

Supporting Information

Calculations of NO Reduction with CO over a Cu₁/PMA Single-Atom Catalyst: A Study of Surface Oxygen Species, Active Sites, and Reaction Mechanism

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2CO@Cu/PMA

O	0.57067	1.27439	-0.02913
O	-1.24026	-0.01362	-1.27197
O	-1.23135	0.03592	1.27265
O	-1.876	-1.2905	3.48923
O	-1.52908	-2.94982	1.36659
O	-1.43888	-2.97051	-1.31337
O	-3.34173	-1.71016	0.00396
O	0.54501	-1.28704	0.01994
O	-3.69242	-0.07031	-2.23291
O	-1.7964	1.24894	-3.51513
O	-1.76128	-1.46445	-3.46419
O	-3.36966	1.55036	-0.08008
O	-1.90808	1.40022	3.40892
O	-4.0678	2.88702	2.38941
O	-1.54017	3.01232	1.17204
O	1.13845	3.55895	1.31109
O	2.8186	0.05935	1.48722
O	1.18112	-3.49402	1.35108
O	-3.79329	0.02295	2.0531
O	-4.0366	2.77425	-2.55583
O	-1.50042	2.97193	-1.38935
O	-0.44989	5.38882	-0.10214
O	1.15377	3.50924	-1.42142
O	3.44162	2.42982	-2.83965
O	0.86673	1.2587	-2.94294
O	2.84761	0.01258	-1.50595
O	3.06392	-2.09966	0.03502
O	3.44488	2.54047	2.74623
O	0.8542	1.3685	2.90043
O	-0.13178	-0.13127	-5.30989
O	0.9231	-1.29067	-2.8915
O	-4.10644	-2.82211	-2.46855
O	-4.14725	-2.69742	2.60238
O	0.85926	-1.23266	2.93986
O	3.43072	-2.60409	-2.72698
O	1.2112	-3.55364	-1.29673
O	-0.66608	-5.29755	0.08241
O	3.38787	-2.50263	2.81536
P	-0.33261	0.00518	-0.00417
O	-0.1459	0.11748	5.28445
Cu	4.31736	-0.10258	0.02524
O	2.98664	2.26954	-0.03372

Mo	-0.39965	-3.60133	0.07255
Mo	-2.97403	-1.71091	-1.8129
Mo	-2.81237	1.79371	-1.85747
Mo	-0.07453	3.71444	-0.07507
Mo	2.22677	1.75982	-1.82017
Mo	2.15583	-2.05054	-1.71185
Mo	-0.51393	-0.11276	-3.63737
Mo	-2.82189	1.8599	1.81273
Mo	-0.43824	0.09343	3.60218
Mo	2.23638	1.8792	1.71881
Mo	-2.95957	-1.61856	1.99666
Mo	2.13385	-1.95294	1.77597
C	5.53858	-1.66055	0.16555
C	5.36312	1.60592	-0.08857
O	6.11078	-2.6472	0.28612
O	5.99876	2.56011	-0.10377
Cs	-0.20291	3.62947	-4.21746
Cs	-0.18392	-3.99375	4.12403
Cs	-0.22029	4.10383	3.85171
TS1			
O	0.63216	1.2453	0.07189
O	-1.22175	0.12184	-1.2678
O	-1.22085	-0.03183	1.27448
O	-1.84112	-1.24871	3.1259
O	-1.54832	-2.67423	0.91924
O	-1.63958	-2.5424	-1.7645
O	-3.40647	-1.30342	-0.34087
O	0.50743	-1.3114	-0.07899
O	-3.82773	0.52923	-2.30943
O	-1.91997	1.89778	-3.62263
O	-1.95833	-0.78823	-3.80296
O	-3.33108	1.95577	-0.11859
O	-1.8091	1.45239	3.29791
O	-3.96714	3.1029	2.40408
O	-1.4234	3.27342	1.24545
O	1.24979	3.70722	1.27061
O	2.76304	0.20943	1.24546
O	1.09614	-3.31575	0.86756
O	-3.72521	0.25825	1.95013
O	-4.01277	3.41604	-2.51274
O	-1.4619	3.41254	-1.32757
O	-0.30516	5.70115	0.0329
O	1.23886	3.86893	-1.43647

O	3.45546	2.84913	-2.96999
O	0.83163	1.78626	-3.16499
O	2.75	0.37226	-1.79432
O	2.98946	-1.80003	-0.40467
O	3.45098	2.51378	2.68681
O	0.8385	1.43914	2.75992
O	-0.21804	0.63724	-5.56794
O	0.77017	-0.82115	-3.26961
O	-4.26888	-2.15605	-2.95971
O	-4.22246	-2.48438	2.08224
O	0.8504	-1.12149	2.56941
O	3.26281	-2.15824	-3.21103
O	1.06507	-3.15595	-1.7631
O	-0.8419	-4.9581	-0.57324
O	3.32848	-2.47293	2.32927
P	-0.32187	0.00798	0.00206
O	-0.17478	-0.05146	5.03688
Cu	4.29429	-0.37778	-0.05228
O	3.14856	2.5101	-0.16496
O	7.05497	-1.62764	-0.20504
C	5.9319	-1.37351	-0.14936
O	5.60801	2.42532	0.17253
C	4.79961	1.57863	0.10139
Mo	-0.53858	-3.27016	-0.4953
Mo	2.02956	-1.62105	-2.14313
Mo	2.06769	-1.85502	1.33664
Mo	-3.04807	-1.13746	-2.31878
Mo	-3.05164	-1.38217	1.48385
Mo	-2.79908	2.32514	-1.99031
Mo	-2.76701	2.11431	1.67802
Mo	0.00077	4.0178	-0.06166
Mo	2.23236	2.19247	-1.96557
Mo	2.20915	1.94329	1.64664
Mo	-0.49396	0.5676	-3.88457
Mo	-0.53834	0.05241	3.36491
Cs	-0.59858	4.74077	-3.72442
Cs	-0.3729	4.12302	4.05781
Cs	-0.12125	-3.7821	3.46302
CO ₂ *			
O	0.84599	-1.31076	0.04762
O	-1.07484	-0.61914	-1.4643
O	0.71642	1.09834	-0.8519
O	1.15174	3.78118	-0.36769

