.581361668
Si 11.029546133 5.112193423 13.139262837
Si 1.539479530 3.553979306 7.791712531
Si 8.805414730 2.801214445 5.549469479
Al 1.047761085 6.668690165 7.066593689
Al 6.218673343 12.406204365 4.004952028
Al 6.018110015 12.274928713 11.652307725
Al 7.078604064 1.628413249 7.892380907
Cu1 3.437482440 8.057373835 6.457761776
Zr2 4.704861818 10.252895374 5.533773927
H 8.006190845 3.088435620 9.564716809
H 7.454514217 11.110651944 10.247161529
C 6.893751268 5.995336805 7.261337694
H 6.772013521 5.140704084 6.586142448
H 7.961419884 6.219085929 7.374888839
H 6.455402523 5.749666924 8.237098363
H 6.378352261 6.863425162 6.833172746
End final coordinates

Products of methane C-H activation: PBE-D3
Cu-O-Co-product-1
Final energy = -6672.3012349249 Ry
13.805446430 0.050682715 -0.013566032
-1.383769987 13.624082572 -0.037628835
-0.007300434 -0.010449264 15.021760751

ATOMIC_POSITIONS (angstrom)
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O 2.254073990 13.786360181 10.684882304
O 5.127022030 11.080240340 3.344119403
O 4.876396866 11.347366395 10.806838414
O 7.889308022 11.533617730 7.575062685
O 7.688451376 11.780832870 0.526448616
O 10.800585719 0.034523837 6.942440324
O 9.451028371 13.467374496 14.507093388
O 8.255275759 2.530959321 7.026004887
O 8.023652111 2.676663897 14.640623002
O 5.202103762 2.233516533 3.644905654
O 5.338579317 2.156511921 11.118900507
O 12.626742099 11.029371315 0.373251296
O 12.974149661 10.686330237 7.859580607
O 2.204178655 7.718441917 0.396793395
O 2.150692015 8.074092925 7.806506891
O 1.562835753 5.339717063 3.285941090
O 1.656174952 4.987843355 11.189858974
O 0.079523150 3.247297980 4.115082446
O 0.135259481 2.858118036 11.657046379
O 11.076576816 5.872609305 4.110545741
O 11.101717778 5.788537648 11.653586299
O 11.425211197 8.671340994 0.094407548
O 11.133219793 8.753204166 7.685649133
O 10.135284546 13.345665403 4.342830318
O 9.501036496 13.192543148 11.869617519
O 7.639228667 2.865920189 4.458413222
O 7.717748300 2.948789881 11.997031740
O 5.497024834 2.022803816 15.064446543
O 5.436224823 1.854246672 7.612333763
O 3.418053269 0.425576439 0.580898443
O 3.153531941 0.539002608 8.110610180
O 5.128411000 11.342672657 0.666409405
O 5.447280833 10.882665394 8.252784112
O 7.860286999 12.101720086 3.695918413
O 7.597434697 11.704306496 10.778461180
O 0.670710012 3.063189325 6.696124626
O 0.509799091 2.771280073 14.296247365
O 10.765029872 6.327162384 6.736960673
O 11.058635688 6.198528958 14.277886665
O 11.209610538 8.452643917 3.504759986
O 11.355067540 8.398537970 11.192165203
O 12.699377158 10.630538196 3.020081920
O 12.519265690 10.740159572 10.492770203
O 2.011564544 7.923904020 3.058848951
O 2.162367736 7.460043534 10.417459361
O 1.613445637 5.299749776 7.827997786
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O 3.097237719 12.214438487 2.131588094
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O 0.929394966 9.630376117 9.601443334
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O 3.689711932 1.320251420 5.672605418
O 3.925731900 1.112860542 13.141523851
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O 9.827033393 12.503226949 1.891307815
O 9.627788997 12.557676120 9.292968093
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O 11.887166781 10.250415180 13.000918106
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O 1.215858278 3.254392569 1.740138690
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O 11.861616658 6.604087147 1.723079812
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O 2.772197584 2.642276738 11.312327624
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O 13.520259733 7.084931192 14.743751403
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O 5.587624029 13.915158900 4.023621452
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O -0.316875871 6.782158925 11.105311065
O 0.467977580 12.358499110 1.861508492
O 0.530671677 12.264457068 9.428851888
O 3.527417518 9.592920396 1.784017090
O 3.606569484 9.472098240 9.477382673
O 12.541586995 1.661787925 5.756337654
O 12.463561191 1.340527750 13.113178558
O 9.541155695 4.323441539 5.562677312
O 9.539573058 4.348209573 13.236026205
O 4.961677777 8.202367307 5.359911830
Si 7.038846339 1.700739832 0.458005285
Si 9.258945650 12.157549374 0.417310682
Si 9.355904383 12.252850495 7.700653051
Si 3.710820811 1.810508432 4.132361957
Si 3.896621544 1.518368832 11.570744625
Si 11.905681105 7.001707786 3.297800099
Si 11.894608283 6.914664682 10.787220480
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Si 1.426637226 3.417802494 10.844401869
Si 1.285056180 6.698198175 14.516847454
Si 11.672694465 10.151279947 7.043443228
Si 11.490188742 10.190589993 14.577192107
Si 6.308169549 11.916740809 7.320594341
Si 6.253781956 12.178456125 14.880160211
Si 3.888379214 1.722893581 7.241760299
Si 3.971536733 1.631574519 14.683760991
Si 6.777772295 1.810273101 3.563419437
Si 6.920079247 1.835771533 11.128649897
Si 9.437661561 12.179834959 3.446284079
Si 9.277769685 12.046466263 10.781360553
Si 1.230463537 6.792391732 3.930061546
Si 1.263233394 6.540441925 11.410806771
Si 11.544344412 9.975291515 3.960075979
Si 11.463267542 9.987839219 11.460585867
Si 11.981176853 7.149705849 0.203275052
Si 11.724392478 7.217179665 7.714841887
Si 1.601909504 3.567254239 0.195586818
Si 1.837992318 13.219729039 1.925518264
Si 1.930230897 13.075780307 9.255088102
Si 4.208871892 11.056069629 1.955093691
Si 4.252919404 10.965989878 9.388185524
Si 11.193860103 0.795121294 5.542433715
Si 11.013826873 0.624305223 13.148425563
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Si -0.159627825 10.803987401 9.340426450
Si 2.141562867 8.739774893 1.667939219
Si 2.208186483 8.669646493 9.339569944
Si 13.281656693 3.094549359 5.606609542
Si 13.225453068 2.778398251 13.088597864
Si 10.907117682 5.190824990 5.580082450
Si 10.983449462 5.080503634 13.113048870
Si 1.644824475 3.705724464 7.829646558
Si 8.839526621 2.852384539 5.561980990
Al 1.108724507 6.767563664 7.088611796
Al 6.219948643 12.327385198 4.122460997
Al 6.015099684 12.260945485 11.701135744
Al 7.095913639 1.509723053 7.795451124
Cu1 3.495556315 8.190642642 6.467578013
Co2 4.989974417 9.980130956 4.978537125
H 8.143513098 2.857427013 9.468924806
H 7.328430209 11.134801331 10.026275128
C 6.955071353 6.683778978 6.760958472
H 6.953253533 5.846365211 6.064766331
H 7.787333748 7.385807224 6.742757282
H 6.312394600 6.644179088 7.639402766
H 5.739642161 7.692171285 5.745698145
End final coordinates

Cu-O-Co-product-2
Final energy = -6672.4061681349 Ry
13.805446430 0.050682715 -0.013566032
-1.383769987 13.624082572 -0.037628835
-0.007300434 -0.010449264 15.021760751

ATOMIC_POSITIONS (angstrom)
O 3.129770909 0.515664851 3.282563634
O 2.298637151 13.730705560 10.731771573
O 5.123939429 10.953375377 3.470470334
O 4.870805456 11.276754434 10.907371959
O 7.977021273 11.529184381 7.600557044
O 7.703342415 11.748670503 0.578117944
O 10.902522140 0.037988220 7.024689969
O 9.485228814 13.442088926 14.577162408
O 8.256339408 2.528192348 7.097401941
O 8.124008656 2.598462213 14.705255260
O 5.226097341 2.138547093 3.673519309
O 5.358536730 2.114656342 11.180473048
O 12.599229376 11.038313099 0.392262447
O 13.063333501 10.621286220 7.880468689

O 2.220073751 7.679098206 0.382221153
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O 1.706723399 4.943345479 11.217830944
O 0.123777935 3.246838709 4.122849728
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O 10.967887158 5.845887306 4.093629363
O 11.187289391 5.699597976 11.666169713
O 11.466978671 8.643494076 0.103567756
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O 5.569301816 2.027836230 15.050173943
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O 3.559554163 0.381079425 0.652882270
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O 5.568438711 10.900196263 8.388431974
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O 0.650132477 3.066541596 6.720081961
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O 10.797786533 6.306690859 6.730505393
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O 12.565393202 10.636662631 10.504259740
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O 1.644742072 5.112171217 14.866827620
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O 9.894330847 1.655922166 12.950319666
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O 0.576775790 12.199904686 9.491756723
O 3.518736681 9.516215818 1.819475883
O 3.691964229 9.416426902 9.453264026
O 12.577819393 1.635402548 5.717001279
O 12.508644731 1.288416538 13.152242002
O 9.520944127 4.292900345 5.605445069
O 9.589587506 4.284450255 13.250509138
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Si 9.272524636 12.118530840 0.466117743
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Si 11.883749150 6.928320668 3.310007427
Si 11.932846883 6.853357343 10.793728218
Si 1.460732017 3.695879855 3.309800422
Si 1.447815875 3.378511844 10.867608430
Si 1.309570833 6.659725239 14.492653657
Si 11.741840650 10.126017287 7.070584639
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Si 6.391981251 11.907796858 7.398007322
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Si 4.039208770 1.596198733 14.727230527
Si 6.804767605 1.723636925 3.602646002
Si 6.936044598 1.775567464 11.198274056
Si 9.439386986 12.110148295 3.498644312
Si 9.304823087 11.983412614 10.837221879
Si 1.199397296 6.734665130 3.931899972
Si 1.309852013 6.502940892 11.383458387
Si 11.608465553 9.948858825 3.981120393
Si 11.491692257 9.919001523 11.479326903
Si 12.003754569 7.114266187 0.204717900
Si 11.744236153 7.181636662 7.730269557
Si 1.654206050 3.535973399 0.205592906
Si 1.890076080 13.157801418 1.972270506
Si 1.972300672 13.016075677 9.306151725
Si 4.225846652 10.957369384 2.075473434
Si 4.308479816 10.926199286 9.455757752
Si 11.220210938 0.766879460 5.589223683
Si 11.061358605 0.565521790 13.199963351
Si 8.842375471 2.849684985 13.278910206
Si -0.217344085 10.899200458 1.690253736
Si -0.095228386 10.733030137 9.373689433
Si 2.116281325 8.711590774 1.642516651
Si 2.287981032 8.622097048 9.313978844
Si 13.291053898 3.083468784 5.597287321
Si 13.267148194 2.729666253 13.127490654
Si 10.880652334 5.164862570 5.575082680
Si 11.031173333 5.023406091 13.137855838
Si 1.658035978 3.672082884 7.844343301
Si 8.837784858 2.815848987 5.626549431
Al 1.141409979 6.739068805 7.121595673
Al 6.218108793 12.224200742 4.169992496
Al 6.019314120 12.196817078 11.787705885
Al 7.111672129 1.489978715 7.859331902
Cu1 3.229476262 8.305597926 6.125215653
Co2 5.281741009 9.827122429 5.226380190
H 8.163391077 2.804943434 9.547870482
H 7.336024288 11.080161941 10.109205085
C 6.589188304 8.716456338 6.108400075
H 6.650534811 7.703827666 5.691891638
H 7.547046112 9.244131237 6.022284290
H 6.233250685 8.699152965 7.150519097
H 4.855273929 7.530390926 4.619854959
End final coordinates

Cu-O-Cr-product-1
Final energy = -6758.5442111758 Ry
13.817593883 0.055273517 0.001137847
-1.380404381 13.613568759 -0.015310522
0.008561982 0.015740211 15.023671420

ATOMIC_POSITIONS (angstrom)
O 3.148349571 0.558368671 3.272755587
O 2.284888026 13.789904431 10.732144812
O 5.211652496 11.012366410 3.400137967
O 4.954085771 11.351720824 10.801416062
O 7.900154915 11.564416163 7.601337117
O 7.696437612 11.744399392 0.549750973
O 10.818848660 0.061951360 6.958772520
O 9.429179947 13.492244014 14.523620141
O 8.254187983 2.539413490 7.058040640
O 8.134059568 2.657262467 14.661419497
O 5.204099555 2.233368774 3.661693375
O 5.356696337 2.175136462 11.177969845
O 12.641688314 11.049343933 0.421300489
O 12.986119018 10.720989159 7.902621668
O 2.230817722 7.690607021 0.425568780
O 2.180520735 8.056799914 7.818111763
O 1.623054829 5.329972608 3.295695851
O 1.691646851 5.002912678 11.205513948
O 0.088053165 3.278384384 4.141218919
O 0.150251588 2.894773444 11.693064324
O 11.001351554 5.909002002 4.147855859
O 11.176263902 5.774561578 11.680935611
O 11.472350869 8.678983603 0.138239966
O 11.149349932 8.779386571 7.716728926
O 10.153209151 13.367714838 4.373411304
O 9.588666617 13.204534603 11.897675741
O 7.631765296 2.866003587 4.492592826
O 7.738939824 2.985930875 12.037615951
O 5.580075207 2.083093835 14.989971814
O 5.433361500 1.890539959 7.660758059
O 3.587272708 0.397651885 0.644724296
O 3.157274724 0.561088547 8.144372046
O 5.132773457 11.317484964 0.735069957
O 5.445943134 10.882339696 8.227356108
O 7.903898127 12.077747785 3.745921922
O 7.648505794 11.712700904 10.863861575
O 0.633991738 3.084184876 6.737514166
O 0.559836379 2.773895869 14.323558015
O 10.766101208 6.344175557 6.784994184
O 11.101878371 6.247388037 14.289376571
O 11.276996361 8.475093477 3.528123273
O 11.395724955 8.398916716 11.269536559
O 12.797117930 10.630524407 3.062478769
O 12.572896245 10.725728840 10.539184768
O 1.910740039 7.933696413 3.078113079
O 2.201528337 7.476793847 10.441943809
O 1.594432188 5.302488857 7.881832254
O 1.651958082 5.152054330 14.923198904
O 3.121814183 12.137468267 2.271528021
O 3.157111124 12.047838295 8.916712880
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O 9.907449727 1.760714091 12.885832665
O 0.927873574 9.765465302 1.430250200
O 0.957254257 9.626644281 9.585047638
O 12.209374398 4.319119307 5.925138991
O 12.221358836 4.015619967 13.394609453
O 3.725064388 1.304517536 5.704588616
O 3.927683172 1.102572460 13.175419909
O 5.921273242 11.666059533 5.785639840
O 6.217794932 11.852148419 13.383995259
O 9.823094901 12.539831279 1.910174890
O 9.648906485 12.558573618 9.326806799
O 7.268033425 2.090804702 2.023456607
O 7.488856715 2.196633137 9.578384585
O 12.142530134 10.018414896 5.525169398
O 11.928639812 10.281756512 13.047182143
O 1.685294168 6.874925830 5.479619220
O 1.623283161 6.967083582 12.971200999
O 1.230417280 3.242063597 1.767978506
O 1.150245066 3.137740760 9.318247880
O 11.833715937 6.592651765 1.754645462
O 11.562920094 6.663617938 9.274981300
O 2.746906665 3.073808570 3.976017637
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O 10.075122190 10.914310484 14.821854451
O 10.479902964 11.247390189 7.169453373
O 10.215098174 10.792672624 3.843848125
O 10.036449491 10.652579480 11.193576608
O 3.121444226 2.958579540 14.938177181
O 3.135945723 3.154857303 7.548824667
O 7.381752200 0.145603249 0.211754376
O 7.441819582 -0.144845181 7.832946843
O 13.569960376 7.077859260 14.824780305
O 13.259735956 7.240199783 7.302257596
O 5.615115477 13.908879587 3.964029707
O 7.330255034 0.372427250 11.500967209
O -0.407039597 6.921746091 3.873864871
O -0.279352262 6.800014626 11.097227043
O 0.514399501 12.366831886 1.845076473
O 0.560293169 12.261014770 9.473738214
O 3.557356394 9.535326124 1.854938656

O 3.633820818 9.483540103 9.493411740
O 12.542257511 1.694347998 5.769674946
O 12.511854813 1.360139100 13.169043135
O 9.528647047 4.335735445 5.613433256
O 9.587363344 4.376727242 13.262700063
O 4.559223805 8.139055523 4.914691548
Si 7.076512301 1.714273888 0.468962372
Si 9.259042522 12.158149992 0.442780017
Si 9.372914965 12.267109902 7.733661754
Si 3.723618383 1.791328705 4.163556656
Si 3.913525372 1.525965942 11.608938033
Si 11.890167169 6.987544460 3.329771435
Si 11.938813368 6.927124153 10.824273663
Si 1.419007816 3.720791633 3.311231040
Si 1.449308994 3.431122343 10.876185605
Si 1.321062461 6.699218605 14.548178203
Si 11.694284270 10.175569903 7.076561072
Si 11.532833615 10.225647410 14.623520628
Si 6.322796816 11.966352156 7.364854820
Si 6.263711743 12.189625366 14.944999873
Si 3.892369869 1.738450292 7.268904217
Si 4.045336052 1.641139761 14.707483506
Si 6.784076855 1.834109049 3.558135484
Si 6.941275447 1.871915058 11.170158952
Si 9.475646113 12.195181819 3.470523514
Si 9.329132990 12.054119305 10.823345321
Si 1.205553123 6.757281835 3.947891169
Si 1.295398847 6.555523184 11.427461627
Si 11.614558429 9.995363562 3.984630144
Si 11.509380503 9.992479167 11.510345180
Si 12.003392823 7.147290165 0.242254984
Si 11.729508725 7.240219254 7.753506367
Si 1.632778038 3.543072209 0.224974737
Si 1.906722702 13.181747581 1.991759463
Si 1.954156897 13.081444576 9.303004388
Si 4.244304432 10.995223295 2.038938847
Si 4.286266051 10.972703919 9.400266410
Si 11.200728214 0.820878208 5.556105237
Si 11.056432181 0.654635431 13.149728372
Si 8.847410370 2.939425087 13.242166569
Si -0.189355371 10.914999160 1.708672119
Si -0.133854170 10.803621897 9.360356516
Si 2.148714654 8.723534120 1.688985681
Si 2.243623434 8.669727063 9.342974510
Si 13.280173521 3.128796270 5.637350554
Si 13.270790507 2.800345676 13.146216482
Si 10.885629331 5.215686883 5.617783305
Si 11.036741794 5.099950091 13.152667599
Si 1.632737784 3.709105222 7.859243155
Si 8.833976064 2.863373818 5.595169637
Al 1.096365747 6.763441670 7.128523324
Al 6.259673636 12.336779252 4.134555797
Al 6.042606098 12.283720948 11.743340286
Al 7.092264211 1.545981994 7.851963389
Cu1 3.385042584 8.148696917 6.342903005
Cr2 5.064156523 9.956602223 5.111407060
H 8.130164139 2.927689099 9.502221522
H 7.377097404 11.092500454 10.155133030
C 6.585287483 6.531121595 6.523746887
H 6.549205052 5.642177820 5.896023379
H 7.485954958 7.141836147 6.530442449
H 5.856090458 6.648126084 7.324151086
H 5.296044736 7.495304128 5.078393700
End final coordinates

Cu-O-Cr-product-2
Final energy = -6758.6777013644 Ry
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-1.380404381 13.613568759 -0.015310522
0.008561982 0.015740211 15.023671420

ATOMIC_POSITIONS (angstrom)
O 3.184650391 0.472562740 3.310109750
O 2.251117706 13.732516684 10.768312495
O 5.248241799 10.960574059 3.440777843
O 4.973256604 11.286549204 10.815551746
O 7.903370188 11.455888798 7.696006379
O 7.747718404 11.642273056 0.532165219
O 10.757374939 -0.040026439 6.973363622
O 9.430828252 13.440773534 14.534584229
O 8.254965067 2.519114189 7.078759577
O 8.161344305 2.548427757 14.689293086
O 5.183134217 2.217972792 3.697842179
O 5.328136626 2.122563606 11.222832891
O 12.759526033 10.929188767 0.411521067
O 12.999363392 10.655043185 7.891129743
O 2.232060082 7.629101999 0.437380517
O 2.165641914 7.966496275 7.883368654
O 1.487710558 5.216241715 3.356752147
O 1.677005424 4.944587131 11.208165250
O 0.025327528 3.117231240 4.164887893
O 0.118555530 2.849068579 11.696769383
O 11.164991540 5.840695344 4.202192756
O 11.180764574 5.674441385 11.698633116
O 11.489860934 8.618232561 0.122922275
O 11.145490551 8.721988315 7.746166171
O 10.171928032 13.341806507 4.392080516
O 9.628227452 13.140666560 11.911259694
O 7.632424836 2.831095540 4.512070200
O 7.718667071 2.920955235 12.083103391
O 5.598555497 1.965703625 14.985086105
O 5.448076035 1.771525794 7.688141290
O 3.585120897 0.310570828 0.675599224
O 3.147336609 0.489769668 8.172029873
O 5.189164064 11.212220929 0.763041082
O 5.412758021 10.844950785 8.224693160
O 7.900153250 12.115528596 3.718796612
O 7.658191074 11.674796704 10.887979852
O 0.694119074 2.967270474 6.729080413
O 0.604859054 2.705092169 14.311597765
O 10.771769242 6.276857630 6.814045521
O 11.094407295 6.190459310 14.288184479
O 11.186407062 8.424672416 3.544448387
O 11.376705881 8.314966911 11.329472038
O 12.723550474 10.579578632 3.064815086
O 12.528189721 10.633728050 10.510134183
O 2.141733007 7.746025393 3.110173552
O 2.193035061 7.438234102 10.512099728
O 1.589074391 5.213825776 7.873766472
O 1.675867068 5.077716444 14.982309222
O 3.175274897 12.067958373 2.284615580
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O 9.915414664 1.689939200 12.871780709
O 0.935756252 9.620813938 1.618204506
O 0.950296086 9.573649774 9.614225251
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O 12.239135210 3.957012843 13.453267715
O 3.711521740 1.257591440 5.736485565
O 3.881373908 1.048629436 13.209291306
O 5.992304579 11.645222351 5.810742815
O 6.214068246 11.841286537 13.408031701
O 9.851025105 12.504195131 1.923715500
O 9.691488387 12.469587277 9.351880472
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O 7.465040552 2.175057127 9.610807389
O 12.126636516 9.930173164 5.530640278
O 11.967388374 10.236581419 13.044242896
O 1.585410353 6.827681668 5.492872837
O 1.575328651 6.874188738 13.011650249
O 1.170972102 3.151653775 1.786099202
O 1.131005891 3.069687608 9.327887751
O 11.733965596 6.536343410 1.762521229
O 11.523507297 6.604274898 9.309007205
O 2.696736032 2.983195193 3.981913254
O 2.757424152 2.591954854 11.380198876
O 10.163185762 10.888569651 14.853532597
O 10.485561850 11.184497422 7.166969518
O 10.172679749 10.765567380 3.894381101
O 10.018475531 10.571832466 11.241145601
O 3.141987954 2.883542703 15.027538689
O 3.167398674 3.084235689 7.614739241
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O 7.507995507 -0.190665117 7.872846016
O 13.567176388 6.977630581 14.912726914
O 13.251852206 7.178170736 7.364291783
O 5.572108607 13.880800603 3.990214523
O 7.306954804 0.320909446 11.495343067
O -0.357890486 7.095204261 3.681086953
O -0.294809690 6.735681465 11.102550575
O 0.564432277 12.247826503 1.910804637
O 0.531692397 12.199821563 9.499529588
O 3.597714008 9.460645505 1.884221064
O 3.628127738 9.425204886 9.525124969
O 12.500134524 1.623181087 5.893417262
O 12.523708857 1.302804695 13.201018463
O 9.587879187 4.268221030 5.589554665
O 9.595774167 4.290034590 13.296836675
O 4.200765465 8.393184275 4.810113868
Si 7.089423366 1.632367743 0.507881520
Si 9.298784173 12.105324905 0.456045216
Si 9.371880677 12.175576867 7.767414029
Si 3.713629346 1.734367103 4.193700280
Si 3.882174635 1.469905148 11.641863191
Si 11.887169787 6.978902997 3.316343367
Si 11.918830452 6.851320901 10.853899529
Si 1.345001879 3.600313841 3.340227200
Si 1.425741400 3.372602199 10.884227622
Si 1.310329783 6.612405733 14.592228165
Si 11.694457059 10.105983265 7.085595109
Si 11.596655372 10.166975446 14.625441565
Si 6.348183568 11.912814004 7.403605848
Si 6.302235397 12.117375453 14.978615603
Si 3.902671026 1.661893402 7.305986589
Si 4.046285032 1.559970625 14.744634825
Si 6.762635886 1.811756620 3.587819901
Si 6.914363503 1.824840661 11.196693278
Si 9.478261361 12.183461905 3.482829617
Si 9.344452041 11.985088669 10.848916484
Si 1.186280048 6.690152455 3.948507688
Si 1.273392756 6.490160217 11.455813785
Si 11.557991523 9.939067269 4.004677630
Si 11.499006937 9.914966650 11.526669548
Si 11.982948560 7.078808841 0.258515319
Si 11.715550164 7.180291904 7.791788459
Si 1.640227342 3.462668501 0.262970171
Si 1.939999746 13.096009958 2.030613856
Si 1.930237078 13.017716750 9.339330281
Si 4.294852331 10.923216410 2.068572717
Si 4.280220373 10.915044904 9.423166654
Si 11.172277824 0.752159731 5.600585900
Si 11.070832063 0.594520829 13.158905122
Si 8.851344669 2.855281066 13.263749065
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Si -0.148633837 10.736978113 9.363881490
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Si 2.236109321 8.611045605 9.392230689
Si 13.279910073 3.025423901 5.695803602
Si 13.280893191 2.742020573 13.167244010
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Si 11.040417900 5.019356164 13.178204078
Si 1.649550044 3.623030426 7.873313122
Si 8.837295040 2.822436741 5.609977615
Al 1.082372709 6.689758233 7.167452410
Al 6.266671064 12.331140800 4.163616831
Al 6.044439848 12.238522560 11.757802026
Al 7.120557596 1.494281836 7.879026328
Cu1 3.246149966 8.252949663 6.363814483
Cr2 5.289661539 9.874427113 5.112751706
H 8.039897362 2.960539697 9.545119302
H 7.384743380 11.053275813 10.180161103
C 7.031742457 8.912555597 5.319054883
H 7.054360632 8.035546101 4.661147214
H 7.897976461 9.563826478 5.154694470
H 6.988360660 8.594888257 6.377356692
H 3.614647745 8.161514455 4.047944936
End final coordinates

Cu-O-Cu-product-1
Final energy = -6723.3541748182 Ry
13.812406654 0.062765001 -0.008803408
-1.372541210 13.620145894 -0.034179750
-0.002136721 -0.006126582 15.018670026

ATOMIC_POSITIONS (angstrom)
O 3.140116704 0.543242099 3.256546793
O 2.256159185 13.777668822 10.701311212
O 5.247145625 11.085862653 3.257268910
O 4.908992076 11.312660992 10.780296668
O 7.902977693 11.556620467 7.648577338

