

XYZ coordinates for all the structures in Fig. 5

1. 1,2-PDO-dehydrogenation path

Str 1

Free energy from VASP is -328.39379400 eV

PBC 10.223900 10.223900 20.000000 90.000000 90.000000

120.000000

H	2.56691945	1.43923141	7.25711903
H	-0.04377945	2.94207071	7.26393275
H	1.94551802	5.59350670	11.35439436
H	1.76263090	6.24853554	8.99010230
H	2.17365364	3.79615525	9.64350942
H	2.56244699	7.54714549	9.93089289
H	3.10591426	3.43031148	11.13626072
H	4.74420331	5.94699531	11.06855044
H	4.19671842	5.57640868	8.76773784
H	4.16467228	3.36776412	8.77649582
C	2.85629577	5.54905729	10.73368286
C	2.67251270	6.51886758	9.55972649
C	3.03096740	4.10086297	10.26669922
O	3.92418748	5.94984188	11.59620540
O	3.83227244	6.50257320	8.68242509
O	4.26507973	4.02136705	9.50131530
Cu	5.10835498	8.84704951	0.00127886
Cu	-2.55543284	8.85212949	0.00592344
Cu	0.00152531	8.85223995	0.00382139
Cu	2.55532374	8.85039728	0.00186300
Cu	8.94196113	2.21496390	0.00537177
Cu	1.27766833	2.21275799	0.01181878
Cu	3.83527190	2.21290275	0.00614283
Cu	6.39109844	2.21514433	0.00009607
Cu	7.66517761	4.42851017	0.00553876
Cu	-0.00407226	4.42907591	0.00459696
Cu	2.55961507	4.43283322	0.00119318
Cu	5.11424490	4.43011061	0.00250585
Cu	6.38824836	6.63671419	0.00238845
Cu	-1.27942586	6.63810758	19.99957806
Cu	1.28003365	6.64250111	0.00191010
Cu	3.83422949	6.64042098	0.00235666
Cu	-0.00423426	1.47161580	2.07977278
Cu	2.55589452	1.47251059	2.08560339
Cu	5.11418136	1.47617222	2.08145297
Cu	7.66551325	1.47261319	2.08871219

Cu	-1.27891381	3.68798736	2.08911201
Cu	1.27788053	3.69337579	2.07727849
Cu	3.83334997	3.69403090	2.09033757
Cu	6.38841629	3.68404943	2.09613188
Cu	-2.55303085	5.90494884	2.09663548
Cu	-0.00047430	5.90443256	2.08853882
Cu	2.55339313	5.90226380	2.09608390
Cu	5.10910155	5.90458536	2.09220622
Cu	-3.83943831	8.11244607	2.09396081
Cu	-1.27932440	8.11161499	2.08182064
Cu	1.28246514	8.11275440	2.09833809
Cu	3.83285494	8.11634263	2.09794856
Cu	1.27193739	0.74587709	4.17299303
Cu	3.83142993	0.73273696	4.15585214
Cu	6.38460431	0.73703332	4.16401753
Cu	8.94420544	0.74866030	4.17545024
Cu	0.01492573	2.93748268	4.15676738
Cu	2.54133091	2.94105598	4.16509683
Cu	5.08758403	2.93410405	4.17473073
Cu	7.67532782	2.94732979	4.17646723
Cu	-1.27503493	5.14946691	4.17670800
Cu	1.26190231	5.15132609	4.17196157
Cu	3.83398467	5.17622035	4.18245299
Cu	6.39091061	5.15895545	4.15547868
Cu	-2.55990830	7.39575798	4.17958269
Cu	-0.00770047	7.37607806	4.16226879
Cu	2.56593376	7.36622985	4.19529103
Cu	5.09781619	7.36443810	4.19058329
Cu	-1.29035035	6.62612545	6.24104059
Cu	3.80857431	6.63558855	6.39840559
Cu	2.55384290	4.42880453	6.20207207
Cu	1.26352078	2.20016581	6.38378922
Cu	1.24265767	6.62351804	6.22606784
Cu	7.63890418	4.42503411	6.24229195
Cu	8.93798225	2.20835420	6.29049756
Cu	-0.01321614	4.40110437	6.29540073
Cu	3.81436428	2.19427375	6.29373834
Cu	5.08698574	8.82344876	6.21786136
Cu	7.64714502	0.00655731	6.23065635
Cu	-2.56704074	8.84244127	6.28868698
Cu	6.38916387	6.62419146	6.23020158
Cu	0.00252283	8.83265511	6.23671930
Cu	5.10719284	4.39874502	6.21703056
Cu	6.37317998	2.20179951	6.24412414

Str 2

Free energy from VASP is -327.58519100 eV

PBC	10.223900	10.223900	20.000000	90.000000	90.000000
120.000000					
H	3.30190534	5.38759710	7.41145086		
H	3.76140143	0.74402440	7.22098851		
H	2.65013308	4.92926800	10.06045620		
H	3.08275476	2.77976466	8.87866706		
H	0.35818124	5.94286582	10.01184763		
H	2.08284369	2.58605063	10.34930056		
H	0.54015517	4.52409100	11.08519452		
H	-0.89270979	4.64857732	8.63452660		
H	1.26135069	8.15339895	7.23313388		
H	0.24590398	2.71820186	8.78167994		
C	1.87306144	4.51587383	9.38328352		
C	2.10330385	3.00064485	9.32539500		
C	0.52090060	4.85515480	10.03478887		
O	1.97586470	5.14590281	8.10993757		
O	1.11501862	2.30614816	8.52591435		
O	-0.60041900	4.16323298	9.44003943		
Cu	-0.03796015	0.00960189	19.97395131		
Cu	2.51283052	0.00703425	-0.02127472		
Cu	5.07269830	0.00571981	19.98560565		
Cu	7.63021066	0.00600369	19.97743390		
Cu	-1.31173878	2.22242498	19.97177770		
Cu	1.23442603	2.22262780	-0.01770096		
Cu	3.78993313	2.22062762	-0.02431419		
Cu	6.35614990	2.22681847	19.96939389		
Cu	-2.59408274	4.43296857	19.97272045		
Cu	-0.03911178	4.42894301	19.97153767		
Cu	2.51454337	4.43198296	19.97231212		
Cu	5.07459226	4.43682499	19.97209283		
Cu	-3.87397023	6.64700201	19.97624598		
Cu	-1.32278514	6.64297628	19.96365952		
Cu	1.23766974	6.64922356	19.97356304		
Cu	3.79719204	6.64671427	19.97360254		
Cu	-0.03982467	1.47774489	2.08100951		
Cu	2.51189354	1.48497714	2.06575532		
Cu	5.07372493	1.49239797	2.04749251		
Cu	7.62734849	1.48374373	2.05377377		
Cu	-1.31253007	3.69408476	2.06281011		
Cu	1.23830940	3.69966073	2.07176914		

Cu	3.78675989	3.69278401	2.06353643
Cu	6.34291398	3.69680745	2.05719604
Cu	-2.60299487	5.91187036	2.05904565
Cu	-0.04079839	5.91258961	2.05246425
Cu	2.51033008	5.90816745	2.05097370
Cu	5.06474170	5.90762756	2.06459517
Cu	-3.87864394	8.12805214	2.06614226
Cu	-1.32145557	8.11478784	2.05026011
Cu	1.23696541	8.12456294	2.06512847
Cu	3.79283342	8.12679436	2.05549702
Cu	1.24804019	0.75237484	4.18310221
Cu	3.81039578	0.72554765	4.10626873
Cu	6.33145656	0.74660010	4.14018272
Cu	8.87873591	0.72771196	4.15151844
Cu	-0.02519619	2.94358592	4.16130176
Cu	2.49758136	2.93594226	4.17893084
Cu	5.05122443	2.96058006	4.15469309
Cu	7.62217059	2.95991600	4.11988455
Cu	-1.32677690	5.16936456	4.11654997
Cu	1.22801200	5.19561875	4.16084027
Cu	3.76861491	5.16018048	4.13274283
Cu	6.32915079	5.16802700	4.14099871
Cu	-2.60716783	7.39209363	4.14194939
Cu	-0.04463229	7.39135729	4.15963200
Cu	2.50906371	7.37344185	4.14431756
Cu	5.06036000	7.38140632	4.13391620
Cu	3.80960276	2.16315439	6.21544372
Cu	-0.09611527	4.43052471	6.17559159
Cu	2.53222952	-0.02578990	6.24465327
Cu	1.19612229	6.66611900	6.30985006
Cu	2.50114909	4.37148924	6.20021301
Cu	1.18441194	2.19020592	6.34768148
Cu	8.86144401	2.20792438	6.19004992
Cu	3.81309958	6.61232434	6.23234225
Cu	-0.06647908	-0.02548224	6.19475013
Cu	-1.35668577	6.60012110	6.19843633
Cu	5.03374383	4.44215431	6.26666822
Cu	-2.62941983	4.43257636	6.21617932
Cu	7.61512418	0.00112277	6.25312771
Cu	-3.88229527	6.64531224	6.21740021
Cu	5.06948032	0.00265429	6.35063611
Cu	6.35123212	2.25710071	6.19205854

Str 3

Free energy from VASP is -328.72559400 eV

PBC 10.223900 10.223900 20.000000 90.000000 90.000000

120.000000

H	1.95798150	3.80416521	8.84076556
H	-2.62416752	7.47263500	7.29149189
H	0.33431610	6.88666390	9.50201089
H	2.60442763	6.56415191	8.64313160
H	-1.26076002	5.00507613	9.77264483
H	2.41202774	5.73825932	10.22037506
H	0.10932251	4.92407534	10.91419647
H	-0.28776040	3.27527952	8.62603433
H	5.12712422	2.92306713	7.22983791
H	5.09102123	5.92821060	7.23214613
C	0.58140473	5.90262430	9.05472003
C	2.10027476	5.73154773	9.16224849
C	-0.17444798	4.83673889	9.85424422
O	0.18498043	5.90124740	7.68203921
O	2.56920559	4.51914033	8.52983801
O	0.17257956	3.49176911	9.46915615
Cu	-0.00083907	0.00751456	19.99872759
Cu	2.55817110	0.00477283	19.99726798
Cu	0.00195778	8.85403772	19.99597183
Cu	7.66575330	0.00097581	19.97696441
Cu	-1.27457727	2.21740341	19.98838933
Cu	1.27590160	2.21978508	19.99341854
Cu	3.83449653	2.21550862	19.99117577
Cu	6.38923679	2.21308353	19.98427728
Cu	-2.54696658	4.42596459	19.98551942
Cu	0.00422366	4.43009278	0.01134248
Cu	2.54722942	4.42948378	0.00157914
Cu	5.11021346	4.42805092	19.99683753
Cu	-3.83345302	6.64165744	0.00816102
Cu	-1.27205498	6.64262930	0.01450922
Cu	1.27539750	6.64020769	0.00542239
Cu	3.83261868	6.64079614	19.99542886
Cu	0.00680039	1.49724197	2.08369372
Cu	2.55488012	1.49804916	2.08404657
Cu	5.10569575	1.48544177	2.07074785
Cu	7.66784221	1.48301423	2.05889780
Cu	-1.27969774	3.70262289	2.09675115
Cu	1.28218223	3.69893802	2.11061100
Cu	3.82767908	3.69579136	2.07456855
Cu	6.39496144	3.69921499	2.05745207

Cu	-2.54963057	5.90348176	2.08720244
Cu	0.00947304	5.90295345	2.11342216
Cu	2.55450640	5.90433969	2.09436750
Cu	5.10325637	5.90148630	2.09038338
Cu	-3.82151969	8.12426351	2.07218493
Cu	-1.27939953	8.12579142	2.09313160
Cu	1.27759183	8.12283487	2.08558086
Cu	3.82833709	8.11867036	2.06425261
Cu	1.29055161	0.74427427	4.14786913
Cu	3.82543065	0.75667387	4.16641781
Cu	6.38080040	0.76388360	4.13981338
Cu	8.94955300	0.75418731	4.11634427
Cu	-0.00217788	2.99164882	4.18232838
Cu	2.57082182	2.97859463	4.20778081
Cu	5.11440190	2.98875172	4.12759511
Cu	7.65155823	2.96031660	4.14828191
Cu	-1.26216003	5.20510624	4.21600431
Cu	1.28899490	5.17411826	4.22720760
Cu	3.82849652	5.15937406	4.19575767
Cu	6.38893838	5.18227471	4.17056101
Cu	-2.55664906	7.37092025	4.18200379
Cu	-0.01545508	7.38636808	4.18327119
Cu	2.56582738	7.37931382	4.16848473
Cu	5.13209634	7.39566909	4.13219627
Cu	-1.33830958	6.70025909	6.39623822
Cu	5.12953376	0.04040658	6.19471735
Cu	-2.54056085	4.40681350	6.19892487
Cu	7.68512576	0.04660754	6.19006843
Cu	6.38954673	2.23014920	6.26987192
Cu	8.93647992	2.21425943	6.21579143
Cu	1.27802025	2.19494966	6.21260257
Cu	-0.01684564	0.04727508	6.18988787
Cu	2.54526225	0.02407214	6.27558425
Cu	5.14656533	4.43157018	6.33694211
Cu	3.85915674	2.21398029	6.26462525
Cu	-3.83994533	6.66322078	6.35587918
Cu	2.56477076	4.42347213	6.33786086
Cu	1.34223575	6.72962271	6.22597889
Cu	3.88140559	6.68012482	6.22668895
Cu	-0.00921655	4.36320710	6.31476621

Str 4

Free energy from VASP is -327.87838600 eV

PBC	10.223900	10.223900	20.000000	90.000000	90.000000
120.000000					
H	4.70448742	3.52312809	7.55213168		
H	-0.04625857	5.96244137	7.23162174		
H	8.08869235	3.46774344	8.63399370		
H	4.65929514	2.28601532	10.71904688		
H	6.68630411	4.06602502	10.45716570		
H	3.74479079	3.53962509	9.82585756		
H	5.84929249	5.10886686	9.26946115		
H	2.58627828	7.39358510	7.24573551		
H	4.19449428	0.93385114	8.78449257		
H	1.31412574	3.64121367	7.22999858		
C	5.65462011	2.94798710	8.96354774		
C	4.36626666	2.64148696	9.70785863		
C	6.43352882	4.18716969	9.38375491		
O	6.31539057	1.96706216	8.47937745		
O	3.58456068	1.65550806	9.04831867		
O	7.64586036	4.34460651	8.63946060		
Cu	0.00547526	0.00177014	-0.00692873		
Cu	2.55323455	0.00060536	-0.00994358		
Cu	5.10990123	0.00402447	-0.01203797		
Cu	7.67086629	0.00335753	-0.00452647		
Cu	8.94772301	2.21189688	-0.00547922		
Cu	1.27911009	2.21018137	-0.00608336		
Cu	3.83550442	2.21318670	-0.00037978		
Cu	6.38942476	2.21647555	-0.00071879		
Cu	-2.55713659	4.43160440	0.00176108		
Cu	-0.00136014	4.42772087	0.00798191		
Cu	2.55958407	4.42037547	-0.00238580		
Cu	5.11703183	4.42711090	-0.00005608		
Cu	6.39241255	6.64319785	0.00103304		
Cu	-1.27931569	6.64187617	0.00751226		
Cu	1.27567092	6.64393448	0.00327459		
Cu	3.84127116	6.64384205	-0.00977776		
Cu	-0.00212387	1.47752412	2.07926476		
Cu	2.55965207	1.47478613	2.08010743		
Cu	5.11784283	1.47703315	2.09060621		
Cu	7.67013017	1.48722992	2.09185000		
Cu	-1.28661271	3.68936436	2.08780689		
Cu	1.28681423	3.68851813	2.08235452		
Cu	3.84510118	3.69063626	2.09298224		
Cu	6.39154835	3.68943328	2.09849474		
Cu	-2.55652728	5.90303832	2.10189372		
Cu	-0.00768778	5.90208169	2.09189721		

Cu	2.56452276	5.90141857	2.05954883
Cu	5.11958389	5.90013621	2.08834667
Cu	-3.83024148	8.11806044	2.09727785
Cu	-1.27696185	8.12930397	2.08555609
Cu	1.27824860	8.12911902	2.06865912
Cu	3.83580177	8.11702687	2.07435348
Cu	1.27796509	0.76559695	4.16316395
Cu	3.83493127	0.76671165	4.17925564
Cu	6.41059941	0.74457796	4.18616367
Cu	8.95028275	0.72810060	4.15406040
Cu	0.00755305	2.98136323	4.15058465
Cu	2.57272749	2.95762779	4.16605182
Cu	5.12849693	2.94449746	4.19389384
Cu	7.65883780	2.96763216	4.20644904
Cu	-1.26490786	5.15086016	4.20314505
Cu	1.29272601	5.17819608	4.16303748
Cu	3.82236724	5.16980136	4.18504272
Cu	6.38957317	5.16382128	4.19337745
Cu	-2.53042605	7.37612623	4.16440208
Cu	0.01754615	7.37993605	4.14808905
Cu	2.53977824	7.36836900	4.12930076
Cu	5.10052835	7.37654202	4.15501569
Cu	0.03364435	0.01502383	6.21826484
Cu	-3.83620582	6.67191889	6.20416184
Cu	3.83156430	6.66062872	6.26849233
Cu	3.85339828	2.24191677	6.32187148
Cu	0.02950814	4.44232864	6.35668544
Cu	-2.55917587	4.45064581	6.30131661
Cu	2.55962164	0.01241747	6.21197180
Cu	1.27578277	2.21960842	6.27000929
Cu	-1.24584121	2.20186226	6.18220926
Cu	1.28075337	6.67659827	6.34954562
Cu	2.56316864	4.41746724	6.28957575
Cu	5.09471669	0.01662643	6.19090197
Cu	5.09528679	4.45024404	6.24931767
Cu	6.45715702	2.16218376	6.31121650
Cu	-1.26861503	6.66626384	6.26382046
Cu	2.59499697	8.82309974	6.24983617

Str 5

Free energy from VASP is -328.29249700 eV

PBC	10.223900	10.223900	20.000000	90.000000	90.000000
120.000000					

H	5.12559278	1.38143336	7.15529302
H	3.81116842	3.72948006	7.16080245
H	7.62525058	2.95332233	7.17158522
H	2.75184695	5.76046369	9.12590879
H	5.03547076	6.97423425	9.09874131
H	2.29010484	6.29090968	10.76171804
H	4.86685909	7.58987125	10.76144238
H	0.05866942	2.95263427	7.15042649
H	0.89955948	7.77275640	9.07603231
H	9.55395389	0.77714758	9.11798801
C	3.12237595	7.83785045	9.53940228
C	2.28506604	6.58869473	9.69274851
C	4.62421074	7.80794324	9.70077130
O	7.68207938	0.04579797	9.23914248
O	0.96569452	6.80260085	9.23164126
O	0.09078908	0.17643221	9.29210749
Cu	5.11768591	8.83412544	19.92276866
Cu	-2.55025140	8.83252476	19.92229991
Cu	0.00183923	8.83382107	19.92113974
Cu	2.56161316	8.83340431	19.91608778
Cu	8.95358157	2.19786787	19.93612267
Cu	1.27907093	2.19887417	19.92868369
Cu	3.83766705	2.19634188	19.92863501
Cu	6.39715931	2.19466098	19.93216456
Cu	-2.54941843	4.41748609	19.92532048
Cu	0.00614669	4.41561978	19.93826528
Cu	2.56083423	4.41376693	19.92652470
Cu	5.11351413	4.41770218	19.92659867
Cu	6.39541510	6.62674255	19.92146139
Cu	-1.27271596	6.62383587	19.92597517
Cu	1.27838330	6.62341798	19.91293774
Cu	3.84004917	6.62651309	19.92228946
Cu	0.00554125	1.45385649	2.01584038
Cu	2.55449897	1.45611584	2.00612340
Cu	5.11289854	1.45596641	2.00782526
Cu	7.67440838	1.45433593	2.00737228
Cu	-1.27961103	3.67660630	2.01434380
Cu	1.28263569	3.67395461	2.01988611
Cu	3.83301586	3.66882989	2.00969438
Cu	6.39874900	3.67605176	2.00334532
Cu	-2.55310098	5.88714569	2.02638842
Cu	0.00203523	5.89003640	2.03355897
Cu	2.54938486	5.89142024	2.00511619
Cu	5.12201636	5.89205523	2.00757943

Cu	-3.83077641	8.10421136	2.01943788
Cu	-1.27517907	8.09728440	2.01620437
Cu	1.27957547	8.09583165	2.00512688
Cu	3.83433098	8.10665016	2.02013997
Cu	1.27729506	0.73207564	4.10885392
Cu	3.83052182	0.74443579	4.09245358
Cu	6.39280910	0.72935185	4.08216348
Cu	8.95137923	0.74756796	4.12841431
Cu	-0.00945152	2.93797550	4.07020749
Cu	2.56611153	2.92071457	4.11231293
Cu	5.12477120	2.93329747	4.08580439
Cu	7.66426612	2.92360806	4.09220989
Cu	-1.27858300	5.12747184	4.11521844
Cu	1.29095603	5.13082543	4.12161954
Cu	3.83262045	5.14736697	4.05628789
Cu	6.37944711	5.13174509	4.11652417
Cu	-2.54895086	7.36294610	4.08403433
Cu	-0.00341852	7.37889196	4.10830200
Cu	2.54475428	7.36068330	4.08162077
Cu	5.11572237	7.36715695	4.08493325
Cu	2.56913712	8.81368965	6.13913912
Cu	5.11621026	8.82417145	6.18868278
Cu	1.26671336	6.62564377	6.17611272
Cu	-1.27972689	2.22449473	6.28372484
Cu	7.63403084	4.41066677	6.20463282
Cu	6.40660953	2.17816873	6.25978668
Cu	-2.56581678	8.83235338	6.14938879
Cu	6.39313277	6.62578850	6.15731272
Cu	3.84178224	2.20109592	6.29075644
Cu	-1.28735782	6.61655394	6.15356817
Cu	5.08495986	4.44594754	6.19997120
Cu	1.26179702	2.19515123	6.19410681
Cu	0.01933635	4.41699960	6.19929530
Cu	-0.01091295	8.83969116	6.18044739
Cu	3.83315804	6.64221275	6.12618521
Cu	2.57641832	4.42133422	6.20154118