O	-1.31877	2.95022	0.03039
O	-3.34454	1.23706	-0.70457
O	-1.62606	2.09809	-2.53808
O	-0.91141	0.28615	0.91332
O	-1.91254	-0.30037	-3.94727
O	-1.70939	-2.78417	-2.90296
O	-3.71983	-1.07758	-1.99119
O	0.86639	-0.00397	-3.61904
O	3.20574	2.11993	-1.24533
O	3.35737	1.30894	-3.95037
O	2.81567	-0.47603	-1.74725
O	3.46946	-1.82399	0.48038
O	1.46946	-0.43902	2.69005
O	-1.40421	2.30651	2.63294
O	1.0837	2.70231	-2.87784
O	-0.15396	-2.10916	-5.25083
O	1.06776	-2.42945	-2.61569
O	3.76587	-3.09158	-2.04112
O	1.72765	-3.72044	-0.14926
O	0.09897	-5.17755	1.57188
O	-1.16045	-3.74585	-0.46524
O	-0.61967	-2.49893	2.10801
O	-1.00419	-0.32187	3.49518
O	4.28216	-1.00477	3.01687
O	3.53263	0.96176	1.13328
O	-3.92657	-3.74756	-1.35014
O	-2.78892	-1.88117	0.48238
O	-4.20138	1.3212	-3.47334
O	-0.78596	4.7679	-2.17856
O	1.24269	2.13959	1.8225
O	-3.34392	-2.05069	3.25519
O	-3.26134	0.42915	1.97442
O	-3.85018	3.11454	1.32825
O	0.56816	1.80715	4.51548
P	-0.09158	-0.14271	-0.34859
O	3.50871	3.79274	1.02973
Cu	0.42276	-1.84216	3.8032
O	2.37425	-3.47878	2.59405
O	1.16893	-3.37299	6.24382
C	0.88104	-2.78582	5.30311
O	4.16477	-4.65274	1.65249
C	3.27065	-4.06034	2.09537
Mo	-2.69229	1.93054	0.8779
Mo	-2.27551	-1.23318	2.20579

Mo	0.02602	1.25406	2.98741
Mo	-2.8929	0.64691	-2.62843
Mo	-0.35413	3.18952	-1.70546
Mo	-0.40022	-1.48247	-3.70241
Mo	2.12269	1.0877	-2.79234
Mo	2.39906	-2.29753	-1.37731
Mo	0.09479	-3.65814	0.78545
Mo	3.09729	-0.64071	1.82022
Mo	-2.71468	-2.54444	-1.35753
Mo	2.43174	2.66354	0.3207
Cs	-0.33775	5.14788	1.94825
Cs	-5.75725	-0.66889	0.32877
Cs	5.69344	0.12725	-1.11289

Cu-O_v/PMA

O	-1.29678	-1.19261	0.17371
P	-0.23212	-0.0569	0.00044
O	0.40042	-0.19173	-1.42841
O	0.87045	-0.21737	1.06567
O	2.36956	0.93959	2.81176
O	1.554	3.11678	1.0412
O	1.08183	2.50635	-1.48602
O	3.00042	0.94315	-0.29486
O	-0.89644	1.35475	0.09498
O	2.73134	-0.67527	-2.39804
O	0.43936	-1.73385	-3.62569
O	0.8737	0.91208	-3.78816
O	2.50551	-2.17125	-0.26424
O	1.99701	-1.74436	2.94744
O	3.30916	-3.93818	1.83052
O	0.51891	-3.68575	1.32642
O	-2.1321	-3.39822	1.61279
O	-2.90809	0.24819	1.90749
O	-1.0626	3.53449	1.28688
O	2.50512	-3.50412	-2.91663
O	0.15356	-3.30054	-1.32026
O	-1.12174	-5.5798	-0.054
O	-2.66887	-3.47127	-1.04688
O	-4.0177	-1.79331	0.65088
O	-5.0075	-2.17102	-1.9293
O	-2.2394	-1.43671	-2.73166
O	-3.57248	0.19032	-1.18636
O	-3.28834	2.4367	0.42619
O	-3.59048	-1.99818	3.5716

O	-0.90093	-1.3082	3.13854
O	-1.47658	-0.2639	-5.15676
O	-1.68849	1.205	-2.75063
O	3.3405	1.98802	-3.10856
O	4.31549	2.63934	1.63453
O	-0.53761	1.28363	2.99696
O	-4.17706	2.72603	-2.20819
O	-1.54556	3.44082	-1.39925
O	0.39595	5.18963	-0.52059
O	-2.90547	2.77669	3.31456
O	0.916	-0.11736	5.04146
Cu	4.06094	-0.56874	-0.67056
O	6.97203	-1.02726	-0.34744
C	5.83758	-0.85256	-0.46177
Mo	1.99955	1.14368	-2.43467
Mo	2.80721	1.86208	1.28516
Mo	-0.07464	3.55541	-0.30477
Mo	-1.02047	-0.34396	-3.50079
Mo	-2.95392	1.94222	-1.29346
Mo	-2.00954	1.9692	2.09974
Mo	0.73937	-0.16767	3.34601
Mo	-2.50987	-1.61597	2.29745
Mo	-3.55936	-1.79011	-1.08967
Mo	2.07358	-2.79281	1.44945
Mo	-1.1142	-3.87451	0.04744
Mo	1.50279	-2.31409	-2.19615
Cs	0.94079	3.57626	3.73134
Cs	-1.47479	-4.14684	-4.02586
Cs	-0.08946	-3.96253	4.00838
NO*			
O	-0.91736	0.57302	0.6591
O	0.93593	0.64545	-1.07006
O	-0.86459	-1.16485	-1.18974
O	-1.52875	-3.58362	-2.02272
O	1.22221	-3.22377	-1.53771
O	3.05097	-1.32185	-1.35089
O	1.17653	-1.21291	-3.3298
O	0.89056	-1.23522	0.66025
O	1.5802	1.48508	-3.49801
O	1.4794	3.30482	-1.52351
O	3.42257	1.38154	-1.59855
O	-1.15183	1.08019	-3.152
O	-3.43351	-1.58623	-1.88395