O 7.694798235 11.797155913 0.542025237
O 10.788741078 0.045176790 6.936787088
O 9.454410579 13.477629863 14.499700887
O 8.225193109 2.565032697 7.010128989
O 8.071397440 2.669901886 14.627581848
O 5.185816564 2.233476638 3.619516023
O 5.347627965 2.145120524 11.126512993
O 12.631707227 11.006608416 0.419741518
O 12.967761354 10.648947761 7.912341362
O 2.214463979 7.702696489 0.420619418
O 2.058714857 8.030418722 7.846452382
O 1.650374988 5.337336313 3.404507637
O 1.681780848 5.001036277 11.204916209
O 0.059290316 3.299019841 4.146802592
O 0.164401334 2.874434025 11.700280553
O 11.081824119 5.929178073 4.165121409
O 11.163437867 5.795077832 11.682491085
O 11.411780824 8.662973591 0.126043282
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O 10.177543885 13.370587499 4.339809050
O 9.555925003 13.196194878 11.869561805
O 7.614139642 2.881406104 4.437682016
O 7.729024529 2.938138687 11.990940087
O 5.527149103 2.068051957 15.005949543
O 5.423927699 1.879923094 7.661254300
O 3.487087713 0.438998641 0.609483069
O 3.144241723 0.541127464 8.126326845
O 5.118062189 11.331672850 0.588800096
O 5.448241803 10.904818784 8.207433537
O 7.909496040 12.138193752 3.679451302
O 7.638987037 11.730032231 10.728745996
O 0.627190325 3.005256865 6.727143186
O 0.516001534 2.763722846 14.344059072
O 10.665899308 6.312047207 6.789682852
O 11.069854290 6.191988104 14.306730050
O 11.276045712 8.490891705 3.501678720
O 11.387502020 8.408453900 11.225675949
O 12.776264695 10.670746567 3.071078413
O 12.549670462 10.758380175 10.544108445
O 2.048874372 7.925410833 3.080670201
O 2.213597909 7.477260770 10.459072399
O 1.554856956 5.269489372 7.780670787
O 1.598124928 5.155975108 14.915947934
O 3.135626131 12.184329781 2.142416965
O 3.131856913 12.027490711 8.889102456
O 9.895062441 1.707711085 5.088295469
O 9.883326430 1.737190914 12.906251556
O 0.911557298 9.737078879 1.497308388
O 0.952730335 9.638341824 9.650175204
O 12.214742404 4.335189644 5.967883673
O 12.190232385 3.993013918 13.350723355
O 3.736258734 1.294051776 5.690290442
O 3.904624280 1.126029083 13.148524030
O 6.008413101 11.606046792 5.717665504
O 6.325889091 11.817685192 13.295180784
O 9.867429911 12.525249344 1.880863061
O 9.701945358 12.567533841 9.297475548
O 7.269162550 2.021260467 1.995700762
O 7.497707693 2.148323644 9.534930730
O 12.134793006 9.999556461 5.517957675
O 11.908011609 10.249464543 13.038033504
O 1.702280383 7.005792427 5.503346483
O 1.591265774 6.970728514 12.963804343
O 1.220044197 3.304269819 1.783121294
O 1.113366710 3.163577795 9.306618657
O 11.857673250 6.594440499 1.755240815
O 11.528334134 6.651514126 9.257927164
O 2.722705537 3.047599703 3.985908245
O 2.793001223 2.653398143 11.300232624
O 10.045419847 10.888578114 14.790777401
O 10.482013701 11.251992106 7.136971605
O 10.192285486 10.794351126 3.847362476
O 10.011786229 10.652616485 11.181207514
O 3.084123582 2.980558393 14.916426162
O 3.121256719 3.131650521 7.548644654
O 7.357311936 0.156699277 0.090981243
O 7.442362335 -0.158063392 7.726667120
O 13.528543326 7.099487849 14.789560595
O 13.159216593 7.192896976 7.216689388
O 5.595866962 13.921574432 3.983309751
O 7.294905899 0.323159013 11.452122271
O -0.347165399 7.012653714 3.838703324
O -0.285128265 6.792738783 11.053367654
O 0.509367938 12.355912708 1.817312385
O 0.531669838 12.260505682 9.428338179
O 3.572075658 9.577336565 1.782334946
O 3.623357006 9.458613864 9.399309915
O 12.485291583 1.710380729 5.750123189
O 12.495360363 1.342414230 13.134307575
O 9.546323456 4.307716385 5.523246118
O 9.555770483 4.357841808 13.213985386
O 4.952680829 8.300855524 5.620879875
Si 7.049825500 1.708998474 0.431217143
Si 9.267294564 12.168747430 0.422158859
Si 9.375652153 12.267265103 7.713828994
Si 3.718638392 1.774667606 4.147511288
Si 3.901360034 1.516991077 11.574061142
Si 11.925165124 7.019087414 3.320969328
Si 11.921524774 6.930423940 10.802287058
Si 1.408431798 3.730472301 3.339819629
Si 1.441021818 3.430687847 10.864039084
Si 1.283584748 6.702751779 14.536655104
Si 11.670657480 10.153651810 7.064870413
Si 11.497754812 10.188211740 14.609874967
Si 6.329205443 11.938032975 7.291823080
Si 6.276937595 12.182554593 14.850939362
Si 3.887405452 1.718733741 7.259075574
Si 3.994656747 1.651319493 14.686275515
Si 6.766428560 1.819146781 3.533604859
Si 6.929983157 1.826194811 11.120841994
Si 9.482419954 12.206044414 3.438106306
Si 9.320729283 12.055230168 10.779036748
Si 1.253908191 6.808415108 3.947994163
Si 1.284131376 6.553614551 11.420299531
Si 11.598223488 10.009700840 3.979878408
Si 11.486030945 9.998324870 11.496182363
Si 11.978129181 7.145812245 0.236188592
Si 11.646785847 7.219770289 7.730968675
Si 1.605735464 3.571676689 0.229243001
Si 1.888269504 13.199496159 1.933073547
Si 1.936432748 13.067853377 9.269053708
Si 4.265627139 11.045143439 1.929168181
Si 4.274934564 10.957168226 9.355593644
Si 11.167253570 0.805691290 5.533990575
Si 11.039519101 0.634130652 13.140986496
Si 8.814358098 2.918842844 13.215986283
Si -0.199690179 10.905309180 1.721619649
Si -0.150668173 10.795317682 9.373581840
Si 2.179157622 8.740338333 1.679662358
Si 2.215232316 8.664784556 9.351726985
Si 13.253472631 3.124636687 5.633792759
Si 13.250395958 2.783840141 13.128392336
Si 10.884787295 5.206956176 5.610073893
Si 11.006845183 5.080809289 13.133689755
Si 1.611200540 3.675617351 7.833057992
Si 8.813224251 2.852896795 5.541413341
Al 1.008812140 6.754913603 7.130835912
Al 6.261712904 12.346526338 4.101568146
Al 6.050773581 12.238755555 11.664486900
Al 7.089375098 1.526525307 7.796018781
Cu1 3.307614729 7.970584418 6.340144538
Cu2 5.274404925 9.899418636 4.805008766
H 8.128999845 2.888873757 9.468737119
H 7.388494366 11.276301523 9.892273631
C 6.827224864 6.322141333 6.800666789
H 6.686427122 5.537488289 6.059438766
H 7.778011593 6.850833832 6.840741656
H 6.133702908 6.397512140 7.636831231
H 5.690084378 7.688650633 5.882134152
End final coordinates

Cu-O-Cu-product-2
Final energy = -6723.4310878517 Ry
13.812406654 0.062765001 -0.008803408
-1.372541210 13.620145894 -0.034179750
-0.002136721 -0.006126582 15.018670026

ATOMIC_POSITIONS (angstrom)
O 3.139315907 0.505986582 3.276096097
O 2.265717798 13.728423024 10.725025448
O 5.192204430 11.003437454 3.394962810
O 4.924367361 11.246135059 10.840312632
O 7.972657332 11.522174403 7.700355818
O 7.714620035 11.733139656 0.563439422
O 10.843235469 0.020033075 6.993331385
O 9.455992669 13.465499087 14.564150149
O 8.222481590 2.548121712 7.062886407
O 8.114600053 2.599491632 14.678873889
O 5.201537230 2.175378030 3.645383461
O 5.341338996 2.101477229 11.155813048
O 12.640919496 10.999084963 0.404874471
O 13.052514548 10.594695691 7.883386713
O 2.206341599 7.670619464 0.409269086
O 2.141292093 7.989255575 7.814005072
O 1.641502231 5.277462589 3.342275277
O 1.691990277 4.942824047 11.200948317
O 0.084328414 3.230955017 4.139152037
O 0.136370467 2.845566933 11.700638992
O 11.005423066 5.874281422 4.130597348
O 11.197253393 5.692645774 11.664511418
O 11.442549590 8.643184422 0.104345745
O 11.134715195 8.731069405 7.700424642
O 10.135244187 13.320444023 4.375718871
O 9.577255839 13.107678970 11.951015565
O 7.623120703 2.827929005 4.479478906
O 7.716348512 2.879546728 12.051809579
O 5.560121261 2.017983268 15.035112097
O 5.426818820 1.797015762 7.696762733
O 3.530456453 0.377246658 0.642766518
O 3.152737456 0.465290375 8.140639852
O 5.146867171 11.269990541 0.718200710
O 5.508609791 10.896117284 8.281612328
O 7.886203174 12.064528960 3.674507684
O 7.653007278 11.674765848 10.810799743
O 0.624684913 3.006074250 6.734943355
O 0.555057030 2.711789042 14.329653951
O 10.730003839 6.299662185 6.764249075
O 11.062511299 6.183890359 14.264019748
O 11.262354124 8.443478648 3.513280039
O 11.389566852 8.323723776 11.271582995
O 12.745782440 10.624869224 3.052611193
O 12.565125169 10.639329170 10.503128226
O 1.955886997 7.864223776 3.062179737
O 2.236140432 7.410063676 10.438716331
O 1.600457811 5.224626401 7.841381133
O 1.627647143 5.104455748 14.921352125
O 3.121278982 12.111128408 2.205272627
O 3.161113223 11.974317571 8.931167833
O 9.900275887 1.676567565 5.157577054
O 9.894342390 1.682138401 12.912673231
O 0.902303241 9.711086368 1.484143354
O 1.014209435 9.581121150 9.637190715
O 12.219026253 4.300784474 5.914262883
O 12.199341080 3.945934052 13.408108171
O 3.745134712 1.241340282 5.707554142
O 3.934644369 1.056530621 13.179804979
O 6.100692058 11.548430037 5.786504087
O 6.271130341 11.741769657 13.367334380
O 9.879530048 12.450671595 1.914561566
O 9.724039142 12.555784039 9.365490052
O 7.291984558 1.950702319 2.042937452
O 7.500319113 2.097817067 9.589075240
O 12.147789724 9.962011057 5.517338446
O 11.931011366 10.228371182 13.019519054
O 1.658386020 6.883074494 5.475770215
O 1.588889357 6.912442812 12.956181422
O 1.245133783 3.217851917 1.774060422
O 1.130059402 3.085956130 9.319553046
O 11.798654137 6.563689592 1.729455439
O 11.520137255 6.607527906 9.259633671
O 2.747468347 3.014864157 3.994347236
O 2.770920711 2.582658386 11.355771993
O 10.063603955 10.868748325 14.775244042
O 10.553290290 11.233427222 7.207391880
O 10.175866954 10.742451798 3.900600223
O 10.029826544 10.580022272 11.170446392
O 3.117844322 2.923165043 14.927129544
O 3.125772692 3.062052880 7.563412175
O 7.368237890 0.091462520 0.143870518
O 7.503720732 -0.174957297 7.746104883

O 13.531127574 7.022976091 14.799038033
O 13.224911488 7.159820514 7.287488077
O 5.604796095 13.865555022 4.050976871
O 7.283890865 0.267908892 11.504099040
O -0.404602645 6.891393224 3.827439977
O -0.269892863 6.742009532 11.032681739
O 0.502833757 12.325267422 1.842636593
O 0.553946204 12.194108452 9.466520529
O 3.554796747 9.509625636 1.824948853
O 3.679887221 9.400276559 9.406723457
O 12.507786047 1.668373144 5.747538812
O 12.506313007 1.296556634 13.162134381
O 9.539108068 4.279603804 5.575675959
O 9.567406152 4.300534403 13.231649280
O 4.435262385 8.408019611 4.850668561
Si 7.076341435 1.646733685 0.475820172
Si 9.280079780 12.125091754 0.447277193
Si 9.442190281 12.247665532 7.776605716
Si 3.728242108 1.730064428 4.166757101
Si 3.900405576 1.462281096 11.609692651
Si 11.874136025 6.958375050 3.302042350
Si 11.932284415 6.859472933 10.802488211
Si 1.425880347 3.667560915 3.324993341
Si 1.436810441 3.371349980 10.878377066
Si 1.290510710 6.648517080 14.534407850
Si 11.723998084 10.116652499 7.075154590
Si 11.518317374 10.169956028 14.591953511
Si 6.405594014 11.919513189 7.374579468
Si 6.269982191 12.110904319 14.924439416
Si 3.892002981 1.651169363 7.279831869
Si 4.028068504 1.590234723 14.715871683
Si 6.781617794 1.760172745 3.580287303
Si 6.921293662 1.773592945 11.171869425
Si 9.464885706 12.147544765 3.466945331
Si 9.338623330 11.998915915 10.831582422
Si 1.200708252 6.721801183 3.928089794
Si 1.297145750 6.497541965 11.406746108
Si 11.590172066 9.961649313 3.986644936
Si 11.503026980 9.921465613 11.488832466
Si 11.973869667 7.113340207 0.215385828
Si 11.694193502 7.183825127 7.739804417
Si 1.636785921 3.516345212 0.226934065
Si 1.897303501 13.143916791 1.966650983
Si 1.952470070 13.009361422 9.298079753
Si 4.259517096 10.965771722 2.039803428
Si 4.303764479 10.910309036 9.407091210
Si 11.177521165 0.771209546 5.571737148
Si 11.052037871 0.587081087 13.187204207
Si 8.828199564 2.860001861 13.252804077
Si -0.206731452 10.876720222 1.719190189
Si -0.105844007 10.720229344 9.366382093
Si 2.153507307 8.695251664 1.682983605
Si 2.271011499 8.601261263 9.334398510
Si 13.265985401 3.088878439 5.623871756
Si 13.257409593 2.740835831 13.145198139
Si 10.880685329 5.175240978 5.597233489
Si 11.018039568 5.026219951 13.136355838
Si 1.626056372 3.629449225 7.854800565
Si 8.812509766 2.824218006 5.593438685
Al 1.068369392 6.692573830 7.136430399
Al 6.242669282 12.277035622 4.117242596
Al 6.045815769 12.187124776 11.737855934
Al 7.098706514 1.500888422 7.842448757
Cu1 3.220170239 8.139835779 6.223084582
Cu2 5.554934936 9.822203684 5.166325074
H 8.151004859 2.822964052 9.537799942
H 7.394123641 11.129452250 10.036411929
C 6.766277739 8.712927036 6.257676799
H 6.899680930 7.759839714 5.737867699
H 7.679158955 9.315554656 6.298742365
H 6.249797757 8.623228765 7.217741593
H 4.852874901 7.591284919 4.522511498
End final coordinates

Cu-O-Fe-product-1
Final energy = -6652.0449010547 Ry
13.807958833 0.043226215 -0.019046104
-1.391379875 13.624553575 -0.029149664
-0.013299265 -0.001666787 15.026550077

ATOMIC_POSITIONS (angstrom)
O 3.133057136 0.601483811 3.224144814
O 2.236628959 13.791961361 10.690079698
O 5.117111043 11.059858913 3.370171042
O 4.887578556 11.350944167 10.796780392
O 7.882475643 11.538700894 7.609543886
O 7.703687667 11.743463609 0.495593341
O 10.796791278 0.029397012 6.941945069
O 9.436176432 13.484568666 14.519005007
O 8.266859892 2.539163569 7.034170995
O 8.022699827 2.682716640 14.644735877
O 5.195848116 2.256225900 3.650794643
O 5.322688833 2.164725254 11.122886798
O 12.660529423 11.025120493 0.357651230
O 12.968639055 10.686737363 7.840062824
O 2.194248402 7.731941862 0.394425557
O 2.150088503 8.073812457 7.803076456
O 1.511606559 5.334062571 3.262373443
O 1.653957829 4.994589114 11.180566032
O 0.069937530 3.223945005 4.109842650
O 0.112801736 2.879840115 11.647132621
O 11.097652731 5.868571381 4.111979895
O 11.088528632 5.789633486 11.644379237
O 11.446161752 8.675265407 0.080452043
O 11.126681215 8.749537408 7.682673703
O 10.114302934 13.341202047 4.346562541
O 9.506416129 13.200266621 11.884629898
O 7.633384123 2.863055972 4.474145777
O 7.701613593 2.960178353 12.005106831
O 5.502592901 1.994174014 15.058312999
O 5.441089496 1.867700796 7.592138953
O 3.421617979 0.404051496 0.575966818
O 3.161963753 0.552342009 8.106733517
O 5.140050271 11.346871163 0.697017102
O 5.426552663 10.885812794 8.236072648
O 7.835736141 12.117956006 3.671020272
O 7.599536940 11.707899725 10.813413270
O 0.678712762 3.062457224 6.688921561
O 0.522572735 2.795058208 14.278291348
O 10.770614830 6.317593385 6.736831893
O 11.045131800 6.219401266 14.263736239
O 11.178473751 8.449453196 3.499214271
O 11.354952947 8.400373604 11.187892695
O 12.654537703 10.636397398 3.006695672
O 12.513978149 10.738841388 10.472983782
O 2.041061871 7.901210232 3.065251352
O 2.147729699 7.471431089 10.421234869
O 1.598080664 5.302109425 7.841848281
O 1.619448744 5.161812205 14.924804556
O 3.103438335 12.220194373 2.155543267
O 3.120304233 12.041403967 8.882062997
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O 9.832795683 1.723613341 12.934181324
O 0.867263551 9.731381510 1.528482537
O 0.919756438 9.635220185 9.586285927
O 12.220340819 4.269816353 5.914435595
O 12.179368647 4.020079572 13.314152821
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O 3.914978134 1.109174420 13.142263201
O 5.936773685 11.585722755 5.760195171
O 6.197242534 11.837651041 13.342554591
O 9.821214636 12.496233851 1.889053378
O 9.626139025 12.565244317 9.309819954
O 7.271758222 2.028335911 2.028047461
O 7.470597176 2.166814562 9.540826414
O 12.078933208 9.993033993 5.480203440
O 11.908877626 10.255016636 12.990041530
O 1.692405468 6.874421717 5.448376690
O 1.603037784 6.954266828 12.952110972
O 1.209276555 3.239746261 1.730200228
O 1.128054331 3.141791194 9.279499391
O 11.829481584 6.603189554 1.713237946
O 11.551442269 6.629374423 9.229060206
O 2.738763036 3.118765511 3.928542618
O 2.752779355 2.641934809 11.324246487
O 10.062187626 10.903215466 14.770433599
O 10.455444075 11.228538401 7.161995138
O 10.099090092 10.758640339 3.856549788
O 9.990681234 10.653879376 11.172795217
O 3.083658870 2.968270294 14.894812826
O 3.156474386 3.157409476 7.561389960
O 7.423637968 0.153790470 0.156142810
O 7.441325758 -0.166695140 7.753420806
O 13.516842007 7.059688729 14.760101981
O 13.254274020 7.225223758 7.260213968
O 5.556893713 13.921056362 4.016999896
O 7.286205920 0.352094543 11.468153882
O -0.378381724 7.099409158 3.801770611
O -0.326710769 6.780807099 11.113362866
O 0.471932971 12.349765525 1.893391972
O 0.522330386 12.270730908 9.415435525
O 3.520898754 9.596614226 1.785822572
O 3.595627214 9.479837427 9.484437504
O 12.545188325 1.645866000 5.761328186
O 12.455143928 1.363173658 13.121641678
O 9.545142509 4.325476049 5.553818118
O 9.537728451 4.350774051 13.235375250
O 4.979867155 8.125259306 5.362422279
Si 7.051915876 1.697870946 0.466418734
Si 9.267716190 12.152145117 0.408746197
Si 9.351876972 12.254473384 7.719631619
Si 3.703415104 1.827141291 4.128851937
Si 3.882034558 1.520956373 11.573393356
Si 11.895725246 7.008993787 3.285272987
Si 11.889610577 6.914072091 10.783223653
Si 1.381092226 3.720276092 3.275858992
Si 1.415843730 3.424022898 10.841226011
Si 1.281870547 6.701408081 14.527210843
Si 11.659682549 10.148556572 7.038371414
Si 11.512092481 10.202390670 14.567031898
Si 6.309635392 11.935699158 7.342706341
Si 6.252428886 12.185364271 14.899994304
Si 3.889721028 1.737515585 7.235102075
Si 3.970620563 1.620729167 14.686495002
Si 6.767863728 1.824175552 3.565356080
Si 6.905766878 1.851273356 11.129976345
Si 9.417512179 12.180826381 3.441699592
Si 9.280065330 12.052994351 10.799210964
Si 1.214681499 6.788068582 3.921460430
Si 1.254994370 6.544700197 11.413433956
Si 11.510556830 9.972630154 3.954259921
Si 11.468985484 9.989593701 11.454263855
Si 11.978963519 7.145585500 0.195257279
Si 11.725122149 7.216376116 7.711790918
Si 1.616113645 3.564444186 0.192599220
Si 1.838095484 13.217419897 1.940956041
Si 1.921482817 13.085025619 9.256166914
Si 4.206038586 11.054561540 1.972965482
Si 4.244444094 10.971200089 9.386316489
Si 11.191840085 0.789171585 5.542224041
Si 11.010211565 0.638315644 13.150675362
Si 8.780315721 2.922386554 13.237757460
Si -0.240225474 10.906148347 1.723678127
Si -0.167013655 10.809701814 9.326125368
Si 2.139360047 8.733817909 1.682155831
Si 2.199971696 8.673389885 9.333908254
Si 13.284799911 3.078486314 5.601748831
Si 13.222680262 2.797364615 13.082527255
Si 10.916271942 5.184725050 5.577729942
Si 10.976969823 5.091038687 13.108701245
Si 1.643164757 3.709323475 7.829478767
Si 8.843674869 2.855796377 5.566108610
Al 1.104309636 6.768193665 7.089175356
Al 6.203442704 12.342974422 4.122293024
Al 6.002084342 12.277685623 11.708685520
Al 7.098261967 1.526267787 7.799987306
Cu1 3.508074599 8.180924567 6.478892318
Fe2 5.098697580 9.932250509 5.021391676
H 8.118552435 2.893242331 9.474973328
H 7.331311714 11.103054248 10.090186902
C 6.691339081 6.378509915 6.865988763
H 6.569478789 5.543720120 6.177556983
H 7.640841983 6.911702082 6.889349272
H 6.007374658 6.470549864 7.708893432
H 5.702221506 7.566720729 5.791671983
End final coordinates

Cu-O-Fe-product-2
Final energy = -6652.1435564329 Ry
13.807958833 0.043226215 -0.019046104

-1.391379875 13.624553575 -0.029149664
-0.013299265 -0.001666787 15.026550077

ATOMIC_POSITIONS (angstrom)
O 3.142299137 0.511991737 3.277804224
O 2.251861471 13.746105399 10.735540323
O 5.148939224 10.969080221 3.451467066
O 4.875987220 11.275146654 10.900148571
O 7.963234072 11.533050028 7.623307482
O 7.709518036 11.743174336 0.577799014
O 10.903526844 0.025979923 7.012338926
O 9.476091785 13.450310928 14.580852664
O 8.256900977 2.533530870 7.085384175
O 8.139781457 2.596376808 14.701152414
O 5.228163079 2.149193930 3.662440434
O 5.357254074 2.101190801 11.159029006
O 12.618475905 11.016404891 0.383145528
O 13.050349924 10.608746210 7.875322856
O 2.222362502 7.677811308 0.395236437
O 2.172750052 8.057759419 7.791486780
O 1.680310334 5.296854618 3.315542685
O 1.698654757 4.952488134 11.218797684
O 0.127400614 3.246507852 4.125327582
O 0.147151127 2.841252757 11.680576918
O 10.971815701 5.855207737 4.095842302
O 11.189278633 5.683333992 11.651330489
O 11.464537299 8.634203042 0.086511618
O 11.167083776 8.716898299 7.686758662
O 10.117294074 13.292440715 4.400070144
O 9.560290824 13.084594967 11.961759546
O 7.648079989 2.786201779 4.504081909
O 7.729863862 2.875974548 12.071152014
O 5.579714537 2.037680520 15.033138929
O 5.441023453 1.801273562 7.687846746
O 3.578595122 0.383447205 0.649145643
O 3.163562314 0.478939467 8.144392767
O 5.156723295 11.281494085 0.779000877
O 5.532124872 10.915838529 8.366414554
O 7.876670085 11.995271087 3.745791574
O 7.619807633 11.654631261 10.853398318
O 0.646655698 3.072337415 6.729474737
O 0.582186953 2.717974467 14.308733991
O 10.780244337 6.295261330 6.735191670
O 11.076805137 6.176197347 14.253668525
O 11.297766214 8.425714527 3.508515011
O 11.387558515 8.312978225 11.258903049
O 12.752773843 10.614874883 3.029434824
O 12.545853686 10.635171668 10.494840150
O 1.874073026 7.892636533 3.037047108
O 2.221678798 7.409362510 10.405323907
O 1.669481116 5.268522571 7.851078746
O 1.645392979 5.115484926 14.892921439
O 3.110101099 12.115478322 2.241575712
O 3.159279757 11.996408778 8.943740811
O 9.948197487 1.680714545 5.180191754
O 9.896801070 1.652096483 12.930592381
O 0.894057831 9.736689183 1.423145087
O 1.003463354 9.595664335 9.642716222
O 12.216065106 4.272748940 5.862301863
O 12.223911509 3.942416159 13.386767437
O 3.738316089 1.248498222 5.708495183
O 3.948460476 1.064917061 13.185957974
O 5.983563555 11.521523196 5.829024390
O 6.229094436 11.737115662 13.409425561
O 9.847012099 12.438241713 1.943449940
O 9.668005298 12.532554353 9.367139918
O 7.307809901 1.948344493 2.052977750
O 7.514358764 2.092307428 9.601157573
O 12.164770432 9.969055320 5.508543569
O 11.890013589 10.233623366 13.010857816
O 1.687820665 6.887830453 5.460360190
O 1.606966744 6.942606513 12.944136925
O 1.268180717 3.235916484 1.752402521
O 1.159340362 3.119684739 9.311026159
O 11.829604572 6.558776663 1.712504324
O 11.537691191 6.594251209 9.243061077
O 2.786702254 3.032741440 3.966942654
O 2.786451127 2.596988451 11.360220442
O 10.034729732 10.848684551 14.804417800
O 10.544678075 11.214945585 7.212194645
O 10.186009568 10.712808627 3.898635930
O 10.004039496 10.557276538 11.155456667
O 3.137290756 2.933625577 14.929271198
O 3.150268387 3.078925626 7.557515578
O 7.375274466 0.092078405 0.154272413
O 7.508087177 -0.173511481 7.751451462
O 13.540100900 7.014133299 14.778142434
O 13.272267344 7.150384067 7.297772335
O 5.614666843 13.836354360 4.041190753
O 7.304823235 0.271937793 11.529799853
O -0.413914357 6.824632615 3.870755330
O -0.270420971 6.744530162 11.049171320
O 0.500776793 12.344435163 1.827172221
O 0.547969763 12.210855227 9.480253178
O 3.531667648 9.513784969 1.826849125
O 3.672782858 9.425992833 9.455349774
O 12.568829812 1.645870213 5.719086114
O 12.512540604 1.286934639 13.146689263
O 9.535837133 4.279886727 5.587223160
O 9.591751747 4.280004863 13.238060099
O 4.316447168 8.402152717 4.686966841
Si 7.098330540 1.650732750 0.483632608
Si 9.279133184 12.114663583 0.463873669
Si 9.434726865 12.239553423 7.767088343
Si 3.741460256 1.733315707 4.166690202
Si 3.912176464 1.472774684 11.615426849
Si 11.878460759 6.929206729 3.292479495
Si 11.931545174 6.847433271 10.790093658
Si 1.461984730 3.687514038 3.302940957
Si 1.452838456 3.384474608 10.875362566
Si 1.303146336 6.661712814 14.518772458
Si 11.729662405 10.113612188 7.065643293
Si 11.494486175 10.168491424 14.587324333
Si 6.383437874 11.922088095 7.401996046
Si 6.249675445 12.121468020 14.961218084
Si 3.902968035 1.661775515 7.278556332
Si 4.048299771 1.602071524 14.720507029
Si 6.806152281 1.735441709 3.589730684
Si 6.936932780 1.774119359 11.186038532
Si 9.452427865 12.112982846 3.497305968
Si 9.307175883 11.978469430 10.838909608
Si 1.199820276 6.719819672 3.929953628
Si 1.301575520 6.509555809 11.401319348
Si 11.608852288 9.947165451 3.977436504
Si 11.483563682 9.911496369 11.476581538
Si 11.997236245 7.104364039 0.196510086
Si 11.734941425 7.172559262 7.724683446
Si 1.665066369 3.525460015 0.204772839
Si 1.895276780 13.157447986 1.973725431
Si 1.944033468 13.027860285 9.307437308
Si 4.234814569 10.961288021 2.066472684
Si 4.290080127 10.934752296 9.454266929
Si 11.222533082 0.763252846 5.580617100
Si 11.064990554 0.564294795 13.191135148
Si 8.845594109 2.845089739 13.268546968
Si -0.212191809 10.897477693 1.697380984
Si -0.113665372 10.738293530 9.373321310
Si 2.126808357 8.705955990 1.661750200
Si 2.268676156 8.628013599 9.331772293
Si 13.295521547 3.087005169 5.595574655
Si 13.271557587 2.728115027 13.120884776
Si 10.885770359 5.164812197 5.571074960
Si 11.034153676 5.017228366 13.126620044
Si 1.661123309 3.672981785 7.851048566
Si 8.841091902 2.810831556 5.613717176
Al 1.126024443 6.726196405 7.124629635
Al 6.231594996 12.246547165 4.154474885
Al 6.020914056 12.197795791 11.782197038
Al 7.110152331 1.502941731 7.853001929
Cu1 3.231020486 8.302489480 6.200705894
Fe2 5.331168360 9.822096248 5.218760861
H 8.194582571 2.789837383 9.543796884
H 7.343675761 11.057813709 10.125106407
C 6.636991475 8.727531239 6.196035712
H 6.751366516 7.745180620 5.723802667
H 7.581412398 9.286007285 6.192089996
H 6.225804408 8.639991476 7.212904054
H 4.725575970 7.548973966 4.454484854
End final coordinates