Str 6

Free energy from VASP is -327.47965900 eV

PBC 10.223900 10.223900 20.000000 90.000000 90.000000

120.000000

H	-0.09150294	5.93329615	7.24584539
H	-0.08431180	2.94320097	7.25350421

H	-1.20228764	8.08142100	8.39797285
H	5.06318333	0.30369328	9.93548238
H	5.06521563	3.88791307	10.46612051
H	3.54482519	1.35780214	10.03186106
H	3.69635221	3.78600614	9.32549370
H	2.60172909	2.97378901	7.22288401
H	6.35137806	4.45160494	8.54035072
H	2.61842520	5.93505418	7.23281220
C	5.25176077	2.26358697	9.07581404
C	4.49178336	1.14207505	9.53371912
C	4.78444649	3.67218373	9.41682898
O	6.38768783	2.14361708	8.48684595
O	3.91787148	0.14688297	8.04016098
O	5.39071295	4.66440290	8.57483386
Cu	0.00261958	-0.00147678	-0.00280253
Cu	2.55555773	-0.00223142	0.00178516
Cu	5.11105538	0.00345985	0.00349747
Cu	7.67212194	0.00185155	-0.00441828
Cu	8.94686445	2.20803889	0.00462315
Cu	1.27740668	2.20549281	-0.00239041
Cu	3.83742930	2.21072361	0.00463109
Cu	6.39158763	2.21387718	0.00237151
Cu	-2.55984458	4.42846594	-0.00836743
Cu	-0.00425613	4.43022170	-0.00367484
Cu	2.56506416	4.42964701	-0.00314565
Cu	5.11700608	4.42848172	-0.00969369
Cu	6.38994431	6.64600346	-0.01908626
Cu	-1.27845414	6.64539107	-0.00426589
Cu	1.28203586	6.64337990	0.00000109
Cu	3.83688562	6.64266554	-0.00806449
Cu	0.00392857	1.47333178	2.09559532
Cu	2.55960312	1.47534495	2.09001613
Cu	5.11768141	1.48489326	2.11071615
Cu	7.65529134	1.47238869	2.10128953
Cu	-1.28476410	3.68429241	2.07130593
Cu	1.27537636	3.69262456	2.05389198
Cu	3.84513628	3.68576666	2.08537375
Cu	6.38968411	3.68846878	2.09591452
Cu	-2.56288042	5.91087009	2.06957703
Cu	0.00546257	5.91798082	2.07767486
Cu	2.56156171	5.90327477	2.08678914
Cu	5.11251064	5.90784054	2.06890036
Cu	-3.83425772	8.12429612	2.10365110
Cu	-1.27332900	8.12590181	2.08994635

Cu	1.27835687	8.13066681	2.08822800
Cu	3.83219147	8.12071037	2.08097548
Cu	1.29389580	0.76559936	4.21004793
Cu	3.82784506	0.75151889	4.18506774
Cu	6.36971684	0.75648301	4.23529618
Cu	8.94968507	0.74452244	4.16012112
Cu	0.00876051	2.97662481	4.15297339
Cu	2.53125023	2.98066821	4.13607804
Cu	5.12523880	2.96356374	4.22572780
Cu	7.66871020	2.93632822	4.18453360
Cu	-1.26988041	5.16463458	4.11954815
Cu	1.26862561	5.15932838	4.17153790
Cu	3.83782605	5.15832999	4.16928583
Cu	6.38041731	5.18161256	4.14931583
Cu	-2.53221682	7.39447881	4.16976744
Cu	0.02181565	7.39470601	4.18665355
Cu	2.53151403	7.37473595	4.15782066
Cu	5.08789488	7.37909990	4.15677759
Cu	-0.00674427	8.88539950	6.28537627
Cu	-1.25459308	2.21098146	6.24486148
Cu	-3.82954084	6.67923177	6.19245482
Cu	5.14184017	4.48787807	6.28954079
Cu	6.40902237	2.23033421	6.38490693
Cu	7.67668450	0.01124718	6.21121856
Cu	7.65143505	4.44953050	6.15594738
Cu	-0.06026811	4.43274974	6.34616047
Cu	3.78240843	2.28704720	6.19025334
Cu	2.56797814	4.45773079	6.30904526
Cu	2.53339232	0.00595884	6.30429867
Cu	1.25681971	2.25769953	6.35211554
Cu	5.10902071	8.84720157	6.21669166
Cu	1.26935249	6.63262982	6.36045195
Cu	3.81748361	6.67754186	6.25315380
Cu	-1.28493649	6.61309871	6.22801502

Str 7

Free energy from VASP is -328.71743700 eV

PBC	10.223900	10.223900	20.000000	90.000000	90.000000
120.000000					
H	3.97089555	5.14059468	7.30354425		
H	1.23690709	5.25246479	7.26104256		
H	3.76833760	8.18945081	8.58817377		
H	7.46500859	1.72760430	8.49952201		

H	3.98883896	3.00594223	9.28692408
H	6.51612955	3.23050117	8.92869875
H	4.66232066	2.14095193	10.68669543
H	-0.09329412	2.89827141	7.24056124
H	3.42080928	0.31721789	9.31266690
H	2.61154240	2.85871398	7.22448621
C	5.37037561	1.42836956	8.80343471
C	6.49462247	2.23779628	8.46715660
C	4.25532395	2.00261358	9.66412981
O	5.20562664	0.21176320	8.42933991
O	3.81158733	8.22163824	7.61682634
O	3.11058860	1.17440011	9.68580713
Cu	5.11271174	8.84989699	19.99434893
Cu	-2.55615163	8.85217081	19.99365316
Cu	-0.00122542	8.85380034	19.99797080
Cu	2.55325385	8.85267969	19.99941215
Cu	8.94480114	2.21346790	19.99971791
Cu	1.27976468	2.20653296	0.00364696
Cu	3.83195715	2.20923728	0.01931793
Cu	6.38623954	2.21121059	19.99153002
Cu	7.66554571	4.42993651	19.98127102
Cu	-0.00300126	4.43181679	0.00221403
Cu	2.55992097	4.42996226	0.00378593
Cu	5.11165663	4.42968681	19.99159007
Cu	-3.83370562	6.64376195	19.98760728
Cu	-1.27828330	6.64447968	19.99224695
Cu	1.27540435	6.64391680	0.00351722
Cu	3.83538322	6.64284845	19.99680503
Cu	-0.00854448	1.47252572	2.08362759
Cu	2.55321127	1.46965611	2.10777199
Cu	5.12496544	1.47284595	2.10015243
Cu	7.65464394	1.47058919	2.09523122
Cu	-1.28731610	3.68612319	2.07378014
Cu	1.27746275	3.69136587	2.06077496
Cu	3.83954174	3.69305267	2.09318575
Cu	6.38924658	3.68649322	2.06713748
Cu	-2.54896795	5.89548567	2.07022137
Cu	0.00629170	5.91285403	2.09503667
Cu	2.54993937	5.91283458	2.08570024
Cu	5.10512160	5.90506773	2.07761285
Cu	-3.84097157	8.12314578	2.08314178
Cu	-1.27079260	8.12036921	2.07925467
Cu	1.27924679	8.12769615	2.11070275
Cu	3.82802069	8.12025767	2.08546363

Cu	1.25780533	0.75254319	4.20556972
Cu	3.85165417	0.74006577	4.17353474
Cu	6.37904072	0.75758921	4.27191769
Cu	8.93576449	0.74051813	4.18188373
Cu	0.01268819	2.96299115	4.13359289
Cu	2.53512180	2.97751554	4.15672095
Cu	5.11286192	2.95874775	4.18509913
Cu	7.65219369	2.94210575	4.17011955
Cu	-1.25028439	5.15037843	4.15979663
Cu	1.29001601	5.14066335	4.16805125
Cu	3.80786575	5.17513299	4.18378753
Cu	6.37431643	5.16210864	4.12980791
Cu	-2.55477947	7.38165454	4.11460844
Cu	0.01070021	7.39887899	4.19006361
Cu	2.55834210	7.37406797	4.20430356
Cu	5.08435642	7.38386344	4.17791712
Cu	3.86141844	6.58498743	6.35585537
Cu	2.58693096	4.43407837	6.49140001
Cu	-1.30294091	6.63169489	6.20326265
Cu	6.38437537	2.30493217	6.36612273
Cu	5.13423283	4.46762717	6.24161592
Cu	-2.54456155	8.82737059	6.19932833
Cu	7.61141895	0.02740037	6.25196317
Cu	1.27894977	2.22160728	6.35730737
Cu	0.08316247	0.02081828	6.29409767
Cu	-2.55796136	4.46787002	6.18765225
Cu	-3.78523688	6.64659270	6.17741572
Cu	-0.00650817	4.42953101	6.36592042
Cu	-0.02254056	8.81808419	6.35329289
Cu	1.23867959	6.59571151	6.22238318
Cu	-1.25306059	2.26204476	6.19419670
Cu	3.79100296	2.21349219	6.18058167

Str 8

Free energy from VASP is -328.29178600 eV

PBC	10.223900	10.223900	20.000000	90.000000	90.000000
	120.000000				

H	-1.05070048	5.03786742	7.51504762
H	3.90490625	0.72856182	7.23652161
H	4.94051142	7.15392666	8.51457439
H	-1.18252420	6.04509757	9.23814093
H	1.60465969	3.59802680	9.54640933
H	-0.70957008	4.30448509	9.68722975

H	2.44218048	4.97227952	10.31474502
H	1.20805112	0.72896665	7.23306137
H	3.70524693	5.25189514	8.43839284
H	6.40305428	3.63804702	7.23577065
C	0.88967231	5.56629023	8.95497774
C	-0.45195817	5.23687023	9.18292268
C	1.99937946	4.60853214	9.37089367
O	1.25404758	6.65457905	8.35929734
O	4.92713426	6.36831545	7.93571572
O	3.04500106	4.49155308	8.39002924
Cu	0.00451295	-0.00804338	-0.00064881
Cu	2.56380279	-0.00751151	0.00863816
Cu	5.11540108	-0.01356778	0.00564514
Cu	7.66682070	-0.01149883	-0.01421766
Cu	8.94765330	2.21215645	-0.01567939
Cu	1.28005469	2.21426364	-0.00712915
Cu	3.83993939	2.20977812	-0.01594652
Cu	6.39518765	2.21372811	-0.01813245
Cu	-2.55153164	4.42467556	-0.00053980
Cu	0.00543965	4.42735915	0.00103992
Cu	2.55556893	4.42923190	-0.00637581
Cu	5.11701055	4.42339370	-0.00640667
Cu	6.39383974	6.63537492	-0.00213179
Cu	-1.26822861	6.63421046	0.00777437
Cu	1.28361109	6.63443554	0.01774344
Cu	3.83096927	6.63304159	-0.00051272
Cu	0.00530028	1.47596051	2.06555541
Cu	2.56318843	1.48572000	2.06995781
Cu	5.11567057	1.46274033	2.05909912
Cu	7.66996867	1.46410097	2.06334020
Cu	-1.26541014	3.68554433	2.07270710
Cu	1.28989824	3.69078265	2.10115398
Cu	3.82926651	3.69113663	2.07494229
Cu	6.39210855	3.68914873	2.07358782
Cu	-2.54494008	5.90715736	2.09844084
Cu	0.01262717	5.89180411	2.12056001
Cu	2.55931791	5.88981999	2.11625838
Cu	5.11258821	5.89385853	2.08981407
Cu	-3.82655960	8.09812503	2.08380138
Cu	-1.27317242	8.09467236	2.10909242
Cu	1.28856602	8.10633058	2.11080908
Cu	3.82982559	8.10238618	2.08286488
Cu	1.30286996	0.73121141	4.11618849
Cu	3.82415241	0.71992509	4.13022827

Cu	6.37627227	0.74821466	4.16801631
Cu	8.96049166	0.72552054	4.12778170
Cu	0.01445129	2.94690356	4.16167307
Cu	2.56543367	2.94690248	4.21091664
Cu	5.10848314	2.92986378	4.12347625
Cu	7.67280798	2.95173854	4.13236325
Cu	-1.28360554	5.14415903	4.16890522
Cu	1.29510071	5.16381562	4.25014660
Cu	3.85412437	5.14791933	4.21380007
Cu	6.41048235	5.17510121	4.17141751
Cu	-2.57145519	7.38148605	4.25883072
Cu	0.01456329	7.35973287	4.21297811
Cu	2.56370833	7.34570515	4.21491100
Cu	5.11986295	7.36975440	4.17825744
Cu	7.67546113	0.03857943	6.17984920
Cu	1.25565949	2.19438892	6.25712492
Cu	3.83981764	6.69014910	6.26328972
Cu	-2.55041459	8.85741420	6.37790442
Cu	-2.51386450	4.40006840	6.36922375
Cu	-0.02716853	4.38359815	6.26698606
Cu	1.29439075	6.68610342	6.35268167
Cu	2.57709426	4.37474215	6.31183910
Cu	3.86658557	2.16187712	6.24009506
Cu	5.17986815	4.33349990	6.19072750
Cu	8.94378381	2.18679278	6.19099118
Cu	0.01911408	0.04231120	6.20883239
Cu	6.42900322	2.20157597	6.27387516
Cu	-1.30335868	6.57698076	6.25813510
Cu	5.09749712	-0.00280983	6.24855103
Cu	6.37799812	6.62429663	6.35999597

Str 9

Free energy from VASP is -329.15574200 eV

PBC 10.223900 10.223900 20.000000 90.000000 90.000000

120.000000

H	-0.90776782	4.60168360	9.10944953
H	3.89770044	0.72511291	7.22735373
H	4.93156353	7.23392914	8.54682965
H	-0.97657910	6.09890028	10.05824758
H	1.69619976	3.55271157	9.52802757
H	-0.30235777	4.57915621	10.78106084
H	2.54094813	4.78836552	10.47871823
H	1.17988631	0.73043824	7.23751478

H	3.75177461	5.38058927	8.51683268
H	6.40532776	3.65504590	7.19102976
C	0.94538396	5.54670819	9.26803744
C	-0.37820670	5.19932346	9.87945341
C	2.10124188	4.57831802	9.48231605
O	1.07332129	6.54037274	8.54036208
O	4.89555443	6.41995238	8.00938154
O	3.08626684	4.60571241	8.46902508
Cu	5.11307489	8.84448603	19.98362139
Cu	-2.55303669	8.84890872	0.00505904
Cu	0.00031712	8.83977998	0.00104402
Cu	2.54933468	8.84041438	19.97207249
Cu	8.94253131	2.21195788	19.95457672
Cu	1.27734488	2.21405131	19.97692450
Cu	3.83481424	2.21207933	19.97835796
Cu	6.38858013	2.21260178	19.95789225
Cu	7.66656600	4.42749257	19.96812487
Cu	0.00420461	4.42997812	19.97995695
Cu	2.55274504	4.43227830	19.98642195
Cu	5.10881072	4.42744132	19.97694889
Cu	6.38867527	6.63627069	19.98474733
Cu	-1.27101514	6.63506875	19.99367021
Cu	1.27955484	6.63502631	0.00704014
Cu	3.82651614	6.63374391	19.98709502
Cu	-0.00613955	1.47010601	2.03930833
Cu	2.55618551	1.48776996	2.06228466
Cu	5.10766910	1.46253807	2.04726948
Cu	7.66034979	1.46161721	2.03621732
Cu	-1.27573662	3.68677822	2.03732735
Cu	1.28287727	3.68929118	2.07989974
Cu	3.82066593	3.69326268	2.07133266
Cu	6.38028345	3.69059758	2.04271302
Cu	-2.55720009	5.90765412	2.07181997
Cu	0.00504869	5.89145919	2.10107501
Cu	2.55713865	5.89464573	2.10569516
Cu	5.09926638	5.89818303	2.07582715
Cu	-3.83959657	8.10043416	2.07684278
Cu	-1.28148869	8.09312309	2.10136743
Cu	1.28406766	8.10241904	2.10576206
Cu	3.82326600	8.10330487	2.07309089
Cu	1.28632809	0.73572711	4.11226005
Cu	3.81102282	0.72012111	4.12305410
Cu	6.36777026	0.74351511	4.15503869
Cu	8.94471742	0.72498973	4.11454550

Cu	-0.00162147	2.93361224	4.11681402
Cu	2.54978259	2.94845983	4.21034552
Cu	5.09668723	2.92651949	4.10884063
Cu	7.65461064	2.94234317	4.08553669
Cu	-1.30366973	5.14599134	4.13931065
Cu	1.29766801	5.15968354	4.19883337
Cu	3.83995073	5.15174566	4.21623693
Cu	6.38220109	5.17625255	4.13857425
Cu	-2.59211709	7.38453486	4.23597109
Cu	0.00624674	7.35985179	4.19123110
Cu	2.56329337	7.34497228	4.21715583
Cu	5.10628300	7.37005573	4.18150400
Cu	7.65722499	0.02304614	6.18084014
Cu	1.23703777	2.20539947	6.26321497
Cu	3.83429041	6.68692953	6.28909811
Cu	2.54104579	0.00701686	6.37692132
Cu	7.67272537	4.39585912	6.24581008
Cu	-0.02214112	4.39416206	6.16383394
Cu	1.26254558	6.63466938	6.32821129
Cu	2.56784733	4.38789921	6.32898946
Cu	3.84920464	2.16124441	6.23372439
Cu	5.15174651	4.33511151	6.18206423
Cu	8.92975945	2.21109165	6.16835487
Cu	-0.00003161	0.04842260	6.20257152
Cu	6.41366710	2.19484645	6.25341986
Cu	-1.30989502	6.59356745	6.20951038
Cu	-0.02207716	8.84131005	6.23782666
Cu	6.37413900	6.61403501	6.36074470

Str 10

Free energy from VASP is -328.46583600 eV

PBC 10.223900 10.223900 20.000000 90.000000 90.000000

120.000000

H	4.27914869	0.04978899	8.66512204
H	2.70614254	1.23042375	8.67209591
H	0.56091382	7.98529710	7.62528845
H	-0.74094936	4.17091971	9.05066694
H	0.91461085	6.65871017	9.80228751
H	-2.12282146	4.49006038	10.10502622
H	-0.29910115	7.47700148	10.79426066
H	-0.43774072	4.70211891	10.73283751
H	1.23525359	5.17303004	7.25434850
H	3.85293567	3.76222003	7.25331846

C	-1.12517934	6.20963799	9.30568764
C	-1.10390743	4.82219159	9.87011597
C	-0.05379752	7.18716588	9.75185291
O	-1.97097059	6.53744642	8.46355503
O	3.35048466	0.81706087	8.06883691
O	0.10001885	8.33984945	8.95049846
Cu	-0.00020433	0.00445074	-0.01854099
Cu	2.55288266	0.00172907	-0.00514296
Cu	5.10727743	0.00159146	-0.01389067
Cu	7.66874039	0.00488774	-0.02285687
Cu	8.94732111	2.21422555	-0.02802259
Cu	1.27436352	2.20943187	-0.01184703
Cu	3.83117450	2.21544586	-0.00483992
Cu	6.39017273	2.21896994	-0.02281508
Cu	-2.55839261	4.43327087	-0.01207279
Cu	-0.00250554	4.42763226	-0.01381508
Cu	2.55587875	4.42812882	-0.00275082
Cu	5.11255353	4.42851898	-0.00636456
Cu	6.39409817	6.64392698	-0.01059891
Cu	-1.28569389	6.64305942	-0.00237249
Cu	1.27360064	6.64227817	-0.01412208
Cu	3.83731466	6.64622897	-0.01581707
Cu	0.00032011	1.47803448	2.07520094
Cu	2.55474999	1.48114522	2.08716016
Cu	5.10407360	1.47912368	2.06258427
Cu	7.67095086	1.48344650	2.04800594
Cu	-1.28287386	3.69769298	2.06283689
Cu	1.28074555	3.69119931	2.06828570
Cu	3.83082148	3.69045691	2.08711348
Cu	6.38316181	3.69154229	2.07593553
Cu	-2.56196303	5.91107324	2.09806644
Cu	-0.00140040	5.89911659	2.06528933
Cu	2.55632945	5.91087394	2.05550515
Cu	5.10785173	5.90843957	2.06796601
Cu	-3.83529539	8.11920099	2.07755998
Cu	-1.28179626	8.12812763	2.08659416
Cu	1.27477356	8.11685211	2.06358578
Cu	3.82777172	8.11931269	2.06582223
Cu	1.28930784	0.73520965	4.16407908
Cu	3.83055405	0.76542020	4.20299554
Cu	6.39774136	0.75092913	4.10125825
Cu	8.93781729	0.74281942	4.13979683
Cu	-0.00045744	2.97464353	4.13444096
Cu	2.56008352	2.96394229	4.19051908

Cu	5.09257626	2.94097313	4.17253080
Cu	7.66884427	2.96118001	4.12593794
Cu	-1.27160574	5.17682326	4.16413966
Cu	1.29951032	5.17263962	4.14685736
Cu	3.81541043	5.17206324	4.15301973
Cu	6.36187992	5.16043589	4.16387408
Cu	-2.55299670	7.41049062	4.18842474
Cu	-0.00504022	7.35399069	4.13828697
Cu	2.53654943	7.37431681	4.15894407
Cu	5.10470752	7.38445331	4.13429974
Cu	7.65964870	4.41904891	6.19374089
Cu	-1.30495264	6.65586469	6.23809302
Cu	1.27339369	6.67127916	6.35995325
Cu	6.35302141	6.64255731	6.19803321
Cu	0.09316573	8.82597545	6.12773937
Cu	3.84361864	6.67353687	6.20233444
Cu	0.01651115	4.43510228	6.23768486
Cu	2.57288528	8.86399630	6.23862670
Cu	8.94026474	2.22873983	6.21125730
Cu	3.85597175	2.22077645	6.40467686
Cu	1.22263886	2.21846336	6.18012693
Cu	2.54675238	4.45157136	6.35594776
Cu	6.42220858	2.21484652	6.18838964
Cu	2.52723094	0.02794264	6.31988746
Cu	5.10125688	4.42958294	6.27193057
Cu	10.20417247	0.00963698	6.21553180