O	-3.69024	0.09934	-4.08206
O	-3.07467	1.00151	-1.39815
O	-3.3568	1.20354	1.34246
O	-1.00982	-1.48501	2.78469
O	1.44823	-3.78817	1.16627
O	-1.44657	-1.56681	-3.82044
O	-0.18626	3.66276	-3.7783
O	-1.07956	2.82932	-1.16601
O	-3.67802	3.5106	-0.31177
O	-1.46595	3.10517	1.48016
O	0.24162	3.25814	3.67047
O	1.19905	2.59667	1.09615
O	1.12994	0.53696	2.86505
O	1.61381	-2.14645	3.31337
O	-3.76696	-0.66871	3.38279
O	-3.01442	-1.49769	0.82876
O	3.69485	3.6148	0.12784
O	3.22614	0.93013	1.02206
O	3.83418	-0.333	-3.81522
O	0.32043	-3.88578	-4.1263
O	-1.29928	-3.44439	0.75543
O	3.80899	-0.18537	3.50214
O	3.38606	-1.82715	1.25879
O	3.77484	-4.00141	-0.48234
O	-0.41102	-4.26926	3.28355
P	0.0162	-0.30019	-0.23534
O	-3.87381	-3.96135	-0.40658
Cu	-0.16023	-0.34224	4.35008
O	-0.79298	0.16611	7.27175
N	1.3062	-1.866	4.51176
Mo	-2.58477	-0.31716	2.19861
Mo	-2.53453	2.23504	-0.17028
Mo	-2.49576	-0.36269	-2.95444
Mo	-2.57901	-2.87443	-0.57371
Mo	-0.02525	-2.79444	-2.88063
Mo	2.51465	-2.91384	-0.12764
Mo	-0.08673	-3.08264	2.11459
Mo	2.67245	-0.3212	2.22793
Mo	-0.17428	2.192	2.39608
Mo	2.56052	2.40196	-0.29669
Mo	2.55237	-0.16772	-2.69386
Mo	0.15039	2.34945	-2.73969
O	-1.42825	1.00643	3.23939
C	-0.56758	0.01096	6.16194

Cs	5.78702	-0.40037	-0.31461
Cs	-0.04633	5.48062	0.05294
Cs	-5.73712	-0.27768	-0.27502

TS₂

O	0.82069000	1.27707300	-0.53297800
P	-0.03399600	-0.02225500	-0.37506200
O	-0.88426100	0.09006200	0.93881000
O	0.92384900	-1.24938300	-0.29296600
O	1.49256400	-3.63032000	-1.33652200
O	-1.19311300	-3.08293900	-1.27192100
O	-3.21111500	-1.78699500	-0.20382400
O	-1.07452700	-2.67515600	1.34372600
O	-0.97450500	-0.19696900	-1.60317000
O	-1.39596700	1.62168000	3.03694700
O	-3.35067500	0.09390700	1.86313700
O	1.14125900	-1.05301500	2.63551200
O	3.40723900	-2.16209100	-0.25817100
O	3.87143500	-2.08888900	2.49060000
O	3.09088500	0.22856500	1.11545100
O	3.39148500	2.06754400	-0.81384100
O	1.04654200	0.89851900	-3.52209100
O	-1.55777000	-1.82904900	-3.75066300
O	1.50516700	-3.25397500	1.38252700
O	0.52109400	0.67395800	4.87622500
O	1.32052200	1.71217200	2.39838100
O	3.79334500	2.97275900	1.86585700
O	1.45929000	3.63402000	0.41921400
O	1.35798000	3.29992000	-2.23793900
O	-0.44950700	5.20508800	-0.89430500
O	-1.26356300	3.01184700	0.62699600
O	-1.26087700	2.63918900	-2.06794400
O	-1.70144500	0.83964900	-3.98433700
O	3.58229400	2.20676300	-3.57871800
O	2.91820900	-0.19363000	-2.09273400
O	-3.71151100	2.92521200	2.06966400
O	-3.14361100	1.48408900	-0.43344300
O	-3.69978000	-2.63252000	2.39835900
O	-0.14451200	-5.24088300	0.29450300
O	1.03508700	-1.71124300	-3.29017800
O	-3.97877800	2.32020000	-2.93127000
O	-3.44694400	-0.39145700	-2.43934200
O	-3.71401600	-3.21066400	-2.61222200

O	0.00015800	-0.47891400	-5.75314000
O	3.67470900	-2.69181600	-3.04402000
O	-1.87433200	-4.68736700	3.07316600
O	-1.43765600	-1.15405300	3.58661000
N	-1.20775800	-4.19580600	3.87828000
N	-0.96238300	-2.17009300	4.16642700
Cu	0.74574900	-2.96599200	3.40845600
Mo	2.41602200	-1.96977800	-2.13717100
Mo	2.57124000	2.17498300	0.98013200
Mo	2.38285600	1.79914600	-2.43440700
Mo	-0.29231400	-0.31311100	-4.08918200
Mo	-0.08943000	3.54653400	-0.76375400
Mo	-2.70486000	1.42249500	-2.22834900
Mo	-2.53026300	1.82604300	1.50609800
Mo	-2.51334700	-2.07941300	-2.18177800
Mo	0.16669000	0.47821800	3.21532700
Mo	-2.60758500	-1.66006100	1.50203400
Mo	0.22192700	-3.60572000	-0.00745000
Mo	2.70430000	-1.58592900	1.33760100
O	2.95535300	-4.52068100	4.89971000
C	2.18363400	-3.93299000	4.29721100
Cs	-5.81634800	-0.14592300	-0.30830100
Cs	5.71226300	-0.03243900	-0.85747800
Cs	-0.00887900	4.52130900	3.13605200

N2O2*

O	-0.87884	1.31694	-0.22271
O	0.91382	0.25687	-1.6654
O	-0.89979	-1.1939	-0.62307
O	-1.6194	-3.57593	0.38353
O	1.03554	-3.03352	0.50606
O	2.99958	-1.54896	-0.55037
O	1.20715	-2.65864	-2.12223
O	0.88841	-0.14494	0.87607
O	1.64144	-0.67137	-4.05668
O	1.64762	1.97823	-3.63123
O	3.49901	0.38	-2.28463
O	-1.12294	-0.68295	-3.65318
O	-3.52398	-1.97211	-0.82809
O	-3.70559	-1.78945	-3.64486
O	-2.96796	0.34797	-1.86608
O	-3.39112	2.20371	-0.02631
O	-1.04185	0.84588	2.74345
O	1.37542	-1.83947	2.86679

O	-1.54159	-3.09894	-2.27856
O	-0.03706	0.96452	-5.7465
O	-1.10208	1.88289	-3.21601
O	-3.67103	2.95829	-2.75172
O	-1.45178	3.70321	-1.08593
O	0.30071	5.21557	0.53616
O	1.28097	3.10933	-1.09197
O	1.13619	2.61248	1.55814
O	1.58648	0.80822	3.59896
O	-3.72716	2.03247	2.73011
O	-2.99604	-0.22326	1.21044
O	3.83745	3.20291	-2.41374
O	3.22307	1.72189	-0.04679
O	3.81122	-2.26749	-3.23589
O	0.13684	-5.13595	-1.17953
O	-1.3574	-1.88955	2.40916
O	3.78495	2.40842	2.57903
O	3.33758	-0.30252	1.8311
O	3.62449	-3.12429	1.69205
O	-0.42897	-0.97117	4.85827
P	0.01869	0.05342	-0.40406
O	-3.99417	-2.86225	1.75187
Cu	-0.38915	2.80912	3.4515
O	-2.32353	3.58171	5.67224
N	1.24282	1.82365	4.26938
Mo	-2.59406	1.61871	1.5112
Mo	-2.37822	2.20422	-1.93253
Mo	-2.43338	-1.40401	-2.57873
Mo	-2.74924	-2.14562	0.81628
Mo	-0.1313	-3.45764	-1.03319
Mo	2.47184	-1.95194	1.18912
Mo	-0.16663	-0.76218	3.17697
Mo	2.6573	1.50071	1.65588
Mo	-0.04888	3.58918	0.18435
Mo	2.6061	2.08082	-2.05952
Mo	2.54162	-1.34234	-2.574
Mo	0.20862	0.68823	-4.10092
O	-1.38964	3.18409	1.60596
C	-1.56264	3.40594	4.83787
Cs	-0.00757	-4.73531	2.83467
Cs	5.77552	-0.14459	-0.27704
Cs	-5.75429	0.23239	-0.62866
O	1.30324	4.57883	3.28206
N	2.34527	4.53168	3.78503