Cu-O-Mn-product-1
Final energy = -6796.8725863847 Ry
13.811943229 0.038263164 -0.014702354
-1.396598396 13.615934446 -0.035287329
-0.008540384 -0.007967288 15.032144927

ATOMIC_POSITIONS (angstrom)
O 3.146289547 0.621832764 3.208750421
O 2.226636975 13.792942546 10.675818121
O 5.112555665 11.058961746 3.360977322
O 4.897813445 11.350597426 10.776827964
O 7.872768962 11.534911697 7.645308186
O 7.708605070 11.720022626 0.470189070
O 10.788271597 0.026682543 6.947405049
O 9.439508534 13.473047946 14.521549642
O 8.268189122 2.539798315 7.030958399
O 8.006572831 2.684284575 14.645070236
O 5.203469946 2.280080332 3.655741081
O 5.324671944 2.167119924 11.126780992
O 12.681704517 11.023467554 0.346595675
O 12.952515599 10.699502921 7.827382553
O 2.190671587 7.731000958 0.393528582
O 2.181194280 8.034344301 7.805505281
O 1.486047318 5.332661431 3.230467478
O 1.647271994 4.995582913 11.168363195
O 0.075174405 3.214480071 4.109915089
O 0.110851042 2.881482082 11.648759802
O 11.132678894 5.845769774 4.111693307
O 11.086546622 5.772168149 11.639503807
O 11.462975557 8.677685567 0.082887362
O 11.128151985 8.745065977 7.686001505
O 10.095927533 13.314094170 4.345579574
O 9.505195976 13.196033416 11.885139978
O 7.647941591 2.877219527 4.466507636
O 7.706525862 2.962188449 12.005221476
O 5.497999313 1.958124267 15.074169508
O 5.441613213 1.869571880 7.584023250
O 3.390981411 0.392783179 0.560059595
O 3.161017184 0.549698017 8.095722794
O 5.139441838 11.343772206 0.680949037
O 5.404319866 10.877677816 8.207639566
O 7.815733045 12.102645060 3.646057001
O 7.608398360 11.709199607 10.798426848
O 0.682147183 3.027909438 6.692177211
O 0.524116197 2.794198865 14.277442300
O 10.796178970 6.313692444 6.733250358
O 11.048777300 6.225419733 14.254147047
O 11.157475722 8.428751434 3.500547492
O 11.342618837 8.386943963 11.194293704
O 12.626866583 10.619255491 2.991632357
O 12.520138754 10.711941888 10.464673467
O 2.062928842 7.894351900 3.066784295
O 2.138849203 7.479971162 10.433894091
O 1.572555142 5.284575655 7.840087253
O 1.629233962 5.152094637 14.935841293
O 3.105854810 12.226575605 2.140133664
O 3.113604352 12.036529226 8.875947563
O 9.946953584 1.725904596 5.103522317
O 9.830351056 1.720071911 12.950489904
O 0.860848386 9.720090778 1.542681312
O 0.911755708 9.622225733 9.535980168
O 12.241554137 4.256313297 5.929957744
O 12.183112713 4.018520366 13.322679386
O 3.676130927 1.343753893 5.659437552
O 3.918862738 1.098682696 13.139819911
O 5.961835038 11.587596144 5.755665240
O 6.199771119 11.833540836 13.330326783
O 9.814410233 12.482322750 1.881849557
O 9.649592885 12.557129329 9.310316080
O 7.272671977 2.028892827 2.026840869
O 7.466580199 2.179910817 9.539606143
O 12.060375192 9.984492179 5.470330552
O 11.927973841 10.240849368 12.986849753
O 1.674998920 6.838825943 5.435096554
O 1.606909888 6.939640175 12.958663261
O 1.209365053 3.221487761 1.724463135
O 1.132996115 3.122956663 9.283132119
O 11.816242527 6.593188244 1.705232987
O 11.564978911 6.623972728 9.230202639
O 2.742557261 3.135113941 3.921699258

O 2.754052388 2.647627839 11.338282479
O 10.084414559 10.896369017 14.763634778
O 10.434548004 11.213694503 7.148763248
O 10.073129990 10.735340424 3.845800219
O 9.998798039 10.651261623 11.181162303
O 3.088359232 2.956598613 14.892586885
O 3.157911732 3.157868469 7.561792284
O 7.446620287 0.154168104 0.158290708
O 7.439451055 -0.162318178 7.774333960
O 13.524618957 7.037662567 14.769367177
O 13.270283465 7.243266812 7.269957294
O 5.548725301 13.927260368 4.022299425
O 7.292492170 0.356570618 11.463476155
O -0.374878316 7.128913476 3.764636631
O -0.333923697 6.784818446 11.130159565
O 0.468371435 12.337029060 1.918357357
O 0.517290934 12.262346270 9.409969863
O 3.517872389 9.601766158 1.779118260
O 3.588742658 9.478172803 9.485759540
O 12.544744333 1.628646258 5.752962658
O 12.455872616 1.363338208 13.128344602
O 9.568805061 4.318227611 5.559122015
O 9.539578255 4.346543917 13.248377390
O 5.047763985 7.985293890 5.423695721
Si 7.049571380 1.692343751 0.466837310
Si 9.270312851 12.141013838 0.397064586
Si 9.346973905 12.246090322 7.725125282
Si 3.709017490 1.844478877 4.122182565
Si 3.883063225 1.523222952 11.574538445
Si 11.899051100 7.001233056 3.276030716
Si 11.888704754 6.904422205 10.788742787
Si 1.377549623 3.717884038 3.265841254
Si 1.415729138 3.421133911 10.843003990
Si 1.286673903 6.689266492 14.534075935
Si 11.648167242 10.143712249 7.030131769
Si 11.534384763 10.194866182 14.564993573
Si 6.305593556 11.936093816 7.339247504
Si 6.261472773 12.170343671 14.890232342
Si 3.889775125 1.738893736 7.228550871
Si 3.965805248 1.602268040 14.686777265
Si 6.772494924 1.837521459 3.566853688
Si 6.908333717 1.855514462 11.129429444
Si 9.399425590 12.162160499 3.430317977
Si 9.289406495 12.048420008 10.798616619
Si 1.211268037 6.784127805 3.906061798
Si 1.249378103 6.542951199 11.419177055
Si 11.488587006 9.955435279 3.945214624
Si 11.473699722 9.976276456 11.454563996
Si 11.981173439 7.142380514 0.191106064
Si 11.739567135 7.216754501 7.715265634
Si 1.616779267 3.559509434 0.189339465
Si 1.830765302 13.212812702 1.931974225
Si 1.914214256 13.080022134 9.245301489
Si 4.209040488 11.058939024 1.962481797
Si 4.240211125 10.967077581 9.375011557
Si 11.187003894 0.777493031 5.542917955
Si 11.012034376 0.638509021 13.160385413
Si 8.777334235 2.920764714 13.244771400
Si -0.245708085 10.897543688 1.723736534
Si -0.174285042 10.803277330 9.306151466
Si 2.141299714 8.730452736 1.682987658
Si 2.200165647 8.662163937 9.327226946
Si 13.295292889 3.057439972 5.605543793
Si 13.225979391 2.795531881 13.088892066
Si 10.942278273 5.173502805 5.581338129
Si 10.978365749 5.085591713 13.110589256
Si 1.638257722 3.692859803 7.830472269
Si 8.852047485 2.855856383 5.565348284
Al 1.106080805 6.755333979 7.078790224
Al 6.188799909 12.344688831 4.118541339
Al 6.009367902 12.273207589 11.695570408
Al 7.098283720 1.531348654 7.801317896
Cu1 3.601588685 8.064366519 6.563481536
Mn2 5.114750508 9.847479513 5.030061559
H 8.113972155 2.906826536 9.474406703
H 7.343963902 11.134128233 10.049086786
C 6.780643423 6.180320867 6.937284341
H 6.613614468 5.397511467 6.198936622
H 7.746166698 6.682812768 6.966349024
H 6.120577262 6.240309129 7.801357105
H 5.769937344 7.450531095 5.868743181
End final coordinates

Cu-O-Mn-product-2
Final energy = -6796.9805282816 Ry
13.811943229 0.038263164 -0.014702354
-1.396598396 13.615934446 -0.035287329
-0.008540384 -0.007967288 15.032144927

ATOMIC_POSITIONS (angstrom)
O 3.173308395 0.512810023 3.291900891
O 2.229574793 13.741911825 10.737307981
O 5.195358896 10.981373371 3.423202178
O 4.913798146 11.292327149 10.823146216
O 7.915829742 11.512349401 7.696684927
O 7.726766827 11.689767413 0.526766514
O 10.829912275 -0.000281894 7.014411783
O 9.442542515 13.445436702 14.554950374
O 8.230294044 2.546433556 7.083979606
O 8.139394121 2.586913432 14.704707543
O 5.201559664 2.221271973 3.661131277
O 5.339683562 2.107258281 11.201825904
O 12.700991353 10.979554055 0.373430573
O 13.002508133 10.626222386 7.862251160
O 2.228820144 7.681875640 0.402670733
O 2.143584209 8.021576469 7.821553658
O 1.556613639 5.255071150 3.306811325
O 1.686007706 4.956883807 11.192398222
O 0.074814522 3.161365494 4.130303504
O 0.138238831 2.851224333 11.689202578
O 11.004656857 5.865256580 4.121925491
O 11.177332661 5.673706403 11.654346862
O 11.481278847 8.634798552 0.098415198
O 11.134031175 8.715720437 7.698051743
O 10.122722774 13.309723432 4.399609147
O 9.563533412 13.103320543 11.940629905
O 7.630341164 2.833746086 4.502883172
O 7.714754394 2.902798231 12.087576235
O 5.584075593 1.988510533 15.016280402
O 5.428767961 1.821923820 7.717004999
O 3.573115989 0.360881497 0.657410904
O 3.142460989 0.510348146 8.156718490
O 5.163879186 11.256884503 0.747628768
O 5.437530697 10.885527663 8.251838452
O 7.861756242 12.076523375 3.697724550
O 7.625135566 11.655423790 10.857146462
O 0.649489571 3.033385374 6.726959406
O 0.584971811 2.719447795 14.310106336
O 10.759803712 6.286387064 6.759805237
O 11.086192654 6.187515027 14.249057830
O 11.218350513 8.432578121 3.490244101
O 11.372740158 8.309974413 11.272400586
O 12.706183196 10.611498178 3.025254589
O 12.512061960 10.640902992 10.486324819
O 1.984133755 7.816874582 3.060059524
O 2.196666837 7.437665188 10.450927962
O 1.594818929 5.252577212 7.879159949
O 1.659451925 5.099478510 14.946436495
O 3.140770355 12.111495752 2.239805365
O 3.127486902 12.010479031 8.929355466
O 9.890103510 1.650522422 5.175681436
O 9.891571355 1.669450526 12.915298735
O 0.910170396 9.694664188 1.531866785
O 0.946565543 9.588049960 9.619517684
O 12.252938564 4.304088271 5.885068145
O 12.226137166 3.948024666 13.402536071
O 3.752620181 1.273327081 5.719427501
O 3.905217520 1.051819338 13.200516508
O 6.030224503 11.577095257 5.797652482
O 6.204145263 11.774942979 13.391950827
O 9.834938509 12.498497088 1.919577578
O 9.686661638 12.501153684 9.369695806
O 7.281510430 2.011537768 2.050885898
O 7.487983116 2.139032476 9.618941223
O 12.099986262 9.958209492 5.495792007
O 11.922569702 10.217971888 13.018999191
O 1.644861655 6.818607107 5.466652924
O 1.594402424 6.901123426 12.974653997
O 1.228439898 3.182934743 1.758758918
O 1.147665601 3.085290638 9.316764338
O 11.782901497 6.546054542 1.717725877
O 11.532506211 6.597320429 9.257780705
O 2.736896120 3.025112985 3.980668022
O 2.775604092 2.605117648 11.372143462
O 10.101073468 10.865847044 14.830060122
O 10.487471174 11.195133250 7.188696399
O 10.139639163 10.737703345 3.861201413
O 9.993201909 10.554213275 11.206002506
O 3.137756227 2.910401691 14.973507014
O 3.141758474 3.106113047 7.563221219
O 7.420204371 0.087441839 0.228427453
O 7.486293924 -0.163552296 7.793098331
O 13.552673130 6.986174768 14.834598400
O 13.246392543 7.172207474 7.299841931
O 5.559380460 13.880706029 4.020557948
O 7.309663964 0.297339268 11.523294536
O -0.416459784 6.957351672 3.807275832
O -0.287812000 6.749770914 11.078660454
O 0.522870264 12.312874827 1.873197087
O 0.520449820 12.213504117 9.467619589
O 3.560722464 9.501396659 1.848014020
O 3.620054107 9.442934735 9.466904093
O 12.493738034 1.663408983 5.807896410
O 12.508054219 1.295340558 13.162003451
O 9.568452177 4.259579232 5.589864073
O 9.590023775 4.288340446 13.260933889
O 4.388069052 8.339115769 4.838890487
Si 7.099087374 1.651571302 0.491550694
Si 9.285540406 12.120854708 0.444486647
Si 9.394617867 12.214182594 7.780157045
Si 3.731805402 1.756349024 4.176544067
Si 3.890638419 1.472303758 11.633515189
Si 11.859745282 6.956521749 3.287235026
Si 11.921400542 6.845977688 10.805856001
Si 1.397168571 3.642772408 3.309634480
Si 1.441600095 3.383223634 10.875373218
Si 1.309095333 6.641009542 14.555909805
Si 11.686345025 10.107528470 7.057558847
Si 11.544621002 10.159365186 14.600375269
Si 6.356390734 11.931355713 7.393923394
Si 6.264948202 12.107493569 14.954655200
Si 3.895162133 1.687111307 7.292171775
Si 4.039576745 1.576844247 14.735947734
Si 6.776443814 1.795578173 3.584925467
Si 6.922042863 1.799043171 11.203752636
Si 9.441728080 12.159812481 3.469627528
Si 9.311638415 11.972215871 10.846871338
Si 1.180601058 6.704399924 3.930652057
Si 1.284404091 6.506258981 11.422938437
Si 11.550560891 9.950008729 3.961832312
Si 11.479253647 9.907472043 11.492650432
Si 11.996137509 7.099328320 0.210513883
Si 11.713722424 7.176525244 7.739006520
Si 1.656478201 3.509450574 0.226780665
Si 1.910697418 13.140188174 1.988889118
Si 1.914335016 13.037622035 9.302995611
Si 4.260401587 10.956011839 2.052559625
Si 4.260495600 10.938829245 9.408975153
Si 11.174674558 0.758488643 5.601183477
Si 11.057318403 0.580844646 13.183382796
Si 8.840455948 2.855769701 13.275004126
Si -0.195052205 10.870537632 1.728521235
Si -0.155244530 10.746698119 9.355262666
Si 2.162603225 8.674847328 1.700730066
Si 2.226329782 8.628220609 9.347745614
Si 13.276084655 3.066234110 5.625127141
Si 13.271803258 2.732511434 13.134585254
Si 10.902898030 5.166696854 5.590100194
Si 11.034352439 5.018709026 13.135471186
Si 1.636333007 3.659347789 7.860001677
Si 8.822008538 2.816840534 5.614247034
Al 1.086677918 6.709869878 7.126823003
Al 6.221873407 12.311101187 4.127684413
Al 6.018852346 12.213519136 11.755713383
Al 7.097918002 1.519296253 7.876960395
Cu1 3.281101083 8.232377888 6.315473333
Mn2 5.475722565 9.797228425 5.188904716
H 8.130758581 2.871297448 9.571370227
H 7.355983850 11.047938156 10.136148235
C 6.994781319 8.740218126 5.949173885

H 7.151847557 7.833972749 5.349789041
H 7.878454855 9.390050131 5.914355273
H 6.733477341 8.480497017 6.984549667
H 4.705934213 7.470931152 4.534846813
End final coordinates

Cu-O-Ni-product-1
Final energy = -6695.9441046587 Ry
CELL_PARAMETERS (angstrom)
13.806335040 0.061323968 -0.011260816
-1.373381928 13.622086156 -0.030072411
-0.004802422 -0.001823208 15.021233550

ATOMIC_POSITIONS (angstrom)
O 3.138732091 0.598930117 3.194617288
O 2.249071092 13.801013653 10.664323596
O 5.176534393 11.102353041 3.300036681
O 4.894233961 11.329370785 10.781130010
O 7.891381729 11.518296199 7.619019894
O 7.704274984 11.750334300 0.503166651
O 10.755197240 0.015334868 6.899498068
O 9.449127756 13.463987563 14.485471906
O 8.249058976 2.539777969 6.999490876
O 7.996155324 2.689707836 14.608430527
O 5.187070449 2.271043889 3.627979689
O 5.330037652 2.172212494 11.104036822
O 12.657726735 11.015358055 0.370902601
O 12.978213509 10.665274754 7.856519983
O 2.206751004 7.735496122 0.385877975
O 2.095187183 8.054827698 7.813676626
O 1.528512100 5.338128656 3.373138372
O 1.631138661 4.999508091 11.175062994
O 0.048090065 3.222948211 4.113546471
O 0.131334626 2.858702465 11.651783179
O 11.120094952 5.890387017 4.136709472
O 11.099834629 5.823725544 11.670802199
O 11.440686644 8.666296928 0.094909728
O 11.112323660 8.754336896 7.683288208
O 10.160097791 13.366767281 4.312224430
O 9.520886209 13.236949520 11.843765644
O 7.624705054 2.892213459 4.436442349
O 7.720659819 2.954991616 11.963951703
O 5.485522499 1.984633683 15.044293369
O 5.435785589 1.847660378 7.586489608
O 3.387096686 0.394719847 0.543398460
O 3.150677830 0.526133418 8.078453366
O 5.130752236 11.339460806 0.624181535
O 5.434166189 10.889283668 8.214061759
O 7.869149095 12.166702057 3.652355649
O 7.613802592 11.739103370 10.743980117
O 0.668400931 3.007915392 6.683205227
O 0.511256406 2.804490278 14.292249784
O 10.716254521 6.310920279 6.759435019
O 11.059294975 6.195460105 14.303291478
O 11.185030457 8.465514975 3.496870886
O 11.342939274 8.427093257 11.177017378
O 12.679475524 10.642160229 3.020801312
O 12.516273400 10.765454819 10.484370697
O 2.067591256 7.897585043 3.049292009
O 2.167354755 7.467532473 10.418616557
O 1.595036944 5.272490739 7.754530343
O 1.635325421 5.171821718 14.909212517
O 3.113790934 12.213232136 2.111204489
O 3.121616345 12.022394002 8.878446560
O 9.922563461 1.728740054 5.064240525
O 9.847477197 1.744568519 12.938080220
O 0.889366567 9.732251800 1.527506361
O 0.937680226 9.643840451 9.617803629
O 12.224458636 4.295252601 5.946886683
O 12.168235798 4.012262343 13.300138734
O 3.689708318 1.313225716 5.647518262
O 3.897212007 1.128760441 13.115909709
O 5.973200745 11.583744438 5.715927523
O 6.271869282 11.842742232 13.301089670
O 9.850803436 12.497985103 1.865937616
O 9.660093419 12.573793396 9.278440670
O 7.260647636 2.029701046 2.001287226
O 7.475656834 2.152379723 9.507718897
O 12.096867609 9.983912697 5.485497787
O 11.918190990 10.249820104 12.997373242
O 1.722330817 7.007853758 5.470838680
O 1.615712049 6.965854205 12.940043283
O 1.194091641 3.299365472 1.744123404
O 1.109479902 3.161359612 9.268011539
O 11.882655909 6.609073598 1.739445706
O 11.541699636 6.637566945 9.241191819
O 2.722984787 3.098766790 3.936296836
O 2.767325592 2.662915107 11.284170830
O 10.063646709 10.884112823 14.765852272
O 10.474630766 11.237777366 7.139602451
O 10.120984662 10.781070612 3.857490051
O 9.994950334 10.685418147 11.182010748
O 3.073229511 2.966961427 14.899926100
O 3.148839941 3.127829893 7.548078278
O 7.406386736 0.153872722 0.126077867
O 7.451564394 -0.179764042 7.713195973
O 13.530176574 7.080146088 14.750006790
O 13.201665462 7.192873787 7.225083536
O 5.572860633 13.940690280 4.009716195
O 7.271536596 0.343789712 11.438807625
O -0.362773220 7.120202237 3.841632005
O -0.322128212 6.809588178 11.099511423
O 0.475680961 12.345382772 1.881771964
O 0.522378867 12.270951063 9.406976556
O 3.550588941 9.595136852 1.779007950
O 3.610115883 9.460634505 9.434848988
O 12.503056522 1.666589948 5.771511759
O 12.466991672 1.360181410 13.129028862
O 9.552510155 4.317506537 5.529816074
O 9.528025013 4.366825695 13.224915715
O 5.049835963 8.332160769 5.654788538
Si 7.031927100 1.695963537 0.442115069
Si 9.271148988 12.145376630 0.398178695
Si 9.355078422 12.248335768 7.695477983
Si 3.705037050 1.815965727 4.111934210
Si 3.885534816 1.532789057 11.544842916
Si 11.912727245 7.029410878 3.307544238
Si 11.887484844 6.941578119 10.791877343
Si 1.370775885 3.724392777 3.303008716
Si 1.412859866 3.428291881 10.830022402
Si 1.297404676 6.710048834 14.512489912
Si 11.668651376 10.146963740 7.041239794
Si 11.518084028 10.192659810 14.572909136
Si 6.318710803 11.913163260 7.295351149
Si 6.276249933 12.184370759 14.861334028
Si 3.888843232 1.710886470 7.217748842
Si 3.954528614 1.619430061 14.665778875
Si 6.761320292 1.837663903 3.542179202
Si 6.911806621 1.846389142 11.098285178
Si 9.447168338 12.203036163 3.422619235
Si 9.294034544 12.078834211 10.769295623
Si 1.228477477 6.824769894 3.932987308
Si 1.256738829 6.555507281 11.405509391
Si 11.524829138 9.986213654 3.960443965
Si 11.468118197 10.012709195 11.459797091
Si 11.989513892 7.143582318 0.213441640
Si 11.683414187 7.213460770 7.717976825
Si 1.604428120 3.578764815 0.198437217
Si 1.846342345 13.208293298 1.912292549
Si 1.929413547 13.072482320 9.241909918
Si 4.235010452 11.062539519 1.933607282
Si 4.259020501 10.955669268 9.362962559
Si 11.167811515 0.792719371 5.515807234
Si 11.014436611 0.645929870 13.135274286
Si 8.777935275 2.932511949 13.215287612
Si -0.229623232 10.898010961 1.721052856
Si -0.158664698 10.804778304 9.333679519
Si 2.166298795 8.742933158 1.667770218
Si 2.203108775 8.669288542 9.328318258
Si 13.263208734 3.084562003 5.614669477
Si 13.225067995 2.799481014 13.089130523
Si 10.909629624 5.190998349 5.591922679
Si 10.975470767 5.096533221 13.119375862
Si 1.635738993 3.679284857 7.804896873
Si 8.829530498 2.857999958 5.533495462
Al 1.059823673 6.764732089 7.107191887
Al 6.231901057 12.361469595 4.108086691
Al 6.023634713 12.264512588 11.668142664
Al 7.097895229 1.506613054 7.767734769
Cu1 3.342359233 8.051522067 6.279346632
Ni2 5.150985046 9.949106357 4.863904077
H 8.103877571 2.895216019 9.431337447
H 7.357608547 11.224982465 9.946799511
C 6.723307223 6.335967164 6.945640329
H 6.422687851 5.547005354 6.257748290
H 7.713295287 6.778212511 6.845334029
H 6.172484780 6.465034708 7.876563243
H 5.765883037 7.755231575 6.049752260
End final coordinates

Cu-O-Ni-product-2
Final energy = -6696.0558002332 Ry
13.793784197 0.062998219 -0.020623402
-1.370440557 13.618808314 -0.037031235
-0.014992104 -0.010569579 15.017798991