Str 11

Free energy from VASP is -329.33652400 eV

PBC	10.223900	10.223900	20.000000	90.000000	90.000000
120.000000					

H	0.48144140	5.44245951	8.89074866
H	1.53457346	7.34810138	8.73071815
H	2.49382683	1.38666212	9.21684665
H	1.84820489	1.58273498	10.85153768
H	0.01778970	3.59155960	10.39812051
H	3.53800154	2.10693704	10.48329657
H	0.15841927	2.56101731	8.95965733
H	2.12750041	6.12193421	9.50578746
H	5.11339663	2.94442185	7.14868615
H	-1.28673274	8.12524452	7.16029748
C	2.01365320	3.39805065	9.68485287
C	2.51205401	2.04457898	10.10457627

C	0.51403475	3.50159178	9.41018632
O	2.76464543	4.36818932	9.56736278
O	1.35548680	6.74004928	9.47658398
O	0.11577247	4.56137542	8.55360576
Cu	5.11000959	8.85408135	19.91030675
Cu	-2.55720875	8.84742076	19.91032729
Cu	0.00097116	8.84320380	19.91009022
Cu	2.56082529	8.85193924	19.91256686
Cu	8.94833145	2.20837755	19.93067884
Cu	1.27133208	2.21033400	19.91387006
Cu	3.83404722	2.21075852	19.91017831
Cu	6.39633246	2.20894610	19.91167225
Cu	-2.54772319	4.41914525	19.91243168
Cu	-0.00029904	4.42013903	19.92372065
Cu	2.55126851	4.42542955	19.91103192
Cu	5.11207443	4.42242362	19.91126546
Cu	6.38999883	6.63445416	19.91076987
Cu	-1.27465202	6.63245208	19.92407806
Cu	1.27839908	6.63155337	19.92163459
Cu	3.83386179	6.63534089	19.91259052
Cu	0.00348913	1.47810000	2.02008485
Cu	2.55323090	1.47112510	1.98826866
Cu	5.11509622	1.46598494	1.98018673
Cu	7.66417613	1.46929837	2.01177868
Cu	-1.27804974	3.68880795	2.02857819
Cu	1.27929071	3.68325943	2.01195264
Cu	3.83044566	3.68541630	1.98455124
Cu	6.39614343	3.68519303	1.98724246
Cu	-2.55057122	5.88643491	2.00841439
Cu	-0.00119422	5.89173682	2.01069705
Cu	2.55352430	5.89345685	2.01065918
Cu	5.11544505	5.89742605	1.99521871
Cu	-3.83554410	8.10940295	1.98559416
Cu	-1.27909621	8.11429792	1.99434567
Cu	1.28106858	8.11691071	1.99721291
Cu	3.83454520	8.11136036	1.99505051
Cu	1.29741649	0.71884170	4.08366467
Cu	3.83867688	0.74336390	4.07645505
Cu	6.36577217	0.73586545	4.11517180
Cu	8.94627795	0.73755850	4.07217673
Cu	-0.00170847	2.96721267	4.10842458
Cu	2.57028115	2.94423983	4.07736816
Cu	5.11606241	2.94525746	4.03304099
Cu	7.65650319	2.94467091	4.08950593

Cu	-1.25722962	5.17709974	4.14747257
Cu	1.26514565	5.15197479	4.10228858
Cu	3.84592002	5.15351906	4.08338582
Cu	6.38816063	5.14785297	4.08419509
Cu	-2.55435586	7.37259140	4.05726088
Cu	-0.00188743	7.38106019	4.06209924
Cu	2.56027080	7.38195074	4.06173339
Cu	5.11479527	7.37903468	4.06762223
Cu	2.55949482	4.43259041	6.13353937
Cu	0.01439344	4.42328508	6.32070427
Cu	-0.00053809	8.83297679	6.21537227
Cu	6.38804613	2.21656371	6.20439824
Cu	6.37180809	6.62925657	6.12610112
Cu	7.67131244	0.00119229	6.15549954
Cu	8.94037930	2.19741332	6.14220557
Cu	-1.28526619	6.66317570	6.19839224
Cu	-2.55406972	8.85073382	6.20057298
Cu	3.84962370	2.23219577	6.18022590
Cu	3.84057496	6.64310924	6.14120017
Cu	1.30588933	6.65305582	6.11043412
Cu	-2.54322704	4.43312762	6.14786443
Cu	5.11842890	4.41748036	6.20370047
Cu	1.29427743	2.19060786	6.11837090
Cu	-5.10849040	8.85172114	6.14734176

Str 12

Free energy from VASP is -314.36578500 eV

PBC	10.223900	10.223900	20.000000	90.000000	90.000000
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120.000000

H	3.18884747	5.13945016	7.66619316
H	4.93091472	2.30516965	8.55724713
H	0.00285243	2.94979073	7.24978107
H	2.83422972	5.88374676	10.16664110
H	2.43386592	3.41324641	9.36180691
H	4.53082722	5.82704721	10.73685407
H	3.83523940	3.18856820	10.44993937
H	4.11459299	6.80297218	9.31039158
C	4.19560637	4.67451393	8.97785775
C	3.88410250	5.87219458	9.84315344
C	3.52850792	3.36592556	9.39790582
O	5.35570339	4.57270748	8.43118547
O	3.95013355	2.24902892	8.60858322
Cu	0.00077155	-0.00555775	-0.00135485

Cu	2.55787549	-0.00270932	0.00815444
Cu	5.11045169	-0.00007331	0.00207384
Cu	7.66721993	-0.00063132	-0.00128725
Cu	8.94514024	2.21166421	0.00488011
Cu	1.27947575	2.20926027	0.00428348
Cu	3.83606007	2.20968632	0.00422142
Cu	6.38753098	2.21175622	0.00039913
Cu	-2.56142345	4.43061647	-0.00032929
Cu	-0.00080913	4.42911681	0.00169912
Cu	2.56196714	4.43030585	0.00553871
Cu	5.11192659	4.42786444	0.00763349
Cu	6.39084974	6.64096083	0.00269385
Cu	-1.27982997	6.64433371	0.00198551
Cu	1.27762064	6.64270422	0.00187242
Cu	3.83525797	6.64029754	0.00649722
Cu	0.00155520	1.46922870	2.07559795
Cu	2.55610007	1.47934916	2.10060112
Cu	5.10999389	1.48178975	2.09694739
Cu	7.66768426	1.47454432	2.08170404
Cu	-1.28146429	3.69372942	2.07150316
Cu	1.28720689	3.68765121	2.07786165
Cu	3.83211452	3.68438690	2.09923476
Cu	6.38829330	3.68391656	2.09830723
Cu	-2.55791163	5.89973219	2.09345931
Cu	0.00253611	5.90277288	2.08276816
Cu	2.55993155	5.89843709	2.09871205
Cu	5.11224943	5.90064822	2.09085597
Cu	-3.83692698	8.11638548	2.09822545
Cu	-1.27946908	8.12162075	2.09857154
Cu	1.28137166	8.11242743	2.08359485
Cu	3.83473725	8.11869102	2.09265077
Cu	1.26899308	0.74549949	4.17424100
Cu	3.83220185	0.75273667	4.18656545
Cu	6.39048143	0.72973986	4.14911156
Cu	8.95138994	0.74890225	4.17391693
Cu	0.00286383	2.95251162	4.11783301
Cu	2.54998599	2.96073686	4.22472023
Cu	5.10119581	2.95550086	4.20487162
Cu	7.68706602	2.94666988	4.16491440
Cu	-1.26557918	5.15769812	4.16335946
Cu	1.28009717	5.15098090	4.18015534
Cu	3.84962118	5.14859070	4.19190151
Cu	6.38091152	5.15389022	4.18025472
Cu	-2.55641236	7.37585443	4.15658188

Cu	0.00487909	7.37395137	4.15962930
Cu	2.55851218	7.36722167	4.16634799
Cu	5.09783387	7.36285238	4.17983077
Cu	-2.56842406	8.83934666	6.22801029
Cu	1.25355742	6.64942711	6.24378781
Cu	-1.26647247	2.20346243	6.29676837
Cu	-3.82123033	6.64898570	6.23255496
Cu	1.24042427	2.20193817	6.26997325
Cu	6.43075319	2.17355273	6.20103200
Cu	5.09998845	8.81414104	6.24011350
Cu	-1.27384800	6.63985390	6.23233006
Cu	2.55068082	4.46734964	6.28943824
Cu	-2.52735265	4.42759773	6.21184467
Cu	-0.00781873	4.41102194	6.28505770
Cu	3.80983829	2.19214614	6.31211282
Cu	3.80270398	6.62636676	6.28418705
Cu	5.19224676	4.39734756	6.32494433
Cu	2.55750380	8.84602421	6.23946508
Cu	0.00779878	8.84104925	6.22896725

Str 13

Free energy from VASP is -315.13369500 eV

PBC	10.223900	10.223900	20.000000	90.000000	90.000000
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120.000000

H	6.50208775	3.64138652	7.25819292
H	1.49152765	1.21876058	8.78810102
H	3.82414618	2.28036676	9.31488730
H	3.47034066	5.31352251	9.70942238
H	1.32391519	4.05328607	9.11930619
H	3.75688600	4.13225986	11.02137600
H	1.67317508	2.88101493	10.42984696
H	5.00803751	4.41414884	9.78270421
C	3.33089876	3.24559027	9.08086489
C	3.92634763	4.34276222	9.95458957
C	1.83516550	3.10852034	9.36334195
O	3.56601497	3.51946787	7.69524136
O	1.16684175	2.11180982	8.55640611
Cu	0.00124075	0.00055852	19.99474357
Cu	2.55484897	0.00020033	19.99666653
Cu	-0.00060682	8.85004162	19.99611525
Cu	2.55285170	8.84790803	19.98798567
Cu	-1.27611419	2.21078886	19.99426688
Cu	1.27982840	2.21274635	0.00253221

Cu	3.82888067	2.21272276	0.00773003
Cu	6.38697436	2.21247032	19.99860700
Cu	7.66653519	4.42731252	0.00335632
Cu	0.00443163	4.43221199	19.99513351
Cu	2.55332790	4.42901193	0.00792961
Cu	5.10856355	4.42701038	0.00789929
Cu	-3.83456321	6.64314273	0.00105361
Cu	-1.27499249	6.64060856	0.01291231
Cu	1.27831152	6.63938534	0.00895387
Cu	3.82902468	6.63967535	19.99340083
Cu	-0.00136469	1.47794697	2.08238915
Cu	2.55353845	1.48050315	2.09602237
Cu	5.11002335	1.47349394	2.08269005
Cu	7.66605112	1.46946724	2.06154704
Cu	-1.26699693	3.68757216	2.07098891
Cu	1.27904376	3.68774311	2.09564094
Cu	3.82275543	3.68823267	2.10442421
Cu	6.37950677	3.68665912	2.08203089
Cu	-2.56565351	5.89648659	2.07992426
Cu	0.00268125	5.89347551	2.10312239
Cu	2.56179353	5.89938323	2.09988819
Cu	5.10202183	5.89870122	2.08359235
Cu	-3.83670722	8.12337532	2.08517661
Cu	-1.28201380	8.12436923	2.08572529
Cu	1.27596876	8.11992999	2.08729633
Cu	3.83194025	8.11550041	2.07144917
Cu	1.27585819	0.75317599	4.18061699
Cu	3.83162753	0.74702898	4.17655629
Cu	6.38806900	0.75769557	4.17329220
Cu	8.93775599	0.73461548	4.14332894
Cu	0.00657024	2.95089668	4.17626486
Cu	2.54265469	2.95247740	4.21641831
Cu	5.09629208	2.95026178	4.18657206
Cu	7.66362600	2.94948324	4.12066179
Cu	-1.31180926	5.15164625	4.16478555
Cu	1.29681325	5.16016096	4.18610743
Cu	3.84773181	5.13345833	4.22922792
Cu	6.36346518	5.14675676	4.17657939
Cu	-2.56219646	7.36581293	4.13811353
Cu	-0.00607171	7.37498353	4.14352649
Cu	2.55098785	7.37595283	4.15097936
Cu	5.10565360	7.37099518	4.13865065
Cu	2.47222431	4.49441848	6.31058503
Cu	6.41437810	2.20240557	6.26989429

Cu	-2.56719879	8.80768544	6.21264460
Cu	0.00323865	8.83424604	6.22860095
Cu	3.81843919	2.11499696	6.26189912
Cu	5.09176501	8.83133738	6.20984579
Cu	-0.04288566	4.45358572	6.20841724
Cu	7.66687467	4.42545329	6.28768551
Cu	2.55016851	8.84937379	6.23092394
Cu	1.25637723	6.66694211	6.23394357
Cu	6.38030091	6.65375747	6.21765584
Cu	5.15465784	4.43639220	6.40166904
Cu	1.22140257	2.19512551	6.32120962
Cu	-1.29179968	6.63924526	6.22466536
Cu	3.82979770	6.66504680	6.21865777
Cu	8.93154075	2.19976854	6.19666883

Str 14

Free energy from VASP is -314.19577500 eV

PBC	10.223900	10.223900	20.000000	90.000000	90.000000
120.000000					
H	4.96958691	3.09542150	7.37222727		
H	1.58928254	1.23549810	8.83651763		
H	3.84543840	2.22324218	9.55039304		
H	3.62035048	5.27587685	9.90322839		
H	1.42757876	4.07232355	9.16149478		
H	3.72310151	4.11504188	11.26056703		
H	1.62778424	2.90271499	10.50504539		
H	5.08443029	4.29101463	10.12457442		
C	3.40417541	3.20868506	9.29960610		
C	3.98960230	4.28578835	10.20709112		
C	1.88653530	3.11573767	9.45459259		
O	3.71225550	3.49824091	7.92704841		
O	1.26835518	2.12860950	8.60026481		
Cu	0.00195489	0.00045008	0.00126044		
Cu	2.55607625	0.00031372	-0.00215015		
Cu	5.11452298	-0.00162019	-0.00229324		
Cu	7.66915875	0.00002653	0.00219736		
Cu	8.94764946	2.21237046	0.00607205		
Cu	1.27975364	2.21396515	0.00497775		
Cu	3.83323979	2.21280674	0.00359600		
Cu	6.39175798	2.21209565	0.00018321		
Cu	-2.55262466	4.42571171	-0.00095050		
Cu	0.00154386	4.42743676	0.00439388		
Cu	2.55360268	4.42742417	0.00477225		

Cu	5.11268571	4.42687984	-0.00034226
Cu	6.39070239	6.64226581	-0.00448841
Cu	-1.27305052	6.63952532	0.00164957
Cu	1.27841883	6.64034353	0.00262922
Cu	3.83377864	6.64043821	-0.00273936
Cu	0.00129742	1.47725586	2.09404935
Cu	2.55410455	1.47817154	2.08983057
Cu	5.11555901	1.47489640	2.08221153
Cu	7.66981892	1.47464530	2.08550419
Cu	-1.27160817	3.68454443	2.09318081
Cu	1.28029600	3.68763670	2.10064256
Cu	3.82767007	3.68821100	2.08858100
Cu	6.39022815	3.68615598	2.07998498
Cu	-2.55046208	5.90126354	2.06587974
Cu	0.01164609	5.89761163	2.09629555
Cu	2.55791644	5.90256666	2.09099826
Cu	5.11027838	5.90384791	2.07363916
Cu	-3.83019601	8.12178016	2.08963073
Cu	-1.27274427	8.11942119	2.07678244
Cu	1.27995853	8.11872839	2.08648655
Cu	3.83380447	8.11696928	2.08443120
Cu	1.27960976	0.75144207	4.18661472
Cu	3.83703344	0.73242582	4.15591471
Cu	6.38921723	0.75071700	4.17737401
Cu	8.94070481	0.73946176	4.16469977
Cu	0.00980271	2.94458887	4.19116704
Cu	2.55151313	2.95090567	4.20732396
Cu	5.10570505	2.95212902	4.15642618
Cu	7.65861634	2.95120755	4.16823289
Cu	-1.27138336	5.16234986	4.15512579
Cu	1.30470083	5.15541698	4.19586241
Cu	3.83840799	5.15631592	4.17627170
Cu	6.40753224	5.17497528	4.13278338
Cu	-2.54352110	7.37169124	4.13991195
Cu	0.00860057	7.37552174	4.15886425
Cu	2.55624751	7.38261854	4.16189326
Cu	5.11633572	7.37672275	4.15255332
Cu	2.56323684	4.45235579	6.32027631
Cu	6.35251840	2.24990810	6.32681260
Cu	-2.55620132	8.81277470	6.21524510
Cu	0.01320267	8.82168751	6.24692564
Cu	3.83209732	2.11236669	6.21465120
Cu	5.09601230	8.84096101	6.23062940
Cu	0.00068665	4.44152172	6.23180163

Cu	-2.52031355	4.44077773	6.24724299
Cu	7.65735886	0.01383174	6.24853077
Cu	1.29078503	6.64439164	6.25395140
Cu	-3.81405668	6.66163034	6.23203542
Cu	5.21552976	4.48301477	6.19226657
Cu	1.24487977	2.19807170	6.32938769
Cu	-1.26614111	6.63773319	6.24418952
Cu	3.84389427	6.66432173	6.22430063
Cu	8.91142286	2.21216730	6.23456273

Str 15

Free energy from VASP is -315.28105400 eV

PBC	10.223900	10.223900	20.000000	90.000000	90.000000
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120.000000

H	5.07611304	3.01154221	8.71284723
H	1.63849745	1.23306128	9.04114981
H	3.63725197	2.08095479	10.43639492
H	3.72484886	5.14926658	10.12896538
H	1.73742157	4.08645510	9.08805681
H	3.39255503	4.27087815	11.64903302
H	1.41346002	3.14259920	10.57315519
H	4.99223086	4.15395931	10.89211927
C	3.43596192	3.01552438	9.87589332
C	3.91516545	4.21883431	10.68318483
C	1.94093967	3.13587788	9.60393219
O	4.10813726	2.93382290	8.59825835
O	1.38311008	2.12698689	8.74161888
Cu	0.00216451	0.00409987	0.00463222
Cu	2.55683678	0.00541139	0.00797226
Cu	5.11234469	0.00238150	19.99655332
Cu	7.66901990	0.00106481	19.99298266
Cu	-1.27355770	2.21432462	0.00455679
Cu	1.28076863	2.21428264	0.01529285
Cu	3.83170936	2.21347705	0.00761679
Cu	6.38969037	2.21329334	19.99695901
Cu	-2.55259214	4.42602769	19.99952067
Cu	0.00417019	4.42565930	0.00473920
Cu	2.55549179	4.42413522	0.00372897
Cu	5.11026492	4.42520581	19.99711008
Cu	-3.83222182	6.64494666	19.99436898
Cu	-1.27578727	6.64472567	19.99616209
Cu	1.27872320	6.64195656	19.99002133
Cu	3.83430880	6.64239249	19.98958812

Cu	0.00521843	1.47959491	2.10025150
Cu	2.55882328	1.48101341	2.11009371
Cu	5.11328100	1.47877571	2.08421734
Cu	7.67232760	1.47699559	2.07448809
Cu	-1.26404796	3.68934358	2.08912380
Cu	1.28540229	3.68650133	2.10608417
Cu	3.82939230	3.68632811	2.09269593
Cu	6.39019374	3.68900675	2.07678716
Cu	-2.54990542	5.90705384	2.06691297
Cu	0.00274090	5.90845205	2.07307857
Cu	2.55766517	5.90711095	2.06885896
Cu	5.11570786	5.90622963	2.06421285
Cu	-3.83000321	8.12722862	2.08754192
Cu	-1.27351083	8.12783256	2.08605947
Cu	1.28028942	8.11860691	2.07126743
Cu	3.83610236	8.11971286	2.07552327
Cu	1.28278933	0.75230460	4.19397710
Cu	3.84335314	0.75233076	4.18519214
Cu	6.39632082	0.73947335	4.14901487
Cu	8.94757672	0.74138231	4.16024050
Cu	0.01951001	2.94826338	4.20034762
Cu	2.55874494	2.94591463	4.22007331
Cu	5.10935082	2.95375118	4.16579422
Cu	7.67899245	2.95788128	4.14587437
Cu	-1.27304953	5.17115818	4.15162967
Cu	1.27795945	5.17769618	4.14824395
Cu	3.83832699	5.17528597	4.13807262
Cu	6.40189618	5.17323819	4.13745552
Cu	-2.54913127	7.38235069	4.14932808
Cu	0.00280752	7.38594803	4.15537369
Cu	2.55794843	7.38493045	4.15096585
Cu	5.11927007	7.38214012	4.14720491
Cu	2.55264192	4.47247716	6.20331448
Cu	6.40967340	2.21769022	6.20916119
Cu	-2.54707707	8.83507326	6.22845192
Cu	5.12497180	0.00013332	6.24178247
Cu	3.84751049	2.21562703	6.30373462
Cu	5.10609372	8.84475562	6.22989663
Cu	-0.00175623	4.44851860	6.22951028
Cu	-2.55413814	4.43257528	6.23492102
Cu	7.66937639	0.00514452	6.23963483
Cu	1.27824618	6.65617630	6.24183958
Cu	-3.82773287	6.64544726	6.23618747
Cu	5.12678910	4.45794506	6.19310534

Cu	1.27428617	2.21329328	6.36463285
Cu	-1.27467138	6.64363514	6.23927356
Cu	3.83689899	6.65557024	6.22631874
Cu	8.93747271	2.21724143	6.24166281

2. 1,3-PDO-dehydrogenation path

Str 1

Free energy from VASP is -328.39379400 eV

PBC	10.223900	10.223900	20.000000	90.000000	90.000000
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120.000000