TS₃

O	-0.92256	-1.32	-0.07547
O	-0.91378	1.16674	-0.61098
O	0.84742	-0.37841	-1.6262
O	3.26196	-0.62698	-2.63805
O	3.00975	1.48854	-0.90904
O	1.19751	3.09356	0.09928
O	0.97487	2.3949	-2.51301
O	0.91746	0.19513	0.86909
O	-1.64695	2.94447	-2.52672
O	-3.52102	1.87756	-0.80149
O	-1.55123	3.61026	0.07483
O	-1.34963	0.40209	-3.49485
O	1.30741	-2.28489	-3.54205
O	-0.46111	-1.28221	-5.58518
O	-1.26422	-2.15196	-2.92455
O	-1.55595	-3.8344	-0.76453
O	1.22062	-2.54416	1.65112
O	3.47684	0.40253	1.50403
O	1.34048	0.31511	-4.16889
O	-3.9328	1.64738	-3.54175
O	-3.11549	-0.52627	-1.84184
O	-3.87261	-3.13597	-2.40518
O	-3.39809	-2.23535	0.26373
O	-3.66143	-1.84674	3.01197
O	-3.00015	0.2873	1.33007
O	-0.90902	-0.76106	2.88279
O	1.75024	-0.41992	3.23993
O	0.24919	-5.19602	0.89822
O	1.1496	-3.24041	-0.9583
O	-3.74641	3.07402	1.783
O	-1.21058	1.9376	2.28305
O	0.16549	5.05838	-1.58562
O	3.61235	2.01259	-3.55882
O	3.11652	-1.73214	-0.19123
O	-0.1021	1.28651	4.76948
O	1.54351	2.08033	2.6241
O	3.76707	3.22849	1.32204
O	3.93811	-2.20792	2.43825
P	-0.01523	-0.08738	-0.36417
O	3.64437	-3.39688	-2.42297
Cu	-0.02826	-2.57589	3.37226
O	1.19993	-2.72126	5.87079

N	2.00689	-1.05194	4.66343
N	1.31217	-1.99217	4.91895
Mo	-0.13678	-3.62144	0.37023
Mo	-2.58509	-2.28556	-1.6687
Mo	-0.0485	-0.87497	-3.98992
Mo	2.43289	-2.25153	-2.06575
Mo	2.42473	1.19795	-2.63916
Mo	2.57543	2.04148	1.02098
Mo	2.71165	-1.39703	1.56676
Mo	0.08423	0.86779	3.12895
Mo	-2.56973	-1.49693	1.74218
Mo	-2.56751	2.19286	0.91933
Mo	-0.11989	3.42102	-1.21367
Mo	-2.65021	1.41284	-2.441
O	-1.35138	-3.07735	1.84695
O	-0.76879	-5.33361	4.74949
C	-0.47398	-4.32964	4.30411
Cs	-5.78287	-0.1997	-0.31983
Cs	0.08971	4.88683	2.50636
Cs	5.7512	-0.1354	-0.79613
N ₂ O*			
O	-1.27337	0.35239	-1.23425
P	-0.3842	0.01525	0.00591
O	0.85027	0.96585	0.01978
O	0.06004	-1.4764	-0.0769
O	0.07839	-3.8497	1.19564
O	0.45915	-1.70124	2.85388
O	1.18793	0.79963	3.0106
O	2.55417	-0.93175	1.44161
O	-1.20917	0.22524	1.31524
O	2.13888	2.94362	-1.329
O	2.1821	2.81536	1.35719
O	2.47223	-0.87178	-1.65846
O	0.01702	-3.7232	-1.42437
O	2.28174	-3.40246	-3.04808
O	0.23157	-1.46133	-3.04803
O	-2.32819	-0.67785	-3.45805
O	-3.73903	-0.71445	0.03802
O	-2.16369	-1.02629	3.48632
O	2.29142	-2.98103	-0.18402
O	3.92371	1.32691	-2.86162
O	1.05848	1.02186	-2.94109
O	-0.34198	0.29619	-5.29275

O	-1.56803	1.9062	-3.3144
O	-3.73483	1.11977	-1.96526
O	-3.17459	3.94059	-2.13659
O	-0.6213	3.27798	-1.11868
O	-2.75629	2.3818	0.23441
O	-3.56648	0.93093	2.29956
O	-4.88741	-1.36915	-2.52605
O	-2.42086	-2.42524	-1.39576
O	1.1447	5.16114	0.11684
O	-0.49494	3.15768	1.47812
O	3.98516	1.15347	2.74559
O	2.53499	-3.66338	2.5359
O	-2.31349	-2.51297	1.29394
O	-2.90789	3.70748	2.78481
O	-1.32323	1.52008	3.59386
O	-0.12109	-0.42665	5.30658
O	-4.80304	-1.56535	2.50147
O	-2.26791	-4.93193	-0.14083
O	6.37055	1.18588	0.34739
O	3.50067	0.97023	-0.08906
N	5.88291	2.26768	0.30337
N	5.44427	3.3181	0.26293
Cu	3.83267	-1.30885	-0.1497
Mo	-1.52615	-3.3828	-0.11671
Mo	-0.56667	0.30285	-3.59715
Mo	-3.42222	-0.6963	-1.94099
Mo	-3.38501	-0.83719	1.86667
Mo	-2.29185	2.56845	-1.61663
Mo	-2.05755	2.40099	2.06835
Mo	0.9408	3.46514	0.04529
Mo	-0.47454	-0.26836	3.6362
Mo	2.61616	1.09949	-1.77284
Mo	2.55689	0.94871	1.80787
Mo	1.48918	-2.74836	1.52432
Mo	1.31029	-2.49775	-1.9575
O	6.68423	-2.12421	-0.24566
C	5.57489	-1.81144	-0.20384
Cs	0.63249	3.91716	-3.97062
Cs	0.77983	3.67953	4.29659
Cs	-1.52373	-3.52578	-4.71269