ATOMIC_POSITIONS (angstrom)
O 3.121302944 0.529536917 3.267912770
O 2.328410647 13.726952532 10.725379552
O 5.170135932 10.999160863 3.382372619
O 4.886354271 11.249516687 10.906000159
O 8.005594873 11.531033994 7.622741902
O 7.684482381 11.763281088 0.616914202
O 10.890090781 0.055854975 6.993257632
O 9.453442728 13.434460927 14.563388074
O 8.256356233 2.524733633 7.075607980
O 8.098306931 2.604813061 14.690027965
O 5.234945917 2.128488284 3.666269918
O 5.354311682 2.135660033 11.145008946
O 12.563891256 11.048871799 0.403037481
O 13.077587487 10.617468087 7.886043550
O 2.218292597 7.680408853 0.397290812
O 2.213168979 8.037822191 7.772949183
O 1.719068226 5.325017882 3.348791697
O 1.692733998 4.936697689 11.233923298
O 0.143243014 3.279251981 4.128112909
O 0.144619048 2.818408904 11.694632871
O 10.958439606 5.865049293 4.093408536
O 11.178845018 5.712521000 11.666864017
O 11.442812103 8.649798303 0.102950562
O 11.170728081 8.749778237 7.688541522
O 10.142126784 13.311855881 4.377380790
O 9.562411145 13.102627173 11.942717597
O 7.649946238 2.801217154 4.491757016
O 7.729811605 2.877689682 12.046783919
O 5.548965776 2.041256191 15.081745832
O 5.445247720 1.791972296 7.663414456
O 3.513490422 0.409336286 0.631069789
O 3.179659441 0.453297166 8.147099855
O 5.118098699 11.280370230 0.700612997
O 5.594538484 10.907441628 8.388279593
O 7.895863670 12.013806356 3.742358389
O 7.632207075 11.681742472 10.796204323
O 0.656455323 3.063719051 6.720710339
O 0.561030776 2.714528588 14.328573294
O 10.781884410 6.326940395 6.728173903
O 11.055808121 6.172401622 14.280086250
O 11.307658340 8.437139274 3.527668394
O 11.383696662 8.332381652 11.266936626
O 12.774743417 10.616775542 3.036967996
O 12.585343688 10.629858529 10.512542240
O 1.836063175 7.934274187 3.030067084
O 2.244555506 7.376099207 10.377881317
O 1.686608533 5.259391724 7.815511222
O 1.624248024 5.122737860 14.862504245
O 3.110679289 12.139617101 2.196177771
O 3.196952089 11.962810526 8.924605822
O 9.965010190 1.725275242 5.161797940
O 9.880227124 1.666626842 12.939668878
O 0.890883529 9.756772233 1.374389363
O 1.051698977 9.576303247 9.632058737
O 12.196978931 4.281857635 5.866570313
O 12.196365531 3.948005959 13.378800992
O 3.708023578 1.254461597 5.708355663
O 3.958131864 1.095130544 13.175595559
O 6.040294840 11.424480909 5.811435459
O 6.307993526 11.721910451 13.376093358
O 9.858857410 12.446844820 1.931521358
O 9.694506276 12.580330014 9.347840671
O 7.324023127 1.889918701 2.064214689

O 7.515869691 2.059120902 9.581898449
O 12.188024876 9.988313199 5.512568600
O 11.866680754 10.250094921 13.017887718
O 1.717395185 6.950554972 5.466999884
O 1.619011332 6.959272683 12.922447054
O 1.276068033 3.282925964 1.760771917
O 1.109919785 3.144337133 9.308261620
O 11.876334328 6.582808808 1.727672733
O 11.511724888 6.619616666 9.247164910
O 2.809232164 3.052739332 3.962829384
O 2.771282834 2.567590482 11.311739991
O 9.984968939 10.829612131 14.794731815
O 10.591399855 11.262525943 7.205991485
O 10.205126227 10.730538769 3.894505633
O 10.024175790 10.589072553 11.119316502
O 3.124551458 2.956534303 14.910081358
O 3.145730925 3.055059455 7.599693670
O 7.340499119 0.099207999 0.101664719
O 7.499351389 -0.200681775 7.682520345
O 13.519068267 7.046260486 14.730680012
O 13.267732031 7.174329043 7.318453882
O 5.647669367 13.828846577 4.103221546
O 7.263331586 0.268133391 11.525852425
O -0.405802226 6.798425086 3.930905861
O -0.261143498 6.739748299 11.026971607
O 0.490268745 12.356292244 1.819892445
O 0.597390614 12.191148056 9.504573510
O 3.522075252 9.532461683 1.819709012
O 3.723339542 9.394469442 9.425673114
O 12.579129207 1.659446086 5.698970880
O 12.490667948 1.290010030 13.168190119
O 9.513316243 4.310203915 5.606513112
O 9.566722045 4.294034580 13.240619346
O 4.407516458 8.288260838 4.667063132
Si 7.080431522 1.646565536 0.489144086
Si 9.255440233 12.117635829 0.467796122
Si 9.461394911 12.269385369 7.751393647
Si 3.740948334 1.734225415 4.164159671
Si 3.922593840 1.477972429 11.599758070
Si 11.882609758 6.940378685 3.310666157
Si 11.920851549 6.867466800 10.793690113
Si 1.483184504 3.714277960 3.312463811
Si 1.434277318 3.372909490 10.873565639
Si 1.299007471 6.671979793 14.493971626
Si 11.754303169 10.140608326 7.068740801
Si 11.457261338 10.174784525 14.590712098
Si 6.418653434 11.882728828 7.364890946
Si 6.246376327 12.110931006 14.926811019
Si 3.901532858 1.646367429 7.280591097
Si 4.027217712 1.617103129 14.717022135
Si 6.815741536 1.714851660 3.606627273
Si 6.928270380 1.774823018 11.170212278
Si 9.466329002 12.128404887 3.487422260
Si 9.318244600 12.007332534 10.808862163
Si 1.209680607 6.747582748 3.929707603
Si 1.309655215 6.501156204 11.388004541
Si 11.623644866 9.962953220 3.983572961
Si 11.488658379 9.931534439 11.476379551
Si 11.991002898 7.125779311 0.203971084
Si 11.723446610 7.200658425 7.731956725
Si 1.654916997 3.548263068 0.205370623
Si 1.886711110 13.170799742 1.951316431
Si 1.994175983 13.003027537 9.306394082
Si 4.240440032 10.982259309 2.031150973
Si 4.332378625 10.911887351 9.448139665
Si 11.223579555 0.788450280 5.562746615
Si 11.039929503 0.570564898 13.194910044
Si 8.822870506 2.855620614 13.265618346
Si -0.215903238 10.907335827 1.689460615
Si -0.069681609 10.722050686 9.385435230
Si 2.121434150 8.731303089 1.644584837
Si 2.312000284 8.606879503 9.318721398
Si 13.288295899 3.108102724 5.588170596
Si 13.245333911 2.732546317 13.130881036
Si 10.871318456 5.182760756 5.574363610
Si 11.010841619 5.029908335 13.134724025
Si 1.656255758 3.662444810 7.852495131
Si 8.837461172 2.828426084 5.607559002
Al 1.126600191 6.726769330 7.134316596
Al 6.240592178 12.217594136 4.153156915
Al 6.042505616 12.188219935 11.759547143
Al 7.112922912 1.474247334 7.823331339
Cu1 3.253532523 8.170952829 6.141008612
Ni2 5.393761150 9.697766842 5.245787845
H 8.168151129 2.782224019 9.515551337
H 7.356940686 11.135290719 10.027140307
C 6.474992355 8.610552407 6.413866003
H 6.586620213 7.608505586 5.981347807
H 7.435113712 9.141116883 6.445650145
H 5.992666480 8.581727688 7.398363004
H 4.888621852 7.448143304 4.536225423
End final coordinates

Cu-O-Ti-product-1
Final energy = -6694.1018005072 Ry
13.797219337 0.031839923 -0.005851243
-1.401561879 13.609961070 -0.014861434
0.000943116 0.015520121 15.005726224

ATOMIC_POSITIONS (angstrom)
O 3.134100526 0.637362502 3.197920481
O 2.228620116 13.834149640 10.665827740
O 5.090950053 11.102890699 3.381458810
O 4.946157598 11.361295623 10.706065957
O 7.843141521 11.514629448 7.613852937
O 7.676634478 11.699538041 0.482336216
O 10.751596126 0.011933524 6.902233005
O 9.409076061 13.448811263 14.474668143
O 8.269534303 2.497460430 7.002832781
O 8.017923950 2.691294186 14.601202495
O 5.190883424 2.298493204 3.624233832
O 5.344569490 2.204015445 11.114444821
O 12.637119348 11.018192783 0.379361894
O 12.924994871 10.719646654 7.849667515
O 2.227539686 7.733068336 0.403359831
O 2.122601996 8.066333221 7.804395251
O 1.484729084 5.343024088 3.254834641
O 1.606385316 5.015851503 11.162073939
O 0.061155788 3.224077832 4.107963558
O 0.139648754 2.855612768 11.632257594
O 11.099609362 5.842352753 4.125435488
O 11.081729720 5.789941377 11.643588856
O 11.445454000 8.655392847 0.131423208
O 11.116567843 8.749638300 7.712736121
O 10.126899404 13.330030253 4.334275117
O 9.524201170 13.242480839 11.832770369
O 7.632512829 2.905963068 4.453094406
O 7.734177163 3.000763814 11.971422150
O 5.505299235 1.984515066 15.034119113
O 5.433867326 1.848249816 7.592592561
O 3.378172974 0.409981380 0.548988456
O 3.131108621 0.563949251 8.068595699
O 5.117215748 11.335515422 0.692118710
O 5.326171741 10.858629498 8.107408001
O 7.843683472 12.111972574 3.672119996
O 7.609966598 11.716936044 10.824535208
O 0.687630879 3.025181371 6.681807014
O 0.546387453 2.817154599 14.263947244
O 10.762386309 6.320446212 6.746463156
O 11.087676014 6.223509484 14.263224053
O 11.151977256 8.423029683 3.506914641
O 11.306250024 8.401995061 11.181061968
O 12.662389597 10.584214462 3.021990473
O 12.486527334 10.739821828 10.484224267
O 2.025596468 7.909617368 3.068012078
O 2.132966314 7.489746926 10.418133462
O 1.567297684 5.289681375 7.826139094
O 1.636031321 5.184356310 14.926484471
O 3.083236477 12.235965712 2.143104964
O 3.091720121 12.056517762 8.880443972
O 9.913701706 1.701716572 5.048577028
O 9.854057418 1.748993885 12.911829557
O 0.881382158 9.741833464 1.497138255
O 0.892190363 9.647970765 9.566087593
O 12.251147965 4.295298537 5.951349503
O 12.197163467 4.020741081 13.293844189
O 3.697838777 1.343091823 5.643334433
O 3.916209186 1.134244423 13.109353042
O 5.909392393 11.692197765 5.751756434
O 6.158176271 11.876548289 13.314468329
O 9.800934758 12.482167271 1.873920159
O 9.627414827 12.533800439 9.285248362
O 7.271005416 2.082125796 2.006161799
O 7.474770972 2.228143640 9.514621957
O 12.063820650 9.963614840 5.489847228
O 11.911102464 10.228031804 12.998380041
O 1.712435771 6.871484601 5.449028347
O 1.638641652 6.964897235 12.946493126
O 1.214109074 3.232716068 1.734890679
O 1.144246387 3.131440876 9.268025913
O 11.855604516 6.572639032 1.738094159
O 11.573651910 6.621698452 9.236761595
O 2.731720096 3.143460355 3.937520273
O 2.787731765 2.708634600 11.310988821
O 10.054104843 10.875576642 14.762885171
O 10.410607034 11.201999212 7.123929810
O 10.103158376 10.747234640 3.844690386
O 9.975892467 10.665506579 11.203191595
O 3.105920648 3.000583174 14.872555237
O 3.163971341 3.169682194 7.536183129
O 7.434221662 0.152349843 0.190155251
O 7.438136214 -0.160648894 7.842841354
O 13.546829888 7.091516364 14.768366523
O 13.237654306 7.235873881 7.245771338
O 5.548240393 13.953368558 3.986619679
O 7.309150400 0.394000027 11.421885997
O -0.382748729 7.118960143 3.835344483
O -0.336786548 6.841823040 11.153927373
O 0.450824835 12.347946906 1.919147316
O 0.501283625 12.288305401 9.434620063
O 3.521492676 9.602614114 1.827984481
O 3.562955755 9.494576409 9.484511678
O 12.497474743 1.661042980 5.771808462
O 12.472352509 1.361332493 13.141994423
O 9.581683077 4.288579401 5.572596078
O 9.554984375 4.369289197 13.256856031
O 4.987854778 8.276143440 5.386628452
Si 7.044502495 1.700409913 0.459417422
Si 9.240929789 12.112583462 0.401996903
Si 9.319664828 12.227008109 7.702171323
Si 3.705797085 1.856609311 4.111699564
Si 3.897741288 1.566961038 11.546372158
Si 11.889816645 6.990590858 3.308050757
Si 11.876101509 6.924728137 10.792787433
Si 1.370600759 3.727712853 3.277261342
Si 1.423366370 3.439691264 10.824936497
Si 1.316944149 6.724139814 14.521070711
Si 11.635534962 10.140335907 7.043251146
Si 11.513350595 10.190821781 14.574484299
Si 6.287371296 11.956860052 7.356555545
Si 6.245341311 12.193389387 14.876713621
Si 3.886793849 1.744684122 7.213651038
Si 3.970355394 1.640859390 14.653436470
Si 6.764709003 1.878069590 3.539807591
Si 6.927595411 1.897581067 11.101476051
Si 9.426488585 12.169468069 3.433073564
Si 9.286906137 12.061883863 10.787924119
Si 1.207929006 6.793951358 3.928019502
Si 1.245197521 6.569760100 11.415870883
Si 11.501684181 9.941583948 3.962426920
Si 11.448873583 9.984504457 11.465624363
Si 11.994871881 7.130678332 0.225922592
Si 11.715532332 7.216662656 7.720133292
Si 1.621973949 3.568984268 0.200682564
Si 1.809011696 13.226472095 1.939627889
Si 1.895540498 13.103471388 9.249077781
Si 4.185146632 11.072946691 1.971097506
Si 4.218710653 10.973359893 9.339083593
Si 11.167413626 0.783061660 5.513847542
Si 11.021516763 0.653109614 13.119169405
Si 8.798227605 2.944438038 13.213593334
Si -0.241117752 10.897846956 1.723372241
Si -0.189431756 10.829368537 9.321176591
Si 2.143013049 8.737535217 1.685767564
Si 2.172073503 8.682251977 9.322974429
Si 13.273717967 3.074251412 5.618033391
Si 13.238283067 2.793936424 13.081395099
Si 10.926153026 5.179477108 5.601595981
Si 10.996641295 5.096777280 13.109807379
Si 1.644441951 3.699429463 7.813678814

Si 8.841825852 2.845157436 5.543877979
Al 1.091105435 6.763180871 7.083382133
Al 6.219638204 12.391842779 4.092280608
Al 6.001755981 12.305831828 11.671145676
Al 7.093733565 1.535722496 7.806777173
Cu1 3.422012928 8.240795543 6.412504477
Ti2 4.858075689 10.085954425 5.131628428
H 8.084132569 2.985215871 9.429352114
H 7.354571047 11.014679426 10.192070575
C 6.921231837 6.701098835 6.784180305
H 6.923339039 5.861454095 6.090879272
H 7.760425449 7.394636008 6.778846389
H 6.260031124 6.674187514 7.649010185
H 5.725147708 7.613215842 5.772291673
End final coordinates

Cu-O-Ti-product-2
Final energy = -6694.2866508434 Ry
13.797219337 0.031839923 -0.005851243
-1.401561879 13.609961070 -0.014861434
0.000943116 0.015520121 15.005726224

ATOMIC_POSITIONS (angstrom)
O 3.221437145 0.557441846 3.260144787
O 2.236787720 13.742914736 10.739365817
O 5.239633745 10.974933350 3.450195466
O 4.902103808 11.302774702 10.871042894
O 7.918410332 11.457473310 7.728696888
O 7.763862930 11.627489817 0.563541879
O 10.774923997 -0.025619767 7.008576589
O 9.424543008 13.466709255 14.582260977
O 8.306053345 2.518228355 7.089147357
O 8.081101630 2.587687147 14.687965840
O 5.215243599 2.290502796 3.725743876
O 5.319517412 2.141306366 11.181683666
O 12.789148646 10.963474675 0.382775470
O 13.028438132 10.616831424 7.847142407
O 2.228624018 7.670058150 0.425561873
O 2.187322201 8.012442163 7.860897747
O 1.387528579 5.237499651 3.324958132
O 1.677647785 4.949271434 11.200292042
O 0.056461611 3.064298705 4.146245968
O 0.085318476 2.874978190 11.647203694
O 11.188686665 5.807619480 4.166875888
O 11.116665459 5.688804167 11.672385512
O 11.523275377 8.644509410 0.099407139
O 11.143350874 8.715986957 7.723984428
O 10.172611662 13.300105932 4.440182705
O 9.540726083 13.122252971 11.961098633
O 7.675772475 2.845769543 4.523384014
O 7.704708180 2.927203032 12.064216003
O 5.559963768 1.900041177 15.065966647
O 5.484381046 1.778440458 7.605503804
O 3.490909838 0.273580551 0.627018321
O 3.189181193 0.499117781 8.134847616
O 5.197234351 11.216245538 0.765527754
O 5.455450378 10.859480896 8.308379329
O 7.854185964 12.174976815 3.738041763
O 7.617254696 11.677916425 10.854870456
O 0.765250667 3.000074605 6.699628538
O 0.602028295 2.759657632 14.250538146
O 10.819924280 6.277183221 6.778786252
O 11.065673047 6.216179066 14.256209203
O 11.109538554 8.399163558 3.563486446
O 11.365966231 8.324609465 11.312158596
O 12.599977587 10.563149174 3.015892391
O 12.488185727 10.637565456 10.453828463
O 2.151922021 7.741732522 3.093862208
O 2.178846433 7.429666248 10.474228026
O 1.640657226 5.243593261 7.870243564
O 1.709295738 5.104338315 14.964695190
O 3.203415892 12.136733162 2.271525750
O 3.137258467 11.987232539 8.951271238
O 9.957024816 1.668820413 5.153725493
O 9.870053901 1.690706393 12.922706209
O 0.890062069 9.608851921 1.660676061
O 0.959762583 9.593724799 9.631407320
O 12.311171027 4.251793418 5.984197415
O 12.197176788 3.971168941 13.410278285
O 3.672531026 1.318163497 5.704648753
O 3.915148817 1.052303974 13.182513611
O 6.016380916 11.558456914 5.833854267
O 6.254412428 11.825689472 13.402930096
O 9.852806883 12.484369583 1.966732667
O 9.687039916 12.500618230 9.387389107
O 7.273468350 2.006528398 2.091894456
O 7.466611237 2.163234770 9.593332831
O 12.079302911 9.947156133 5.507286618
O 11.973024718 10.265351221 13.005487595
O 1.600966500 6.833422144 5.472779769
O 1.601900908 6.893218104 12.986187452
O 1.162234275 3.164189719 1.753535790
O 1.153535704 3.086132157 9.303777713
O 11.733527649 6.567205735 1.743967345
O 11.512312655 6.608858605 9.291730396
O 2.729789579 3.068295350 3.925321512
O 2.734035050 2.585150130 11.386872954
O 10.180654471 10.915917676 14.838529141
O 10.504269654 11.201330852 7.216783172
O 10.067393233 10.725025660 3.922297907
O 9.990076531 10.574967890 11.244469701
O 3.133540677 2.876617110 14.993585354
O 3.219584651 3.110398761 7.633879203
O 7.475090018 0.056515185 0.315997856
O 7.528730387 -0.190773279 7.832339695
O 13.552807398 6.950461545 14.862315996
O 13.279309346 7.186223656 7.384938647
O 5.512932107 13.899555325 4.105159683
O 7.286580807 0.325329321 11.500745111
O -0.365809266 7.184887756 3.691923095
O -0.306283958 6.733177206 11.121335077
O 0.565941396 12.231287344 2.026234350
O 0.529821273 12.217637543 9.463655375
O 3.559903339 9.516483492 1.879180251
O 3.632512998 9.430253985 9.536090034
O 12.530266857 1.610294109 5.922155787
O 12.487561237 1.317276248 13.171052112
O 9.632247534 4.261604058 5.595404537
O 9.555261487 4.302439463 13.302009647
O 4.114341517 8.463673225 4.716372904
Si 7.085852690 1.610773675 0.543315888
Si 9.310302033 12.108026688 0.489989852
Si 9.381793860 12.188702178 7.803898933
Si 3.728591955 1.808339488 4.167668686
Si 3.881980175 1.479625775 11.618540054
Si 11.867321714 6.988265027 3.304125466
Si 11.891304001 6.852990269 10.840453203
Si 1.336893168 3.616563987 3.305737280
Si 1.419507860 3.381125461 10.866053835
Si 1.322927352 6.631854224 14.563416143
Si 11.690292589 10.104323968 7.074237586
Si 11.612092663 10.196286722 14.589057022
Si 6.360097166 11.896141006 7.424869800
Si 6.319391670 12.106828033 14.973256812
Si 3.926881857 1.685452927 7.273367001
Si 4.017731528 1.534902186 14.730831948
Si 6.777600333 1.823274230 3.633714446
Si 6.903971474 1.827705097 11.178899252
Si 9.437072764 12.176666784 3.517482954
Si 9.303727827 11.986518802 10.866631639
Si 1.163119778 6.713074895 3.940191986
Si 1.270849735 6.494957439 11.439903245
Si 11.471741467 9.922871180 3.998023662
Si 11.480742415 9.926258447 11.498197436
Si 11.983092308 7.094556534 0.235561854
Si 11.734417110 7.182825275 7.778215531
Si 1.649744168 3.484587751 0.238089192
Si 1.923982024 13.114160965 2.033084636
Si 1.932807345 13.027593429 9.308036610
Si 4.295630168 10.959734047 2.074584670
Si 4.270424971 10.925666668 9.453010514
Si 11.200339710 0.742617554 5.626437687
Si 11.037165018 0.602779549 13.186051197
Si 8.806864830 2.868780763 13.274290142
Si -0.190518862 10.823470781 1.790065538
Si -0.138762225 10.748980308 9.340848382
Si 2.188556686 8.649218398 1.723554202
Si 2.238274927 8.626416675 9.383381074
Si 13.313361284 3.004257847 5.681663293
Si 13.239839910 2.758257560 13.118652527
Si 10.986442661 5.137777270 5.636043796
Si 10.995503022 5.035910051 13.154969184
Si 1.698443643 3.652368952 7.864183082
Si 8.881699269 2.819977757 5.617975754
Al 1.124807187 6.713949098 7.155424101
Al 6.218091280 12.347758969 4.206063288
Al 6.023507099 12.238655414 11.765289651
Al 7.146155780 1.494173922 7.851525168
Cu1 3.265020708 8.378449693 6.352783302
Ti2 5.454623478 9.697360078 5.101468055
H 8.077432797 2.921898160 9.532686865
H 7.348450822 11.112109427 10.098421380
C 7.157341224 8.600634794 5.494807905
H 7.152809164 7.611013491 5.016084330
H 8.095054617 9.126309957 5.263145892
H 7.093439227 8.461031768 6.594361910
H 3.449771160 8.168815112 4.029267600
End final coordinates

Cu-O-V-product-1
Final energy = -6724.4080483871 Ry
13.897745499 -0.012636249 -0.007300503
-1.455514333 13.642598006 -0.026166584
-0.000430949 0.003140602 15.103261880

ATOMIC_POSITIONS (angstrom)
O 3.188495929 0.620380502 3.146707632
O 2.117804166 13.927169650 10.664119814
O 5.103118873 11.134954878 3.316727308
O 4.918108545 11.342393658 10.755522129
O 7.785381545 11.551164457 7.581956935
O 7.672911038 11.763779983 0.391764651
O 10.839207794 -0.034815499 6.909777229
O 9.510622691 13.404721428 14.492429116
O 8.230209687 2.538854877 6.973766988
O 8.002912011 2.661269914 14.613395438
O 5.232436873 2.275618035 3.673330754
O 5.370954773 2.179288769 11.182018189
O 12.670871512 10.969326765 0.366050354
O 12.873459431 10.745066478 7.896384170
O 2.160100035 7.766526704 0.363705490
O 2.106809053 8.057643309 7.841909267
O 1.483281241 5.343942522 3.284422763
O 1.563697217 5.071075260 11.188559902
O 0.094203782 3.193570338 4.116611977
O 0.191772475 2.852916406 11.690607869
O 11.129156086 5.873993474 4.135201376
O 11.077160775 5.818129885 11.692673004
O 11.480454084 8.617881912 0.011443421
O 11.150990004 8.710754459 7.657943637
O 10.105446154 13.344286334 4.309029789
O 9.526481595 13.244144742 11.841347234
O 7.708772912 2.896542708 4.386526423
O 7.806936277 2.932683066 11.967324271
O 5.485823559 1.979106943 15.033475589
O 5.408109843 1.864699359 7.550777969
O 3.395807484 0.396330244 0.492097937
O 3.133034294 0.540859471 8.056613134
O 5.115025055 11.330298633 0.637680961
O 5.292661918 10.924928352 8.151571320
O 7.843534602 12.080832731 3.666228337
O 7.601686331 11.695660396 10.875826720
O 0.613339411 3.022317581 6.724831580
O 0.469733285 2.852576561 14.339271403
O 10.835986986 6.249648967 6.781182237
O 11.128251250 6.140710039 14.331352127
O 11.227335249 8.447615924 3.527777997
O 11.358430741 8.423310734 11.245348906
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O 12.557189222 10.742996014 10.551450851
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O 1.561548384 5.296202182 7.784758803
O 1.624358878 5.193174938 14.973945091
O 3.073574476 12.255644772 2.067368556
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O 12.278097223 4.018422540 13.239313660
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O 12.074057427 10.044664743 5.493328983
O 11.885827224 10.290993971 13.056352504
O 1.612628344 6.931014876 5.436659713
O 1.521070376 6.991369954 13.009224439
O 1.172403173 3.276534001 1.708858198
O 1.133370729 3.180730383 9.299306576
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O 2.760449456 3.129788255 3.859858607
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O 10.063125244 10.829902081 14.900370518
O 10.344171893 11.142382274 7.157822426
O 10.142654217 10.767700363 3.782668633
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O 3.116580077 3.147744100 7.524105274
O 7.415739303 0.149264066 0.180479265
O 7.440768131 -0.144967687 7.765828376
O 13.579421028 7.003654841 14.894612570
O 13.301593678 7.191014393 7.315715217
O 5.585822397 13.979518777 3.896174397
O 7.332025930 0.347313160 11.391689318
O -0.424997852 7.116144714 3.738160596
O -0.418747054 6.854173143 11.180319186
O 0.428876203 12.368587524 1.856313833
O 0.451835674 12.315797712 9.434116483
O 3.483606737 9.624522286 1.790607076
O 3.488349261 9.547841455 9.495464974
O 12.541005080 1.637091512 5.749423285
O 12.518939855 1.361199098 13.138290650
O 9.645197093 4.260697575 5.558357665
O 9.620196646 4.288532286 13.278468997
O 4.976934763 8.210595644 5.455291070
Si 7.020264598 1.706811895 0.395671012
Si 9.252323886 12.122765874 0.359526023
Si 9.277471809 12.216510156 7.698603561
Si 3.722578127 1.839075461 4.083847858
Si 3.885410725 1.605436121 11.573764179
Si 11.921813885 7.000334705 3.285088111
Si 11.892197674 6.937068703 10.836665552
Si 1.375947927 3.729092077 3.260758847
Si 1.433370328 3.487468404 10.854704422
Si 1.249824498 6.729516711 14.593171043
Si 11.620348198 10.145104145 7.048301127
Si 11.525988790 10.170720679 14.640720378
Si 6.222200769 11.983684748 7.311917688
Si 6.213863360 12.219226379 14.924403102
Si 3.855954848 1.732686437 7.189985968
Si 3.938724407 1.635037711 14.690037468
Si 6.804921310 1.872482441 3.495983450
Si 6.949376963 1.856937461 11.107745991
Si 9.419888839 12.178200080 3.401373895
Si 9.276871608 12.061292621 10.799252734
Si 1.165672789 6.812046673 3.904589997
Si 1.164940964 6.613748246 11.464054547
Si 11.547913409 9.981838943 3.951889787
Si 11.480307284 10.012410888 11.512523931
Si 12.011306309 7.094294430 0.189054650
Si 11.765914499 7.187959912 7.742866644
Si 1.578368160 3.590594516 0.168319877
Si 1.794006014 13.240974178 1.874274457
Si 1.836568302 13.150536193 9.260776762
Si 4.179834541 11.086583201 1.925114926
Si 4.182043131 11.016053539 9.374139548
Si 11.213524083 0.748316571 5.518214243
Si 11.092030012 0.604917939 13.154984932
Si 8.832772206 2.878309314 13.245375895
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Si -0.272273761 10.872569587 9.337864526
Si 2.101406013 8.758317501 1.661950940
Si 2.104414059 8.720849857 9.346763297
Si 13.348951523 3.032446912 5.604244260
Si 13.316210443 2.777779975 13.102737429
Si 10.992102052 5.154100245 5.588187790
Si 11.039690591 5.061536702 13.132093086
Si 1.609437367 3.704877798 7.818887707
Si 8.872745863 2.829455007 5.528033797
Al 1.054628604 6.782625415 7.082381909
Al 6.212131615 12.399607599 4.062059542
Al 5.979013244 12.303501582 11.699728951
Al 7.068878962 1.543004602 7.770483259
Cu1 3.495957101 8.208420169 6.568315296
V2 4.963027483 10.016971197 5.012988564
H 8.091495602 2.936012308 9.428969193
H 7.331371811 11.027717507 10.212050912
C 6.921231837 6.701098835 6.784180305
H 6.923339039 5.861454095 6.090879272
H 7.760425449 7.394636008 6.778846389
H 6.260031124 6.674187514 7.649010185
H 5.727729516 7.614829676 5.774979298
End final coordinates