H	2.56691945	1.43923141	7.25711903
H	-0.04377945	2.94207071	7.26393275
H	1.94551802	5.59350670	11.35439436
H	1.76263090	6.24853554	8.99010230
H	2.17365364	3.79615525	9.64350942
H	2.56244699	7.54714549	9.93089289
H	3.10591426	3.43031148	11.13626072
H	4.74420331	5.94699531	11.06855044
H	4.19671842	5.57640868	8.76773784
H	4.16467228	3.36776412	8.77649582
C	2.85629577	5.54905729	10.73368286
C	2.67251270	6.51886758	9.55972649
C	3.03096740	4.10086297	10.26669922
O	3.92418748	5.94984188	11.59620540
O	3.83227244	6.50257320	8.68242509
O	4.26507973	4.02136705	9.50131530
Cu	5.10835498	8.84704951	0.00127886
Cu	-2.55543284	8.85212949	0.00592344
Cu	0.00152531	8.85223995	0.00382139
Cu	2.55532374	8.85039728	0.00186300
Cu	8.94196113	2.21496390	0.00537177
Cu	1.27766833	2.21275799	0.01181878
Cu	3.83527190	2.21290275	0.00614283
Cu	6.39109844	2.21514433	0.00009607
Cu	7.66517761	4.42851017	0.00553876
Cu	-0.00407226	4.42907591	0.00459696
Cu	2.55961507	4.43283322	0.00119318
Cu	5.11424490	4.43011061	0.00250585
Cu	6.38824836	6.63671419	0.00238845
Cu	-1.27942586	6.63810758	19.99957806
Cu	1.28003365	6.64250111	0.00191010
Cu	3.83422949	6.64042098	0.00235666
Cu	-0.00423426	1.47161580	2.07977278
Cu	2.55589452	1.47251059	2.08560339
Cu	5.11418136	1.47617222	2.08145297
Cu	7.66551325	1.47261319	2.08871219
Cu	-1.27891381	3.68798736	2.08911201
Cu	1.27788053	3.69337579	2.07727849
Cu	3.83334997	3.69403090	2.09033757

Cu	6.38841629	3.68404943	2.09613188
Cu	-2.55303085	5.90494884	2.09663548
Cu	-0.00047430	5.90443256	2.08853882
Cu	2.55339313	5.90226380	2.09608390
Cu	5.10910155	5.90458536	2.09220622
Cu	-3.83943831	8.11244607	2.09396081
Cu	-1.27932440	8.11161499	2.08182064
Cu	1.28246514	8.11275440	2.09833809
Cu	3.83285494	8.11634263	2.09794856
Cu	1.27193739	0.74587709	4.17299303
Cu	3.83142993	0.73273696	4.15585214
Cu	6.38460431	0.73703332	4.16401753
Cu	8.94420544	0.74866030	4.17545024
Cu	0.01492573	2.93748268	4.15676738
Cu	2.54133091	2.94105598	4.16509683
Cu	5.08758403	2.93410405	4.17473073
Cu	7.67532782	2.94732979	4.17646723
Cu	-1.27503493	5.14946691	4.17670800
Cu	1.26190231	5.15132609	4.17196157
Cu	3.83398467	5.17622035	4.18245299
Cu	6.39091061	5.15895545	4.15547868
Cu	-2.55990830	7.39575798	4.17958269
Cu	-0.00770047	7.37607806	4.16226879
Cu	2.56593376	7.36622985	4.19529103
Cu	5.09781619	7.36443810	4.19058329
Cu	-1.29035035	6.62612545	6.24104059
Cu	3.80857431	6.63558855	6.39840559
Cu	2.55384290	4.42880453	6.20207207
Cu	1.26352078	2.20016581	6.38378922
Cu	1.24265767	6.62351804	6.22606784
Cu	7.63890418	4.42503411	6.24229195
Cu	8.93798225	2.20835420	6.29049756
Cu	-0.01321614	4.40110437	6.29540073
Cu	3.81436428	2.19427375	6.29373834
Cu	5.08698574	8.82344876	6.21786136
Cu	7.64714502	0.00655731	6.23065635
Cu	-2.56704074	8.84244127	6.28868698
Cu	6.38916387	6.62419146	6.23020158
Cu	0.00252283	8.83265511	6.23671930
Cu	5.10719284	4.39874502	6.21703056
Cu	6.37317998	2.20179951	6.24412414

Free energy from VASP is -327.36260600 eV

PBC	10.223900	10.223900	20.000000	90.000000	90.000000
120.000000					
H	2.99761186	5.67667921	7.35343176		
H	1.60759316	8.32430256	11.03827891		
H	-0.38146860	7.98926225	9.07584354		
H	2.81936316	7.96068304	8.94543691		
H	-0.44654041	7.04479669	11.60641624		
H	2.94570645	6.55287705	10.04685761		
H	0.98204320	5.97254351	11.56912339		
H	0.02181787	2.95474206	7.23472821		
H	-2.55001116	7.39393356	7.24696705		
H	0.28432576	5.57142050	9.30615621		
C	1.12828456	7.69907180	10.26412171		
C	2.25516666	7.11497658	9.38825906		
C	0.31093138	6.59626227	10.94645737		
O	0.27833819	8.57114733	9.50719074		
O	1.75220394	6.23552838	8.38851008		
O	-0.39579869	5.80814486	9.98429453		
Cu	-0.00186215	-0.00095479	-0.00359628		
Cu	2.56375801	-0.00088330	0.01120208		
Cu	5.11818975	0.00005989	0.00646399		
Cu	7.66596244	0.00179656	0.00742814		
Cu	8.94490656	2.21388197	0.00675079		
Cu	1.28130255	2.21678448	0.00643400		
Cu	3.83796900	2.21075465	-0.00377055		
Cu	6.39337867	2.21121290	-0.00136893		
Cu	-2.55695606	4.42393441	-0.00865433		
Cu	0.00394233	4.42801551	0.01359926		
Cu	2.56031667	4.43097038	0.00098756		
Cu	5.11317256	4.42819338	-0.00572953		
Cu	6.39236778	6.64099181	0.00078626		
Cu	-1.27281953	6.64438205	0.01540542		
Cu	1.27915726	6.64447940	0.01584997		
Cu	3.83399084	6.63863284	0.00424822		
Cu	0.01041790	1.46945035	2.08267990		
Cu	2.56419037	1.47682674	2.09183854		
Cu	5.11458810	1.47548848	2.09330505		
Cu	7.66884893	1.47447978	2.09205948		
Cu	-1.27778280	3.69901585	2.08640013		
Cu	1.28744899	3.69980902	2.09148781		
Cu	3.83924374	3.68087992	2.07766272		
Cu	6.39595316	3.68852840	2.08546715		
Cu	-2.54915733	5.89388649	2.08177947		

Cu	0.00758899	5.90625906	2.11460005
Cu	2.55452138	5.90513297	2.10172733
Cu	5.11940825	5.90236748	2.07516663
Cu	-3.83265719	8.12048400	2.07922951
Cu	-1.25754030	8.11265138	2.10601864
Cu	1.27899719	8.11188572	2.11314132
Cu	3.83378583	8.11562760	2.09694334
Cu	1.29545610	0.73977070	4.18450084
Cu	3.84009936	0.72195290	4.18497603
Cu	6.39318377	0.73700460	4.17226242
Cu	8.95918831	0.74834685	4.17004952
Cu	0.01127120	2.95492295	4.12460999
Cu	2.55281232	2.95827218	4.18230773
Cu	5.11858866	2.95336109	4.15697516
Cu	7.68928276	2.95091993	4.17371514
Cu	-1.26451345	5.17315950	4.19746134
Cu	1.28434540	5.17686696	4.23433390
Cu	3.84631409	5.15802074	4.13100997
Cu	6.40090579	5.17673964	4.17097444
Cu	-2.54388865	7.37697873	4.12651172
Cu	0.02777238	7.36338391	4.26232999
Cu	2.55341609	7.36821717	4.19953490
Cu	5.12718055	7.37202582	4.16957636
Cu	-3.80514954	6.65141414	6.28631260
Cu	1.28697015	2.22296026	6.28072785
Cu	7.65873592	4.41857577	6.23630419
Cu	3.84568885	2.20275187	6.22819423
Cu	-1.28745943	6.64524450	6.30347991
Cu	2.56405644	-0.00199837	6.29157032
Cu	5.13637038	4.42526990	6.24311762
Cu	7.69200978	0.03439102	6.22293099
Cu	6.40555407	2.22694689	6.23673069
Cu	3.88405737	6.61309641	6.23593343
Cu	5.14311452	0.03830730	6.27742508
Cu	5.10664622	8.84303748	6.21964887
Cu	8.97022682	2.22121414	6.29427998
Cu	1.27528161	6.67890696	6.46646459
Cu	-0.00484630	4.40772219	6.27282966
Cu	2.63185840	4.42231460	6.25119226

Str 3

Free energy from VASP is -328.45724400 eV

PBC	10.223900	10.223900	20.000000	90.000000	90.000000
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120.000000

H	2.53812477	5.90776665	7.24483954
H	2.53256387	1.45778952	7.25969997
H	-2.58990461	5.68963354	9.15885972
H	-1.92490572	5.18095000	11.51986597
H	-1.83050090	3.38099427	9.61605004
H	-0.22847705	5.57601744	11.13765444
H	-0.12451520	3.84593230	9.36999028
H	0.14598346	6.28290093	8.63205560
H	5.14198897	2.96490280	7.25421477
H	-1.15008911	7.72599262	10.55801283
C	-1.53418860	5.49853229	9.41160431
C	-1.28299456	5.81270339	10.88754905
C	-1.16402289	4.05780910	9.05389477
O	-0.81764086	6.47427948	8.60210791
O	-1.59856339	7.16009802	11.21488450
O	-1.27788975	3.79329527	7.65689366
Cu	-5.10994155	8.85221241	19.99387207
Cu	-2.55787954	8.85368343	0.01126952
Cu	-0.00104520	8.84807800	19.99004678
Cu	2.55804614	8.85331380	19.99386471
Cu	8.94359882	2.21621149	19.99645285
Cu	1.27714079	2.20703946	19.99830438
Cu	3.83273814	2.20960225	0.00330008
Cu	6.39516362	2.21657622	0.00132612
Cu	-2.55223127	4.42828566	0.00987633
Cu	-0.00686745	4.42766945	0.00063345
Cu	2.55290338	4.43369056	19.99401729
Cu	5.11791559	4.42889300	19.99820875
Cu	-3.83124345	6.64086739	19.99077175
Cu	-1.28143337	6.63842408	19.99524588
Cu	1.27997607	6.64015881	19.99963196
Cu	3.83333349	6.64287162	0.01069541
Cu	-0.00454936	1.47912508	2.08131310
Cu	2.55570926	1.47933100	2.09250699
Cu	5.11462578	1.47104277	2.06906082
Cu	7.67089245	1.47507497	2.09260328
Cu	-1.27650765	3.68766463	2.10761023
Cu	1.27852975	3.68083061	2.07700820
Cu	3.83266633	3.69157652	2.06610281
Cu	6.38917455	3.68793360	2.09388489
Cu	-2.55775208	5.90672902	2.10630929
Cu	-0.00494907	5.90440710	2.08158704
Cu	2.55337223	5.89637134	2.09046373

Cu	5.12264052	5.90323761	2.08678303
Cu	-3.82853178	8.10359476	2.09585009
Cu	-1.27626368	8.11331913	2.09528260
Cu	1.26912684	8.12036966	2.08096802
Cu	3.84049267	8.13150351	2.08473240
Cu	1.28028348	0.72898686	4.13651911
Cu	3.83605904	0.74967136	4.16355651
Cu	6.38705520	0.75107002	4.15842502
Cu	8.95312716	0.76481184	4.19250643
Cu	0.01396812	2.93649174	4.19894017
Cu	2.57236896	2.97270112	4.18976747
Cu	5.08760781	2.93820093	4.14166669
Cu	7.66862993	2.95630636	4.20978528
Cu	-1.28379126	5.16512459	4.19243394
Cu	1.26373221	5.14722391	4.15866965
Cu	3.84640243	5.15946280	4.15914117
Cu	6.39874959	5.14333629	4.19589801
Cu	-2.53656692	7.39545315	4.20885031
Cu	0.01361777	7.34970991	4.19010720
Cu	2.56524459	7.38464641	4.12595416
Cu	5.09167570	7.36518208	4.17059414
Cu	6.34763197	2.19586004	6.25871791
Cu	7.66702437	0.01145597	6.21371976
Cu	2.56382456	4.45357458	6.27714080
Cu	3.84033093	6.63931377	6.29072671
Cu	5.10396463	8.83150202	6.22101936
Cu	1.33474013	6.65038735	6.23723373
Cu	2.55385131	0.00913860	6.28536804
Cu	8.95225324	2.15076564	6.32435987
Cu	3.83659038	2.20441771	6.37626943
Cu	0.05901437	4.43540380	6.23424991
Cu	5.10496061	4.40511458	6.26829470
Cu	-1.26507289	6.67602121	6.31394997
Cu	0.02594192	8.83185114	6.19785416
Cu	1.31529636	2.18329018	6.25163153
Cu	6.36781070	6.65654809	6.21520728
Cu	7.60842733	4.47895825	6.28636084

Str 4

Free energy from VASP is -327.43789200 eV

PBC	10.223900	10.223900	20.000000	90.000000	90.000000
	120.000000				
H	2.58149359	7.46096329	7.15743205		

H	-0.00822561	2.99471049	7.15653662
H	5.03260084	2.71809775	10.30936154
H	2.67876924	2.19705920	10.85056394
H	6.44587900	1.26397829	8.84669494
H	2.82460004	2.35009567	9.07344164
H	5.19111038	2.38312332	7.62736091
H	4.40584801	0.10641803	11.13405165
H	-0.02775985	5.96931766	7.15156908
H	-2.05099768	8.84351981	9.12140158
C	4.64038387	1.71633569	10.07921237
C	3.11739306	1.74121050	9.95154594
C	5.34373823	1.15224744	8.83817409
O	5.03789594	0.85781962	11.16010645
O	2.59216606	0.41122231	9.87646306
O	4.83069989	0.11523202	8.26017452
Cu	-0.01514696	0.08314908	19.91756219
Cu	2.53732583	0.08656602	19.92209939
Cu	5.09029425	0.09128490	19.92880849
Cu	7.65153399	0.08624585	19.92677080
Cu	-1.29553695	2.29452030	19.92578457
Cu	1.26163495	2.29258370	19.92949493
Cu	3.81948320	2.29523082	19.93355043
Cu	6.36698064	2.29869181	19.93224775
Cu	-2.57800831	4.51206527	19.91521408
Cu	-0.01805515	4.51193717	19.93938790
Cu	2.54221372	4.50859725	19.91389763
Cu	5.09579915	4.51011341	19.92089009
Cu	-3.85412922	6.72798209	19.90947835
Cu	-1.29431519	6.72831866	19.92655386
Cu	1.25916616	6.72912938	19.93124718
Cu	3.81964672	6.72884711	19.91610604
Cu	-0.01929354	1.55573349	2.00934940
Cu	2.55414962	1.55512984	2.02905623
Cu	5.09972560	1.55615996	2.03461395
Cu	7.64025088	1.55760065	2.03196540
Cu	-1.30315665	3.76046406	2.00525952
Cu	1.27354768	3.76715882	2.00715240
Cu	3.81690812	3.77486925	2.01799351
Cu	6.37981004	3.77075642	2.01632680
Cu	-2.57320555	5.98601996	1.99995064
Cu	-0.01411509	5.99367383	2.01486591
Cu	2.54480978	5.98156015	1.99694770
Cu	5.09910568	5.98394963	2.00215188
Cu	-3.84658904	8.19811187	2.01102446

Cu	-1.29260861	8.20587055	2.02148231
Cu	1.26256026	8.21189776	2.01600494
Cu	3.81798737	8.20370493	2.00551897
Cu	1.25814823	0.82688621	4.08209536
Cu	3.84559197	0.82385775	4.15104411
Cu	6.36807575	0.81888460	4.17956287
Cu	8.93004150	0.81872708	4.10262095
Cu	-0.01051824	3.04801852	4.06756039
Cu	2.55354192	3.01627792	4.12409065
Cu	5.10349655	3.03448917	4.09342882
Cu	7.64531100	3.01444895	4.13798549
Cu	-1.28187122	5.22538557	4.07047458
Cu	1.26276310	5.24142912	4.09399806
Cu	3.82371348	5.25794192	4.09626603
Cu	6.37684378	5.24425706	4.08326227
Cu	-2.54410990	7.44723222	4.08811371
Cu	0.00395568	7.46779308	4.11607489
Cu	2.52580884	7.44954943	4.06373711
Cu	5.08833289	7.46497419	4.08001563
Cu	5.10843165	4.54001755	6.18040239
Cu	1.29644984	6.67958488	6.26451393
Cu	2.58114469	4.48982654	6.14181964
Cu	3.86151658	2.33086077	6.25167359
Cu	-3.84330445	6.72479641	6.14472865
Cu	3.82674417	6.72652348	6.20196724
Cu	2.52614505	0.07600212	6.13335682
Cu	6.35822006	2.32786251	6.28066823
Cu	1.27170279	2.29466339	6.20448573
Cu	-1.28421031	2.29137989	6.20351611
Cu	7.69241968	0.05990352	6.19276529
Cu	-0.00619201	4.48799954	6.27312744
Cu	5.08486259	0.01838931	6.24948575
Cu	0.01533529	0.07140912	6.15351877
Cu	-1.29716585	6.66859926	6.17273954
Cu	-2.59153629	4.51308939	6.14424206

Str 5

Free energy from VASP is -327.85242000 eV

PBC	10.223900	10.223900	20.000000	90.000000	90.000000
120.000000					
H	5.47993481	1.31077895	8.95922969		
H	-0.03866856	7.38160203	7.24882144		
H	5.80627676	3.77715025	11.52827660		

H	7.17033289	3.55693650	9.43746515
H	3.64181604	2.55697718	11.82487868
H	7.16398993	2.05272929	10.40731108
H	3.86310907	8.18614933	7.24440531
H	2.52677415	5.85765405	7.28685928
H	2.56481080	2.91213436	7.25756118
H	4.27290585	3.87542080	9.12511857
C	5.39437547	3.27701813	10.63649369
C	6.54248630	2.73057144	9.79651586
C	4.39705156	2.20929506	11.07986702
O	4.59594902	4.26301389	9.96716508
O	6.05920475	2.03694307	8.62933932
O	4.32979769	1.08866634	10.58675242
Cu	10.21896655	0.00091238	19.99962844
Cu	2.55058134	0.00130147	19.99989339
Cu	5.10598141	0.00443807	0.00710070
Cu	7.66721504	0.00636994	0.00636163
Cu	8.93938352	2.21277317	0.00068318
Cu	1.27533965	2.21065130	0.00091900
Cu	3.83106052	2.21414409	0.02370404
Cu	6.38481418	2.21567586	0.00789562
Cu	7.66153340	4.42762354	19.99805264
Cu	-0.01116468	4.42455368	19.99051752
Cu	2.55525844	4.42477930	0.01565437
Cu	5.11101317	4.42493913	0.00464138
Cu	6.38729412	6.64100176	19.99398626
Cu	-1.28537230	6.64183038	19.99557490
Cu	1.27272166	6.64326437	0.00930364
Cu	3.83137488	6.64251450	0.00910089
Cu	-0.00772280	1.47702599	2.08257177
Cu	2.54634131	1.47445580	2.10294001
Cu	5.11309648	1.47709482	2.11358105
Cu	7.65346607	1.47844845	2.10185965
Cu	-1.29042255	3.68499033	2.09843592
Cu	1.26423922	3.69012992	2.07900059
Cu	3.83699649	3.69227989	2.10609140
Cu	6.38200935	3.68618003	2.10559121
Cu	-2.56631102	5.90176849	2.08015645
Cu	-0.00796378	5.89677681	2.07306492
Cu	2.54747235	5.90220970	2.09632154
Cu	5.10313268	5.90218355	2.08697255
Cu	-3.84300908	8.11736575	2.09222721
Cu	-1.28505331	8.11939320	2.08707812
Cu	1.27096633	8.12965638	2.09072467

Cu	3.82737586	8.11731475	2.09198650
Cu	1.25767710	0.73620277	4.19068424
Cu	3.82968916	0.73862668	4.18107506
Cu	6.38981619	0.73539903	4.24185624
Cu	8.93924039	0.73686019	4.15404604
Cu	0.00844161	2.94278135	4.16729757
Cu	2.54889752	2.97466968	4.15290952
Cu	5.10038749	2.94094288	4.21205259
Cu	7.64456287	2.93997531	4.19430936
Cu	-1.28373301	5.17669887	4.16303445
Cu	1.27605255	5.16476529	4.18537104
Cu	3.81698109	5.17959391	4.20284077
Cu	6.38059181	5.16766800	4.15774719
Cu	-2.55217374	7.38096168	4.16368616
Cu	0.00974960	7.36269591	4.14276606
Cu	2.53461708	7.37771348	4.17969709
Cu	5.08334814	7.36758998	4.17694329
Cu	-1.26985713	2.22689027	6.22120578
Cu	-0.03724808	4.40054444	6.21427089
Cu	3.82021028	6.64322726	6.39668800
Cu	2.56028915	4.41668199	6.37554659
Cu	-3.82423901	6.63150358	6.21753171
Cu	1.28140813	2.21253930	6.28985788
Cu	-5.10769476	8.85190020	6.28959142
Cu	-0.01812424	8.81237924	6.25351389
Cu	1.25093142	6.61438502	6.36246027
Cu	3.80682008	2.20831746	6.26664706
Cu	5.13756951	4.44913203	6.21854595
Cu	6.37787412	2.20996303	6.36573470
Cu	-2.55713213	4.43593781	6.22800876
Cu	-2.57977138	8.83735774	6.22705852
Cu	-1.28151202	6.63338620	6.28455607
Cu	7.69858053	0.01679387	6.27682993