CO@Cu₁/PMA

O	0.85933	-1.27243	0.52729
O	-0.95079	-1.04862	-1.24449

O	0.89735	0.68152	-1.09443
O	1.49333	3.22531	-1.45338
O	-1.13253	2.96501	-1.0763
O	-3.09085	1.08228	-1.227
O	-1.23664	1.21008	-3.05029
O	-0.89959	0.58405	0.70475
O	-1.65667	-1.43248	-3.77839
O	-1.68022	-3.4682	-2.06128
O	-3.51393	-1.49582	-1.77344
O	0.98556	-1.13539	-3.37378
O	3.37329	1.26156	-1.71295
O	3.69197	-0.35133	-3.99522
O	2.9583	-1.47505	-1.5613
O	3.39963	-2.01105	1.08137
O	1.13599	0.48679	2.88512
O	-1.45715	3.0268	1.63905
O	1.47292	1.50884	-3.56106
O	0.10114	-3.72055	-4.26417
O	1.06831	-3.24755	-1.68778
O	3.68421	-4.11676	-0.75906
O	1.42944	-3.87004	0.95328
O	-0.32348	-4.31506	3.1698
O	-1.24264	-3.35106	0.65034
O	-1.08819	-1.61734	2.73827
O	-1.36055	0.87488	3.36173
O	3.80783	-0.44158	3.38461
O	3.02706	0.68497	0.93113
O	-3.91037	-3.85518	-0.31354
O	-3.02483	-1.46191	0.90432
O	-3.83314	0.33221	-3.89167
O	-0.15757	3.78601	-3.65235
O	1.21306	2.57098	1.17327
O	-3.77181	-0.69392	3.48103
O	-3.39309	1.18772	1.48572
O	-3.70435	3.56668	-0.10503
O	0.33058	3.18355	3.74777
P	-0.02307	-0.26879	-0.26645
O	3.79861	3.32505	0.20521
Cu	-0.066	-0.56359	4.23607
O	1.50437	-2.12656	2.96967
O	0.42804	-1.31436	7.0856
C	0.23448	-1.02065	5.99722
Mo	2.54858	-0.64968	2.24622
Mo	-0.09166	2.11436	2.47815

Mo	2.50455	-2.97897	-0.30277
Mo	2.58099	2.18764	-0.20397
Mo	-2.50445	2.33807	-0.04902
Mo	2.50984	-0.1435	-2.78499
Mo	0.18809	2.43592	-2.66697
Mo	-2.5756	-0.1705	-2.85157
Mo	-2.63163	-2.75452	-0.55496
Mo	-2.59495	-0.27182	2.31348
Mo	-0.14229	-2.67664	-2.94929
Mo	0.00657	-3.05978	2.0729
Cs	-5.75198	-0.14073	-0.11585
Cs	5.74223	-0.25307	-0.22929
Cs	0.29123	5.43305	0.38594
TS ₄			
O	-0.44334	0.52453	-1.21432
O	1.16744	1.15346	0.64304
O	1.28095	-1.16635	-0.44161
O	2.03447	-3.65278	-0.17426
O	1.41417	-2.40273	2.26658
O	1.26585	-0.05552	3.35385
O	3.27864	-0.54166	1.57024
O	-0.6521	-0.57688	1.10541
O	3.65961	2.05727	1.13557
O	1.8001	3.79	0.28668
O	1.67546	2.66004	2.73582
O	3.41046	0.77967	-1.3213
O	2.12319	-2.51487	-2.63148
O	4.42009	-1.04286	-3.31957
O	1.74215	0.11552	-3.17773
O	-0.93845	0.32432	-3.81392
O	-2.56931	-1.40492	-0.78535
O	-1.34332	-2.7323	2.43575
O	3.90601	-1.80464	-0.6869
O	4.24609	3.46762	-1.19894
O	1.57779	2.53423	-2.00344
O	0.94568	2.32036	-4.73071
O	-1.08688	2.67845	-2.66376
O	-3.35529	3.49984	-1.25324
O	-0.87281	3.15519	0.05166
O	-2.71785	1.23542	0.57004
O	-3.445	-1.1174	2.01466
O	-3.04135	-1.52972	-3.69992
O	-0.56681	-2.14173	-2.5121

O	0.06532	4.93301	2.13521
O	-0.98592	2.28638	2.48669
O	3.75982	1.09441	3.86975
O	4.02593	-3.33028	1.79661
O	-0.7522	-3.40057	-0.21148
O	-3.5668	1.56627	3.26302
O	-1.43175	-0.26023	3.59712
O	0.11086	-2.31341	4.83782
O	-3.39377	-3.71363	0.72828
P	0.33711	-0.01397	0.02682
O	0.52812	-4.85243	-2.28128
Cu	-4.11447	-0.07957	-0.71386
O	-6.54641	-0.07627	0.41392
N	-4.73136	-0.79446	1.82393
N	-5.13931	-1.06045	0.68509
Mo	-1.8454	-0.8137	-2.69842
Mo	0.62418	1.56301	-3.22465
Mo	3.15948	-1.02262	-2.15816
Mo	0.68955	-3.33676	-1.51527
Mo	2.81842	-2.37886	1.04717
Mo	-0.06588	-1.59862	3.29736
Mo	-2.14114	-2.54721	0.69123
Mo	-2.23289	0.97461	2.35968
Mo	-2.08503	2.35309	-1.17502
Mo	0.4355	3.39371	1.48432
Mo	2.61317	0.92816	2.60637
Mo	3.04921	2.42983	-0.5422
O	-2.97131	0.80108	-2.04705
O	-6.6511	1.43141	-1.24426
C	-6.04971	0.60143	-0.59753
Cs	0.45087	-1.91421	-5.25785
Cs	0.19831	2.06055	5.4296
Cs	0.59286	-5.45335	1.90146
N ₂ *+CO ₂ *			
O	-0.7916	-1.03774	-0.01506
O	1.26304	-0.21559	-1.27263
O	1.25075	-0.24104	1.27538
O	2.13512	0.8554	3.50487
O	2.22002	2.60918	1.36233
O	2.24624	2.61833	-1.22228
O	3.67051	0.76173	0.0686
O	-0.16273	1.45118	0.00779
O	3.73646	-0.85723	-2.06716