Cu-O-V-product-2
Final energy = -6724.5642236969 Ry
13.897745499 -0.012636249 -0.007300503
-1.455514333 13.642598006 -0.026166584
-0.000430949 0.003140602 15.103261880

ATOMIC_POSITIONS (angstrom)
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O 2.118866870 13.868494625 10.730099129
O 5.213296743 11.007105921 3.376394909
O 4.961378735 11.270114368 10.809580983
O 7.819134705 11.501667946 7.693490038
O 7.741713609 11.685566839 0.425162515
O 10.849872621 -0.078298474 6.999450817
O 9.565350290 13.372554364 14.568559066
O 8.275075112 2.506233445 7.038879955
O 8.073226240 2.564983215 14.683295797
O 5.258819708 2.260574330 3.722822498
O 5.400893513 2.093122741 11.249315489
O 12.784451320 10.909193209 0.399418472
O 12.909073604 10.681225496 7.930449605
O 2.172526769 7.673410516 0.425321527
O 2.122969455 7.948858030 7.929298247
O 1.490301154 5.257537500 3.346948261
O 1.638315877 5.023740557 11.221976359
O 0.108456194 3.113769755 4.188676336
O 0.217883089 2.841855444 11.746714140
O 11.236392563 5.811723430 4.205785290
O 11.124962500 5.714315868 11.726287584
O 11.569500745 8.577951510 0.032523783
O 11.154897538 8.670530837 7.691189455
O 10.135102853 13.268425174 4.403844873
O 9.578730462 13.147086000 11.926499271
O 7.741435939 2.834634888 4.447340032
O 7.828881839 2.857934485 12.043129280
O 5.548230409 1.897880834 15.072783727
O 5.450897300 1.814786927 7.617854048
O 3.501504638 0.272675539 0.564649809
O 3.176038343 0.487616884 8.116434090
O 5.181420637 11.231905336 0.702990010
O 5.315961849 10.884638256 8.197987923
O 7.853911409 12.071714159 3.715726091
O 7.645010179 11.622201032 10.940021251
O 0.651928241 2.903692599 6.794285611
O 0.525116592 2.763445707 14.387601738
O 10.860500378 6.192293349 6.835763000
O 11.139933322 6.116239175 14.337743322
O 11.229931757 8.391775729 3.597276987
O 11.418053633 8.344552438 11.366552502
O 12.712445025 10.557919393 3.046932285
O 12.581879316 10.660700233 10.578113301
O 2.118234386 7.804163219 3.107504079
O 2.080773415 7.541919687 10.585788688
O 1.547864649 5.203289733 7.823232649
O 1.690913188 5.094619207 15.030144420
O 3.159601787 12.145641612 2.175513881
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O 12.317834949 3.959514609 13.345380820
O 3.700409296 1.274328415 5.678593823
O 3.875894636 1.076947248 13.206651241
O 5.952831399 11.627441906 5.768868044
O 6.150451821 11.871988304 13.418560205
O 9.793267251 12.498484532 1.913854983
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O 7.254827311 2.062707975 2.001883962
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O 12.089609601 10.008037476 5.532093124
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O 1.495053299 6.875155395 5.479690668
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O 1.176162921 3.196044330 1.769969085
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O 11.689892381 6.549933042 1.745183494
O 11.535950322 6.632213186 9.340515432
O 2.769817376 3.041383228 3.915429140
O 2.870396122 2.742754340 11.409641455
O 10.160387798 10.803827636 14.984395935
O 10.376461039 11.111079704 7.204929293
O 10.134783313 10.708374100 3.830691670
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O 7.476120322 -0.186071799 7.802111618
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O 0.518201566 12.271234214 1.949606848
O 0.474246145 12.258435066 9.473220892
O 3.538068791 9.525376237 1.833349722
O 3.523760396 9.488684104 9.531420257
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O 9.658093446 4.212754044 13.334618443
O 4.083380204 8.613728660 4.860010242
Si 7.074760045 1.624223107 0.462212732
Si 9.313315855 12.081255655 0.425297093
Si 9.311752982 12.168315251 7.781550175
Si 3.766212063 1.777184741 4.143192304
Si 3.912392980 1.532902511 11.648532579
Si 11.923542324 6.956204948 3.300122033
Si 11.917412538 6.864948929 10.890834293
Si 1.385200573 3.638515575 3.323383719
Si 1.484614302 3.435755906 10.918068538
Si 1.261175690 6.620956326 14.666828203
Si 11.641792702 10.100788782 7.090334103
Si 11.611652956 10.137544398 14.686039059
Si 6.264413866 11.937587128 7.379222771
Si 6.268060476 12.137998513 14.989487549
Si 3.902927106 1.676967728 7.249074175
Si 3.997836370 1.533252149 14.763626972
Si 6.824229886 1.826948910 3.556997260
Si 6.981784816 1.783867850 11.170212163
Si 9.432762604 12.137534108 3.466540727
Si 9.321548751 11.979327269 10.870855490
Si 1.154560504 6.731782164 3.925724833
Si 1.192758205 6.549938202 11.515589679
Si 11.547704871 9.932678748 3.997919306
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Si 11.761366851 7.147916226 7.805114455
Si 1.622184767 3.492104667 0.235957824
Si 1.888307502 13.138347089 1.958150731
Si 1.861703817 13.094593852 9.320317455
Si 4.266557502 10.976287152 2.006796968
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Si 11.141564247 0.541429159 13.210773679
Si 8.875815731 2.799173070 13.302397190

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Si -0.239295852 10.809652360 9.373630569
Si 2.150102856 8.670405909 1.713312273
Si 2.140477646 8.657963069 9.408931927
Si 13.378302133 2.959991046 5.685193673
Si 13.356789249 2.723178419 13.162144776
Si 11.051942778 5.093676334 5.654156313
Si 11.073555967 4.990994083 13.181068474
Si 1.642551994 3.616292295 7.875682006
Si 8.908471342 2.774688246 5.584209804
Al 1.043425019 6.701115632 7.162437432
Al 6.213366252 12.361088992 4.115045352
Al 6.018866230 12.232055558 11.757394437
Al 7.113911763 1.503746152 7.828476116
Cu1 3.187837380 8.354441312 6.436282582
V2 5.500384298 9.806727021 5.053170661
H 8.099616900 2.905262124 9.503099618
H 7.375338430 10.960081096 10.269984966
C 7.153932867 8.701277201 5.382743273
H 7.236686837 7.851195376 4.689171738
H 8.052224383 9.333907825 5.303359762
H 7.046727326 8.329062221 6.419597171
H 3.491987348 8.388223724 4.095445302
End final coordinates

Cu-O-Ag-product-1
Final energy = -6865.5243975287 Ry
CELL_PARAMETERS (angstrom)
13.801609146 0.028376461 -0.004955632
-1.405466785 13.632444982 -0.034248132
0.001903557 -0.005789397 15.025718342

ATOMIC_POSITIONS (angstrom)
O 3.122602483 0.576569694 3.268736003
O 2.179510646 13.830275109 10.725829330
O 5.191554052 11.109545985 3.222637785
O 4.855868768 11.353069836 10.834622545
O 7.878273584 11.655812288 7.755543038
O 7.668448630 11.822608296 0.538194319
O 10.858316876 0.080256381 6.995751892
O 9.465585398 13.508988640 14.561348582
O 8.238275608 2.621717599 7.030369471
O 8.038966960 2.750176279 14.656766502
O 5.181024528 2.251665058 3.650612512
O 5.333927758 2.162638599 11.167920903
O 12.606446366 11.014876861 0.413811269
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O 2.174364532 7.757530088 0.412591670
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O 1.658499063 5.057499012 11.189633778
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O 11.164243534 5.887652389 4.171486728
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O 0.633443415 2.966369044 6.729397291
O 0.531728455 2.804109407 14.347451847
O 10.657522593 6.294693307 6.781854376
O 11.041382420 6.212617345 14.317030964
O 11.250904704 8.457703720 3.537206854
O 11.340785125 8.418633173 11.204162566
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O 12.542901434 10.748090188 10.558653945
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O 2.214641848 7.530129276 10.458295527
O 1.502625822 5.286410242 7.709458183
O 1.581997009 5.211013441 14.909217981
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O 1.092333807 3.218769042 9.303163197
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O 2.730338842 3.094301741 3.972272085
O 2.792281988 2.717529237 11.283067282
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O 7.309928315 0.353535634 11.404999214
O -0.303486956 7.095309363 3.816517932
O -0.289158145 6.872224928 11.047792617
O 0.466746022 12.382690689 1.855532429
O 0.502330419 12.297251797 9.406367663
O 3.531707396 9.660031717 1.703980836
O 3.610143723 9.514955895 9.398028810
O 12.490796965 1.692692764 5.650688714
O 12.477133093 1.374215671 13.148586275
O 9.575606493 4.284778808 5.478788282
O 9.564931962 4.367215420 13.208377110
O 5.132670768 8.212547187 6.346570181
Si 7.039518729 1.747611816 0.438654881
Si 9.244968875 12.179394317 0.442742928
Si 9.371493506 12.317227746 7.775107982
Si 3.705260663 1.805964740 4.157481866
Si 3.871172609 1.558416804 11.589982952
Si 11.949397984 7.015676616 3.324301434
Si 11.906781140 6.948913586 10.795436779
Si 1.422485924 3.794751267 3.336550180
Si 1.430723314 3.483700374 10.858785001
Si 1.264434534 6.755514131 14.524483539
Si 11.610858096 10.160048332 7.076586742
Si 11.469428535 10.195461602 14.620646589
Si 6.308377955 12.040101595 7.345010428
Si 6.273183561 12.248801773 14.841956652
Si 3.886138793 1.769027823 7.264018417
Si 3.962911188 1.690454896 14.704117443
Si 6.755031226 1.814997780 3.540079014
Si 6.918441473 1.859867024 11.134018760
Si 9.401391407 12.158339720 3.456507250
Si 9.304685925 12.087554074 10.815092020
Si 1.291856910 6.874172341 3.926443818
Si 1.277140224 6.612735155 11.413611660
Si 11.524374954 9.994372890 3.992669087
Si 11.461887283 10.003914437 11.503917996
Si 11.954592528 7.162541742 0.235451208
Si 11.624157135 7.225764570 7.719802840
Si 1.601919488 3.629131096 0.228517825
Si 1.832018065 13.251183038 1.939608761
Si 1.904009918 13.118061147 9.284821460
Si 4.233019824 11.122435286 1.890368420
Si 4.255395147 11.016956022 9.388973961
Si 11.167435763 0.775717239 5.544288380
Si 11.031695307 0.646219509 13.191890361
Si 8.803479004 2.940455082 13.247350045
Si -0.251341366 10.940085699 1.739130968
Si -0.169746509 10.826937815 9.361730871
Si 2.156813087 8.801219562 1.663840699
Si 2.219473080 8.704087348 9.335210077
Si 13.257908350 3.107996216 5.632578917
Si 13.246231513 2.805006460 13.141898655
Si 10.911181454 5.180935757 5.614408007
Si 11.008327886 5.101705760 13.140608205
Si 1.593448635 3.696218846 7.820793180
Si 8.821694487 2.839134004 5.546519292
Al 0.987771917 6.805953248 7.122389847
Al 6.189889836 12.333916520 4.131547934
Al 6.043238462 12.284227215 11.649569473
Al 7.089324173 1.598105325 7.823661971
Cu1 3.363440039 7.785188160 6.300880196
Ag2 5.240112441 9.560115866 4.738560228
H 8.103269689 2.981697662 9.514952167
H 7.400730543 11.415789952 9.812648055
C 7.039395363 5.930623617 6.914527997
H 6.825464278 5.343108876 6.024020883
H 7.900998928 6.596809702 6.929260510
H 6.498469431 5.722479368 7.835814966
H 5.774911871 7.463115469 6.410713135
End final coordinates

Cu-O-Ag-product-2
Final energy = -6865.5870593901 Ry
CELL_PARAMETERS (angstrom)
13.801609146 0.028376461 -0.004955632
-1.405466785 13.632444982 -0.034248132
0.001903557 -0.005789397 15.025718342

ATOMIC_POSITIONS (angstrom)
O 3.166678788 0.501574035 3.294138108
O 2.151331831 13.779989346 10.728193070
O 5.150199503 11.028544008 3.383528668
O 4.964005012 11.279773565 10.745959361
O 7.854095248 11.597704212 7.928987585
O 7.740005608 11.677583399 0.477455604
O 10.787855997 -0.027855990 7.000498672
O 9.451255248 13.477265785 14.558519567
O 8.202874939 2.603474948 7.066628484
O 8.116116418 2.590061795 14.692388027
O 5.181963849 2.229876506 3.651836966
O 5.309621413 2.103801480 11.195509599
O 12.705842537 10.969555101 0.362323528
O 12.884721654 10.668084970 7.845531168
O 2.184934032 7.739492655 0.371263765
O 2.208631489 7.913745198 7.789005160
O 1.519724463 5.261901199 3.356682076
O 1.664326836 4.996605732 11.110828942
O 0.051416994 3.145864060 4.106985281
O 0.104454182 2.916344700 11.671820756
O 11.092945768 5.840102928 4.129942148
O 11.176983587 5.677389682 11.668004873
O 11.449375642 8.642038101 0.110149787
O 11.063622533 8.698586418 7.685929864
O 10.045285762 13.272190920 4.383898892
O 9.636942402 13.148338821 11.946757812
O 7.607827198 2.839554481 4.475784646
O 7.701285446 2.876248092 12.077004152
O 5.571422484 1.916342930 14.991251611
O 5.404056147 1.862478337 7.707596167
O 3.444214104 0.416246307 0.647514885
O 3.131048355 0.509353259 8.140308665
O 5.163474353 11.268984257 0.689570272
O 5.348964449 10.943306565 8.129399347
O 7.798569331 12.106970428 3.523937500
O 7.682405360 11.772441570 10.760825909
O 0.639823425 2.911981346 6.697290905
O 0.631769183 2.778564129 14.273345996
O 10.745180186 6.252272294 6.758105979
O 11.037461378 6.193562407 14.272466002
O 11.168796428 8.412719388 3.498664004
O 11.310441263 8.304934840 11.256728826
O 12.609589221 10.623098872 3.013541824

O 12.551727331 10.573717544 10.480400818
O 2.063621891 7.811565119 3.039293535
O 2.186216793 7.494222591 10.439572652
O 1.484172485 5.202623646 7.775482059
O 1.667345407 5.155225594 14.962885390
O 3.133763998 12.171405638 2.126227607
O 3.092272865 12.032193509 8.957953245
O 9.828169930 1.608352278 5.170405855
O 9.893139560 1.668033043 12.913051093
O 0.865344851 9.684069558 1.603728011
O 0.951775892 9.588316134 9.427193951
O 12.266206200 4.267705814 5.927541594
O 12.218131786 3.978507490 13.442948204
O 3.733241582 1.285353572 5.712702534
O 3.832334316 1.088435149 13.184123930
O 6.251320628 11.654482952 5.773083440
O 6.252871747 11.779489357 13.327589386
O 9.873357853 12.457106287 1.885875228
O 9.807848569 12.543989777 9.371387253
O 7.250810525 1.965028424 2.035173603
O 7.456745321 2.162543346 9.606863427
O 12.014445927 9.961837918 5.485921512
O 11.966071926 10.180145005 13.003847610
O 1.667819988 6.893283361 5.460835990
O 1.605727661 6.902028526 12.943968805
O 1.226848263 3.221640369 1.746524999
O 1.091190373 3.082571409 9.291619552
O 11.825216599 6.557585308 1.724683043
O 11.520632220 6.588715781 9.253282569
O 2.717332068 3.024779563 3.972377427
O 2.747135464 2.643071941 11.333465231
O 10.122850558 10.891029540 14.752637302
O 10.343308022 11.141222197 7.157933917
O 10.039824480 10.704416810 3.849920384
O 10.023812168 10.600649142 11.213896632
O 3.173931854 2.980073202 14.967269576
O 3.111495668 3.110296034 7.564783685
O 7.460138498 0.070959082 0.175942621
O 7.452421054 -0.114466696 7.770622635
O 13.522378349 6.998517876 14.768007270
O 13.206188382 7.218002528 7.277519436
O 5.519584019 13.894549656 4.044053156
O 7.269705339 0.278504404 11.475537034
O -0.377941967 7.066910205 3.800215922
O -0.298090481 6.803905681 11.060437141
O 0.492790191 12.314160150 1.904543794
O 0.486309691 12.218326266 9.426711604
O 3.537216141 9.554692019 1.799074744
O 3.627635565 9.450248551 9.386704157
O 12.436402306 1.622098604 5.753615640
O 12.521567013 1.336558639 13.198155031
O 9.590141565 4.236023326 5.527696398
O 9.574043284 4.281898164 13.245141434
O 4.793625816 7.818699099 5.028650948
Si 7.085072272 1.615011047 0.471540935
Si 9.293568987 12.121053853 0.411560892
Si 9.371484278 12.238334616 7.820159702
Si 3.715897293 1.755688219 4.166633490
Si 3.844805859 1.494878407 11.614941040
Si 11.885974297 6.973451972 3.292185962
Si 11.897679721 6.852600382 10.805513186
Si 1.379417747 3.647684116 3.306773813
Si 1.408635240 3.415091620 10.839600491
Si 1.300067489 6.678666071 14.526099812
Si 11.590906619 10.102416887 7.043110005
Si 11.558480323 10.159195142 14.577685326
Si 6.337401112 12.000715158 7.374925580
Si 6.290493052 12.104539222 14.896951713
Si 3.874774786 1.695910569 7.283699577
Si 4.004817924 1.597828389 14.720726722
Si 6.752019723 1.779554679 3.575966719
Si 6.892251101 1.786854602 11.187675974
Si 9.385275706 12.140507114 3.413641554
Si 9.371906401 12.029905261 10.845796286
Si 1.208331766 6.747940991 3.909625262
Si 1.275369530 6.541661685 11.390908780
Si 11.467238521 9.945231902 3.950746801
Si 11.484250344 9.897184282 11.485394125
Si 11.971386924 7.108272037 0.207109190
Si 11.675829004 7.172710009 7.734592294
Si 1.673523590 3.559779012 0.221503141
Si 1.869180369 13.168227963 1.969264989
Si 1.874970128 13.057881942 9.295083954
Si 4.256739468 11.001917776 2.008544760
Si 4.250813428 10.958091499 9.354796538
Si 11.116710003 0.715304252 5.572840572
Si 11.080693270 0.604235064 13.193877287
Si 8.827473382 2.845637228 13.264998159
Si -0.228901639 10.877396012 1.740846963
Si -0.171911765 10.746497028 9.289841743
Si 2.159772694 8.706852689 1.688497866
Si 2.244037313 8.621921946 9.272208752
Si 13.251162306 3.007343449 5.611150549
Si 13.271383730 2.776556122 13.145998580
Si 10.928679651 5.135218807 5.587346119
Si 11.012813200 5.028104381 13.151123907
Si 1.583190378 3.613692698 7.822416311
Si 8.798517600 2.814993039 5.586982196
Al 1.037451511 6.711531566 7.108459450
Al 6.189257965 12.313784128 4.089730910
Al 6.056310496 12.209614111 11.688184508
Al 7.074388369 1.566103705 7.858576278
Cu1 3.402262462 7.776623109 6.252214715
Ag2 5.838344936 9.603164308 5.198678428
H 8.096055780 2.898126733 9.579779436
H 7.468167031 11.474064312 9.838825344
C 7.194763993 8.637130760 6.530735544
H 7.501769719 7.713000316 6.033969713
H 7.988271015 9.384160707 6.610270509
H 6.607248387 8.500406715 7.441586766
H 5.372828914 7.034603153 5.065624506
End final coordinates

Cu-O-Mo-product-2
Final energy = -6874.2378569164 Ry
CELL_PARAMETERS (angstrom)
13.819673438 0.045295416 -0.002364200
-1.390263873 13.591441107 -0.029913170
0.004859519 -0.000703465 15.016638838

ATOMIC_POSITIONS (angstrom)
O 3.154173227 0.552514237 3.293461974
O 2.272892282 13.735335585 10.734247193
O 5.204460968 10.965511771 3.422271557
O 4.908236074 11.297923637 10.847985312
O 7.892837511 11.495534675 7.612052587
O 7.687336538 11.651269763 0.574577856
O 10.788137337 0.037626502 6.994382066
O 9.370687693 13.420099471 14.535165650
O 8.228319721 2.508690989 7.091644140
O 8.132146065 2.584240944 14.691093235
O 5.186422622 2.245120286 3.718586170
O 5.322251125 2.166047828 11.213336221
O 12.660910357 11.017532294 0.408775913
O 12.985431508 10.690770635 7.882491212
O 2.223831795 7.651597061 0.449455776
O 2.224871394 7.979294710 7.821080888
O 1.545962302 5.292575569 3.285908589
O 1.637150598 4.948230440 11.222837423
O 0.050133277 3.223511283 4.148966692
O 0.097968567 2.832146602 11.698586253
O 10.984674835 5.850429304 4.151985705
O 11.172033870 5.680466774 11.679075865
O 11.486100694 8.650042600 0.138572291
O 11.144341407 8.754406000 7.742036766
O 10.129425102 13.325426637 4.396075881
O 9.575472520 13.123484265 11.913506001
O 7.623993904 2.858636583 4.522960788
O 7.713312390 2.947512541 12.074975523
O 5.578396673 1.999908207 14.999258650
O 5.411901781 1.822998051 7.691375556
O 3.570590684 0.353105837 0.665452221
O 3.129109938 0.502568479 8.162851511
O 5.120751587 11.242811529 0.748427244
O 5.457139409 10.834112974 8.290976559
O 7.866280897 12.067133419 3.764652101
O 7.615666529 11.666691184 10.867526289
O 0.639641064 3.052523552 6.734960468
O 0.579814271 2.715956618 14.311245319
O 10.778970368 6.331731998 6.784276186
O 11.093059779 6.211264147 14.273094977
O 11.203700551 8.425304454 3.539437268
O 11.343394556 8.316863697 11.312228629
O 12.734980790 10.565125918 3.045108612
O 12.543741089 10.607306223 10.509503463
O 1.905042105 7.885479514 3.107010389
O 2.180127400 7.416566532 10.453245977
O 1.569000214 5.261294250 7.908759039
O 1.649078862 5.095972451 14.943338355
O 3.125204752 12.103161462 2.293530369
O 3.141540974 11.983819557 8.928750897
O 9.915724567 1.719816738 5.154027555
O 9.890386817 1.706334678 12.890345062
O 0.911603631 9.718808096 1.463340570
O 0.941117616 9.546439863 9.547966699
O 12.220348254 4.304834114 5.945288469
O 12.218817846 3.959983237 13.436950723
O 3.686567101 1.290613674 5.733344263
O 3.894656653 1.063937820 13.194027242
O 5.903589067 11.585157779 5.806553196
O 6.206749622 11.810168053 13.404270826
O 9.797030995 12.496310381 1.932093198
O 9.634423088 12.494590511 9.338143691
O 7.236655932 2.075748843 2.064278670
O 7.455330209 2.161007449 9.609944951
O 12.114339740 9.963870656 5.520347362
O 11.912699467 10.241487823 13.034082341
O 1.641195463 6.801695325 5.488496266
O 1.602213012 6.910380352 12.987914810
O 1.198135790 3.188174351 1.778765233
O 1.099093023 3.090406143 9.329655874
O 11.786875638 6.556942403 1.758733630
O 11.540894105 6.622327820 9.286232098
O 2.715082312 3.061551767 3.993348190
O 2.740067685 2.598878001 11.369179634
O 10.079568632 10.860670949 14.836463188
O 10.474695420 11.217748994 7.161387208
O 10.164461027 10.750753009 3.872652173
O 10.004942193 10.578124708 11.190509943
O 3.128384840 2.911341044 14.983364342
O 3.120651646 3.109337314 7.608434725
O 7.396562024 0.096660487 0.307008711
O 7.447910961 -0.185863471 7.842917044
O 13.562821891 7.004425631 14.857377475
O 13.264811772 7.229398095 7.346187685
O 5.566743638 13.878039770 4.004378275
O 7.282097092 0.342931238 11.533973294
O -0.447329296 6.934893201 3.871008233
O -0.307103962 6.772961421 11.119146373
O 0.507002577 12.311274511 1.902021000
O 0.547461074 12.183435499 9.515792312
O 3.542467961 9.487553319 1.898241233
O 3.622383955 9.425683141 9.521112902
O 12.511018695 1.673234332 5.816640804
O 12.491364932 1.300475730 13.220404917
O 9.532142798 4.301322175 5.666069037
O 9.581859205 4.315236388 13.294574258
O 4.603156643 7.754295258 4.902331550
Si 7.073931308 1.669871249 0.513893344
Si 9.241031732 12.101165333 0.465087457
Si 9.355647040 12.213821721 7.743800167
Si 3.702610758 1.787930933 4.197064389
Si 3.883573725 1.494461889 11.628974481
Si 11.846876701 6.950205867 3.334107245
Si 11.912169595 6.862577816 10.839865355
Si 1.375768758 3.680031516 3.319671910
Si 1.399124404 3.377054565 10.888562873
Si 1.309328563 6.640609841 14.566445152
Si 11.683797392 10.140024212 7.075497726
Si 11.536639452 10.179311017 14.614895294
Si 6.312798019 11.893967608 7.384826193
Si 6.256479409 12.110431268 14.971177240
Si 3.867832169 1.691800484 7.304883015
Si 4.034178079 1.584866438 14.728653366
Si 6.761324967 1.827922499 3.603574836
Si 6.904111250 1.844901925 11.202551600
Si 9.440635839 12.161038550 3.492574703
Si 9.302382275 11.984683794 10.829458997
Si 1.159077372 6.718755757 3.959230159
Si 1.266049373 6.507357995 11.441577667