Str 6

Free energy from VASP is -327.19932700 eV

PBC	10.223900	10.223900	20.000000	90.000000	90.000000
120.000000					
H	3.15365806	6.50222251	8.71723547		
H	-2.65980174	7.44632140	7.24320863		
H	5.03035693	5.75584961	10.07817072		
H	5.32779114	3.40385137	10.79396633		
H	3.11242521	2.91633503	9.10481922		

H	3.67520215	3.82803283	11.28107152
H	0.09383796	7.44348343	7.25696378
H	-1.32161436	5.11814358	7.28082904
H	5.67796978	3.44489789	8.41841504
H	0.01577563	2.85203234	7.21570408
C	4.40104288	4.97416835	9.64714341
C	4.33631376	3.67226235	10.40242159
C	3.28149873	5.41733246	8.90325274
O	5.67097127	4.40494284	8.19762169
O	3.87893990	2.56975245	9.61774163
O	2.41443188	4.59733188	8.39263537
Cu	-0.00209900	0.00009436	-0.01220240
Cu	2.55285519	0.00264962	-0.00345039
Cu	5.11339288	0.00102786	-0.00525913
Cu	7.66693934	0.00133804	-0.01146299
Cu	8.94609212	2.21074733	-0.00694757
Cu	1.27571768	2.21335743	0.00001113
Cu	3.83364800	2.21431793	-0.00470114
Cu	6.38957439	2.21182411	-0.00926050
Cu	-2.56154129	4.42556983	-0.00345792
Cu	0.00118887	4.42448051	0.00698450
Cu	2.55950206	4.42820105	-0.00109482
Cu	5.10862067	4.42903064	0.00374112
Cu	6.38477003	6.63912235	0.00347452
Cu	-1.27629593	6.64023449	0.01239292
Cu	1.27840243	6.64097727	0.00518439
Cu	3.83207697	6.63838931	-0.00329319
Cu	0.00235328	1.47795887	2.07446788
Cu	2.56070296	1.48494600	2.09384332
Cu	5.10755470	1.48421586	2.08416136
Cu	7.66021911	1.48044225	2.07671401
Cu	-1.28425385	3.69771858	2.08029014
Cu	1.28442749	3.69193670	2.09176861
Cu	3.82545511	3.68839586	2.09844173
Cu	6.38818350	3.68767261	2.08772703
Cu	-2.56290889	5.89307577	2.09228704
Cu	0.00140507	5.89345584	2.09901687
Cu	2.55407872	5.88967946	2.10230763
Cu	5.10118882	5.89272224	2.09571768
Cu	-3.83289815	8.11845474	2.07813003
Cu	-1.28417971	8.12487870	2.07446972
Cu	1.27173018	8.11182704	2.07654157
Cu	3.82869405	8.11414245	2.07731238
Cu	1.27901125	0.73822316	4.16072502

Cu	3.83163948	0.72743044	4.17888268
Cu	6.37651571	0.72510217	4.14516451
Cu	8.94337489	0.74819705	4.14490772
Cu	-0.01105601	2.97017475	4.13172225
Cu	2.54341991	2.96978888	4.20452524
Cu	5.10768370	2.96331070	4.16610478
Cu	7.68060383	2.97089861	4.17619886
Cu	-1.28652764	5.18127082	4.20506269
Cu	1.26073386	5.15480234	4.23826963
Cu	3.82364584	5.14335394	4.22398146
Cu	6.38258422	5.16449986	4.20427303
Cu	-2.53955264	7.36646159	4.15010433
Cu	-0.03028630	7.36950230	4.15165006
Cu	2.53446963	7.36833459	4.14873950
Cu	5.11742220	7.37506708	4.14795605
Cu	2.53441773	0.00740079	6.26672301
Cu	3.82652386	6.67758820	6.19842302
Cu	-3.84134644	6.69506889	6.23932245
Cu	3.82473603	2.18763087	6.21073790
Cu	5.12172355	0.00476399	6.27454695
Cu	8.94323279	2.17631159	6.27301427
Cu	6.40366278	2.17921698	6.17908855
Cu	2.52012955	4.43862804	6.35895301
Cu	7.64256424	4.41779376	6.32756025
Cu	7.67763176	0.00842050	6.21162416
Cu	-1.28414327	6.65166409	6.50331559
Cu	1.25397203	2.19564080	6.23963004
Cu	1.25453008	6.68215553	6.23939969
Cu	5.08513355	8.84811821	6.21826196
Cu	5.11430334	4.42315627	6.29092466
Cu	-0.06836232	4.38311150	6.34644907

Str 7

Free energy from VASP is -328.59621000 eV

PBC	10.223900	10.223900	20.000000	90.000000	90.000000
120.000000					
H	5.04854718	2.88640712	7.19599296		
H	7.68269308	2.78025709	7.25718725		
H	5.85779102	0.56763981	8.97829260		
H	3.48764166	0.54838325	10.18125761		
H	-3.18707668	5.55298773	8.55097718		
H	3.57710384	1.69579049	8.82012340		
H	0.96639197	7.03717182	8.56236093		

H	0.07936616	2.94562140	7.19371641
H	2.62967707	5.87358160	7.19783185
H	-2.34986478	7.84466292	8.52999078
C	4.95532846	0.02361972	8.68817152
C	3.63628613	0.63121350	9.08857888
C	-0.04744488	7.48920231	8.55114497
O	6.53259311	5.38655647	7.73222331
O	-2.59265692	8.81571900	8.44816199
O	-1.07040194	6.67120932	8.43650886
Cu	-5.10155146	8.84707423	19.97537045
Cu	-2.54953494	8.84939634	0.01109830
Cu	-0.00503873	8.85035672	0.01175499
Cu	7.66651178	0.00133332	0.00271532
Cu	8.94342565	2.21345877	0.00432269
Cu	1.28572412	2.20816466	19.97967693
Cu	3.83624209	2.20695569	19.98720233
Cu	6.39233319	2.20914244	0.00948646
Cu	-2.55367340	4.43235782	19.99955256
Cu	0.00011116	4.43182505	19.99285786
Cu	2.56096979	4.42997267	19.96513615
Cu	5.11424078	4.42853770	19.98592878
Cu	-3.82776658	6.64121000	19.99829688
Cu	-1.27816267	6.64546147	0.01593999
Cu	1.27707592	6.64166908	0.00072243
Cu	3.83809200	6.63843005	19.97603757
Cu	0.01992046	1.46381273	2.05949735
Cu	2.57031822	1.47182722	2.09111109
Cu	5.10316114	1.47224907	2.10267178
Cu	7.66288269	1.47323573	2.10065218
Cu	-1.27983760	3.69973177	2.07712785
Cu	1.28626519	3.68347844	2.04833989
Cu	3.83869220	3.68211561	2.05803847
Cu	6.39706498	3.69462149	2.08067555
Cu	-2.55501440	5.90551522	2.12146026
Cu	-0.00864219	5.91031376	2.10020397
Cu	2.56631544	5.89613297	2.05985944
Cu	5.12615629	5.90123128	2.06841868
Cu	-3.81879500	8.10984864	2.10014948
Cu	-1.27596387	8.11227883	2.13521698
Cu	1.26461918	8.11849796	2.09182204
Cu	3.85205708	8.11842906	2.06191353
Cu	1.30809152	0.73365613	4.16984714
Cu	3.84935844	0.71579238	4.23931720
Cu	6.36420586	0.73226553	4.21155218

Cu	8.96335329	0.75538211	4.14364511
Cu	-0.00331073	2.94284458	4.09545562
Cu	2.56362490	2.96351652	4.15660139
Cu	5.13775218	2.95631738	4.14223945
Cu	7.67670813	2.95912350	4.18463915
Cu	-1.28516296	5.15733255	4.22940141
Cu	1.27979592	5.15427257	4.12384228
Cu	3.86153588	5.14909881	4.14161455
Cu	6.39724754	5.14575197	4.21058769
Cu	-2.54020546	7.37403587	4.24511163
Cu	0.00733715	7.37324111	4.26070519
Cu	2.56673900	7.38402121	4.10085814
Cu	5.12822478	7.35381794	4.16796409
Cu	5.09539736	8.84927226	6.17990286
Cu	1.27650058	2.23075340	6.20718001
Cu	5.06994307	4.39608843	6.32368861
Cu	3.84116775	2.23841282	6.20499631
Cu	6.36187623	6.68575084	6.26376738
Cu	-1.25659406	2.20040324	6.33116844
Cu	3.83416389	6.64800454	6.22233027
Cu	6.39487133	2.19169999	6.31616573
Cu	2.59475110	8.85144737	6.17069338
Cu	-1.23750876	6.56615982	6.32585100
Cu	2.56524579	4.43743528	6.25080908
Cu	2.53571974	0.04694405	6.30531699
Cu	0.05192298	8.83268864	6.44333624
Cu	7.68414287	4.36798450	6.37066857
Cu	0.04373227	4.38453919	6.21790861
Cu	1.35764355	6.61837267	6.22195264

Str 8

Free energy from VASP is -327.94651900 eV

PBC 10.223900 10.223900 20.000000 90.000000 90.000000

120.000000

H	5.19622623	5.91530916	7.22780059
H	1.36520298	3.44274997	7.57973461
H	-0.74424030	3.60203857	11.04435665
H	0.83077527	1.85284205	10.46526275
H	2.53966301	5.93002533	7.26261553
H	0.04471047	1.62841715	8.87510107
H	-2.28212292	4.59177035	9.47769167
H	2.26623401	2.33191957	8.72358854
H	-0.00715570	7.42933614	7.25192249

H	3.90062988	0.85119517	8.51798654
C	-0.63826150	3.33902179	9.99117011
C	0.42528503	2.38132333	9.59135013
C	-1.50240558	3.90640540	9.12379117
O	3.18051822	1.25574753	7.99618052
O	1.57644860	3.06040043	8.95754542
O	-1.48527971	3.71310445	7.78612353
Cu	0.00531367	0.01033350	0.00784008
Cu	2.55302730	0.00855577	0.01596440
Cu	5.10804733	0.00998129	0.01716419
Cu	7.66961029	0.01264527	-0.00442437
Cu	8.94791189	2.22084534	0.00561829
Cu	1.27745774	2.21693845	0.00418319
Cu	3.83386698	2.21530621	0.00590007
Cu	6.39015729	2.22015681	-0.00047643
Cu	-2.55750466	4.43415290	0.01462360
Cu	-0.00226768	4.42726715	0.00021655
Cu	2.55589919	4.43255205	0.00589684
Cu	5.11473501	4.43555067	0.00807846
Cu	6.39036870	6.64954224	0.01383176
Cu	-1.28163465	6.65090005	0.00354479
Cu	1.27813919	6.64983112	0.00727605
Cu	3.83536922	6.64670341	0.02994852
Cu	0.00637339	1.48340146	2.09871079
Cu	2.56247891	1.48754473	2.10666687
Cu	5.11061516	1.49372603	2.10617678
Cu	7.66894898	1.49257406	2.09524037
Cu	-1.28339152	3.71181389	2.09139716
Cu	1.28304436	3.69808534	2.09550318
Cu	3.84001106	3.69814719	2.08323354
Cu	6.38454647	3.69365296	2.10768668
Cu	-2.55012971	5.92632451	2.11165789
Cu	-0.00760830	5.91090466	2.07712920
Cu	2.54996259	5.91256360	2.09507382
Cu	5.12144192	5.91150360	2.10604181
Cu	-3.83062802	8.12323812	2.11249957
Cu	-1.28371191	8.13076680	2.11227683
Cu	1.28967406	8.12883146	2.08118440
Cu	3.83227704	8.13783537	2.09717169
Cu	1.30415197	0.75064834	4.18462524
Cu	3.83890091	0.75221979	4.21475829
Cu	6.39081701	0.74368930	4.15878492
Cu	8.95260511	0.77677097	4.18447868
Cu	-0.01877442	2.98105668	4.16017450

Cu	2.58052340	2.98401874	4.18109342
Cu	5.09540408	2.98174337	4.22162744
Cu	7.67725216	2.98398528	4.18803389
Cu	-1.27166059	5.19479224	4.21507955
Cu	1.25836819	5.18763734	4.18423712
Cu	3.82372402	5.17898579	4.16441360
Cu	6.40888109	5.18341205	4.18230554
Cu	-2.55825376	7.42226544	4.25131190
Cu	0.02499342	7.38415461	4.13493577
Cu	2.56880460	7.37466340	4.19298178
Cu	5.09059660	7.38290273	4.17395725
Cu	-1.24745603	6.70596801	6.26208895
Cu	5.11404970	8.88182861	6.21197421
Cu	2.51595051	4.44696258	6.31608244
Cu	5.12079476	4.45903984	6.27219100
Cu	6.39212609	2.21133679	6.20435496
Cu	8.94051849	2.17967681	6.31203164
Cu	0.07224868	8.84195583	6.23170382
Cu	1.29483819	6.67781525	6.37049077
Cu	2.53903958	0.05037101	6.39538130
Cu	7.62951036	4.50010137	6.27611367
Cu	0.02847358	4.43924544	6.31529641
Cu	3.88405505	2.25057139	6.32800079
Cu	1.25326757	2.27626025	6.16053854
Cu	-3.83376990	6.69899623	6.29526340
Cu	3.84139311	6.64807256	6.37851008
Cu	7.70571386	0.02590892	6.22323841

Str 9

Free energy from VASP is -328.59621000 eV

PBC 10.223900 10.223900 20.000000 90.000000 90.000000
120.000000

H	5.04854718	2.88640712	7.19599296
H	7.68269308	2.78025709	7.25718725
H	5.85779102	0.56763981	8.97829260
H	3.48764166	0.54838325	10.18125761
H	-3.18707668	5.55298773	8.55097718
H	3.57710384	1.69579049	8.82012340
H	0.96639197	7.03717182	8.56236093
H	0.07936616	2.94562140	7.19371641
H	2.62967707	5.87358160	7.19783185
H	-2.34986478	7.84466292	8.52999078
C	4.95532846	0.02361972	8.68817152

C	3.63628613	0.63121350	9.08857888
C	-0.04744488	7.48920231	8.55114497
O	6.53259311	5.38655647	7.73222331
O	-2.59265692	8.81571900	8.44816199
O	-1.07040194	6.67120932	8.43650886
Cu	-5.10155146	8.84707423	19.97537045
Cu	-2.54953494	8.84939634	0.01109830
Cu	-0.00503873	8.85035672	0.01175499
Cu	7.66651178	0.00133332	0.00271532
Cu	8.94342565	2.21345877	0.00432269
Cu	1.28572412	2.20816466	19.97967693
Cu	3.83624209	2.20695569	19.98720233
Cu	6.39233319	2.20914244	0.00948646
Cu	-2.55367340	4.43235782	19.99955256
Cu	0.00011116	4.43182505	19.99285786
Cu	2.56096979	4.42997267	19.96513615
Cu	5.11424078	4.42853770	19.98592878
Cu	-3.82776658	6.64121000	19.99829688
Cu	-1.27816267	6.64546147	0.01593999
Cu	1.27707592	6.64166908	0.00072243
Cu	3.83809200	6.63843005	19.97603757
Cu	0.01992046	1.46381273	2.05949735
Cu	2.57031822	1.47182722	2.09111109
Cu	5.10316114	1.47224907	2.10267178
Cu	7.66288269	1.47323573	2.10065218
Cu	-1.27983760	3.69973177	2.07712785
Cu	1.28626519	3.68347844	2.04833989
Cu	3.83869220	3.68211561	2.05803847
Cu	6.39706498	3.69462149	2.08067555
Cu	-2.55501440	5.90551522	2.12146026
Cu	-0.00864219	5.91031376	2.10020397
Cu	2.56631544	5.89613297	2.05985944
Cu	5.12615629	5.90123128	2.06841868
Cu	-3.81879500	8.10984864	2.10014948
Cu	-1.27596387	8.11227883	2.13521698
Cu	1.26461918	8.11849796	2.09182204
Cu	3.85205708	8.11842906	2.06191353
Cu	1.30809152	0.73365613	4.16984714
Cu	3.84935844	0.71579238	4.23931720
Cu	6.36420586	0.73226553	4.21155218
Cu	8.96335329	0.75538211	4.14364511
Cu	-0.00331073	2.94284458	4.09545562
Cu	2.56362490	2.96351652	4.15660139
Cu	5.13775218	2.95631738	4.14223945

Cu	7.67670813	2.95912350	4.18463915
Cu	-1.28516296	5.15733255	4.22940141
Cu	1.27979592	5.15427257	4.12384228
Cu	3.86153588	5.14909881	4.14161455
Cu	6.39724754	5.14575197	4.21058769
Cu	-2.54020546	7.37403587	4.24511163
Cu	0.00733715	7.37324111	4.26070519
Cu	2.56673900	7.38402121	4.10085814
Cu	5.12822478	7.35381794	4.16796409
Cu	5.09539736	8.84927226	6.17990286
Cu	1.27650058	2.23075340	6.20718001
Cu	5.06994307	4.39608843	6.32368861
Cu	3.84116775	2.23841282	6.20499631
Cu	6.36187623	6.68575084	6.26376738
Cu	-1.25659406	2.20040324	6.33116844
Cu	3.83416389	6.64800454	6.22233027
Cu	6.39487133	2.19169999	6.31616573
Cu	2.59475110	8.85144737	6.17069338
Cu	-1.23750876	6.56615982	6.32585100
Cu	2.56524579	4.43743528	6.25080908
Cu	2.53571974	0.04694405	6.30531699
Cu	0.05192298	8.83268864	6.44333624
Cu	7.68414287	4.36798450	6.37066857
Cu	0.04373227	4.38453919	6.21790861
Cu	1.35764355	6.61837267	6.22195264

Str 10

Free energy from VASP is -328.37892700 eV

PBC 10.223900 10.223900 20.000000 90.000000 90.000000
120.000000

H	4.42686535	4.46797073	8.81027586
H	-2.57392591	7.37878826	7.23746711
H	-0.39633337	3.77590532	9.56049525
H	1.95032209	4.25312700	10.68193789
H	0.58314060	3.59943336	7.64523063
H	2.00891339	2.91673131	9.49843519
H	-0.90064353	6.05268745	8.83043206
H	5.66909786	3.47928404	8.74736891
H	2.56891771	1.52161883	7.27339427
H	2.40153980	5.62620403	8.71381495
C	0.42923298	4.36856446	9.16032449
C	1.81734672	3.99405347	9.61402669
C	0.15060436	5.71367563	8.84828978

O	5.38695191	4.38518401	8.52473185
O	2.80526133	4.70435792	8.83736088
O	1.07317522	6.57483880	8.51552441
Cu	-0.00898161	0.00447285	-0.00298502
Cu	2.55453440	0.00613061	0.01082327
Cu	5.11937827	0.00451293	-0.00645644
Cu	7.66530953	0.00362141	-0.00382528
Cu	8.94044686	2.21926729	-0.00201283
Cu	1.27573239	2.22197720	0.01604182
Cu	3.83336736	2.22096078	0.00788944
Cu	6.39240699	2.21982466	-0.00781698
Cu	-2.55834495	4.42708380	0.00377108
Cu	-0.00136717	4.43107181	0.01165193
Cu	2.55412317	4.43476544	0.02007252
Cu	5.11155156	4.43091004	0.00198059
Cu	6.38679829	6.63882963	0.00819946
Cu	-1.27668903	6.63840431	0.00872677
Cu	1.28024776	6.64357786	0.01137089
Cu	3.82781915	6.64216060	0.00496623
Cu	-0.00302113	1.48424503	2.08555918
Cu	2.55103842	1.48733746	2.09535288
Cu	5.10862152	1.48983903	2.08486797
Cu	7.66350801	1.48126439	2.07632549
Cu	-1.27594105	3.69717659	2.09578048
Cu	1.27208051	3.70483866	2.11424268
Cu	3.83446681	3.69698902	2.09925483
Cu	6.38022902	3.69562988	2.09742365
Cu	-2.55943770	5.90179203	2.09596353
Cu	0.00647565	5.90616128	2.10801669
Cu	2.55406614	5.90168680	2.12670181
Cu	5.09863031	5.90360170	2.09658090
Cu	-3.84674378	8.12774944	2.06990115
Cu	-1.26842790	8.11860990	2.07299365
Cu	1.27164291	8.11665106	2.09095730
Cu	3.82230028	8.11599446	2.09147208
Cu	1.27947658	0.75760453	4.19017905
Cu	3.81712227	0.73419662	4.15583350
Cu	6.38085156	0.74584184	4.14259655
Cu	8.93914747	0.74665248	4.14654639
Cu	0.01217160	2.94953504	4.18728300
Cu	2.54226924	2.96735287	4.18435454
Cu	5.08679505	2.96333589	4.20417867
Cu	7.66457330	2.96146167	4.14322813
Cu	-1.27389341	5.17536529	4.18151386

Cu	1.27422291	5.18372025	4.25183829
Cu	3.83922825	5.15339533	4.22330221
Cu	6.37678592	5.18361520	4.18573975
Cu	-2.56731480	7.41871025	4.12139589
Cu	-0.00653208	7.37520086	4.19928056
Cu	2.52902257	7.38083663	4.19036971
Cu	5.11665612	7.38931608	4.15587526
Cu	6.39583707	2.20602516	6.20295262
Cu	10.18016415	0.02583391	6.21658116
Cu	1.24265703	2.25733501	6.40165009
Cu	2.53386584	0.03104204	6.37391390
Cu	5.14186046	4.43717631	6.34108176
Cu	3.83899894	6.68206899	6.20279837
Cu	7.66311013	0.02885902	6.23354564
Cu	2.56895775	4.45156064	6.29784041
Cu	1.25769590	6.70252980	6.37385967
Cu	3.81707285	2.19892144	6.25754891
Cu	-3.83930384	6.69431873	6.25146161
Cu	7.66687857	4.41143307	6.19467939
Cu	-0.03858189	4.40691380	6.29752882
Cu	5.12332406	0.03703761	6.20620365
Cu	8.92127084	2.20742451	6.22906218
Cu	-1.33798055	6.66518620	6.22430003