O	1.54182	-1.68044	-3.4703
O	2.24913	0.92111	-3.41629
O	2.84535	-2.4026	0.00474
O	1.44343	-1.74442	3.46523
O	3.36472	-3.6393	2.48409
O	0.71716	-3.16798	1.34484
O	-2.00983	-3.05433	1.2905
O	-2.60239	0.74606	1.55398
O	-0.23703	3.75433	1.37513
O	3.64865	-0.87711	2.20225
O	3.40266	-3.58682	-2.56257
O	0.78593	-3.18503	-1.34966
O	-0.60482	-5.23597	-0.03214
O	-1.97019	-3.02758	-1.32159
O	-3.83912	-1.57102	-2.81282
O	-1.068	-0.96325	-2.96445
O	-2.59443	0.76409	-1.54861
O	-2.364	2.90215	0.01613
O	-3.92165	-1.60268	2.7192
O	-1.14049	-0.99174	2.93048
O	0.25424	0.12403	-5.2937
O	-0.41707	1.5796	-2.92758
O	4.69992	1.86076	-2.38405
O	4.63234	1.82153	2.54443
O	-0.43073	1.50858	2.94336
O	-2.66188	3.33429	-2.79624
O	-0.24087	3.80087	-1.32493
O	1.80367	5.17573	0.04011
O	-2.65081	3.27108	2.84522
P	0.38118	-0.00843	0.00061
O	0.15561	-0.06042	5.30676
Cu	-3.96227	0.89769	-0.02112
O	-6.31373	-1.16997	-0.13575
N	-6.50785	2.44757	0.14324
N	-5.55452	1.85856	0.08461
Mo	-2.54041	-1.36639	1.72083
Mo	-0.43413	-3.52739	-0.03261
Mo	2.52837	-2.28545	1.84313
Mo	0.49615	-0.13712	3.62917
Mo	3.19755	1.1523	1.88392
Mo	1.05043	3.63723	0.01932
Mo	-1.63399	2.36269	1.79999
Mo	-1.64857	2.43797	-1.74099
Mo	-2.47484	-1.32099	-1.79568

Mo	0.52126	0.04259	-3.60804
Mo	3.25031	1.163	-1.79561
Mo	2.52624	-2.23612	-1.97221
O	-3.45279	-1.13868	-0.03151
O	-5.4279	-3.33312	-0.11225
C	-5.81748	-2.23241	-0.12235
Cs	-0.96532	-3.65179	3.9999
Cs	1.43803	3.8462	-4.16664
Cs	-0.66225	-3.55447	-4.15687
Cu ₁ /PMA			
O	-0.94677	1.33506	-0.15388
O	0.9607	0.26058	1.14285
O	0.97341	0.23844	-1.41455
O	1.74832	-1.27241	-3.43645
O	1.4934	-2.87627	-1.31812
O	1.48376	-2.85372	1.37756
O	3.1908	-1.43314	0.0262
O	-0.6971	-1.19654	-0.13082
O	3.5171	0.31126	2.14358
O	1.53338	1.46171	3.46521
O	1.71653	-1.21383	3.47118
O	2.96732	1.75127	-0.00137
O	1.5664	1.40308	-3.47598
O	3.55063	3.15638	-2.44765
O	0.98318	3.08956	-1.32351
O	-1.78914	3.31675	-1.37538
O	-2.97398	-0.29673	-1.81229
O	-1.14238	-3.65617	-1.26539
O	3.53737	0.27404	-2.11775
O	3.52619	3.19863	2.42781
O	0.97044	3.11295	1.27978
O	-0.29388	5.36307	-0.04833
O	-1.80183	3.34047	1.29968
O	-3.8317	2.26408	2.85851
O	-1.16716	1.21682	3.00022
O	-2.98698	-0.26517	1.79347
O	-3.14025	-2.24226	0.00627
O	-3.80639	2.21254	-2.92984
O	-1.14145	1.16205	-3.03166
O	-0.04146	0.02384	5.32986
O	-0.93583	-1.43458	3.00416
O	4.12784	-2.38378	2.54359
O	4.14933	-2.42871	-2.46498

O	-0.90846	-1.48704	-2.98847
O	-3.34618	-2.93208	2.85847
O	-1.15232	-3.63414	1.31952
O	0.8968	-5.25988	0.04916
O	-3.32195	-2.97919	-2.83518
P	0.07696	0.15631	-0.13925
O	0.00785	-0.06473	-5.33091
Cu	-3.60397	-0.35806	-0.01052
O	-3.5325	1.57399	-0.02682
Mo	-2.56244	1.67394	-1.88325
Mo	-2.15148	-2.23771	-1.82093
Mo	-0.41763	3.6621	-0.03423
Mo	0.27747	-0.01488	-3.64226
Mo	0.49632	-3.58831	0.03204
Mo	2.40932	2.03348	-1.83833
Mo	2.88812	-1.42316	-1.88125
Mo	2.87053	-1.38998	1.93223
Mo	0.24138	0.04624	3.64278
Mo	-2.16948	-2.20854	1.83852
Mo	2.39059	2.06548	1.82659
Mo	-2.57949	1.70752	1.83128
Cs	0.46546	-4.04144	3.99886
Cs	-0.31907	4.02886	-3.94806
Cs	-0.3329	3.81876	4.02529
N ₂ O*			
O	-1.01987	0.62964	0.43975
O	0.99955	0.38175	-1.10752
O	-0.61707	-1.58778	-0.74345
O	-0.91622	-4.33955	-0.67772
O	1.66389	-3.53742	-0.30205
O	3.18033	-1.32625	-0.51433
O	1.70302	-2.28272	-2.55056
O	0.94417	-0.85614	1.10562
O	1.94854	0.30483	-3.57648
O	1.58076	2.62081	-2.37294
O	3.69034	0.9907	-1.62567
O	-0.61965	-0.37212	-3.38626
O	-2.9269	-2.66824	-1.39999
O	-3.27341	-1.52588	-3.90049
O	-2.82926	0.12218	-1.7329
O	-3.55427	1.11191	0.81298
O	-1.33861	-0.44133	2.99603
O	1.70846	-2.9144	2.47506