Si 11.561991764 9.943224242 3.989124931
Si 11.477386392 9.915753049 11.507076756
Si 11.993207938 7.111791982 0.251084898
Si 11.727066856 7.216969674 7.773479364
Si 1.631969302 3.502420024 0.246019621
Si 1.895788403 13.136650940 2.013858007
Si 1.933522955 13.011243786 9.315854628
Si 4.229477299 10.948255847 2.052976482
Si 4.270094579 10.916387695 9.433131915
Si 11.174259700 0.796563381 5.593786392
Si 11.034571895 0.598916718 13.176874808
Si 8.833593945 2.882195967 13.267681167
Si -0.209290067 10.869856262 1.726403043
Si -0.147951723 10.730273776 9.354079173
Si 2.131430544 8.675940898 1.717651929
Si 2.244000382 8.600942992 9.343773613
Si 13.266462411 3.093908731 5.654911117
Si 13.256097740 2.736678846 13.166032303
Si 10.884789559 5.185551252 5.637293274
Si 11.031114693 5.036274174 13.165212334
Si 1.611816633 3.669021093 7.883678774
Si 8.817275391 2.840344144 5.634140829
Al 1.085535381 6.724053159 7.147242923
Al 6.226528275 12.313775795 4.183540439
Al 6.011655006 12.234325949 11.764198256
Al 7.075498793 1.499395391 7.880238487
Cu1 3.476764869 7.930005071 6.375428624
Mo2 5.297331090 9.632355274 5.046193611
H 8.089600313 2.898173539 9.530735893
H 7.334570029 11.055958640 10.153109169
C 7.207770540 8.813558550 5.374135217
H 7.464661562 8.055846905 4.617930115
H 7.977239193 9.596683137 5.378248423
H 7.173890951 8.336514818 6.370828969
H 5.205607199 6.987564685 4.860324698
End final coordinates

Cu-O-Nb-product-2
Final energy = -6844.6923262139 Ry
CELL_PARAMETERS (angstrom)
13.808252686 0.049255984 -0.012798476
-1.385324889 13.609471515 -0.011664165
-0.006727656 0.018258231 14.993339083

ATOMIC_POSITIONS (angstrom)
O 3.215615552 0.515858443 3.300724831
O 2.225383611 13.739287221 10.762932423
O 5.247825988 10.987807906 3.444400518
O 4.875019155 11.293997860 10.894373079
O 7.901507351 11.470398903 7.706823674
O 7.764784443 11.648520076 0.580273866
O 10.746795828 -0.005100942 7.006252334
O 9.411012678 13.489156861 14.567598257
O 8.266327595 2.562530806 7.095338682
O 8.109996202 2.561305329 14.681124028
O 5.179657563 2.291207733 3.727799838
O 5.303280804 2.137830346 11.175114291
O 12.805324044 10.932071867 0.386714517
O 13.006267564 10.661377355 7.846253108
O 2.216970711 7.662219549 0.454022396
O 2.188796118 7.991774723 7.851601402
O 1.382147845 5.218279889 3.301791853
O 1.655013885 4.950775921 11.192422257
O 0.013502386 3.073869014 4.148289275
O 0.076065255 2.863714701 11.652544175
O 11.166379445 5.847566374 4.170903517
O 11.136171363 5.676931652 11.655358349
O 11.482430483 8.644814158 0.102188656
O 11.133321805 8.742916112 7.741069621
O 10.166890583 13.334067723 4.444568696
O 9.545543278 13.112319369 11.952090102
O 7.635091604 2.864176713 4.535044085
O 7.681418436 2.925248983 12.070186668
O 5.561271198 1.951567619 15.036435990
O 5.446105675 1.791759736 7.651304002
O 3.513095500 0.316599158 0.662769749
O 3.143737286 0.515520794 8.163949700
O 5.200203737 11.192760918 0.760933110
O 5.450351300 10.897097118 8.335460753
O 7.856945740 12.178545115 3.771525547
O 7.601607153 11.676053570 10.848558066
O 0.730600734 3.011873847 6.697629928
O 0.593477767 2.734436513 14.249993072
O 10.792098086 6.307524550 6.782675454
O 11.070737514 6.213145743 14.236610770
O 11.126804185 8.428019287 3.538498585
O 11.344120074 8.320636433 11.304232856
O 12.625336221 10.595922555 3.029139402
O 12.485054852 10.630394716 10.452975576
O 2.166006600 7.715889443 3.121026703
O 2.173810235 7.439856702 10.483796721
O 1.580654516 5.247604744 7.906477966
O 1.651355798 5.101150349 14.980172760
O 3.192682183 12.107131855 2.257099070
O 3.123851227 12.000855174 8.963034246
O 9.914132367 1.687414385 5.160805400
O 9.870722545 1.698872959 12.871443843
O 0.917174849 9.616811607 1.709924227
O 0.937838041 9.575539945 9.599968280
O 12.289764561 4.289341382 5.982426780
O 12.192895394 3.959625088 13.410689648
O 3.666787212 1.310058053 5.730903567
O 3.897909709 1.072623907 13.190340496
O 5.987331918 11.574814530 5.832012183
O 6.258730102 11.848700612 13.405688093
O 9.839295261 12.524977678 1.975894112
O 9.667432889 12.499492999 9.376774776
O 7.252045438 2.046209581 2.094885016
O 7.457365769 2.168962374 9.595138515
O 12.074103777 9.948706875 5.510625389
O 11.949179733 10.263211482 12.999173995
O 1.577251553 6.769334393 5.476217387
O 1.600889121 6.883420070 12.996527406
O 1.150266018 3.127529744 1.764190710
O 1.121059907 3.071546872 9.306736785
O 11.729530264 6.569136529 1.740136945
O 11.539282821 6.617131447 9.281680874
O 2.686380530 3.033077540 3.952285126
O 2.725001838 2.595146472 11.377082978
O 10.182720036 10.948295082 14.843858406
O 10.480532706 11.213701907 7.191754095
O 10.086223420 10.755306455 3.916220793
O 9.975862341 10.568617892 11.225539304
O 3.124140031 2.909071560 14.992168678
O 3.180738186 3.124526586 7.633288809
O 7.424126493 0.054023431 0.358184716
O 7.512907939 -0.161191434 7.801315938
O 13.541065991 6.999860258 14.848605040
O 13.262367468 7.228000222 7.343442877
O 5.506801632 13.913794329 4.087999183
O 7.267409862 0.322948189 11.487484525
O -0.369432335 7.168256972 3.681312910
O -0.312315125 6.750644634 11.139868346
O 0.561882875 12.244284027 1.989889468
O 0.520105755 12.205808287 9.490369891
O 3.585804727 9.484065945 1.909140036
O 3.616824790 9.436934178 9.519950861
O 12.489562974 1.651140626 5.928725624
O 12.485202977 1.310475971 13.153516955
O 9.610947130 4.285568056 5.588785015
O 9.553768235 4.302887232 13.281106155
O 4.325698702 8.080278642 4.779407211
Si 7.081492767 1.625682337 0.549737664
Si 9.309556826 12.134398468 0.498278973
Si 9.364173034 12.201415412 7.791454725
Si 3.704257657 1.788584707 4.189794149
Si 3.865569413 1.485334063 11.622488547
Si 11.870539807 7.005845393 3.296216548
Si 11.898814619 6.859008164 10.835466474
Si 1.310036837 3.598596360 3.312478317
Si 1.401491615 3.380203286 10.864444243
Si 1.299129861 6.635800927 14.572934122
Si 11.677775640 10.125359972 7.073429448
Si 11.597541021 10.199321456 14.584954171
Si 6.341669819 11.916132959 7.424026467
Si 6.307952631 12.116559894 14.977974937
Si 3.892629460 1.694933219 7.299568874
Si 4.015073336 1.571151018 14.732552075
Si 6.747833969 1.842834323 3.632199278
Si 6.887820137 1.827592504 11.175792390
Si 9.437571062 12.202363975 3.526814944
Si 9.289973027 11.981923572 10.855918764
Si 1.158186423 6.688001710 3.938711035
Si 1.265889445 6.499551426 11.446596691
Si 11.486299405 9.946217114 3.993523735
Si 11.465885092 9.922503026 11.489431302
Si 11.975301049 7.104174789 0.233322159
Si 11.726634522 7.208985923 7.770728283
Si 1.632819884 3.476592756 0.253356646
Si 1.930161031 13.111850503 2.041514159
Si 1.914100915 13.031455804 9.329775607
Si 4.297708843 10.942674929 2.070710142
Si 4.251915545 10.935008816 9.466052225
Si 11.168012742 0.772200578 5.628757006
Si 11.028266291 0.606532422 13.160831324
Si 8.807385209 2.866594845 13.257056144
Si -0.180083365 10.819228442 1.800636396
Si -0.157092882 10.742182020 9.344390952
Si 2.199176184 8.632385137 1.762108698
Si 2.229051663 8.618983860 9.370175689
Si 13.284997379 3.036975467 5.678676201
Si 13.240000860 2.751661384 13.113313830
Si 10.961791748 5.170163458 5.636012654
Si 10.999724767 5.029651463 13.139909815
Si 1.656662055 3.657657654 7.872023948
Si 8.848053989 2.848692650 5.622665524
Al 1.095403971 6.712451500 7.154629818
Al 6.210879541 12.364185622 4.205621428
Al 6.010919129 12.237120611 11.765506961
Al 7.116587009 1.519958590 7.852810973
Cu1 3.385624205 8.185823471 6.388665756
Nb2 5.579152235 9.585841614 5.087077787
H 8.062717555 2.931905233 9.531290153
H 7.329035084 11.118413831 10.087332446
C 7.415407443 8.579889094 5.435323125
H 7.740516980 7.879560084 4.651919978
H 8.202294296 9.337144295 5.587902690
H 7.275445256 8.023059170 6.384597748
H 3.683519658 7.884668857 4.047992167
End final coordinates

Cu-O-Pd-product-1
Final energy = -6841.2568168277 Ry
CELL_PARAMETERS (angstrom)
13.808256237 0.049015168 -0.003796070
-1.385703312 13.639772435 -0.028786205
0.003244735 0.000376318 15.034469166

ATOMIC_POSITIONS (angstrom)
O 3.101794628 0.536912162 3.244990817
O 2.228341816 13.822106126 10.707741250
O 5.162324146 11.071204959 3.293312120
O 4.836940120 11.339064509 10.873277268
O 7.934919858 11.574457920 7.620275174
O 7.689944154 11.849493859 0.546293684
O 10.854467220 0.054108728 6.979458343
O 9.522055866 13.495912350 14.551768426
O 8.211390798 2.611994212 7.024626048
O 8.042860238 2.726051796 14.649163145
O 5.185933306 2.178712256 3.613919438
O 5.364110437 2.139579483 11.147887401
O 12.606333896 10.999984621 0.394674787
O 13.003457811 10.618459524 7.914176460
O 2.202113696 7.731991313 0.375114943
O 2.070319691 8.044019935 7.859841140
O 1.701126687 5.359996208 3.453292544
O 1.679701524 5.031950314 11.200139822
O 0.077165405 3.340905611 4.150009224
O 0.203233548 2.879111911 11.696665538
O 11.116138013 5.888255512 4.152894140
O 11.164260547 5.811205734 11.672620962
O 11.382997968 8.655749342 0.109544414
O 11.098731965 8.752355463 7.665569119
O 10.097382460 13.333495385 4.371327693
O 9.498955296 13.197169281 11.918480806
O 7.608583121 2.837226406 4.440347516
O 7.750758023 2.926327850 12.002392754
O 5.508774472 2.065961110 15.027847559
O 5.424384583 1.848847068 7.646680666
O 3.446981812 0.444598764 0.595585144

O 3.138159687 0.535538587 8.121118530
O 5.119822291 11.404241428 0.636721651
O 5.517914294 11.000901766 8.347077512
O 7.859973695 12.061441661 3.675869431
O 7.603060807 11.723483548 10.759579152
O 0.618444278 2.977682097 6.729949889
O 0.505617230 2.783277460 14.355763120
O 10.673033877 6.299649084 6.771125242
O 11.075921359 6.187219641 14.304061338
O 11.270987263 8.463504601 3.541086825
O 11.372680215 8.418787758 11.192944974
O 12.730220697 10.651659145 3.047243890
O 12.529842588 10.769294278 10.536817369
O 2.058956967 7.939665612 3.024706977
O 2.236195369 7.499949723 10.463843275
O 1.587604400 5.274254307 7.660398081
O 1.595722732 5.183356031 14.895922530
O 3.083439582 12.202184548 2.131677111
O 3.145314958 12.074038970 8.911040225
O 9.887039389 1.690705950 5.136831958
O 9.876840062 1.723122209 12.989791520
O 0.887173983 9.756220779 1.479788346
O 0.961806686 9.652503902 9.681507865
O 12.190977518 4.285830468 5.983059499
O 12.206682625 4.003047883 13.320717952
O 3.717925240 1.278361121 5.679284056
O 3.877286424 1.158181865 13.152782457
O 5.973545603 11.616120236 5.772023130
O 6.313801346 11.826002624 13.331522909
O 9.854470754 12.487558786 1.912627293
O 9.670830563 12.591401164 9.338401710
O 7.261749709 1.993392944 1.993817721
O 7.496934116 2.150791264 9.545620993
O 12.138744358 10.022718339 5.519894957
O 11.881678060 10.241338057 13.034747715
O 1.721244825 7.135369791 5.467260528
O 1.577767653 7.001779809 12.952280609
O 1.206661924 3.370381114 1.778245616
O 1.125653273 3.225874411 9.288301883
O 11.844623264 6.601542455 1.745029462
O 11.541347945 6.647255847 9.237217525
O 2.738592947 3.047135470 3.959331948
O 2.823603841 2.697056795 11.269089680
O 10.023296917 10.888960348 14.805801962
O 10.520985526 11.268403933 7.199999097
O 10.159857843 10.757886237 3.878026750
O 9.990070293 10.663337162 11.194792585
O 3.073398451 3.001048570 14.935056187
O 3.129336661 3.122717100 7.529886538
O 7.374565973 0.188365252 0.037195293
O 7.513974856 -0.124052485 7.696878988
O 13.519702141 7.113844217 14.796353357
O 13.170599224 7.169713850 7.182634877
O 5.598343304 13.893762793 3.979097142
O 7.314525825 0.315787072 11.462629731
O -0.330185493 7.016416740 3.806019100
O -0.281597533 6.827386764 11.032795981
O 0.460798237 12.371811419 1.806935914
O 0.533143052 12.272189347 9.435525291
O 3.552759324 9.605512205 1.725182914
O 3.624248978 9.501455350 9.412911827
O 12.506167571 1.675283016 5.674811366
O 12.497101319 1.347585118 13.105064069
O 9.533148628 4.306060607 5.490821432
O 9.570518408 4.356401020 13.207054686
O 4.921903052 8.683378138 6.586647418
Si 7.035975531 1.722960689 0.422861956
Si 9.271171951 12.174789661 0.437551746
Si 9.401460027 12.287452590 7.744991583
Si 3.707886797 1.754984920 4.135716499
Si 3.901318924 1.538245164 11.574624997
Si 11.928749120 7.003008407 3.315431457
Si 11.921167640 6.941587391 10.782687239
Si 1.426396181 3.758359606 3.340933964
Si 1.460129594 3.463314923 10.848739228
Si 1.274624327 6.729819035 14.520606180
Si 11.690867979 10.154700585 7.074530000
Si 11.473216940 10.187096160 14.607268819
Si 6.355860403 11.972262830 7.340077293
Si 6.276575865 12.232524243 14.875610409
Si 3.885194675 1.703278813 7.246836147
Si 3.973693499 1.665709802 14.696273675
Si 6.768841464 1.773612007 3.533132472
Si 6.944285236 1.818074813 11.135976466
Si 9.436007638 12.160175084 3.460366115
Si 9.283552201 12.063916795 10.812510742
Si 1.269902527 6.845416179 3.915837018
Si 1.286324245 6.586214141 11.407603675
Si 11.578402233 9.994366527 3.991203135
Si 11.467453162 10.005203921 11.487719998
Si 11.962847522 7.144348054 0.222042599
Si 11.660469266 7.208328427 7.706440878
Si 1.590704435 3.597108861 0.216878761
Si 1.837565077 13.218696533 1.922403650
Si 1.928796655 13.094161136 9.279363823
Si 4.224006946 11.073107537 1.933683174
Si 4.268332490 10.997825536 9.416054343
Si 11.167122875 0.784004613 5.545280991
Si 11.048098252 0.626114430 13.173331195
Si 8.817195687 2.924762446 13.243954594
Si -0.235016990 10.915591866 1.701205579
Si -0.139953498 10.802149698 9.381539457
Si 2.162886532 8.767971832 1.630747429
Si 2.228662586 8.685818435 9.350098264
Si 13.253745093 3.103061478 5.627181341
Si 13.261121230 2.785112592 13.118974311
Si 10.884431086 5.182752639 5.601141581
Si 11.017230344 5.086814932 13.120051293
Si 1.622471676 3.685089846 7.796523077
Si 8.803644637 2.850117881 5.548608780
Al 1.039847485 6.801551587 7.116966243
Al 6.223022512 12.301787326 4.120260858
Al 6.025369172 12.252169365 11.705726059
Al 7.097130873 1.543811906 7.798955322
Cu1 3.291420158 8.013362436 6.133608584
Pd2 5.053899861 9.815442158 4.980837670
H 8.149552155 2.873607394 9.488526435
H 7.340139847 11.250821650 9.937530235
C 6.744992546 6.478605665 6.948680055
H 6.469956109 5.942539274 6.041996500
H 7.703893006 6.993362987 6.990234912
H 6.212317512 6.260949068 7.873551874
H 5.647856017 7.986838856 6.663820095
End final coordinates

Cu-O-Pd-product-2
Final energy = -6841.3961583891 Ry
CELL_PARAMETERS (angstrom)
13.808256237 0.049015168 -0.003796070
-1.385703312 13.639772435 -0.028786205
0.003244735 0.000376318 15.034469166

ATOMIC_POSITIONS (angstrom)
O 3.126087270 0.518212741 3.253605312
O 2.295904597 13.767205128 10.732641519
O 5.101382829 11.031140063 3.370564898
O 4.894270643 11.265192882 10.919530525
O 7.987979244 11.556591728 7.657627598
O 7.674734503 11.774917518 0.596226898
O 10.910535245 0.038328944 6.989901469
O 9.490959763 13.438241212 14.577644889
O 8.242585929 2.539867569 7.060876234
O 8.093371318 2.607621651 14.685763820
O 5.244566662 2.111064591 3.682165255
O 5.372572706 2.130210922 11.154094126
O 12.550352192 11.038645091 0.404622024
O 13.049315570 10.653857916 7.894899526
O 2.190173894 7.716339049 0.361647059
O 2.285003469 8.034412834 7.730484030
O 1.733057826 5.333970858 3.365417033
O 1.687509797 4.967270684 11.229493154
O 0.161522485 3.276786804 4.116395347
O 0.173213009 2.828570359 11.696969205
O 10.989694566 5.856252837 4.104136200
O 11.189951241 5.726306070 11.693850657
O 11.423849305 8.636090999 0.093064326
O 11.187720067 8.738982244 7.692509734
O 10.087433474 13.297669327 4.377468851
O 9.587126342 13.130458642 11.950445617
O 7.668902905 2.793013789 4.469497387
O 7.761074321 2.868125229 12.038934263
O 5.546472178 2.030291894 15.076383953
O 5.438339762 1.785365625 7.641169386
O 3.444027644 0.448472979 0.607523146
O 3.176805717 0.443809923 8.141452426
O 5.113446775 11.284766195 0.679386890
O 5.579795252 10.937903980 8.395095087
O 7.855740054 11.970377617 3.720331534
O 7.654546926 11.701981169 10.804816067
O 0.643069622 3.024751479 6.718931984
O 0.568304113 2.748913510 14.335184935
O 10.828963254 6.302129065 6.744282324
O 11.070685454 6.152599009 14.319744680
O 11.317757308 8.431348161 3.543535789
O 11.376559719 8.338306825 11.288110902
O 12.754120880 10.625243429 3.041724634
O 12.622090360 10.602204177 10.532832208
O 1.823651397 7.947326595 2.997002124
O 2.230576159 7.392075841 10.340454268
O 1.691104032 5.253479138 7.739241334
O 1.625878660 5.164940936 14.851458862
O 3.082642756 12.177901643 2.113350736
O 3.193112575 11.994240921 8.953699553
O 9.967935421 1.711993991 5.170672276
O 9.897355810 1.650525327 12.967524899
O 0.860615915 9.779105048 1.368254582
O 1.046066069 9.576852176 9.542361454
O 12.219417897 4.251579783 5.866414432
O 12.223412219 3.953558584 13.379874069
O 3.687451625 1.242085204 5.697615407
O 3.934811872 1.122374884 13.168436980
O 6.029702308 11.478832095 5.830792047
O 6.321477120 11.762756223 13.375159535
O 9.838092913 12.430711872 1.934802863
O 9.713652081 12.598047059 9.353896808
O 7.302226024 1.892188571 2.045542827
O 7.508381163 2.088521071 9.566136704
O 12.176895324 9.997379213 5.520048531
O 11.878493570 10.257811211 13.035261537
O 1.726932280 7.003947234 5.447426589
O 1.626347626 7.000232393 12.904578880
O 1.285254274 3.319581626 1.742654070
O 1.104887588 3.186648154 9.299322858
O 11.905511516 6.591104047 1.736124911
O 11.531369594 6.625551617 9.265833514
O 2.823488815 3.048837565 3.938170012
O 2.798388623 2.609247729 11.278043983
O 9.991130435 10.829360000 14.812304901
O 10.554161391 11.240974363 7.211610745
O 10.184171009 10.717720938 3.900824131
O 10.051635974 10.615713120 11.128287685
O 3.138728617 3.006760188 14.892152748
O 3.137800065 3.043899997 7.588676538
O 7.336714770 0.090826094 0.094048643
O 7.512606902 -0.185755652 7.703912070
O 13.528859628 7.065758520 14.722142373
O 13.304483021 7.184253816 7.348959175
O 5.657633968 13.836208354 4.089172952
O 7.293063490 0.266685978 11.485646499
O -0.398780374 6.810728123 3.929349528
O -0.267820091 6.774163135 11.031645017
O 0.450879496 12.380166589 1.811085613
O 0.592391570 12.198075726 9.513155807
O 3.491779067 9.561737963 1.795900245
O 3.721941010 9.420079028 9.435466301
O 12.588622066 1.626023466 5.657753146
O 12.517904010 1.299439374 13.181497548
O 9.535996914 4.301372487 5.602854813
O 9.589183812 4.281590629 13.250660238
O 4.452758995 7.938672473 4.559421299
Si 7.061916852 1.637249944 0.472552193
Si 9.249093302 12.112957028 0.462761829
Si 9.453203287 12.277155920 7.762977245
Si 3.742466424 1.721966170 4.153979155
Si 3.924900111 1.498351165 11.590973773
Si 11.903399907 6.940125636 3.321432696
Si 11.928156100 6.879109835 10.815474642
Si 1.497406677 3.722755394 3.301061326
Si 1.446125998 3.402038036 10.863091598
Si 1.297254036 6.712173551 14.475085342

Si 11.740069610 10.144330015 7.076132408
Si 11.463445981 10.175727984 14.606438729
Si 6.404662076 11.918204348 7.380371874
Si 6.255080903 12.137948128 14.928312536
Si 3.892905875 1.634906721 7.267991240
Si 4.015286239 1.646815197 14.707982887
Si 6.825459766 1.701425433 3.596215083
Si 6.948367996 1.776479279 11.157818481
Si 9.427923696 12.105765976 3.485617362
Si 9.340899947 12.031797484 10.819088110
Si 1.216058097 6.766019552 3.908880395
Si 1.305799886 6.532940153 11.374505813
Si 11.610414274 9.964767248 3.992008853
Si 11.503805536 9.937157951 11.493514784
Si 11.989147086 7.118571516 0.203553851
Si 11.753335814 7.195611836 7.747816269
Si 1.649343593 3.580181938 0.182434784
Si 1.844866959 13.202920107 1.924947495
Si 1.979922528 13.025586801 9.318488242
Si 4.208703645 11.012935936 1.996270631
Si 4.329562972 10.938554454 9.463257023
Si 11.223317864 0.764054465 5.551492510
Si 11.073350552 0.566949052 13.205649283
Si 8.839967525 2.845718326 13.270603291
Si -0.249057163 10.927613995 1.678481400
Si -0.077158718 10.733133711 9.365004523
Si 2.096664641 8.756592995 1.616569730
Si 2.325640571 8.620423256 9.278161572
Si 13.305803351 3.073935042 5.583659111
Si 13.275964922 2.739808226 13.145422840
Si 10.901088808 5.164774639 5.581267246
Si 11.028502443 5.028153504 13.155126753
Si 1.649409650 3.658080393 7.827416062
Si 8.844657685 2.825006891 5.598073427
Al 1.144678433 6.750156099 7.118996951
Al 6.206445593 12.205950803 4.160073937
Al 6.058355828 12.211639734 11.754323132
Al 7.107981105 1.484200298 7.815038258
Cu1 3.326975103 8.084584127 6.055398615
Pd2 5.352685591 9.596606366 5.218749862
H 8.152345923 2.818094035 9.491730022
H 7.383702502 11.175512596 10.020268028
C 6.381804865 8.505603000 6.591873972
H 6.508658327 7.483719649 6.211026379
H 7.345817246 9.029289446 6.630517016
H 5.872516105 8.525495887 7.560660047
H 5.021362195 7.145913868 4.628780021
End final coordinates

Cu-O-Rh-product-2
Final energy = -6980.4474984796 Ry
CELL_PARAMETERS (angstrom)
13.814331180 0.069158007 0.005757228
-1.366364585 13.599312344 -0.012363006
0.013549734 0.019460677 15.002118280