Str 11

Free energy from VASP is -329.06902500 eV

PBC	10.223900	10.223900	20.000000	90.000000	90.000000
120.000000					
H	7.62560968	1.44938853	7.24604306		
H	4.75457599	6.04799064	9.54405999		
H	2.78734073	5.56520417	11.10616243		
H	1.29316137	3.84601557	10.13939578		
H	1.07918266	6.10969786	11.06760754		
H	0.67397768	4.98710737	8.91853772		
H	1.52674444	7.70366402	9.23760343		
H	5.66925824	4.97706529	8.84576623		
H	0.00136672	2.96453387	7.23225956		
H	3.50646460	4.49817020	8.98180070		
C	1.96137944	5.87588176	10.45036426		
C	1.55931413	4.71638170	9.51629613		
C	2.35570311	7.11337662	9.69586122		
O	4.97979741	5.08430560	9.53301278		
O	2.59020087	4.34804881	8.58902887		

O	3.51691369	7.47897028	9.53852530
Cu	-5.10738779	8.85211422	19.97799833
Cu	2.55884316	0.00267511	19.98068642
Cu	5.11392196	0.00201962	19.97958121
Cu	7.66980029	0.00143551	19.98148403
Cu	-1.27451025	2.21563805	19.98762102
Cu	1.28473044	2.21958645	19.99817581
Cu	3.83347560	2.21998062	19.99202549
Cu	6.39118575	2.21515831	19.98338109
Cu	-2.55624852	4.43263585	19.97907811
Cu	0.00884607	4.42976822	19.99631172
Cu	2.56130978	4.43014771	0.01325832
Cu	5.10842671	4.42999943	19.99478449
Cu	-3.83415532	6.64219110	19.98156646
Cu	-1.27496851	6.64389263	19.97914938
Cu	1.28370925	6.63851160	19.98827414
Cu	3.83470521	6.63744215	19.99252090
Cu	0.00287356	1.47589175	2.06146357
Cu	2.55914877	1.48329748	2.08415623
Cu	5.11254062	1.48048880	2.06196040
Cu	7.67085066	1.47804340	2.06220887
Cu	-1.27710545	3.69325414	2.05881821
Cu	1.28119345	3.69122773	2.09676003
Cu	3.83507775	3.68613831	2.10320925
Cu	6.39231812	3.68840771	2.06569256
Cu	-2.55099170	5.90351972	2.05869029
Cu	0.00805124	5.90373396	2.07771377
Cu	2.55398578	5.90654905	2.09965009
Cu	5.10641908	5.90205540	2.07747605
Cu	-3.83349335	8.12356784	2.06252749
Cu	-1.27501603	8.12024474	2.05986847
Cu	1.28291652	8.11621239	2.05986512
Cu	3.83410466	8.12073460	2.06422773
Cu	1.27339654	0.75167132	4.15582487
Cu	3.83426936	0.74198792	4.14297419
Cu	6.38956783	0.74025463	4.13280635
Cu	8.94621983	0.75091196	4.15653428
Cu	-0.02386329	2.93989635	4.14307359
Cu	2.53965826	2.96721109	4.20951584
Cu	5.12992239	2.93796130	4.16727256
Cu	7.67732958	2.94841822	4.15682889
Cu	-1.27307831	5.15893620	4.14793507
Cu	1.28200877	5.14595536	4.20155320
Cu	3.81219583	5.15374458	4.18215760

Cu	6.38579825	5.16488035	4.12942098
Cu	-2.55738372	7.38090460	4.12943152
Cu	0.00110026	7.38056814	4.13583154
Cu	2.55408046	7.40183076	4.16393289
Cu	5.10670615	7.37821437	4.13567923
Cu	6.38850188	2.20978062	6.28412277
Cu	1.24434341	2.19898113	6.26656354
Cu	5.12326255	8.82094067	6.20739084
Cu	3.83736915	2.19913227	6.21664692
Cu	1.25871141	6.65543096	6.20542156
Cu	5.12324891	4.42256142	6.20211974
Cu	-0.02155581	8.84437418	6.21136594
Cu	2.56152599	4.44215209	6.39510021
Cu	-2.55983794	8.85387743	6.21364270
Cu	-0.03886856	4.41284022	6.25240441
Cu	7.63707403	4.45905762	6.20944700
Cu	7.65868429	0.00786031	6.26849903
Cu	-1.28384092	6.64160842	6.21147583
Cu	6.38906468	6.64018424	6.21327720
Cu	8.92884702	2.20891979	6.37007295
Cu	3.83282348	6.65438148	6.20817781

Str 12

Free energy from VASP is -313.93075600 eV

PBC	10.223900	10.223900	20.000000	90.000000	90.000000
120.000000					
H	5.19677997	4.69811258	10.04495515		
H	3.11288667	4.15510808	8.70243031		
H	4.28141750	5.94159869	10.91492019		
H	2.87697752	3.90750344	10.44761858		
H	5.69384871	6.96023243	9.07344276		
H	5.32516724	5.66366103	7.65875958		
H	5.11669953	2.87894361	7.27009562		
H	2.17597769	6.33891502	9.20382858		
C	4.36219578	5.40868405	9.94604473		
C	3.04320611	4.68248694	9.68441915		
C	4.70318691	6.48133460	8.93466133		
O	1.91164281	5.54614090	9.72313755		
O	3.74700417	7.20296224	8.43198097		
Cu	-0.00195990	0.00108220	0.01493144		
Cu	2.55238692	0.00069426	0.01593916		
Cu	5.10991462	-0.00341589	0.02383608		
Cu	7.66860906	-0.00165018	0.01558623		

Cu	8.94712618	2.21391733	0.00484828
Cu	1.27464014	2.21503770	0.00565031
Cu	3.83069525	2.21582736	0.02873736
Cu	6.38774613	2.21227606	0.01572993
Cu	-2.55360286	4.43152359	0.00826360
Cu	-0.00009361	4.43006148	0.00674656
Cu	2.54989434	4.43145839	0.01479716
Cu	5.10890403	4.43195465	0.03514031
Cu	6.38593714	6.64416951	0.02598254
Cu	-1.27698175	6.64286365	0.01212638
Cu	1.27683296	6.64086625	0.01759173
Cu	3.83189780	6.64459693	0.03003075
Cu	-0.00310578	1.47867424	2.09622075
Cu	2.54907128	1.47770770	2.09775012
Cu	5.10843994	1.48025135	2.10252829
Cu	7.66889263	1.47649001	2.09420982
Cu	-1.28165642	3.68845229	2.09414799
Cu	1.27800293	3.68901023	2.09710648
Cu	3.82845691	3.70280818	2.11393307
Cu	6.39329624	3.69089954	2.09132797
Cu	-2.56004178	5.90150175	2.10151071
Cu	-0.00195656	5.90134293	2.09673846
Cu	2.56118674	5.90148438	2.11855795
Cu	5.10687563	5.90666249	2.12705019
Cu	-3.84082859	8.11316166	2.11469613
Cu	-1.28845556	8.11724790	2.10892729
Cu	1.28243783	8.11588034	2.10783706
Cu	3.83390826	8.11622015	2.11572106
Cu	1.27437378	0.73729485	4.17419139
Cu	3.82906968	0.75063014	4.18200312
Cu	6.37669612	0.74902013	4.17781914
Cu	8.94186619	0.73958422	4.17576321
Cu	0.00013575	2.95291394	4.16786324
Cu	2.56769160	2.95032057	4.18553634
Cu	5.10983402	2.97561381	4.17132105
Cu	7.65177570	2.94724030	4.18036810
Cu	-1.28025273	5.16459008	4.16899853
Cu	1.27530399	5.16357623	4.17108925
Cu	3.84911741	5.17573023	4.26428347
Cu	6.37938500	5.14979922	4.19684091
Cu	-2.57896707	7.36249504	4.19686861
Cu	-0.00838331	7.38256873	4.16538943
Cu	2.56422666	7.37110316	4.20158543
Cu	5.10075910	7.37156354	4.23231875

Cu	6.37951974	2.21546532	6.29538537
Cu	5.12996272	4.42361180	6.42722758
Cu	1.27941530	2.20855799	6.24765366
Cu	3.83776103	2.21681382	6.29490327
Cu	-1.28971382	6.63781955	6.25632407
Cu	-0.00496020	4.42047921	6.25879446
Cu	7.63833006	0.03855815	6.23151657
Cu	6.38225051	6.59749982	6.31105516
Cu	-2.51611643	4.41780552	6.23873934
Cu	-0.01891881	8.83410432	6.24235109
Cu	3.76835799	6.69146285	6.36929396
Cu	8.94548789	2.21775564	6.24502329
Cu	-2.56968938	8.84482121	6.25074452
Cu	1.23607068	6.63901771	6.23753068
Cu	2.51412150	4.42244172	6.24570169
Cu	0.00145113	0.02956024	6.25444323

Str 13

Free energy from VASP is -314.75637300 eV

PBC	10.223900	10.223900	20.000000	90.000000	90.000000
120.000000					
H	2.86388000	2.96051755	8.47209078		
H	5.10301519	4.81156428	10.19522746		
H	2.63250765	4.87544325	10.28912645		
H	4.16425155	2.55522421	10.51737582		
H	3.20928498	6.06662171	9.09696124		
H	5.51673600	2.41457440	9.36361182		
H	5.07914440	4.63602584	8.43623462		
H	-0.00347217	7.36070181	7.25968413		
C	4.52937018	4.36356772	9.36705037		
C	3.12769267	4.98235013	9.30364451		
C	4.51519668	2.84606119	9.51088484		
O	2.29282763	4.34432781	8.33391041		
O	3.61361513	2.23539923	8.54744469		
Cu	0.00339831	0.00533133	19.99894727		
Cu	2.55678912	0.00698127	0.01904112		
Cu	5.11375347	0.00519204	0.01861323		
Cu	7.67503813	0.00498982	19.98735101		
Cu	-1.27199344	2.21307221	19.99994149		
Cu	1.28379549	2.21502310	0.02747745		
Cu	3.83597548	2.21876405	0.04090475		
Cu	6.39065369	2.21640302	0.00828025		
Cu	-2.55471441	4.42695916	0.00943303		

Cu	0.00639989	4.42330454	0.01533705
Cu	2.56334779	4.42457209	0.03906776
Cu	5.11234742	4.42640268	0.01931125
Cu	-3.83181043	6.64183862	0.00589334
Cu	-1.27510811	6.64429749	0.02283823
Cu	1.28232819	6.64102892	0.01266792
Cu	3.83841983	6.64013523	0.00106419
Cu	0.00620867	1.47795525	2.09216631
Cu	2.56849156	1.48632910	2.13478535
Cu	5.11635427	1.48089264	2.11773657
Cu	7.66968051	1.47520553	2.07975035
Cu	-1.27057925	3.69180417	2.09172086
Cu	1.29450183	3.69062518	2.12744501
Cu	3.83898524	3.68881956	2.13435966
Cu	6.38788341	3.68411589	2.10439618
Cu	-2.55194278	5.90313815	2.09273418
Cu	0.01506338	5.89618693	2.09473139
Cu	2.56445527	5.90488091	2.10426804
Cu	5.10966119	5.90222400	2.09642524
Cu	-3.82578888	8.11860620	2.08968623
Cu	-1.27514194	8.13325863	2.10321840
Cu	1.28960940	8.12253498	2.07815974
Cu	3.83557045	8.11696215	2.07710890
Cu	1.29038806	0.73797172	4.16769433
Cu	3.85263346	0.75337115	4.24962239
Cu	6.39209965	0.72794653	4.17724181
Cu	8.95272457	0.73797213	4.14999065
Cu	0.01375652	2.95612283	4.16989046
Cu	2.58666533	2.96567565	4.27437805
Cu	5.10530752	2.94160009	4.23017900
Cu	7.67696141	2.94982353	4.15206993
Cu	-1.25902466	5.17807838	4.17465424
Cu	1.30195761	5.16781727	4.22819272
Cu	3.82593924	5.15878300	4.21236261
Cu	6.39319862	5.16357412	4.16226151
Cu	-2.53167581	7.38119450	4.17354418
Cu	0.01228257	7.38028912	4.13321063
Cu	2.55100154	7.37840410	4.17307797
Cu	5.12020602	7.38088202	4.14735449
Cu	-3.81756295	6.64385228	6.22581223
Cu	7.70513253	0.01251680	6.23721780
Cu	5.15221956	4.44384860	6.23886394
Cu	3.89619769	2.17605151	6.44099496
Cu	2.56596212	4.47652752	6.39964779

Cu	-2.57658151	8.84282796	6.24805732
Cu	1.27690607	6.66934068	6.29283757
Cu	-1.26467647	6.64465240	6.28745983
Cu	-0.01994552	4.40179365	6.24777773
Cu	1.25529962	2.18265060	6.22612786
Cu	6.43604845	2.20109193	6.23235292
Cu	-2.54354836	4.42832857	6.22681406
Cu	3.85702183	6.67700164	6.21658589
Cu	-1.27125538	2.20687986	6.23874371
Cu	-5.10467331	8.84918882	6.24143010
Cu	0.03475721	8.82318040	6.30250255

Str 14

Free energy from VASP is -313.67465900 eV

PBC	10.223900	10.223900	20.000000	90.000000	90.000000
120.000000					
H	1.30895640	2.55554427	11.23083277		
H	0.09948611	1.85765989	9.31351001		
H	2.51948182	4.57278264	11.58183302		
H	-0.43984411	3.52671366	9.60987535		
H	0.91177777	5.04661534	10.99016069		
H	1.24740925	4.53387608	7.42507555		
H	2.00136330	5.40948723	8.91680865		
H	2.48848864	2.63182435	9.91084647		
C	1.57507058	3.10252845	10.30907923		
C	0.43023894	2.90989987	9.32040483		
C	1.86178889	4.55422257	10.70119341		
O	0.80220693	3.23623417	7.96027451		
O	2.55575533	5.33014124	9.71831189		
Cu	0.00190070	0.00052632	0.00184647		
Cu	2.55496734	0.00088468	0.00409961		
Cu	5.11339082	0.00172950	0.00447888		
Cu	7.66756248	0.00163715	0.00370963		
Cu	8.94622381	2.21494120	0.00143405		
Cu	1.27844815	2.21154692	0.00205842		
Cu	3.83454824	2.21481136	0.00084539		
Cu	6.39022129	2.21485417	0.00036869		
Cu	-2.55667016	4.42770090	-0.00241368		
Cu	-0.00061065	4.42807388	0.00219714		
Cu	2.55767309	4.42861006	0.00244426		
Cu	5.11296146	4.42718747	-0.00060998		
Cu	6.39049472	6.64402645	0.00403165		
Cu	-1.27960637	6.64311884	0.00112096		

Cu	1.27867381	6.64319955	0.00341294
Cu	3.83552554	6.64270269	0.00215451
Cu	0.00128451	1.47682910	2.08954755
Cu	2.55523392	1.47669885	2.09166311
Cu	5.11041037	1.47577830	2.08754868
Cu	7.66890133	1.47521855	2.08766659
Cu	-1.27832823	3.68730646	2.08320398
Cu	1.27762108	3.68713831	2.08163873
Cu	3.83178452	3.68591502	2.08573974
Cu	6.38939742	3.69028872	2.08784411
Cu	-2.55505650	5.90178321	2.08134475
Cu	-0.00252559	5.90605798	2.08272253
Cu	2.55410772	5.90418366	2.08618527
Cu	5.11051244	5.90315417	2.07632770
Cu	-3.83526291	8.12574628	2.09660065
Cu	-1.27683282	8.11687876	2.08832632
Cu	1.27742958	8.11781720	2.08701921
Cu	3.83139284	8.11678710	2.08773799
Cu	1.27571542	0.75458233	4.19543070
Cu	3.83200332	0.73465658	4.16418111
Cu	6.38697824	0.73440597	4.16706096
Cu	8.94453596	0.73346355	4.16244285
Cu	0.00470368	2.95086945	4.17958389
Cu	2.53980567	2.95280806	4.18736017
Cu	5.10688232	2.94999699	4.16488244
Cu	7.66530717	2.95037212	4.16427084
Cu	-1.28526771	5.16319485	4.16201542
Cu	1.26807363	5.16073888	4.15215379
Cu	3.83426042	5.16495464	4.15647491
Cu	6.38262036	5.16927888	4.15368938
Cu	-2.56003728	7.37761870	4.15755037
Cu	0.00298157	7.37258209	4.17584820
Cu	2.54674764	7.37003374	4.17532782
Cu	5.10661588	7.37382265	4.15979863
Cu	1.28390824	2.13320569	6.32600036
Cu	5.11363907	-0.01603624	6.24893183
Cu	-1.30530297	6.65181533	6.24552408
Cu	3.84008510	6.64506680	6.25579493
Cu	5.09278379	8.82439054	6.23796089
Cu	1.27079461	6.60716166	6.30261169
Cu	-2.55017185	8.83116319	6.24455542
Cu	6.38017365	6.63297711	6.24575670
Cu	7.63391472	4.42452148	6.23026667
Cu	3.84562482	2.20211813	6.22849039

Cu	5.10707913	4.42217192	6.23935249
Cu	2.54087386	8.83614484	6.25126441
Cu	6.37918357	2.20487175	6.25550411
Cu	-0.06725963	4.47022514	6.22894367
Cu	8.90645614	2.19097409	6.21756430
Cu	2.57393980	4.47359266	6.22834649

Str 15

Free energy from VASP is -315.05615700 eV

PBC 10.223900 10.223900 20.000000 90.000000 90.000000

120.000000

H	6.30055975	2.15328358	8.53010910
H	6.22150780	1.75802999	10.25165557
H	4.21078227	2.99328516	9.56669657
H	8.49602698	2.51841057	9.44676606
H	5.14001842	3.99820573	10.70845018
H	7.86844505	3.47433834	10.82643404
H	-1.49422828	4.71637459	8.87876477
H	6.02309020	5.02815329	8.76628143
C	6.33907572	2.59750767	9.54569727
C	5.15245581	3.54263530	9.70233780
C	7.70902892	3.22287968	9.76321432
O	5.13502057	4.60681705	8.71694197
O	-2.42573394	4.43846964	8.97476084
Cu	5.11194552	8.85127755	19.99105937
Cu	-2.55758212	8.85209664	19.99254484
Cu	-0.00085888	8.85372147	19.99470046
Cu	2.55661110	8.85209552	19.99144659
Cu	8.94530363	2.21279157	19.99005346
Cu	1.27781247	2.21201952	19.98741790
Cu	3.83429515	2.21499740	19.99876813
Cu	6.38858067	2.21597676	0.00184053
Cu	7.66386251	4.42548434	0.00803146
Cu	-0.00139125	4.42483028	19.99241265
Cu	2.55869473	4.42515989	19.99910826
Cu	5.11253456	4.42582990	0.01458113
Cu	6.38781264	6.63572448	0.01022168
Cu	-1.28170997	6.63655428	0.00081513
Cu	1.27889193	6.63635485	19.99708951
Cu	3.83657921	6.63574944	0.00477498
Cu	0.00014420	1.47163397	2.06782031
Cu	2.55329593	1.47256524	2.07186555
Cu	5.10961325	1.47888346	2.08350427

Cu	7.66819710	1.47410140	2.07260959
Cu	-1.27989620	3.68396336	2.07808142
Cu	1.27737486	3.68474546	2.06958162
Cu	3.83374127	3.68650062	2.09687206
Cu	6.38638295	3.68676047	2.10368817
Cu	-2.56544002	5.89260661	2.10119206
Cu	-0.00420697	5.89469583	2.07613687
Cu	2.56247462	5.89298188	2.08809095
Cu	5.11271131	5.89333303	2.10965964
Cu	-3.83617538	8.11256432	2.07899390
Cu	-1.28056098	8.11105563	2.07088154
Cu	1.27798501	8.10995077	2.06866500
Cu	3.83425554	8.11034687	2.07408890
Cu	1.27525927	0.73143228	4.15438471
Cu	3.82970386	0.72901025	4.14656830
Cu	6.38788404	0.72830261	4.14090362
Cu	8.94585465	0.72956314	4.14474843
Cu	0.00078878	2.94461383	4.14736869
Cu	2.54745979	2.94357158	4.15552481
Cu	5.10432830	2.95738603	4.19328531
Cu	7.66863244	2.94737584	4.16476192
Cu	-1.28570072	5.15370149	4.16596957
Cu	1.27584013	5.15707041	4.15008568
Cu	3.84201513	5.14818422	4.20595260
Cu	6.37609986	5.14262286	4.22328646
Cu	-2.55781315	7.37149129	4.15520768
Cu	-0.00227803	7.36839293	4.14453470
Cu	2.55427115	7.36745048	4.15103797
Cu	5.10863718	7.37343193	4.16153678
Cu	8.95395819	2.19470820	6.21827634
Cu	0.00041893	4.41629606	6.23025331
Cu	3.80970312	2.18576207	6.22300042
Cu	7.67620794	4.41043883	6.28331826
Cu	2.52746898	4.41149840	6.23789427
Cu	3.82246767	6.64614548	6.23849808
Cu	5.08367537	4.40436284	6.40286175
Cu	-0.00514440	8.83893261	6.22068575
Cu	-3.83440539	6.65256525	6.22650749
Cu	-1.27640840	6.63526928	6.23002490
Cu	5.10763502	8.84841359	6.24008723
Cu	1.27119774	6.63085021	6.23252457
Cu	-2.56000456	8.84321083	6.23867413
Cu	2.55281559	8.84302339	6.22280827
Cu	6.38783250	2.18380479	6.20678228

Cu	1.26828414	2.20005943	6.24168430
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3. 1,2-PDO-dehydration path

Str 1

Free energy from VASP is -328.39379400 eV

PBC	10.223900	10.223900	20.000000	90.000000	90.000000
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120.000000