O	-0.86279	-2.95209	-3.03958
O	-0.03431	2.17136	-4.63719
O	-1.12812	2.05667	-2.10439
O	-3.82755	2.83161	-1.45535
O	-1.74246	3.2095	0.44473
O	-0.23927	4.58578	2.3644
O	1.08222	3.47779	0.13788
O	0.54205	1.83567	2.49438
O	1.19477	-0.42287	3.67969
O	-4.165	-0.07573	3.21828
O	-3.25013	-1.69753	1.12995
O	3.74234	3.61204	-0.79898
O	2.72538	1.50621	0.90671
O	4.26435	-1.29544	-3.17123
O	0.93596	-5.06711	-2.67291
O	-1.0019	-2.9754	1.78256
O	3.30423	1.44755	3.65435
O	3.50013	-0.8607	2.11943
O	4.13963	-3.45963	1.06659
O	-0.26761	-2.74756	4.52395
P	0.06979	-0.35036	-0.08688
O	-3.29363	-4.4769	0.84364
Cu	-0.29864	0.93651	4.17695
Mo	2.68954	-2.56853	0.8556
Mo	2.42108	0.51037	2.52527
Mo	0.08292	-2.03872	3.02221
Mo	-0.13246	3.15255	1.41823
Mo	-2.92149	-0.16659	2.03884
Mo	-2.59598	1.85512	-0.78288
Mo	0.22173	1.32567	-3.17075
Mo	-2.14975	-1.38217	-2.61989
Mo	2.80361	-0.84051	-2.39811
Mo	0.37124	-3.6699	-1.89066
Mo	2.66408	2.28359	-0.87522
Mo	-2.20373	-3.287	0.31486
C	-0.86829	1.71783	5.72966
O	-1.22871	2.20911	6.69903
N	-3.44215	3.22704	2.74833
O	-2.56766	2.56811	3.23043
N	-4.27125	3.85008	2.28845
Cs	5.9353	-0.31373	0.17887
Cs	-5.60199	-1.07036	-0.91801
Cs	-0.38569	5.06815	-2.146

TS₅

O	-1.01987	0.62964	0.43975
O	0.99955	0.38175	-1.10752
O	-0.61707	-1.58778	-0.74345
O	-0.91622	-4.33955	-0.67772
O	1.66389	-3.53742	-0.30205
O	3.18033	-1.32625	-0.51433
O	1.70302	-2.28272	-2.55056
O	0.94417	-0.85614	1.10562
O	1.94854	0.30483	-3.57648
O	1.58076	2.62081	-2.37294
O	3.69034	0.9907	-1.62567
O	-0.61965	-0.37212	-3.38626
O	-2.9269	-2.66824	-1.39999
O	-3.27341	-1.52588	-3.90049
O	-2.82926	0.12218	-1.7329
O	-3.55427	1.11191	0.81298
O	-1.33861	-0.44133	2.99603
O	1.70846	-2.9144	2.47506
O	-0.86279	-2.95209	-3.03958
O	-0.03431	2.17136	-4.63719
O	-1.12812	2.05667	-2.10439
O	-3.82755	2.83161	-1.45535
O	-1.74246	3.2095	0.44473
O	-0.23927	4.58578	2.3644
O	1.08222	3.47779	0.13788
O	0.54205	1.83567	2.49438
O	1.19477	-0.42287	3.67969
O	-4.165	-0.07573	3.21828
O	-3.25013	-1.69753	1.12995
O	3.74234	3.61204	-0.79898
O	2.72538	1.50621	0.90671
O	4.26435	-1.29544	-3.17123
O	0.93596	-5.06711	-2.67291
O	-1.0019	-2.9754	1.78256
O	3.30423	1.44755	3.65435
O	3.50013	-0.8607	2.11943
O	4.13963	-3.45963	1.06659
O	-0.26761	-2.74756	4.52395
P	0.06979	-0.35036	-0.08688
O	-3.29363	-4.4769	0.84364
Cu	-0.29864	0.93651	4.17695
Mo	2.68954	-2.56853	0.8556
Mo	2.42108	0.51037	2.52527
Mo	0.08292	-2.03872	3.02221

Mo	-0.13246	3.15255	1.41823
Mo	-2.92149	-0.16659	2.03884
Mo	-2.59598	1.85512	-0.78288
Mo	0.22173	1.32567	-3.17075
Mo	-2.14975	-1.38217	-2.61989
Mo	2.80361	-0.84051	-2.39811
Mo	0.37124	-3.6699	-1.89066
Mo	2.66408	2.28359	-0.87522
Mo	-2.20373	-3.287	0.31486
C	0.5263	2.39972	4.90108
O	1.03907	3.31862	5.35231
N	-3.21895	3.10583	2.62912
O	-2.10263	2.0995	2.79626
N	-3.89041	3.75522	3.25869
Cs	5.9353	-0.31373	0.17887
Cs	-5.60199	-1.07035	-0.91801
Cs	-0.38569	5.06815	-2.146
C	-1.0809	0.09729	5.60162
O	-1.62296	-0.34777	6.46892
N ₂ *			
O	-0.94648	0.75962	0.15841
O	0.93938	-0.22761	-1.28324
O	-0.85034	-1.74839	-0.27501
O	-1.53516	-4.20898	0.71685
O	1.14061	-3.70307	0.80756
O	2.95552	-1.8944	-0.17847
O	1.23487	-3.28596	-1.79791
O	0.87874	-0.63606	1.22244
O	1.64658	-1.18561	-3.60999
O	1.68502	1.52452	-3.17683
O	3.62263	-0.12634	-2.02453
O	-1.11877	-1.19564	-3.15679
O	-3.39994	-2.46153	-0.37496
O	-3.72792	-2.40203	-3.18977
O	-3.01257	-0.07791	-1.6687
O	-3.31088	1.80032	0.35755
O	-1.24653	0.64366	2.90649
O	1.4195	-2.18895	3.20598
O	-1.52112	-3.70647	-1.95595
O	-0.05547	0.52864	-5.16824
O	-0.92924	1.45734	-2.57992
O	-3.48647	2.61256	-2.3587
O	-1.33237	3.29382	-0.63155

O	0.39979	5.02757	0.74079
O	1.48861	3.14733	-1.05823
O	0.86144	2.37443	1.68933
O	1.33911	0.60228	3.5401
O	-3.89444	1.60031	3.05311
O	-3.42721	-0.76636	1.64637
O	4.08258	2.58143	-2.08216
O	2.89998	1.27655	0.22862
O	3.85216	-2.84119	-2.74885
O	0.1828	-5.80171	-0.96674
O	-1.28307	-2.09439	2.58217
O	3.64279	2.03258	2.81396
O	3.41559	-0.66422	2.15283
O	3.6732	-3.51358	2.05384
O	-0.37637	-1.06882	5.11586
P	-0.00442	-0.45537	-0.0563
O	-3.74411	-3.53614	2.26778
Cu	0.5082	2.50492	3.80756
Mo	2.35254	-2.54478	1.56468
Mo	2.56236	0.91708	2.07307
Mo	-0.02474	-0.93611	3.46034
Mo	0.28867	3.37566	0.24951
Mo	-2.80298	0.87787	1.93486
Mo	-2.40437	1.63523	-1.44006
Mo	0.21453	0.07282	-3.54521
Mo	-2.46725	-2.08334	-2.08706
Mo	2.53204	-1.98886	-2.0863
Mo	-0.10603	-4.16109	-0.68867
Mo	2.82362	1.47539	-1.72125
Mo	-2.53951	-2.78739	1.32352
C	1.8303	3.96798	3.91201
O	2.52691	4.86983	3.89193
Cs	5.76143	-0.82232	0.1419
Cs	-5.7954	-0.60338	-0.36291
Cs	-0.0127	4.12725	-3.65345
C	-1.05078	2.41739	4.93885
O	-1.96436	2.31691	5.61459
O	-1.7961	3.52243	2.20843
N	-3.22738	4.78478	1.40669
N	-4.00973	5.47664	0.96649
cis-N2O2			
O	-1.22117	0.40465	-1.22443
P	-0.33142	0.03465	0.00349