ATOMIC_POSITIONS (angstrom)
O 3.122908403 0.540179977 3.262696994
O 2.341119320 13.721747808 10.727650516
O 5.153324165 10.973393370 3.413017972
O 4.877608535 11.274227566 10.940006857
O 8.004832674 11.526725914 7.586502906
O 7.666789221 11.716336731 0.641930747
O 10.884729468 0.079522874 6.978331594
O 9.435630089 13.436538309 14.558706842
O 8.265586614 2.509253376 7.071846921
O 8.124696720 2.621470114 14.676896918
O 5.231664683 2.151284049 3.661796506
O 5.358860010 2.155273958 11.140914574
O 12.566793550 11.066417318 0.415588497
O 13.083542780 10.652872826 7.893377841
O 2.208187276 7.672892012 0.382331167
O 2.263880508 8.056528720 7.727879711
O 1.716783940 5.337728879 3.340891733
O 1.690947952 4.944790217 11.227285840
O 0.132322206 3.298543089 4.116277853
O 0.139363533 2.829583756 11.676749291
O 10.939441286 5.852717122 4.100876752
O 11.210888083 5.721855152 11.675189993
O 11.465301803 8.649430694 0.139745126
O 11.196617057 8.763061543 7.705632700
O 10.134390199 13.306585557 4.390443421
O 9.579892266 13.121961855 11.935585342
O 7.650456868 2.806081315 4.495750876
O 7.735973839 2.922206821 12.045714626
O 5.569579939 2.067248218 15.045229592
O 5.447331832 1.810801965 7.660319191
O 3.523818456 0.396428299 0.630987383
O 3.184271700 0.463693783 8.128240729
O 5.101393302 11.255185956 0.731337637
O 5.632427885 10.884482791 8.448397123
O 7.884652981 11.980900557 3.814605419
O 7.640320461 11.682409766 10.817901879
O 0.636712711 3.076641289 6.712215311
O 0.568315526 2.731873258 14.308175671
O 10.815023517 6.345170815 6.733092408
O 11.091307437 6.203185739 14.286140670
O 11.315344833 8.425192094 3.549727042
O 11.399338115 8.342225204 11.277559844
O 12.791565528 10.584683896 3.038200571
O 12.615405363 10.627461401 10.522155009
O 1.732214138 7.953457480 3.002082347
O 2.240828481 7.364803161 10.326490010
O 1.696423180 5.272013404 7.786580413
O 1.646822587 5.142602935 14.819708645
O 3.086883025 12.103954037 2.235990794
O 3.219380984 11.959353089 8.928001239
O 9.984000046 1.761011303 5.142947142
O 9.903400827 1.710481938 12.907755516
O 0.896258747 9.783599454 1.313744388
O 1.048669817 9.562041416 9.576029526
O 12.190170500 4.278912015 5.880266778
O 12.215250608 3.964456476 13.399642392
O 3.721196922 1.263072983 5.697034206
O 3.965175919 1.098725466 13.157122063
O 5.946447444 11.476805994 5.869478472
O 6.313121384 11.742664056 13.392338800
O 9.815475262 12.439765610 1.958596694
O 9.684993549 12.565631406 9.343333517
O 7.308165830 1.920938626 2.061636005
O 7.513939517 2.109998938 9.582359879
O 12.206929685 9.988512378 5.521375273
O 11.890573080 10.263342990 13.026264573
O 1.698052911 6.977434587 5.450259278
O 1.628062803 6.988185654 12.888282440
O 1.267057119 3.294624848 1.751309455
O 1.113671901 3.163080219 9.292858186
O 11.897313454 6.572570927 1.749847111
O 11.530243477 6.627557968 9.256343867
O 2.796593265 3.060023148 3.957994616
O 2.768612992 2.573731754 11.300545320
O 10.015555345 10.845700974 14.812874907
O 10.593770804 11.265301061 7.197411108
O 10.219869197 10.725905506 3.905033347
O 10.047466663 10.602547484 11.131852588
O 3.134953094 2.968088189 14.883770214
O 3.138787946 3.064211421 7.573362166
O 7.327078181 0.092776943 0.138314593
O 7.500581251 -0.189068451 7.765886304
O 13.558820949 7.068763166 14.734335485
O 13.301407135 7.198805886 7.350335449
O 5.642034807 13.813785007 4.100953108
O 7.289360993 0.310821572 11.525395802
O -0.441189374 6.750734009 3.957140970
O -0.258893330 6.754289248 11.003785491
O 0.469856764 12.357466962 1.841470453
O 0.615529015 12.178869206 9.504578291
O 3.504388559 9.501738535 1.849422527
O 3.729353996 9.397460295 9.462591352
O 12.596088507 1.663230593 5.689638475
O 12.507201668 1.308252589 13.178713270
O 9.502605086 4.328441986 5.642198289
O 9.584637853 4.330391052 13.248482990
O 4.340568771 8.012300275 4.518707847
Si 7.068010524 1.648335589 0.492445624
Si 9.232901683 12.094295117 0.491342794
Si 9.456503588 12.263861070 7.744487377
Si 3.739505529 1.748983602 4.156547280
Si 3.926781098 1.488788606 11.582699061
Si 11.880081501 6.924685990 3.334317178
Si 11.943177210 6.880962425 10.800527973
Si 1.474939657 3.726597355 3.303033595
Si 1.433612747 3.382580423 10.859756528
Si 1.317287239 6.693578584 14.460629407
Si 11.767951983 10.153972698 7.075956166
Si 11.491702653 10.201613839 14.601517820
Si 6.408491839 11.883033119 7.410107395
Si 6.260488593 12.118763805 14.944356980
Si 3.906422391 1.659589235 7.268133546
Si 4.046723800 1.635019743 14.692349024
Si 6.810702337 1.728943550 3.604279639
Si 6.937711798 1.814283534 11.170179981
Si 9.450572262 12.113465874 3.520124396
Si 9.327301109 12.012308419 10.815088770
Si 1.174424524 6.748859078 3.919297149
Si 1.311982164 6.512195495 11.359019553
Si 11.635332929 9.953132369 3.995364252
Si 11.511207742 9.941398492 11.485368044
Si 12.003870535 7.120497266 0.227468074
Si 11.751024462 7.215125437 7.744956571
Si 1.639815889 3.540213696 0.191210611
Si 1.876923206 13.153655016 1.978332267
Si 2.010847740 12.993167288 9.309197730
Si 4.215871697 10.953521043 2.049707821
Si 4.345493923 10.910185312 9.478909935
Si 11.229101409 0.808475682 5.550079516
Si 11.048633247 0.600115320 13.173647842
Si 8.841458334 2.890775811 13.253605505
Si -0.227631653 10.906698509 1.670980416
Si -0.066766947 10.719241612 9.362089959
Si 2.091351015 8.727853828 1.624172730
Si 2.328265618 8.610333496 9.284229940
Si 13.294628556 3.119516839 5.599349961
Si 13.265289286 2.750729632 13.142311417
Si 10.869735608 5.187595246 5.591332675
Si 11.036655431 5.052845833 13.147267648
Si 1.651989532 3.675241082 7.831938301
Si 8.841124398 2.839574020 5.609522550
Al 1.139342469 6.750531144 7.128277400
Al 6.223986659 12.199796052 4.209551594
Al 6.051696297 12.207611212 11.774640066
Al 7.112917047 1.487884618 7.840436996
Cu1 3.259737953 8.155253131 6.034690651
Rh2 5.179181768 9.642071445 5.236798367
H 8.174940469 2.824074287 9.508589268
H 7.355976558 11.132229188 10.053736509
C 6.403515237 8.497488127 6.377695075
H 6.538807109 7.496572273 5.940685295
H 7.365951079 9.024158739 6.422025242
H 5.956139875 8.427314372 7.380508224
H 4.914224608 7.220688032 4.591812941
End final coordinates

Cu-O-Ru-product-2
Final energy = -6941.9185482771 Ry
CELL_PARAMETERS (angstrom)
13.817316730 0.054757312 0.001174593
-1.380843176 13.603132927 -0.017820998
0.008604928 0.012972424 15.006350271

ATOMIC_POSITIONS (angstrom)
O 3.135494844 0.505195549 3.308966792
O 2.295330990 13.715011485 10.753913392
O 5.185445481 10.928324919 3.463145449
O 4.890917242 11.281120584 10.893188004
O 7.935683580 11.530655353 7.568382858
O 7.675596093 11.681839250 0.601829678
O 10.859003705 0.063911731 7.020654986
O 9.409771272 13.438521455 14.560481184
O 8.241865645 2.514280617 7.106871727
O 8.176247866 2.582941817 14.693766934
O 5.191037294 2.184030681 3.690470934
O 5.329271125 2.140674580 11.211963267
O 12.614683024 11.028406879 0.424445769
O 13.028451387 10.653213924 7.901893869
O 2.211933035 7.636929598 0.433540237
O 2.224548770 8.003866673 7.786849517
O 1.662484847 5.296204166 3.322705682
O 1.685168389 4.935763491 11.223232757
O 0.080575852 3.272076897 4.139232836

O 0.112355376 2.841249876 11.693341578
O 10.932504401 5.861794059 4.136976283
O 11.221627882 5.682249528 11.683558368
O 11.477727972 8.636693088 0.143726597
O 11.154477354 8.748180374 7.723393164
O 10.116641646 13.294684949 4.427205879
O 9.584243679 13.090774090 11.948310273
O 7.612282218 2.805952005 4.538877393
O 7.715773943 2.925668272 12.086624406
O 5.602885096 2.051423456 14.966315406
O 5.422593000 1.823502862 7.704004361
O 3.638799028 0.357643213 0.695666810
O 3.148800169 0.490693900 8.170359136
O 5.115729848 11.252549399 0.803404218
O 5.539603627 10.862562152 8.360703684
O 7.874358212 11.990038983 3.811709630
O 7.616319395 11.642822178 10.899171746
O 0.616046809 3.056048388 6.735975677
O 0.587445527 2.698363701 14.311999036
O 10.769119464 6.323213820 6.774594481
O 11.089651093 6.196374453 14.284442793
O 11.300335568 8.426191486 3.545984334
O 11.393223795 8.314143674 11.313502625
O 12.786338898 10.592261168 3.059991406
O 12.576354298 10.614452231 10.529174357
O 1.783825778 7.910364583 3.067363027
O 2.229606289 7.391542295 10.407951464
O 1.607033207 5.254065045 7.873780587
O 1.650066129 5.097325910 14.886357425
O 3.093557263 12.053323067 2.329306293
O 3.176538404 11.980833084 8.933970826
O 9.922002675 1.706737713 5.170187466
O 9.905804988 1.689189346 12.876510078
O 0.911159968 9.745082986 1.392538477
O 0.991238376 9.548257046 9.581468096
O 12.191316823 4.293962246 5.914337171
O 12.225120363 3.946980702 13.447003365
O 3.721534943 1.252220694 5.734510653
O 3.907666983 1.048884361 13.198853242
O 5.872061395 11.646753857 5.857605544
O 6.189915717 11.807858970 13.432242897
O 9.787685301 12.481890877 1.963052689
O 9.617534710 12.516201657 9.362497281
O 7.250672476 2.082510903 2.058490468
O 7.467957282 2.165066822 9.625322786
O 12.153403055 9.987089610 5.533628694
O 11.888596175 10.253386417 13.040074918
O 1.673419181 6.867627452 5.485502780
O 1.620283985 6.930517366 12.947918764
O 1.229036241 3.222604931 1.777042382
O 1.115781492 3.099446808 9.321512966
O 11.843004410 6.552863161 1.762814593
O 11.534163489 6.620495529 9.279395120
O 2.735691822 3.020142830 3.998188696
O 2.745168323 2.564493051 11.360853180
O 10.048823285 10.855922111 14.847235888
O 10.525738419 11.237968061 7.208258844
O 10.200109326 10.724573806 3.875916871
O 10.019962220 10.561491572 11.160013222
O 3.139284616 2.913679894 14.963269318
O 3.117770511 3.085335885 7.576117930
O 7.360889814 0.095814945 0.298680501
O 7.480557053 -0.168009884 7.891603692
O 13.560529101 7.016445773 14.796655290
O 13.263707535 7.198607943 7.338552505
O 5.603007169 13.842428949 3.957938848
O 7.291729781 0.319960281 11.528212935
O -0.449180765 6.775346663 3.937090741
O -0.263507215 6.750643742 11.050727278
O 0.501881246 12.337348064 1.842413927
O 0.575092701 12.176568266 9.513181000
O 3.526357239 9.459317628 1.885416028
O 3.669152016 9.415197917 9.481665538
O 12.536889897 1.669536528 5.738860048
O 12.506185186 1.290546944 13.192369862
O 9.507541251 4.295408781 5.645956984
O 9.597411348 4.307989136 13.257696199
O 4.375374122 8.022891113 4.646163121
Si 7.082793457 1.675890137 0.509691228
Si 9.235150225 12.102205898 0.490951455
Si 9.394716524 12.240652762 7.759315241
Si 3.714264971 1.739221411 4.194864970
Si 3.893152272 1.467177253 11.630542270
Si 11.865573360 6.921953645 3.344111756
Si 11.945585383 6.858920825 10.824789674
Si 1.425009155 3.687419206 3.322273151
Si 1.420367905 3.369077285 10.883082638
Si 1.313659028 6.646462709 14.521757758
Si 11.715154903 10.141337771 7.089652569
Si 11.510586595 10.185058621 14.619406081
Si 6.348258254 11.930943843 7.419516223
Si 6.239888232 12.130467300 14.994940880
Si 3.884101041 1.673249823 7.302335015
Si 4.063571977 1.597123335 14.723409663
Si 6.771964724 1.786946177 3.587752851
Si 6.911941008 1.824286265 11.209433414
Si 9.442125533 12.125035506 3.520999162
Si 9.301850811 11.972566484 10.844966727
Si 1.168122196 6.705611186 3.955667558
Si 1.305604807 6.498478378 11.404837383
Si 11.616516133 9.951978711 3.997362175
Si 11.494299642 9.915873664 11.505949819
Si 11.999054903 7.101874516 0.245950028
Si 11.723111977 7.204651338 7.762407822
Si 1.641715339 3.495965697 0.231431154
Si 1.907684179 13.123928232 2.023813971
Si 1.964132105 13.002634186 9.327025624
Si 4.217669146 10.911984681 2.095566246
Si 4.303059970 10.915645612 9.451705537
Si 11.191855558 0.789835360 5.589652388
Si 11.049775055 0.583606795 13.174582856
Si 8.855706054 2.870781893 13.258796483
Si -0.206521986 10.887711851 1.702420673
Si -0.110761498 10.717718230 9.370565360
Si 2.104990799 8.681410055 1.684432524
Si 2.282756167 8.600146584 9.321691472
Si 13.265998750 3.107836193 5.630234351
Si 13.266596694 2.730983136 13.161895850
Si 10.857884709 5.181625969 5.619081644
Si 11.048081351 5.031112830 13.162634308
Si 1.619276677 3.659044422 7.865460427
Si 8.814264448 2.823187179 5.638909283
Al 1.096259705 6.722183134 7.149852322
Al 6.226488560 12.269116032 4.192586992
Al 6.008215749 12.223801354 11.789757044
Al 7.088398338 1.511604302 7.900032784
Cu1 3.318430286 8.071932277 6.181336933
Ru2 5.161137187 9.755789033 5.208386862
H 8.112156259 2.894513777 9.562127543
H 7.326437624 11.032270563 10.187467691
C 6.935369063 8.828098030 5.475232281
H 7.038192633 7.898115834 4.894607935
H 7.748395470 9.516978932 5.206838976
H 6.961775902 8.611524009 6.561069286
H 5.026274140 7.290461707 4.639075874
End final coordinates

Cu-O-Zr-product-2
Final energy = -6817.7967346217 Ry
CELL_PARAMETERS (angstrom)
13.816672096 0.026776249 -0.011828930
-1.408406185 13.617810460 -0.022343649
-0.005569044 0.006669328 15.015412987

ATOMIC_POSITIONS (angstrom)
O 3.216966589 0.537057481 3.282743538
O 2.206734604 13.764699655 10.748781269
O 5.202004346 10.965620279 3.456383171
O 4.870454940 11.308551430 10.899932011
O 7.896770423 11.493191122 7.727513441
O 7.754385338 11.646276058 0.548765781
O 10.780913221 -0.007200527 7.036213033
O 9.421391012 13.474701644 14.585109842
O 8.267368791 2.568045005 7.104123431
O 8.100090509 2.558884529 14.704487449
O 5.198296991 2.283540306 3.735673529
O 5.310970193 2.141832756 11.198858561
O 12.793506159 10.946446462 0.376320026
O 12.995446712 10.666917802 7.848010643
O 2.202941052 7.693202909 0.412651044
O 2.226490952 8.009456125 7.831740629
O 1.361608475 5.222074553 3.327707197
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O 3.160403347 0.508211968 8.154351810
O 5.198510978 11.200177438 0.770281964
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O 7.604040294 11.676338567 10.864308725
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O 11.942242911 10.271807551 13.010962712
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O 7.281080618 0.321752511 11.497161942
O -0.388920599 7.176477495 3.705717313
O -0.324164490 6.756328561 11.149621694
O 0.560100936 12.247272792 1.985591850
O 0.517481561 12.216499137 9.486062464
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Si 11.896363442 6.854961874 10.845754185
Si 1.320161872 3.602564714 3.305006705
Si 1.403480078 3.393235255 10.866643969
Si 1.295117578 6.640806667 14.562901384
Si 11.673203639 10.122775838 7.072221502
Si 11.594133954 10.191197148 14.596594148
Si 6.338875449 11.933037321 7.432520048
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Si 3.897114615 1.695052064 7.291195859
Si 4.008815137 1.562327142 14.740174113
Si 6.762081756 1.826304708 3.637422763
Si 6.894562169 1.826567340 11.191277089
Si 9.400165589 12.181690552 3.517902367
Si 9.293212414 11.983008288 10.868188201
Si 1.141926890 6.701442759 3.938001275
Si 1.257312610 6.512252473 11.438364877
Si 11.473420215 9.949688770 3.987556849
Si 11.474552111 9.920352441 11.498406309
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Si 1.638054337 3.499857028 0.236838821
Si 1.914746792 13.133364526 2.021311957
Si 1.908765153 13.043741213 9.319648756
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Si 4.249584051 10.947971216 9.471844026
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Si 11.041400599 0.593762215 13.191218458
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Si -0.205391281 10.837664493 1.790373576
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Si 13.248212111 2.750031584 13.118154455
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Si 11.000469898 5.024673767 13.151604473
Si 1.661948562 3.667423114 7.863867261
Si 8.858066962 2.842139054 5.633183067
Al 1.131741492 6.738784496 7.141920633
Al 6.180917319 12.350327992 4.210230339
Al 6.005835543 12.245624909 11.774241983
Al 7.116554742 1.528059415 7.860878612
Cu1 3.433815083 8.315511247 6.338384171
Zr2 5.554004668 9.519877578 5.115529771
H 8.071084191 2.928125882 9.547019854
H 7.329712444 11.118857799 10.103398794
C 7.472475502 8.525425383 5.499550263
H 7.766539499 7.785113170 4.739775243
H 8.280109518 9.270207771 5.588214077
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End final coordinates

Cluster models from Priroda

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29 18.36889027 23.94515655 5.07109760
8 16.50438712 14.47916382 3.27736062
8 15.24114349 28.40572375 3.28092802
8 17.21109978 14.28087517 10.78738011
8 18.55096125 24.96542095 3.34628994
8 18.29420172 25.49155371 10.96284459
8 21.31641023 26.04651284 7.31670080
8 23.09031844 28.08428793 7.01984306
8 24.53388410 13.48991886 14.58995361
8 21.30476766 16.41558405 6.75147860
8 21.72843815 16.88588735 14.94758259
8 18.71188104 16.04606880 3.93885337
8 18.92638482 16.32304778 11.61188045
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8 26.24910207 24.81141635 8.08081646
8 15.33433080 21.80134047 0.44167311
8 15.34170737 22.08652675 7.86060863
8 15.33886715 19.53624206 3.31395536
8 15.21534482 19.11298206 11.10970274
8 13.67901176 17.55094018 4.33307893
8 13.63269766 17.05624993 12.05708305
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8 23.32607306 27.52618664 4.28071221
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14 17.12140495 15.70153615 4.24464914
14 17.47131510 15.60631030 11.81447436
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14 25.47049881 20.99585994 10.73242561
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13 19.55719391 26.25102709 4.09202626
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1 17.82366752 13.52125506 10.81497377
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29 19.03716443 23.82422037 6.31434315
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8	15.61028607	28.42026453	0.65034792
8	16.52644543	14.49176840	8.22101033
8	18.32258920	25.53422622	0.46460623
8	19.08707878	25.26308303	8.54177727
8	21.26495280	25.61408154	3.96199109
8	21.22296193	25.44698001	10.93257392
8	13.59019832	16.99827246	6.97116844
8	27.51194420	16.59829213	14.82826877
8	24.18928364	20.42318147	6.65883419
8	25.22250721	20.17063192	14.22711144
8	25.11933137	22.48550551	3.58716448
8	24.94988893	22.43639942	11.39181842
8	12.32044491	24.72944811	2.96694424
8	26.27425832	24.76418698	2.92470436
8	26.45357989	24.72304065	10.80322441
8	15.13144101	22.21631028	3.13906817
8	15.77639696	21.63570081	10.50159241
8	14.69238049	19.25652214	7.92927917
8	16.46270822	26.30760726	2.22168409
8	16.53285894	26.20814923	9.13506285
8	23.54990439	15.93192841	5.57448910
8	23.55621822	15.75906018	13.50419569
8	14.21272476	24.00341337	1.21889750
8	14.47287564	23.91010909	9.72853480
8	25.50575145	18.22053330	5.71328656
8	25.88133242	17.89645213	13.07640948
8	16.83201362	15.15182869	5.70875735
8	17.40360253	15.06331428	13.40155978
8	19.15657421	25.71048723	5.89906231
8	20.09603195	26.28954861	13.31033985
8	22.91635337	26.51846933	1.88216076
8	23.08194887	26.80292961	9.44206460
8	20.73320575	15.52038933	1.97976571
8	20.66489250	16.56992255	9.61983795
8	25.64644572	24.31815391	5.53244881
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8	14.99753132	21.07392748	5.54029907
8	14.82232770	21.09474761	12.96529192
8	14.67819495	17.49946170	1.79877517
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8	25.70220312	20.45711344	1.81684601
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8	23.86923199	25.58860485	7.11713921
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8	23.73756883	24.74884902	11.13875676
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8	19.19118223	27.84602768	7.72415353
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8	20.75834485	14.06574011	4.22720864
8	19.22514958	27.82704630	3.89341469
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8	13.15491587	20.91194039	10.83341684
8	27.11782926	20.88649272	10.92518674
8	13.79329925	26.66077779	1.73645216
8	16.83599971	23.62875979	1.66984228
8	17.16564512	23.62928194	9.29025087
8	26.12295889	15.13647893	13.05410380
8	22.76184419	18.46798213	5.55968581
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14	25.52016779	20.89728935	3.40094853
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14	14.99178288	17.91621118	3.37969633
14	14.88323579	17.47016252	11.03974921
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14	14.57196243	20.88171487	3.96362442
14	14.71206485	20.66310195	11.36388427
14	25.17217676	24.08683729	3.95878145
14	25.19672567	24.05749429	11.63137818
14	25.06910591	21.43872624	7.63636452
14	15.26185741	27.41476345	1.92951143
14	17.55861893	25.10418174	1.88861068
14	17.78546897	25.16577730	9.55940709
14	24.59923991	14.50302097	13.27398528
14	22.47809481	16.98443879	13.46490366
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14	15.35644954	22.88565208	1.64869977
14	15.71745347	22.85909433	9.41897025
14	26.87899909	16.59118883	13.29441220
14	24.22060091	19.26018155	5.49113810
14	24.74279563	19.07859539	13.07045933
14	14.79361515	17.64267042	7.97337050
14	22.21100021	16.92636113	5.58774633
13	14.22824592	20.71488352	7.07930629
13	19.36696548	26.11628026	4.19785670
13	19.67534574	26.45292296	11.62716690
13	20.22245855	15.72205888	8.14166854
1	24.36638056	13.92094168	15.44585509
1	23.34430071	13.61054990	11.63862691
1	27.54826560	17.45788383	15.27375858
1	27.87819150	16.09613168	11.40203794
1	24.79597177	21.04263718	14.22937773
1	21.01169118	17.52230449	15.06640037
1	15.49980362	28.08483841	-0.25562718
1	14.45459690	28.34142296	3.85055800
1	11.40931963	25.05461271	3.01846970
1	11.83592223	24.51738359	-0.19371730
1	23.40769796	15.01357539	5.86245059
1	25.26195714	17.27527718	5.69547702

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   1   18.33474370  27.98704241   3.53769590
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   1   19.63200776  28.38177424  10.11409711
   1   11.91270545  20.56472942   7.63347223
   1   20.40584090  13.42911613   7.58191765
   1   27.51123065  19.99481141  10.93070219
   1   26.80148253  21.28175909   6.20908324
   1   27.08541520  19.62113180   4.38188995
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   1   27.05896121  24.30217307   7.90712399
   1   26.57357100  25.65252524   3.17157305
   1   22.33202453  27.91505737  12.10383543
   1   22.68535453  28.90156919   7.37359433
   1   23.22437378  27.65662055   5.25382269
   1   23.04241581  27.46722075   1.70385250
   1   18.67611056  28.32658400   7.05001719
   1   12.45783569  20.85721420   4.60977289
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   1   13.75966977  17.32736855   5.29777459
   1   16.27300881  13.68147040   3.79203569
   1   20.26371908  16.07772685   1.33477694
   1   20.79288631  13.33112100   3.59471099
   1   16.76335754  14.49633061   9.18931011
   1   12.76358325  17.06253769  11.61571016
   1   17.82366752  13.52125506  10.81497377
   1   16.50396243  14.79386895  13.63236268
   1   15.73897318  21.15544942  13.28128602
   1   12.87522754  21.84768062  10.82714231
   1   13.38087340  16.05556130   7.08542247
   1   20.81878872  14.00932731  10.32809275
$end

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multip=3
cartesian
   8   -0.10852515  -0.15189316  -0.00000077
   8    0.86786215   0.61452398   0.00000081
$end

Water-PBE-Priroda
$molecule
charge=0
multip=1
cartesian
   8    0.00000000  -0.07247149  -0.00000002
   1    0.75901377   0.53221960   0.00000001
   1   -0.75901377   0.53221960   0.00000001
$end