H	2.56691945	1.43923141	7.25711903
H	-0.04377945	2.94207071	7.26393275
H	1.94551802	5.59350670	11.35439436
H	1.76263090	6.24853554	8.99010230
H	2.17365364	3.79615525	9.64350942
H	2.56244699	7.54714549	9.93089289
H	3.10591426	3.43031148	11.13626072
H	4.74420331	5.94699531	11.06855044
H	4.19671842	5.57640868	8.76773784
H	4.16467228	3.36776412	8.77649582
C	2.85629577	5.54905729	10.73368286
C	2.67251270	6.51886758	9.55972649
C	3.03096740	4.10086297	10.26669922
O	3.92418748	5.94984188	11.59620540
O	3.83227244	6.50257320	8.68242509
O	4.26507973	4.02136705	9.50131530
Cu	5.10835498	8.84704951	0.00127886
Cu	-2.55543284	8.85212949	0.00592344
Cu	0.00152531	8.85223995	0.00382139
Cu	2.55532374	8.85039728	0.00186300
Cu	8.94196113	2.21496390	0.00537177
Cu	1.27766833	2.21275799	0.01181878
Cu	3.83527190	2.21290275	0.00614283
Cu	6.39109844	2.21514433	0.00009607
Cu	7.66517761	4.42851017	0.00553876
Cu	-0.00407226	4.42907591	0.00459696
Cu	2.55961507	4.43283322	0.00119318
Cu	5.11424490	4.43011061	0.00250585
Cu	6.38824836	6.63671419	0.00238845
Cu	-1.27942586	6.63810758	19.99957806
Cu	1.28003365	6.64250111	0.00191010
Cu	3.83422949	6.64042098	0.00235666
Cu	-0.00423426	1.47161580	2.07977278
Cu	2.55589452	1.47251059	2.08560339
Cu	5.11418136	1.47617222	2.08145297
Cu	7.66551325	1.47261319	2.08871219
Cu	-1.27891381	3.68798736	2.08911201
Cu	1.27788053	3.69337579	2.07727849
Cu	3.83334997	3.69403090	2.09033757

Cu	6.38841629	3.68404943	2.09613188
Cu	-2.55303085	5.90494884	2.09663548
Cu	-0.00047430	5.90443256	2.08853882
Cu	2.55339313	5.90226380	2.09608390
Cu	5.10910155	5.90458536	2.09220622
Cu	-3.83943831	8.11244607	2.09396081
Cu	-1.27932440	8.11161499	2.08182064
Cu	1.28246514	8.11275440	2.09833809
Cu	3.83285494	8.11634263	2.09794856
Cu	1.27193739	0.74587709	4.17299303
Cu	3.83142993	0.73273696	4.15585214
Cu	6.38460431	0.73703332	4.16401753
Cu	8.94420544	0.74866030	4.17545024
Cu	0.01492573	2.93748268	4.15676738
Cu	2.54133091	2.94105598	4.16509683
Cu	5.08758403	2.93410405	4.17473073
Cu	7.67532782	2.94732979	4.17646723
Cu	-1.27503493	5.14946691	4.17670800
Cu	1.26190231	5.15132609	4.17196157
Cu	3.83398467	5.17622035	4.18245299
Cu	6.39091061	5.15895545	4.15547868
Cu	-2.55990830	7.39575798	4.17958269
Cu	-0.00770047	7.37607806	4.16226879
Cu	2.56593376	7.36622985	4.19529103
Cu	5.09781619	7.36443810	4.19058329
Cu	-1.29035035	6.62612545	6.24104059
Cu	3.80857431	6.63558855	6.39840559
Cu	2.55384290	4.42880453	6.20207207
Cu	1.26352078	2.20016581	6.38378922
Cu	1.24265767	6.62351804	6.22606784
Cu	7.63890418	4.42503411	6.24229195
Cu	8.93798225	2.20835420	6.29049756
Cu	-0.01321614	4.40110437	6.29540073
Cu	3.81436428	2.19427375	6.29373834
Cu	5.08698574	8.82344876	6.21786136
Cu	7.64714502	0.00655731	6.23065635
Cu	-2.56704074	8.84244127	6.28868698
Cu	6.38916387	6.62419146	6.23020158
Cu	0.00252283	8.83265511	6.23671930
Cu	5.10719284	4.39874502	6.21703056
Cu	6.37317998	2.20179951	6.24412414

Free energy from VASP is -327.55689300 eV

PBC	10.223900	10.223900	20.000000	90.000000	90.000000
120.000000					
H	0.41803939	3.78330425	9.08754491		
H	2.58304673	2.83799530	11.57251313		
H	-0.00935142	3.99196046	11.51408969		
H	2.57227681	5.05842209	10.42006097		
H	0.76966359	1.19468379	11.15693051		
H	2.92490548	3.70592893	9.28587146		
H	1.81427403	1.40729991	9.70755324		
H	1.30934761	4.77421857	7.81179170		
H	-0.20052064	1.72910747	8.82017480		
H	-0.02218211	7.40968325	7.25539596		
C	1.69330947	3.15089279	11.00030645		
C	2.16345321	4.15825345	9.94539963		
C	1.08179799	1.89767883	10.36929725		
O	0.81995222	3.74417010	11.96353382		
O	1.02959254	4.59771141	9.12340272		
O	-0.08657991	2.31094164	9.60586383		
Cu	0.00103464	0.00020449	0.00498014		
Cu	2.55388503	-0.00035608	0.00389075		
Cu	5.11369406	0.00007407	0.00906814		
Cu	7.67019607	0.00281001	0.00331187		
Cu	8.94612973	2.21248154	0.00501377		
Cu	1.27749488	2.21182995	0.00640117		
Cu	3.83638904	2.21495120	0.00410722		
Cu	6.39104634	2.21481048	0.00217394		
Cu	-2.55768036	4.42638791	0.00297858		
Cu	0.00044275	4.42337431	0.00737437		
Cu	2.55853829	4.42710207	0.00848962		
Cu	5.11374617	4.42757513	0.00395788		
Cu	6.38950041	6.64037184	0.00381682		
Cu	-1.28002554	6.64241800	0.00989594		
Cu	1.27895243	6.64206727	0.01295945		
Cu	3.83824963	6.64033868	0.00475765		
Cu	-0.00065265	1.47569516	2.08670002		
Cu	2.55963849	1.47520768	2.09089661		
Cu	5.11155533	1.47772152	2.09209824		
Cu	7.66602117	1.47504143	2.09310697		
Cu	-1.27980954	3.69286595	2.08965462		
Cu	1.27997465	3.69263233	2.09114912		
Cu	3.83514189	3.68840663	2.09095273		
Cu	6.39127465	3.69025617	2.09351264		
Cu	-2.55563402	5.90121518	2.09412554		

Cu	-0.00180717	5.89946513	2.08696000
Cu	2.55955831	5.90315864	2.09322563
Cu	5.11147808	5.90348390	2.09387526
Cu	-3.83172579	8.11298182	2.09395953
Cu	-1.27837213	8.11731485	2.09046041
Cu	1.28182602	8.11884072	2.08954108
Cu	3.82974791	8.11294205	2.09309416
Cu	1.27646734	0.73955373	4.16293213
Cu	3.83987643	0.72952745	4.18119147
Cu	6.38165076	0.73166993	4.18407901
Cu	8.94518533	0.73599219	4.16362037
Cu	-0.00039965	2.95466907	4.16091509
Cu	2.55246963	2.96032142	4.17178047
Cu	5.10920389	2.95347013	4.17362688
Cu	7.66781375	2.95290389	4.16729680
Cu	-1.26881736	5.17318913	4.19146074
Cu	1.27612863	5.17809886	4.17546949
Cu	3.82418423	5.16028670	4.18287516
Cu	6.38683924	5.16545622	4.17212526
Cu	-2.54619568	7.37561517	4.18164547
Cu	0.00541994	7.37274743	4.15565931
Cu	2.53911925	7.37243475	4.19580596
Cu	5.10704640	7.37872682	4.17022380
Cu	7.68290796	0.00985619	6.24906452
Cu	5.09911467	4.42746926	6.25297936
Cu	10.21785667	0.00345240	6.26767126
Cu	3.82951700	2.21916083	6.24226143
Cu	8.94096379	2.21385089	6.24470335
Cu	1.27252236	2.20055032	6.24684583
Cu	2.51996402	4.43997012	6.31613412
Cu	-1.28225646	6.65269021	6.29963189
Cu	1.26719283	6.62201043	6.37210452
Cu	2.53110439	0.01332520	6.24701981
Cu	0.00042469	8.84812409	6.29750586
Cu	6.38344018	2.21640864	6.24961137
Cu	6.38463227	6.63868751	6.24895517
Cu	3.83072900	6.64127644	6.25428041
Cu	-2.55466295	4.43040392	6.24533020
Cu	0.02162526	4.40704171	6.26262435

Str 3

Free energy from VASP is -327.56297700 eV

PBC 10.223900 10.223900 20.000000 90.000000 90.000000

120.000000

H	4.03164058	7.40356701	8.30825541
H	5.11781924	1.47279123	7.24750026
H	3.88825496	5.15628085	11.81522686
H	2.62848272	4.21761305	9.90646425
H	4.79982512	5.59411861	9.52635366
H	1.48101069	4.74582987	11.18967905
H	5.15378743	6.98079370	10.63162587
H	2.63439274	6.83399642	9.15823536
H	2.28447344	7.48575402	11.51299896
H	1.25882659	5.55657620	8.70015795
C	3.35080929	5.85653851	11.15500804
C	2.22879840	5.08223894	10.45683418
C	4.36615340	6.39577016	10.14484068
O	2.85617972	6.87902056	12.01919352
O	1.58852373	6.01472918	9.52097943
O	3.62374919	7.32401269	9.25461929
Cu	-5.10958122	8.85408695	0.00602150
Cu	-2.55698881	8.85355534	0.00577642
Cu	5.10997423	0.00200725	0.00928024
Cu	7.66958929	0.00089629	0.00453084
Cu	-1.27447937	2.21828257	0.00667681
Cu	1.27516370	2.21565721	0.00500999
Cu	3.83481789	2.21097297	0.01030999
Cu	6.38943168	2.21352618	0.01217257
Cu	-2.55028320	4.42763061	0.00716398
Cu	-0.00143228	4.42608428	0.01868685
Cu	2.55113608	4.42543481	0.00327553
Cu	5.11358745	4.42721790	0.00597714
Cu	-3.83250921	6.64168497	0.00755031
Cu	-1.27768659	6.63581663	0.00542577
Cu	1.27446458	6.63569229	0.00323715
Cu	3.83689233	6.64171639	0.00566668
Cu	0.00226066	1.47592422	2.09283913
Cu	2.55278205	1.47724492	2.09087763
Cu	5.11252571	1.47462639	2.09404490
Cu	7.67273933	1.47848715	2.08883751
Cu	-1.28127012	3.68582560	2.10702553
Cu	1.28357064	3.68392212	2.10195800
Cu	3.83133297	3.68761189	2.08299529
Cu	6.39550934	3.69120445	2.09132232
Cu	-2.55483190	5.90260789	2.09578060
Cu	0.00017274	5.90748018	2.10180168
Cu	2.55702479	5.90063380	2.07886869

Cu	5.11467994	5.89899668	2.08749076
Cu	-3.82772004	8.11898485	2.09283929
Cu	-1.27837965	8.11136178	2.08918385
Cu	1.27631117	8.11374904	2.07862363
Cu	3.83507831	8.11910303	2.08440587
Cu	1.27603685	0.73999423	4.17808980
Cu	3.83493834	0.73680470	4.16396895
Cu	6.39565482	0.73425145	4.16197845
Cu	8.95341659	0.73827348	4.16842636
Cu	0.00479895	2.95542288	4.17414153
Cu	2.58036982	2.93948585	4.19907029
Cu	5.11400192	2.95234885	4.16321087
Cu	7.65072734	2.93808959	4.19988861
Cu	-1.26905917	5.16143865	4.17423017
Cu	1.28152078	5.15972719	4.16031830
Cu	3.83170315	5.16107942	4.15939610
Cu	6.39448494	5.16526964	4.17409412
Cu	-2.55174167	7.37246874	4.17735342
Cu	0.00274803	7.40192947	4.19021453
Cu	2.55706067	7.37343055	4.14801468
Cu	5.11866883	7.37857921	4.15948639
Cu	3.84096167	2.21243058	6.31027217
Cu	-1.26984703	6.63629848	6.25690652
Cu	1.28166736	2.21271497	6.25904646
Cu	2.55610982	4.42974891	6.26433048
Cu	6.38709660	6.63856385	6.27376422
Cu	5.11190937	4.44705687	6.24242742
Cu	1.28466894	6.63212713	6.23165417
Cu	5.11872447	0.00042256	6.30388017
Cu	6.39127664	2.20917590	6.30388687
Cu	0.01322833	4.42992599	6.27833292
Cu	5.10999718	8.83888199	6.27927305
Cu	3.84445504	6.63893499	6.22931403
Cu	-2.57001162	8.84155116	6.23939607
Cu	-2.54902882	4.42607640	6.25320150
Cu	2.58064169	8.83445432	6.23130703
Cu	-1.26968803	2.21178084	6.24969774

Str 4

Free energy from VASP is -326.87855200 eV

PBC	10.223900	10.223900	20.000000	90.000000	90.000000
120.000000					
H	5.11348022	7.37666432	7.24283537		

H	-0.67588916	7.94941975	8.66219704
H	6.68263393	0.21712320	11.88925362
H	7.06193449	1.64366742	9.56583531
H	0.21003374	7.38660727	10.87713135
H	6.48272701	2.72583429	10.98363608
H	1.40215081	8.00422432	9.68028676
H	4.25132086	1.56663883	11.46915232
H	4.53724651	2.98085437	8.77680860
H	4.24415133	1.48646306	9.17011991
C	5.90755679	0.59402436	11.17847758
C	6.48320335	1.75886769	10.48379930
C	0.49316004	8.25239455	10.25781197
O	4.79429434	0.94459145	11.99853165
O	4.20949204	2.42080167	9.51052710
O	-0.59109780	8.60674956	9.38529820
Cu	-0.00065261	0.00131123	0.00743859
Cu	2.55918766	0.00237251	-0.00287104
Cu	5.11192946	0.00105428	-0.00047904
Cu	7.66419713	0.00265585	-0.00089622
Cu	8.94639115	2.21583504	0.00069816
Cu	1.27654994	2.21605181	-0.00007903
Cu	3.83465343	2.21323174	0.00019346
Cu	6.38911649	2.21303316	0.00056583
Cu	-2.55340435	4.42647529	0.00010595
Cu	-0.00059910	4.42722202	0.00019870
Cu	2.55297822	4.42660481	0.00060971
Cu	5.11174839	4.42264104	-0.00118539
Cu	6.39021140	6.64048777	0.00676471
Cu	-1.27633082	6.63869935	-0.00007198
Cu	1.27589745	6.63895807	0.00128823
Cu	3.83294086	6.64063762	0.00768069
Cu	0.00005460	1.47775877	2.08822173
Cu	2.55157983	1.47486969	2.08322221
Cu	5.11212655	1.47528391	2.07733197
Cu	7.67175001	1.47502142	2.08598747
Cu	-1.27868518	3.68787566	2.08676884
Cu	1.27763505	3.68884344	2.08655752
Cu	3.83222486	3.69250576	2.08483511
Cu	6.39182021	3.69263055	2.08500769
Cu	-2.55438759	5.90097441	2.08501749
Cu	-0.00001146	5.90258655	2.08694649
Cu	2.55394223	5.90144705	2.08735380
Cu	5.11200202	5.89684226	2.07876404
Cu	-3.82965223	8.11918019	2.07817560

Cu	-1.28064952	8.11336475	2.08288249
Cu	1.28107758	8.11405392	2.08482823
Cu	3.82899047	8.11851686	2.07999994
Cu	1.27031216	0.72825213	4.17662564
Cu	3.83399008	0.73760861	4.15119258
Cu	6.39071323	0.73878859	4.15528980
Cu	8.95426290	0.72803816	4.17648369
Cu	-0.00036927	2.95213447	4.16796521
Cu	2.55468391	2.95169331	4.15711436
Cu	5.11346133	2.95093436	4.15202397
Cu	7.66778830	2.95091849	4.16043055
Cu	-1.27769921	5.16266706	4.16521404
Cu	1.27780803	5.16364360	4.16827720
Cu	3.83787733	5.17510820	4.17707449
Cu	6.38720421	5.17522268	4.17690566
Cu	-2.56731382	7.37360369	4.17225987
Cu	0.00090870	7.37720890	4.15416181
Cu	2.56748605	7.37463629	4.17727271
Cu	5.11255709	7.37681126	4.13191723
Cu	2.57655899	0.00711966	6.22957463
Cu	7.64860320	0.01077817	6.23539753
Cu	6.38563154	6.64221696	6.29626577
Cu	-5.11240151	8.84420881	6.29488044
Cu	8.94697759	2.21143184	6.24077136
Cu	3.84073774	6.64286145	6.29676974
Cu	2.55597116	4.42881717	6.24440012
Cu	-0.00027875	4.42634915	6.25093112
Cu	3.83200158	2.21643554	6.22803341
Cu	-1.27689646	6.63737981	6.23759423
Cu	0.00198731	8.85120421	6.22982928
Cu	1.27524963	2.21147820	6.23952772
Cu	6.38953120	2.21543463	6.24571380
Cu	1.27722263	6.63874143	6.24361396
Cu	-2.55421325	4.42755818	6.24347138
Cu	5.11282695	4.40152178	6.23774564

Str 5

Free energy from VASP is -328.45969500 eV

PBC	10.223900	10.223900	20.000000	90.000000	90.000000
120.000000					
H	3.85636566	5.15592326	7.24168009		
H	0.44748235	7.33659282	8.82923624		
H	2.36688496	3.72072307	9.03560459		

H	2.35903231	2.14400099	11.01331194
H	1.98373804	1.21775575	8.72514396
H	1.79532918	3.79158925	11.41108122
H	0.23182292	1.51112597	8.75840380
H	0.14049972	1.52360049	11.02890700
H	-0.37015685	3.86346430	9.72833886
H	0.77053440	5.78543552	8.90398992
C	1.44505025	3.20279521	9.34489393
C	1.55405930	2.88055669	10.84513487
C	1.20383736	1.96319004	8.49651670
O	0.37715121	4.18036791	9.17935207
O	0.29779227	2.42309212	11.37049013
O	1.12231785	6.67311366	8.59378194
Cu	10.21970541	0.00474158	0.00109052
Cu	2.55570584	0.00192151	19.99766900
Cu	0.00009755	8.85216912	19.99250826
Cu	7.66261730	0.00099499	19.99624368
Cu	-1.27952869	2.21860190	19.99474901
Cu	1.27252472	2.21871501	0.01004402
Cu	3.83125794	2.21295344	19.98639448
Cu	6.39013768	2.21552415	19.98204191
Cu	-2.55680751	4.42916313	19.99366618
Cu	-0.00338876	4.43099564	0.01301965
Cu	2.55110830	4.43240854	0.01306099
Cu	5.11158525	4.43013859	19.99607824
Cu	-3.83247543	6.64226784	19.99331363
Cu	-1.27595858	6.64319295	0.00328789
Cu	1.27062434	6.64676083	0.00638541
Cu	3.82764727	6.64309520	0.00636447
Cu	-0.00600599	1.48625540	2.08729160
Cu	2.54759473	1.48747565	2.07823037
Cu	5.10867289	1.48400045	2.06589454
Cu	7.66309521	1.48144276	2.07042745
Cu	-1.27760378	3.69394512	2.09338057
Cu	1.27160435	3.70197817	2.11361271
Cu	3.82383726	3.68605175	2.07542696
Cu	6.38749135	3.69220382	2.07081996
Cu	-2.55824732	5.90310487	2.08424131
Cu	0.00164625	5.90453518	2.10709089
Cu	2.53894537	5.91035233	2.09777051
Cu	5.10967384	5.90913400	2.06927314
Cu	-3.84419289	8.12571197	2.07940491
Cu	-1.27451704	8.11905068	2.08090213
Cu	1.27723179	8.11816399	2.09260905

Cu	3.81989375	8.11915906	2.09296045
Cu	1.26835504	0.76596192	4.17157107
Cu	3.82262597	0.75004734	4.13399887
Cu	6.38375345	0.74756750	4.13879904
Cu	8.93907017	0.74726055	4.15329999
Cu	0.01211039	2.94904102	4.20874025
Cu	2.52788508	2.95435665	4.20886335
Cu	5.09787235	2.96902162	4.15631070
Cu	7.66565439	2.95669926	4.15252815
Cu	-1.27661545	5.16416809	4.16889355
Cu	1.27583301	5.17858272	4.24416062
Cu	3.82494820	5.16474977	4.12149137
Cu	6.37127280	5.16668909	4.15655897
Cu	-2.56429888	7.39039270	4.13875587
Cu	0.00963298	7.37745295	4.18305280
Cu	2.53997648	7.36245269	4.21698879
Cu	5.09613597	7.37528930	4.16228581
Cu	8.91602404	2.21324066	6.23142336
Cu	3.84299358	2.19485223	6.21284653
Cu	2.58818990	4.43421106	6.26544129
Cu	-1.30676209	6.64947498	6.21650539
Cu	1.26012063	2.20533256	6.48265144
Cu	5.11236306	4.43376230	6.28224846
Cu	-0.02661103	4.42090117	6.27330228
Cu	7.65027652	4.43137938	6.22445853
Cu	5.08905115	8.84462200	6.20557485
Cu	3.84869661	6.63126127	6.28573849
Cu	6.38157286	2.22493780	6.22406997
Cu	-2.55512749	8.85363079	6.20697500
Cu	7.65898237	0.01739710	6.21931592
Cu	5.10068498	0.02624708	6.20468593
Cu	1.24598012	6.66524246	6.39740848
Cu	-3.82048460	6.65610590	6.21687274

Str 6

Free energy from VASP is -328.03457400 eV

PBC	10.223900	10.223900	20.000000	90.000000	90.000000
120.000000					
H	3.08991344	3.79401319	8.94383019		
H	3.46367717	1.54600804	8.72561869		
H	1.59664376	2.80518994	10.17234878		
H	0.65139041	7.15818934	9.12796431		
H	0.17932056	4.09380247	8.76288658		