O	0.80286	1.10631	0.16399
O	0.29091	-1.37288	-0.24245
O	0.60174	-3.83393	0.74379
O	0.63386	-1.88235	2.67994
O	1.02703	0.6194	3.28958
O	2.63968	-0.64411	1.43831
O	-1.18882	-0.02031	1.30364
O	1.77826	3.35595	-0.8645
O	1.79511	2.89895	1.82811
O	2.64012	-0.18221	-1.58063
O	0.55603	-3.41338	-1.86155
O	2.86685	-2.57067	-3.25283
O	0.53842	-0.95125	-3.16231
O	-2.1607	-0.53865	-3.59085
O	-3.60292	-1.14534	-0.15261
O	-2.06372	-1.70983	3.28227
O	2.66591	-2.51863	-0.43515
O	3.69269	2.27056	-2.65143
O	0.97507	1.59919	-2.89544
O	-0.3312	0.81784	-5.29725
O	-1.74235	2.08933	-3.14119
O	-3.78825	0.88294	-1.92459
O	-3.55189	3.77634	-1.79017
O	-0.98346	3.3216	-0.72721
O	-3.02878	1.97467	0.40191
O	-3.66865	0.18261	2.28098
O	-4.62864	-1.63732	-2.80054
O	-2.04865	-2.47658	-1.72195
O	0.49393	5.23368	0.83348
O	-0.91514	2.87609	1.83744
O	3.72545	1.33601	3.14736
O	2.97377	-3.46044	2.19437
O	-1.95103	-2.8815	0.92204
O	-3.43407	2.96085	3.05804
O	-1.59719	0.90852	3.7188
O	-0.23637	-1.06266	5.28133
O	-4.58537	-2.45761	2.13336
O	-1.52354	-5.0799	-0.79523
O	5.94559	0.59934	0.41462
O	3.57146	1.47614	0.18176
N	5.76416	1.88061	0.47317
N	4.66833	2.44939	0.36263
Cu	4.18934	-0.41985	-0.13349
Mo	-1.01106	-3.45934	-0.56251

Mo	-0.55813	0.62844	-3.61639
Mo	-3.26605	-0.86626	-2.10333
Mo	-3.25863	-1.48787	1.64377
Mo	-2.50424	2.47622	-1.41365
Mo	-2.40718	1.87074	2.22329
Mo	0.5003	3.55032	0.54781
Mo	-0.5489	-0.71064	3.63374
Mo	2.38143	1.72919	-1.69574
Mo	2.35173	1.08373	2.15172
Mo	1.80777	-2.57488	1.29625
Mo	1.71712	-1.97724	-2.12325
O	5.68381	-3.02224	-0.76768
C	5.11742	-2.05157	-0.55092
Cs	0.30742	3.29472	4.56109
Cs	-0.87845	-3.17252	-4.74182
Cs	0.32888	4.42929	-3.41245

TS4

O	1.05557	0.21664	-1.19249
P	0.10947	-0.37157	-0.09973
O	-0.99481	0.69814	0.24095
O	0.94495	-0.70333	1.17023
O	1.60456	-2.5986	2.95523
O	-1.01809	-2.71192	2.07656
O	-3.07953	-1.48155	1.06294
O	-1.45337	-0.18863	2.89695
O	-0.56418	-1.67342	-0.6209
O	-1.8109	3.1258	-0.42915
O	-3.60626	1.07985	0.16417
O	0.51381	2.0059	2.2751
O	3.30892	-0.66669	2.36047
O	3.18229	1.85295	3.5504
O	2.83095	1.57261	0.79197
O	3.68945	0.72403	-1.63229
O	1.90577	-2.55185	-2.08518
O	-0.78484	-4.36981	-0.13583
O	1.03461	-0.03587	3.73811
O	-0.49403	4.62879	1.56335
O	0.96478	3.08659	-0.25641
O	3.57727	3.54525	-1.22429
O	1.64886	2.18298	-2.80265
O	2.1026	-0.32137	-3.64501
O	0.21489	1.42366	-5.07386
O	-1.09446	1.64561	-2.62912

O	-0.51158	-0.88814	-3.41909
O	-0.66856	-3.43837	-2.63681
O	4.48888	-1.61613	-2.90848
O	3.38742	-1.49754	-0.23914
O	-3.7995	2.47046	-2.31422
O	-2.77009	-0.26946	-2.00041
O	-4.23581	0.36849	2.81096
O	-0.44865	-2.19277	4.81495
O	1.66051	-3.48075	0.35298
O	-2.98861	-2.24841	-3.92204
O	-2.81323	-2.90298	-1.19249
O	-3.25167	-4.31142	1.20692
O	1.28574	-5.29852	-1.9068
O	4.14737	-3.31582	1.71183
O	-4.42309	3.72578	4.23189
O	-2.19562	2.32486	2.1163
N	-3.82037	3.18404	3.32259
N	-2.56034	3.07384	3.20349
Cu	-0.51074	1.37553	3.97683
Mo	2.78943	-2.37401	1.27057
Mo	2.51047	2.22368	-1.06841
Mo	3.05879	-0.97661	-2.23154
Mo	0.65832	-3.79802	-1.42006
Mo	0.40099	0.86265	-3.47605
Mo	-1.963	-1.8148	-2.6257
Mo	-2.60901	1.67591	-1.37947
Mo	-2.08349	-3.25086	0.55963
Mo	-0.44792	3.03019	0.97454
Mo	-2.89286	0.19128	1.76221
Mo	0.06228	-1.67499	3.27524
Mo	2.29471	0.88189	2.4583
O	-1.51603	2.67877	6.4755
C	-1.11145	2.16992	5.53331
Cs	-5.52397	-1.33796	-0.84214
Cs	5.81933	0.15718	0.62361
Cs	-0.33924	4.72812	-2.75042