Cu3O3-cluster-model-doublet
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  29   18.19287226  23.23195755   3.84955310
   8   18.08383644  22.48714520   7.01856792
  29   18.98510634  23.86400816   6.37224769
   8   19.70106790  23.17754851   4.85612142
   8   16.53001164  14.47440479   3.28752934
   8   15.19115032  28.47622134   3.23624714
   8   17.23490669  14.29672477  10.76691420
   8   18.61927711  25.11948333   3.12000907
   8   18.42021239  25.53202257  10.91027822
   8   21.30298871  26.20123742   7.82407393
   8   23.14915518  28.08822314   7.10020764
   8   24.46445994  13.48461797  14.58243352
   8   21.34505611  16.57406522   6.88730222
   8   21.58855799  16.77944886  14.84405884
   8   18.78479454  15.95860909   3.83341001
   8   18.91761209  16.32978781  11.60072893
   8   12.19967401  25.34168905   0.17008066
   8   26.25677737  24.81678234   8.10978325
   8   15.65676130  21.87660656   0.46177639
   8   15.43563476  22.04861433   7.84646235
   8   15.39670936  19.47163978   3.35713564
   8   15.18290131  19.10790840  11.12201003
   8   13.76227341  17.37909115   4.30710983
   8   13.64285696  16.99553444  12.03129004
   8   28.05567401  16.69111322  12.14865891
   8   24.30709559  19.93540257   3.99130287
   8   24.63020085  19.76179247  11.57413156
   8   24.34147700  22.91454569   7.64179449
   8   23.57493628  27.45633734   4.36023107
   8   24.28391927  13.62809631  11.88151554
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   8   21.47781715  16.96919014  12.10766265
   8   18.57056121  16.20472403   7.84543979
   8   15.36975998  28.48341330   0.61844353
   8   16.41490176  14.55144715   8.26126048
   8   18.15685828  25.35759553   0.37049751
   8   18.91531835  25.16642187   8.25775846
   8   21.38631879  25.88035824   3.82086852
   8   21.27890391  25.48679736  10.91678979
   8   13.46161601  17.02039041   6.99584982
   8   27.49571415  16.59462812  14.83735999
   8   24.17417456  20.40760692   6.66712747
   8   25.19028733  20.15620460  14.26555973
   8   25.17036533  22.47406632   3.58300523
   8   24.94227281  22.41882472  11.39147462
   8   12.22434957  24.55694051   2.82930005
   8   26.45641754  24.69690395   3.06202337
   8   26.45271463  24.72335165  10.80761059
   8   14.83868251  22.12547438   3.09475697
   8   15.74837035  21.65547349  10.50440262
   8   14.59365099  19.27286041   7.91715863
   8   16.43116455  26.40800476   2.06828177
   8   16.51702487  26.22681095   9.09760903
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   8   23.49623923  15.73039191  13.41559567
   8   14.34083171  24.05373906   1.23950964
   8   14.43212554  23.87724722   9.61526636
   8   25.50596268  18.22015472   5.74109070
   8   25.84122376  17.87471243  13.09857704
   8   17.07225657  15.13995146   5.79766946
   8   17.38840411  15.10895055  13.38681875
   8   19.39805739  25.79069088   5.87528856
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   8   23.26148903  26.54091367   1.88748063
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   8   20.77168138  16.54561351   9.60746379
   8   25.63748011  24.23569780   5.59667974
   8   25.52832870  24.23242291  13.26952165
   8   14.95172918  21.07188034   5.56914311
   8   14.82182646  21.06974146  12.97283714
   8   14.80256542  17.44274752   1.82915596
   8   14.43679724  17.05517081   9.48070133
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   8   25.01358775  20.80734044   9.18943741
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   8   23.74750674  24.73578392   3.75397948
   8   23.74754291  24.73403881  11.23773714
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   8   12.93463409  20.40795548   3.89597711
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   8   27.10000587  20.87205607  11.02016144
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   8   16.82594982  23.67061719   2.16984715
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   1   11.40931963  25.05461271   3.01846970
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   1   25.26195714  17.27527718   5.69547702
   1   18.98001022  24.86496617   0.21240233
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   1   27.08541520  19.62113180   4.38188995
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$end



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   8   18.14171646  22.46812068   7.05154876
  29   19.12940887  23.63224641   6.14593003
   8   19.91712886  23.04330878   4.62379733
   8   16.52153242  14.47718270   3.28792151
   8   15.18717147  28.48409282   3.23336665
   8   17.23076661  14.29370003  10.76886040
   8   18.62901570  25.10901877   3.10977236
   8   18.32295403  25.52127981  11.06604414
   8   21.31034972  26.14195180   7.62349753
   8   23.15035988  28.09473970   7.08456585
   8   24.45976235  13.48560928  14.58139605
   8   21.35135464  16.57829303   6.89361614
   8   21.59258674  16.78203695  14.84597864
   8   18.78040627  15.95764465   3.81744621
   8   18.91562076  16.32862314  11.59736812
   8   12.18903300  25.34368237   0.17561041
   8   26.25842596  24.81975113   8.09930903
   8   15.63145800  21.87128358   0.44447808
   8   15.45022886  22.06414345   7.85582678
   8   15.40569982  19.47577585   3.37269937
   8   15.18403513  19.10965895  11.11802302
   8   13.75796315  17.38877802   4.30757249
   8   13.64521957  16.99318947  12.02555684
   8   28.05540920  16.69097663  12.14889305
   8   24.30378954  19.93763789   3.99248390
   8   24.63002752  19.76994277  11.57247417
   8   24.34320626  22.92167698   7.62225247
   8   23.54654464  27.45413055   4.34822617
   8   24.28409846  13.63002157  11.88040265
   8   23.01778672  27.21998802  12.13922090
   8   21.31965856  16.68967258   4.15799167
   8   21.47456354  16.96831251  12.11029330
   8   18.57563330  16.20320212   7.84647827
   8   15.39267106  28.48691029   0.61984938
   8   16.41898849  14.55075306   8.25964465
   8   18.17870235  25.39201389   0.37231436
   8   19.01232952  25.23766342   8.49273262
   8   21.33637624  25.87869768   3.94469381
   8   21.23883372  25.46292614  10.92452009
   8   13.46830841  17.01967430   6.99001123
   8   27.49022012  16.59513883  14.83727771
   8   24.17456221  20.40739950   6.66987016
   8   25.18969807  20.15584035  14.26507791
   8   25.15215943  22.47786308   3.56844022
   8   24.94113922  22.42818486  11.39516559
   8   12.23346951  24.56950312   2.83776451
   8   26.40067333  24.71097427   3.02188267
   8   26.44515022  24.72947332  10.80833775
   8   14.88023702  22.13344114   3.09398206
   8   15.75714760  21.65737952  10.51176511
   8   14.61079048  19.27717572   7.89831964
   8   16.43812439  26.41265785   2.08020529
   8   16.51401161  26.21260640   9.14003727
   8   23.59398744  15.90503906   5.52006542
   8   23.49676144  15.73287916  13.41346558
   8   14.33357191  24.05434774   1.23567527
   8   14.43905294  23.87957999   9.62934187
   8   25.50580264  18.22011967   5.74174675
   8   25.83966647  17.87617186  13.09236028
   8   17.08290506  15.13855583   5.79608567
   8   17.38575656  15.11588448  13.38641927
   8   19.26590629  25.62962533   5.92311648
   8   20.11836376  26.30156681  13.31323514
   8   23.10411036  26.51794297   1.89352772
   8   23.14414459  26.82585861   9.48730387
   8   20.59467153  15.34552296   1.88139456
   8   20.77457602  16.54503103   9.60979751
   8   25.63412678  24.24110839   5.57278904
   8   25.48315634  24.26422527  13.26180418
   8   14.97628892  21.10835856   5.57576667
   8   14.82143409  21.06626573  12.97426269
   8   14.80202088  17.44394117   1.83274721
   8   14.43659704  17.06410403   9.47327769
   8   25.73282828  20.42846461   1.82602320
   8   25.01165599  20.82303105   9.18990368
   8   16.47738645  17.13554711   4.00570260
   8   16.25707651  16.69643556  11.45384307
   8   23.86250542  25.54906410   7.17928699
   8   23.69962364  24.73010659   3.75681722
   8   23.73078858  24.73798210  11.18743957
   8   16.16193401  17.14731404   7.35620799
   8   20.57183634  14.04373436   8.32155925
   8   19.23949302  27.86165633   7.69227988
   8   12.48507773  21.15845301   7.11236175
   8   26.64504147  21.54365247   7.14305656
   8   20.73987698  14.06004797   4.23164383
   8   19.08895136  27.85262497   4.12919120
   8   20.86181015  14.39751962  11.23138877
   8   20.03690396  28.05531575  10.93564410
   8   12.95556193  20.43151847   3.89629655
   8   26.91012743  20.58521066   4.34596220
   8   13.14328357  20.90860941  10.84367981
   8   27.10038134  20.87304598  11.02061606
   8   13.73849657  26.63744694   1.87194417
   8   16.83656534  23.67073183   2.10925638
   8   17.13758308  23.63330547   9.41328067
   8   26.09966692  15.13121197  13.08513285
   8   22.75736806  18.43438403   5.55727272
   8   23.21779549  18.46660716  13.42159550
   8   17.36678830  21.84378783   4.56374504
  14   22.85333987  26.64459404   7.86449798
  14   17.20689451  15.67380262   4.23584522
  14   17.42904628  15.60989731  11.80474384
  14   25.53065907  20.88990617   3.40773880
  14   25.45982918  20.98211243  10.77581899
  14   15.07997549  17.82381992   3.42918482
  14   14.86529127  17.49208103  11.00931933
  14   24.99383944  24.35273616   7.08481718
  14   19.68461219  26.27727723   7.40570792
  14   17.08702417  15.75675016   7.34923506
  14   20.33920060  15.51931306   3.51644242
  14   20.48469671  16.00814001  11.23458642
  14   22.88156576  26.17594742   3.51583142
  14   22.86375712  26.10045227  10.94425461
  14   14.57417072  20.76072746   3.97834547
  14   14.71168184  20.67858821  11.35983265
  14   25.18945012  24.07884986   3.96589899
  14   25.20394224  24.04678939  11.63976426
  14   25.06670190  21.40229588   7.63879234
  14   15.16957516  27.48041593   1.91396016
  14   17.51632262  25.20721142   1.87732222
  14   17.74905671  25.15786828   9.58651736
  14   24.58137743  14.48965144  13.26473528
  14   22.47247795  16.99337745  13.45963509
  14   13.11371573  25.13270442   1.54196639
  14   15.38078717  22.87870082   1.73056412
  14   15.69880083  22.82169143   9.34111388
  14   26.86118895  16.58898294  13.30283019
  14   24.19669419  19.23123565   5.49798772
  14   24.73163225  19.08621295  13.08303462
  14   14.71184852  17.66661107   7.93975204
  14   22.21179566  16.87276070   5.54615017
  13   14.20445827  20.83396811   7.22402021
  13   19.65381310  26.19528254   4.19179988
  13   19.71000276  26.47266927  11.62962187
  13   20.24314595  15.74025675   7.92841677
   1   24.36638056  13.92094168  15.44585509
   1   23.34430071  13.61054990  11.63862691
   1   27.54826560  17.45788383  15.27375858
   1   27.87819150  16.09613168  11.40203794
   1   24.79597177  21.04263718  14.22937773
   1   21.01169118  17.52230449  15.06640037
   1   15.49980362  28.08483841  -0.25562718
   1   14.45459690  28.34142296   3.85055800
   1   11.40931963  25.05461271   3.01846970
   1   11.83592223  24.51738359  -0.19371730
   1   23.40769796  15.01357539   5.86245059
   1   25.26195714  17.27527718   5.69547702
   1   18.98001022  24.86496617   0.21240233
   1   15.68417467  20.92546602   0.65726132
   1   14.64884221  24.79084273   9.34111451
   1   16.72596318  27.10839426   9.45565630
   1   18.33474370  27.98704241   3.53769590
   1   19.73374121  26.87224256  13.99021208
   1   19.63200776  28.38177424  10.11409711
   1   11.91270545  20.56472942   7.63347223
   1   20.40584090  13.42911613   7.58191765
   1   27.51123065  19.99481141  10.93070219
   1   26.80148253  21.28175909   6.20908324
   1   27.08541520  19.62113180   4.38188995
   1   26.31520253  24.80897135   9.83131222
   1   26.03841283  25.04280623  13.43643477
   1   26.33548474  20.96700052   1.28720631
   1   27.05896121  24.30217307   7.90712399
   1   26.57357100  25.65252524   3.17157305
   1   22.33202453  27.91505737  12.10383543
   1   22.68535453  28.90156919   7.37359433
   1   23.22437378  27.65662055   5.25382269
   1   23.04241581  27.46722075   1.70385250
   1   18.67611056  28.32658400   7.05001719
   1   12.45783569  20.85721420   4.60977289
   1   14.35920276  16.58776973   1.73656295
   1   13.75966977  17.32736855   5.29777459
   1   16.27300881  13.68147040   3.79203569
   1   20.26371908  16.07772685   1.33477694
   1   20.79288631  13.33112100   3.59471099
   1   16.76335754  14.49633061   9.18931011
   1   12.76358325  17.06253769  11.61571016
   1   17.82366752  13.52125506  10.81497377
   1   16.50396243  14.79386895  13.63236268
   1   15.73897318  21.15544942  13.28128602
   1   12.87522754  21.84768062  10.82714231
   1   13.38087340  16.05556130   7.08542247
   1   20.81878872  14.00932731  10.32809275
$end
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Table SI1: Relative Energies of optimized periodic [Cu-O-M]-H_2MOR species. These are the analogues of the $[Cu_2O]^{2+}$ active site balancing the charges of two aluminate tetrahedra. Total energies are given in Rydberg while relative energies are in kcal/mol.

	Cu-O-M-species					Relative Energies			
CuCoO	singlet	quintet	triplet			singlet	quintet	triplet	
	-6649.13895918	-6649.16392267	-6649.15621300			7.83233243	0.00000000	2.41892053	
CuCrO	doublet	quartet	sextet			doublet	quartet	sextet	
	-6735.40470457	-6735.46251885	-6735.37304465			18.13931707	0.00000000	28.07266446	
CuFeO	doublet	quartet	sextet			doublet	quartet	sextet	
	-6628.85506953	-6628.91369765	-6628.90833941			18.39466059	0.00000000	1.68115584	
CuMn	singlet	triplet	quintet	septet		singlet	triplet	quintet	septet
	-6773.64508998	-6773.68930493	-6773.74378436	-6773.69596147		30.96550977	17.09300288	0.00000000	15.00450
CuNiO	doublet	quartet				doublet	quartet		
	-6672.79068119	-6672.79327276				0.81310897	0.00000000		
CuTiO	doublet	quartet				doublet	quartet		
	-6671.08978812	-6670.93884271				0.00000000	47.35934881		
CuVO	singlet	quintet	triplet			singlet	quintet	triplet	
	-6701.35476836	-6701.23672954	-6701.35596816			0.37643905	37.41129588	0.00000000	
CuMoO	doublet	quartet	sextet			doublet	quartet	sextet	
	-6851.01384159	-6851.04281346	-6850.90367902			9.08996767	0.00000000	43.65363925	
CuNbO	singlet	quintet	triplet			singlet	quintet	triplet	
	-6821.49822742	-6821.34280957	-6821.51553789			5.43118593	54.19376949	0.00000000	
CuPdO	doublet	quartet				doublet	quartet		
	-6818.09783595	-6818.06904377				0.00000000	9.03358966		
CuRhO	singlet	quintet	triplet			singlet	quintet	triplet	
	-6957.18730449	-6957.13088496	-6957.17935418			0.00000000	17.70171217	2.49442169	
CuRuO	doublet	quartet	sextet			doublet	quartet	sextet	
	-6918.68209148	-6918.66409850	-6918.61353991			0.00000000	5.64532446	21.50815791	
CuAgO	singlet	triplet				singlet	triplet		
	-6842.31584042	-6842.31905484				1.00852910	0.00000000		
CuZrO	doublet	quartet				doublet	quartet		
	-6794.59885944	-6794.41575114				0.00000000	57.45050379		

Table SI2: Relative Energies of optimized periodic [Cu-M]-H_2MOR species. These are the species formed after auto-reduction. Total energies are given in Rydberg while relative energies are in kcal/mol.

	Cu-M-species					Relative Energies			
CuCo	singlet	quintet	triplet			singlet	quintet	triplet	
	-6607.35040809	-6607.41622096	-6607.40865544			20.64888668	0.00000000	2.37369325	
CuCr	doublet	quartet	sextet			doublet	quartet	sextet	
	-6693.51284138	-6693.63650651	-6693.66096976			38.80012004	0.00000000	-7.67538138	
CuFe	doublet	quartet	sextet			doublet	quartet	sextet	
	-6587.07702161	-6587.14554689	-6587.16292051			26.95090872	5.45099934	0.00000000	
CuMn	singlet	triplet	quintet	septet		singlet	triplet	quintet	septet
	-6731.83122940	-6731.87338205	-6731.97524723	-6731.99190552		50.41237366	37.18691650	5.22656347	0.000000
CuNi	doublet	quartet				doublet	quartet		
	-6631.07119572	-6631.06060100				0.00000000	3.32410929		
CuTi	doublet	quartet				doublet	quartet		
	-6629.20444056	-6629.18063127				0.00000000	7.47020045		
CuV	singlet	quintet	triplet			singlet	quintet	triplet	
	-6659.49467789	-6659.48709896	-6659.50010348			1.70228700	4.08018766	0.00000000	
CuMo	doublet	quartet	sextet			doublet	quartet	sextet	
	-6809.15805137	-6809.20164694	-6809.19776479			13.67817548	0.00000000	1.21803039	
CuNb	singlet	quintet	triplet			singlet	quintet	triplet	
	-6779.59697570	-6779.59435247	-6779.61977216			7.15242352	7.97546587	0.00000000	
CuPd	doublet	quartet				doublet	quartet		
	-6776.43300587	-6776.37435324				0.00000000	18.40235064		
CuRh	singlet	quintet	triplet			singlet	quintet	triplet	
	-6915.45567299	-6915.41183315	-6915.45926442			1.12681655	14.88163211	0.00000000	
CuRu	doublet	quartet	sextet			doublet	quartet	sextet	
	-6876.90270013	-6876.90941863	-6876.88831765			2.10793945	0.00000000	6.62046413	
CuAg	singlet	triplet				singlet	triplet		
	-6800.71698889	-6800.67482063				0.00000000	13.23035483		
CuZr	doublet	quartet				doublet	quartet		
	-6752.70457574	-6752.65495525				0.00000000	15.56850317		

Table SI3: Relative Energies of optimized periodic [Cu_6W]-H_2MOR species. These are the species with hexaaquo metal centers (prior to calcination but after ion-exchange). Total energies are given in Rydberg while relative energies are in kcal/mol.

	Cu6W-species				Relative Energies		
Co	doublet	quartet			doublet	quartet	
	-6659.04529343	-6659.07849562			10.41723692	0.00000000	
Cr	singlet	triplet	quintet		singlet	triplet	quintet
	-6745.22929817	-6745.25858467	-6745.34383377		35.93571630	26.74703300	0.000000
Fe	singlet	triplet	quintet		singlet	triplet	quintet
	-6638.75725890	-6638.75544932	-6638.82150539		20.15743261	20.72519105	0.000000
Mn	doublet	quartet	sextet		doublet	quartet	sextet
	-6783.52968123	-6783.56074570	-6783.66339987		41.95442388	32.20789982	0.000000
Ni	singlet	triplet			singlet	triplet	
	-6682.68940671	-6682.73256451			13.54082449	0.00000000	
Ti	singlet	triplet			singlet	triplet	
	-6680.88866648	-6680.91623556			8.64984020	0.00000000	
V	doublet	quartet			doublet	quartet	
	-6711.17056505	-6711.22935985			18.44695669	0.00000000	
Mo	singlet	triplet	quintet		singlet	triplet	quintet
	-6860.77014621	-6860.78957941	-6860.85687653		27.21176800	21.11457235	0.000000
Nb	doublet	quartet			doublet	quartet	
	-6831.26276288	-6831.30452419			13.10267365	0.00000000	
Pd	singlet	triplet			singlet	triplet	
	-6828.01300509	-6827.96956677			0.00000000	13.62883806	
Rh	doublet	quartet			doublet	quartet	
	-6967.06682832	-6967.01023873			0.00000000	17.75506875	
Ru	singlet	triplet	quintet		singlet	triplet	quintet
	-6928.57576417	-6928.54104566	-6928.48096993		0.00000000	10.89298459	29.741834
Ag	doublet	quartet			doublet	quartet	
	-6852.21388454	-6851.87994351			0.00000000	104.77449907	
Zr	singlet	triplet			singlet	triplet	
	-6804.36823641	-6804.34758551			0.00000000	6.47925085	

Table SI4: Relative Energies of optimized periodic [Cu-O-M](CH_4)-H_2MOR species. These are the adduct complexes between the active sites and methane. Total energies are given in Rydberg while relative energies are in kcal/mol.

	CuOM-Methane-adduct					differences		
CuCoO	singlet	quintet	triplet			singlet	quintet	triplet
	-6672.35857719	-6672.38387431	-6672.37659351			7.93700935	0.00000000	2.2843619
CuCrO	doublet	quartet	sextet			doublet	quartet	sextet
	-6758.62477163	-6758.68239103	-6758.59467749			18.07817318	0.00000000	27.5202547
CuFeO	doublet	quartet	sextet			doublet	quartet	sextet
	-6652.07541910	-6652.13503884	-6652.12841982			18.70578285	0.00000000	2.0767274
CuMn	singlet	triplet	quintet	septet		singlet	triplet	quintet
	-6796.86102647	-6796.90916728	-6796.96530749	-6796.91834076		32.71832645	17.61407510	0.0000000
CuNiO	doublet	quartet				doublet	quartet	
	-6696.01288342	-6696.01304830				0.05173135	0.00000000	
CuTiO	doublet	quartet				doublet	quartet	
	-6694.31169160	-6694.15891399				0.00000000	47.93420430	
CuVO	singlet	quintet	triplet			singlet	quintet	triplet
	-6724.57981133	-6724.46059479	-6724.57690335			0.00000000	37.40436825	0.9123830
CuMoO	doublet	quartet	sextet			doublet	quartet	sextet
	-6874.23555073	-6874.26303238	-6874.12580473			8.62240891	0.00000000	43.0553810
CuNbO	singlet	quintet	triplet			singlet	quintet	triplet
	-6844.71850758	-6844.56440171	-6844.73623118			5.56080609	53.91175396	0.0000000
CuPdO	doublet	quartet				doublet	quartet	
	-6841.31789894	-6841.29212235				0.00000000	8.08744378	
CuRhO	singlet	quintet	triplet			singlet	quintet	triplet
	-6980.40760570	-6980.35300737	-6980.39937064			0.00000000	17.13030793	2.5837624
CuRuO	doublet	quartet	sextet			doublet	quartet	sextet
	-6941.90220739	-6941.89775284	-6941.83041381			0.00000000	1.39762174	22.5253434
CuAgO	singlet	triplet				singlet	triplet	
	-6865.53882610	-6865.53600823				0.00000000	0.88411094	
CuZrO	doublet	quartet				doublet	quartet	
	-6817.82094636	-6817.62924805				0.00000000	60.14563231	

Overall, we find that there are near-degenerate states for CuOCo (triplet and quintet), CuOFe (sextet and quaret), CuONi.(doublet and quartet, CuOV (singlet and triplet), CuORh (singlet and triplet), CuORu (doublet and quartet) as well as CuOAg (singlet and triplet). For these species, we have also examined the impact of spin-crossover on the methane C-H activation barriers.

On Spin-State Relative Energies.

To consider the relative spin state energies of the various species, we employed in all cases 5 different strategies in the periodic DFT calculations:

1) We specified only the overall multiplicity or total_magnetization.
2) We specified the total_magnetization and initial starting spin polarizations for each atom type. For example:
   tot_magnetization = 0.0
   starting_magnetization(1) = 0.00000e+00
   starting_magnetization(2) = 0.00000e+00
   starting_magnetization(3) = 0.00000e+00
   starting_magnetization(4) = 5.00000e-01
   starting_magnetization(5) = 5.00000e-01
3) We changed the different starting magnetizations for the Cu and M centers in the active site. Specifically, we used also ±0.2 and ±0.7
4) The optimized geometries and cell parameters of the high-spin (HS) states were used as staring points to re-optimize the low-spin (LS) and intermediate-spin (IS) states. The converse calculations were also performed, i.e. optimized structures of the LS and IS were used for the other spin states.
5) The optimized structures of the dicopper species as well as the analogous Cu-Rh heterometallic were used as starting points in the re-optimization of the LS, IS and HS states of each species.
6) For the lowest energy structures obtained with the 5-steps above, we considered then 3 more possibilities: A) we perturbed the atomic positions and reused the same SCF convergence algorithm. B) We perturbed the atomic positions and lowered the mixing beta to 0.1. C) We perturbed the atomic positions and removed random atomic orbitals from the initial charge density guess.

This 6-level protocol indicates at least 10 computations for each spin state.

Spin Crossover and Methane C-H Activations

Cu-O-Co-triplet: The C-H activation barriers via the separated CH_3 and surface-stabilized CH_3 pathways are 24.1 and 27.6 kcal/mol, respectively. These are for the triplet state and are to be compared to 25.5 and 28.1 kcal/mol for the quartet state (Table 3). Given that the adduct complex with methane prefers the quartet state by 2.3 kcal/mol (Table SI4), then spin crossover is not crucial here.

Cu-O-Fe-sextet: The C-H activation barriers via the separated CH_3 and surface-stabilized CH_3 pathways are 27.9 and 30.7 kcal/mol, respectively. These are for the sextet state and are to be compared to 28.7 and 30.3 kcal/mol for the quartet state (Table 3). Given that the adduct complex with methane prefers the quartet state by 2.1 kcal/mol (Table SI4), then spin crossover is not crucial here.

Cu-O-Ni-doublet: The C-H activation barriers via the separated CH_3 and surface-stabilized CH_3 pathways are 27.0 and 24.8 kcal/mol, respectively. These are for the doublet state and are to be compared to 23.5 and 24.0 kcal/mol for the quartet state (Table 3). Given that the adduct complex with methane prefers the quartet state by about 0.1 kcal/mol (Table SI4), then spin crossover is not crucial here.

Cu-O-V-triplet: The triplet state of the methane adduct is 0.9 kcal/mol less stable than the singlet state (Table SI4). The surface-stabilized singlet intermediate is +5.9 kcal/mol higher in energy than the adduct. The triplet is 4.0 kcal/mol higher in energy than the adduct (Table 3). Based on these, there is no reason to even consider the C-H activation barrier for this species.

Cu-O-Rh-triplet: The C-H activation barriers via surface-stabilized CH_3 pathways is 10.2 kcal/mol. This is for the triplet state and is to be compared to 9.1 kcal/mol for the singlet state (Table 3). Given that the adduct complex with methane prefers the singlet state by about 2.6 kcal/mol (Table SI4), then spin crossover is not crucial here.

Cu-O-Ru-quartet: The C-H activation barriers via surface-stabilized CH_3 pathways is 20.5 kcal/mol. This is for the quartet state and is to be compared to 24.7 kcal/mol for the singlet state (Table 3). Given that the adduct complex with methane prefers the singlet state by about 1.4 kcal/mol (Table SI4), then spin crossover is important here as it can reduce the barrier by almost 2.8 kcal/mol.

Cu-O-Ag-triplet: The C-H activation barriers via the separated CH_3 and surface-stabilized CH_3 pathways are 9.0 and 9.4 kcal/mol, respectively. These are for the triplet state and are to be compared to 5.0 and 5.1 kcal/mol for the singlet state (Table 3). Given that the adduct complex with methane prefers the singlet state by about 0.9 kcal/mol (Table SI4), then spin crossover is not crucial here.

Table SI6: Relative spin-state energies of species examined with periodic DFT and cluster-models.

Species		Cluster-model	Periodic model
Isolated $[Cu\text{-}OH]^+$	Only doublet state is considered		
Paired $[Cu\text{-}OH]^+$	Singlet & triplet states	Triplet favored by 2.5 kcal/mol	Triplet favored by 1.0 kcal/mol
$[Cu_2O]^{2+}$	Singlet & triplet states	Singlet favored by 3.8 kcal/mol	Singlet favored by 1.7 kcal/mol
$[Cu_3O_3]^{2+}$	Doublet & quartet states	Doublet favored by 0.3 kcal/mol	Doublet favored by 2.1 kcal/mol

Overall, the relative spin-state energies from the cluster-models are not far off from the periodic DFT calculations.

For the cluster model calculations, we ensured lowest-energy configurations by carrying out short TD-DFT calculations (stability-analyses). The lack of imaginary excitations indicate the lowest possible electron arrangement for that spin state.