H	2.32077718	7.30978474	8.52659034
H	-0.09545086	5.10295639	10.21282303
H	2.37265897	5.61891002	10.25570799
H	0.20020524	6.11178433	7.42234875
H	4.12411192	1.92024497	10.09863633
C	1.84214241	5.35428186	9.31813379
C	1.46099026	6.63080436	8.61190516
C	0.64894379	4.47762129	9.69758361
O	2.80223407	4.63273646	8.49580956
O	3.35257706	2.10244587	9.53147692
O	0.96907783	3.42581675	10.59577568
Cu	0.00370380	0.00117560	0.00872804
Cu	2.55709173	0.00157365	0.00985177
Cu	5.11463396	0.00084607	0.00700898
Cu	7.67205638	0.00095052	0.00594050
Cu	8.94787825	2.21457823	0.00496665
Cu	1.28027663	2.21368533	0.00587088
Cu	3.83671952	2.21535927	0.00230959
Cu	6.39388577	2.21595137	-0.00300374
Cu	-2.55396836	4.42659053	0.00447551
Cu	0.00273663	4.42922320	0.01615511
Cu	2.55798348	4.42860711	0.01352579
Cu	5.11564780	4.42717068	-0.00005738
Cu	6.39190030	6.64183514	0.00798479
Cu	-1.27412336	6.64025271	0.01420115
Cu	1.28102409	6.63975002	0.02171229
Cu	3.83577928	6.64188055	0.00946489
Cu	0.00627153	1.48212038	2.08841224
Cu	2.56063806	1.48753843	2.09007687
Cu	5.11878277	1.47666004	2.08038067
Cu	7.67218473	1.47953828	2.08427982
Cu	-1.27093051	3.69186714	2.09498719
Cu	1.28372525	3.69935254	2.10634198
Cu	3.83722701	3.69352037	2.08940608
Cu	6.39650941	3.69229674	2.08123509
Cu	-2.54761578	5.90652979	2.09321961
Cu	0.01117514	5.90150125	2.11449913
Cu	2.55964787	5.90409700	2.10839317
Cu	5.11258777	5.90016596	2.09250628
Cu	-3.82593302	8.11768890	2.08854022
Cu	-1.26544085	8.11207809	2.09388226
Cu	1.28543844	8.11681087	2.09554097
Cu	3.83158444	8.11410392	2.10092752
Cu	1.29211199	0.74229081	4.15481507

Cu	3.84000392	0.73796398	4.14480416
Cu	6.39791455	0.74300729	4.15789686
Cu	8.96256495	0.74531511	4.15369760
Cu	0.01120004	2.96961535	4.17763532
Cu	2.56478623	2.97502242	4.18971722
Cu	5.12365751	2.95435656	4.15359777
Cu	7.67673980	2.95556704	4.16397737
Cu	-1.26242502	5.17372712	4.17750308
Cu	1.30259249	5.17770803	4.24493011
Cu	3.83305465	5.16048577	4.18936480
Cu	6.40265719	5.17323558	4.15798858
Cu	-2.52936297	7.38064235	4.17639349
Cu	0.02685658	7.37416097	4.20645552
Cu	2.54068478	7.36987062	4.20921725
Cu	5.12943311	7.38574649	4.15406439
Cu	2.57934457	0.00911879	6.25028879
Cu	7.69708945	0.04136679	6.21209346
Cu	-1.25526570	6.64134774	6.29528640
Cu	5.11990329	0.04896162	6.22853614
Cu	1.32750287	6.67444296	6.43846333
Cu	3.86420081	2.20141904	6.21490748
Cu	6.41229176	2.22568635	6.24849076
Cu	-1.25936859	2.22288575	6.24514218
Cu	1.28851205	2.20728652	6.22819386
Cu	3.89070448	6.66589100	6.20358916
Cu	5.16498384	4.42661933	6.21931139
Cu	-2.54480547	4.43177568	6.24517478
Cu	0.02748073	0.01253118	6.24104214
Cu	2.60926578	4.40746003	6.35462629
Cu	-0.01124697	4.43641372	6.28057941
Cu	-3.80227779	6.65296844	6.24189973

Str 7

Free energy from VASP is -329.44101400 eV

PBC	10.223900	10.223900	20.000000	90.000000	90.000000
120.000000					
H	1.03598457	1.20423790	8.59718619		
H	2.83900058	7.21080868	9.62265514		
H	2.33526895	3.13306881	9.66778464		
H	4.20728410	6.11285542	9.92660468		
H	0.55888029	6.27800600	9.20461303		
H	2.93893787	6.29537281	11.16192062		
H	0.53636850	5.13322204	10.58669760		

H	0.27680859	3.43147690	8.99980615
H	0.88904866	1.19260048	10.16770073
H	2.61060222	5.10445803	8.33703065
C	2.37005445	5.10339973	9.44001376
C	3.12859422	6.25408272	10.07956619
C	0.85464823	5.27226326	9.53870434
O	2.82816338	3.89918847	10.03720662
O	1.02126461	1.77707411	9.40045086
O	0.11684798	4.35649089	8.69143886
Cu	10.22364868	0.00007844	0.00495902
Cu	-2.55524295	8.85373875	0.00434309
Cu	5.11212969	0.00049225	0.00389059
Cu	7.66758463	0.00021738	0.00440042
Cu	-1.27839707	2.21443242	0.00493334
Cu	1.27773295	2.21434347	0.00459320
Cu	3.83523655	2.21353467	0.00197383
Cu	6.38970196	2.21387198	0.00327777
Cu	7.66800968	4.42693021	0.00537097
Cu	0.00011782	4.42754206	0.00411261
Cu	2.55534271	4.42754895	0.00387282
Cu	5.11257703	4.42670236	0.00353503
Cu	-3.83322512	6.63970298	0.00427077
Cu	-1.27779167	6.63996055	0.00426915
Cu	1.27762361	6.63971877	0.00448686
Cu	3.83366778	6.64033655	0.00320745
Cu	-0.00068927	1.48294777	2.09245600
Cu	2.55739922	1.47671073	2.08506748
Cu	5.11208910	1.47587615	2.08778474
Cu	7.66734966	1.47659534	2.08726817
Cu	-1.27668988	3.69162621	2.09472991
Cu	1.27629181	3.69105870	2.09122911
Cu	3.83508604	3.68968998	2.08515619
Cu	6.39040934	3.68949889	2.08967816
Cu	-2.54925601	5.89927326	2.09654271
Cu	-0.00031641	5.89992002	2.09513340
Cu	2.55089193	5.89982275	2.09396244
Cu	5.11258245	5.90282237	2.08577360
Cu	-3.83373497	8.11418853	2.08153530
Cu	-1.27813529	8.11602515	2.08540093
Cu	1.27817189	8.11645606	2.08836745
Cu	3.83459185	8.11540999	2.08431021
Cu	1.27816836	0.73271105	4.15068513
Cu	3.83305140	0.73692690	4.16738415
Cu	6.39138488	0.73968359	4.16822928

Cu	8.94994076	0.73771716	4.16141782
Cu	-0.00037083	2.97341644	4.19480308
Cu	2.56180370	2.95351998	4.15789815
Cu	5.11412613	2.95207365	4.16825614
Cu	7.66847952	2.95205422	4.16704926
Cu	-1.25858816	5.15688780	4.20811079
Cu	1.26307759	5.15673404	4.19829047
Cu	3.83874308	5.16875968	4.16121870
Cu	6.39511047	5.16923116	4.16602960
Cu	-2.55640173	7.38031022	4.16393069
Cu	-0.00217170	7.38311385	4.16020431
Cu	2.56088185	7.38044327	4.16046527
Cu	5.11672869	7.38181040	4.16253299
Cu	7.67578086	0.00718194	6.25439340
Cu	5.12691282	4.43118851	6.24825586
Cu	3.84754259	6.65557949	6.23548071
Cu	2.57941784	4.43235507	6.22516294
Cu	2.55409463	0.00579943	6.26429118
Cu	7.66589738	4.42930466	6.24582627
Cu	3.84295019	2.21362283	6.25206337
Cu	8.94521709	2.20454720	6.23593070
Cu	5.11485628	0.00860908	6.25436177
Cu	6.39546378	2.21506400	6.25367056
Cu	-3.82897722	6.64823352	6.25604823
Cu	1.28355932	6.67268471	6.21584628
Cu	1.29340111	2.20093437	6.20347893
Cu	-1.27847357	6.66156553	6.23904403
Cu	0.01437255	4.43332327	6.41347691
Cu	0.01022543	0.00649629	6.26005713

4. 1,3-PDO-dehydration path

Str 1

Free energy from VASP is -328.39379400 eV

PBC	10.223900	10.223900	20.000000	90.000000	90.000000
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120.000000

H	2.56691945	1.43923141	7.25711903
H	-0.04377945	2.94207071	7.26393275
H	1.94551802	5.59350670	11.35439436
H	1.76263090	6.24853554	8.99010230
H	2.17365364	3.79615525	9.64350942
H	2.56244699	7.54714549	9.93089289
H	3.10591426	3.43031148	11.13626072
H	4.74420331	5.94699531	11.06855044
H	4.19671842	5.57640868	8.76773784
H	4.16467228	3.36776412	8.77649582
C	2.85629577	5.54905729	10.73368286
C	2.67251270	6.51886758	9.55972649
C	3.03096740	4.10086297	10.26669922
O	3.92418748	5.94984188	11.59620540
O	3.83227244	6.50257320	8.68242509
O	4.26507973	4.02136705	9.50131530
Cu	5.10835498	8.84704951	0.00127886
Cu	-2.55543284	8.85212949	0.00592344
Cu	0.00152531	8.85223995	0.00382139
Cu	2.55532374	8.85039728	0.00186300
Cu	8.94196113	2.21496390	0.00537177
Cu	1.27766833	2.21275799	0.01181878
Cu	3.83527190	2.21290275	0.00614283
Cu	6.39109844	2.21514433	0.00009607
Cu	7.66517761	4.42851017	0.00553876
Cu	-0.00407226	4.42907591	0.00459696
Cu	2.55961507	4.43283322	0.00119318
Cu	5.11424490	4.43011061	0.00250585
Cu	6.38824836	6.63671419	0.00238845
Cu	-1.27942586	6.63810758	19.99957806
Cu	1.28003365	6.64250111	0.00191010
Cu	3.83422949	6.64042098	0.00235666
Cu	-0.00423426	1.47161580	2.07977278
Cu	2.55589452	1.47251059	2.08560339
Cu	5.11418136	1.47617222	2.08145297
Cu	7.66551325	1.47261319	2.08871219
Cu	-1.27891381	3.68798736	2.08911201
Cu	1.27788053	3.69337579	2.07727849
Cu	3.83334997	3.69403090	2.09033757

Cu	6.38841629	3.68404943	2.09613188
Cu	-2.55303085	5.90494884	2.09663548
Cu	-0.00047430	5.90443256	2.08853882
Cu	2.55339313	5.90226380	2.09608390
Cu	5.10910155	5.90458536	2.09220622
Cu	-3.83943831	8.11244607	2.09396081
Cu	-1.27932440	8.11161499	2.08182064
Cu	1.28246514	8.11275440	2.09833809
Cu	3.83285494	8.11634263	2.09794856
Cu	1.27193739	0.74587709	4.17299303
Cu	3.83142993	0.73273696	4.15585214
Cu	6.38460431	0.73703332	4.16401753
Cu	8.94420544	0.74866030	4.17545024
Cu	0.01492573	2.93748268	4.15676738
Cu	2.54133091	2.94105598	4.16509683
Cu	5.08758403	2.93410405	4.17473073
Cu	7.67532782	2.94732979	4.17646723
Cu	-1.27503493	5.14946691	4.17670800
Cu	1.26190231	5.15132609	4.17196157
Cu	3.83398467	5.17622035	4.18245299
Cu	6.39091061	5.15895545	4.15547868
Cu	-2.55990830	7.39575798	4.17958269
Cu	-0.00770047	7.37607806	4.16226879
Cu	2.56593376	7.36622985	4.19529103
Cu	5.09781619	7.36443810	4.19058329
Cu	-1.29035035	6.62612545	6.24104059
Cu	3.80857431	6.63558855	6.39840559
Cu	2.55384290	4.42880453	6.20207207
Cu	1.26352078	2.20016581	6.38378922
Cu	1.24265767	6.62351804	6.22606784
Cu	7.63890418	4.42503411	6.24229195
Cu	8.93798225	2.20835420	6.29049756
Cu	-0.01321614	4.40110437	6.29540073
Cu	3.81436428	2.19427375	6.29373834
Cu	5.08698574	8.82344876	6.21786136
Cu	7.64714502	0.00655731	6.23065635
Cu	-2.56704074	8.84244127	6.28868698
Cu	6.38916387	6.62419146	6.23020158
Cu	0.00252283	8.83265511	6.23671930
Cu	5.10719284	4.39874502	6.21703056
Cu	6.37317998	2.20179951	6.24412414

Free energy from VASP is -327.61250800 eV

PBC	10.223900	10.223900	20.000000	90.000000	90.000000
120.000000					
H	1.90929166	5.85345239	9.22242785		
H	1.80301577	4.62822239	7.93863158		
H	2.55322887	4.62634726	11.12465670		
H	3.21111864	2.62979439	8.88980700		
H	4.51889806	4.88820423	8.76152877		
H	3.92478997	2.57168954	10.52031635		
H	4.91276785	5.03625008	10.50620582		
H	-1.29688721	3.68084890	7.24092131		
H	4.15551149	7.02220119	8.96133507		
H	1.15162637	2.33831277	9.95206780		
C	2.88562568	4.39015593	10.10144563		
C	3.03501307	2.88652150	9.95315777		
C	4.12832601	5.19934365	9.74773441		
O	1.77075893	4.86772865	9.23671538		
O	1.93878323	2.16251529	10.49767662		
O	3.72353756	6.57605790	9.72035543		
Cu	5.11416412	8.85310367	19.98109789		
Cu	-2.55382651	8.85585100	19.97774993		
Cu	0.00032452	8.85734478	19.97044293		
Cu	2.55831442	8.85394984	19.97234552		
Cu	8.94659073	2.21639048	-0.01121834		
Cu	1.28197955	2.21294773	-0.01261144		
Cu	3.83591587	2.21289126	19.97639748		
Cu	6.39040673	2.21387307	19.97452356		
Cu	7.67086155	4.42910755	19.98842523		
Cu	0.00107289	4.42870594	-0.00373031		
Cu	2.55923970	4.43079275	19.99004407		
Cu	5.11214690	4.43201681	19.97859591		
Cu	6.38995902	6.64400810	-0.01536613		
Cu	-1.27868451	6.64594957	19.98206202		
Cu	1.28273178	6.64390543	19.98427088		
Cu	3.83689802	6.64262071	-0.00637720		
Cu	0.00240930	1.47806015	2.06443601		
Cu	2.55834363	1.47911401	2.06398386		
Cu	5.11441792	1.47923020	2.05861806		
Cu	7.67075843	1.47565074	2.05662981		
Cu	-1.27492098	3.69274246	2.07178457		
Cu	1.28305921	3.69292415	2.06993529		
Cu	3.83780517	3.68988629	2.05982455		
Cu	6.38976658	3.69366739	2.05761708		
Cu	-2.55097723	5.90525467	2.06697520		

Cu	0.00342301	5.90831133	2.06499275
Cu	2.55389140	5.90271331	2.07245992
Cu	5.11802575	5.90112676	2.07397699
Cu	-3.82853821	8.12150058	2.06583695
Cu	-1.27261924	8.11860689	2.06263024
Cu	1.27851119	8.12135465	2.05601829
Cu	3.83460705	8.12531771	2.06840709
Cu	1.27944554	0.74493793	4.14673411
Cu	3.83721696	0.74112042	4.14037629
Cu	6.39667615	0.73982115	4.13610834
Cu	8.94990022	0.76478217	4.16387024
Cu	0.00494587	2.96115861	4.15550191
Cu	2.55992403	2.96496927	4.14698063
Cu	5.11376158	2.95958399	4.13549792
Cu	7.67221974	2.95526440	4.13541119
Cu	-1.25978516	5.16233418	4.16078792
Cu	1.26267248	5.15495879	4.16847400
Cu	3.82325750	5.16491781	4.14629004
Cu	6.41654687	5.15802559	4.16128788
Cu	-2.55243123	7.37934589	4.14045241
Cu	0.01122333	7.37826823	4.14502221
Cu	2.55804637	7.37868913	4.13363040
Cu	5.11237081	7.38011660	4.13220903
Cu	3.84164433	2.21865255	6.21014433
Cu	2.53493870	4.43584748	6.28967178
Cu	-2.55041442	8.85553476	6.21967033
Cu	5.11637717	4.43248946	6.20136122
Cu	1.28852655	6.63686888	6.22974564
Cu	6.37884775	2.20898626	6.20290097
Cu	8.94952289	2.22125566	6.28178744
Cu	3.84137678	6.65044456	6.20779346
Cu	6.39095558	6.64325374	6.21765902
Cu	-1.27197001	6.66283784	6.21091169
Cu	7.67265161	0.00180520	6.21615652
Cu	10.22572927	0.00141890	6.22305583
Cu	0.03349349	4.42590934	6.38223534
Cu	5.12001429	0.00086378	6.21776618
Cu	7.68496820	4.42995113	6.27808979
Cu	1.30263746	2.20286557	6.22095993

Str 3

Free energy from VASP is -327.65664800 eV

PBC	10.223900	10.223900	20.000000	90.000000	90.000000
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120.000000

H	3.30615826	6.44492500	9.18135047
H	2.37805109	5.33564790	8.34226188
H	3.18900038	4.89135801	11.09600215
H	3.64815822	3.10234589	8.62974467
H	5.35448241	4.72992863	8.89412169
H	3.90231518	2.65785111	10.33492914
H	5.56676875	5.14979685	10.63238998
H	-1.28462492	3.68619659	7.21477680
H	5.15192597	6.85014576	8.54919188
H	1.52946118	2.80041721	8.89802584
C	3.48830437	4.71879251	10.05409094
C	3.27523563	3.26547333	9.65785009
C	4.91161660	5.25380056	9.75830040
O	2.58603215	5.65205122	9.29728281
O	1.92573281	2.85693144	9.79423557
O	4.75007046	6.66006671	9.44216181
Cu	5.11518484	8.84106039	19.93681415
Cu	-2.55006546	8.84306793	19.93030122
Cu	0.00132920	8.84411062	19.93073087
Cu	2.55861073	8.84204987	19.93779667
Cu	8.94835394	2.20309448	19.95598128
Cu	1.28265702	2.19909804	19.94281529
Cu	3.83820837	2.19784902	19.92871810
Cu	6.39241927	2.19984645	19.94237922
Cu	7.67333390	4.41405809	19.95081576
Cu	0.00045690	4.41428173	19.95160941
Cu	2.56004534	4.41734879	19.93157125
Cu	5.11542494	4.41690858	19.92968719
Cu	6.39256883	6.63100751	19.93226301
Cu	-1.27546992	6.63205789	19.93816158
Cu	1.28217617	6.63138219	19.93353056
Cu	3.83733181	6.63033433	19.94468193
Cu	0.00226231	1.46382313	2.02800539
Cu	2.55890396	1.46347308	2.01795135
Cu	5.11520568	1.46471115	2.02118338
Cu	7.67190038	1.46377617	2.03056877
Cu	-1.27585659	3.68136840	2.03635651
Cu	1.28205412	3.67998210	2.01962213
Cu	3.83819735	3.67564380	2.00467313
Cu	6.39168837	3.68106092	2.02185677
Cu	-2.55249511	5.89452271	2.02359555
Cu	0.00212489	5.89567541	2.02197590
Cu	2.55134827	5.89057900	2.01862801

Cu	5.12236502	5.89053309	2.01847188
Cu	-3.82762828	8.10730882	2.01656403
Cu	-1.27414479	8.10512797	2.02015583
Cu	1.27742931	8.10834974	2.01736877
Cu	3.83629032	8.11511544	2.02545113
Cu	1.27923454	0.72435900	4.09733145
Cu	3.83564448	0.72299107	4.09590240
Cu	6.39527035	0.72370467	4.09916290
Cu	8.95117837	0.75169207	4.13858572
Cu	0.00169666	2.94373242	4.10825948
Cu	2.55886429	2.94569109	4.08298701
Cu	5.11392121	2.94513111	4.08659916
Cu	7.67305808	2.94249829	4.10931044
Cu	-1.27141198	5.15176632	4.11467254
Cu	1.25724764	5.14211432	4.11667270
Cu	3.83422062	5.15524397	4.07030641
Cu	6.41650166	5.14573650	4.11959060
Cu	-2.55533419	7.36662722	4.09718624
Cu	0.00764919	7.36463093	4.09959671
Cu	2.55926537	7.36741097	4.08287658
Cu	5.11356929	7.36819042	4.08169531
Cu	3.83492653	2.20428957	6.15482535
Cu	2.55254657	4.42174797	6.17279082
Cu	-2.55508181	8.84323232	6.18489973
Cu	5.11368549	4.42077843	6.15444682
Cu	1.28884028	6.62035130	6.18319749
Cu	6.37329462	2.19346641	6.16512338
Cu	-1.27372086	2.21051907	6.26562150
Cu	3.83897536	6.62662320	6.15548236
Cu	6.38591325	6.63164513	6.18336963
Cu	-1.27561506	6.65150611	6.17067172
Cu	2.55959721	8.83953761	6.18076313
Cu	5.11455851	8.83715536	6.18948217
Cu	0.00872595	4.41376725	6.28572100
Cu	0.00473161	8.84074413	6.17897926
Cu	7.67313609	4.41791712	6.25862177
Cu	1.29932409	2.19309383	6.16535537

Str 4

Free energy from VASP is -326.93793800 eV

PBC	10.223900	10.223900	20.000000	90.000000	90.000000
120.000000					
H	3.67593051	3.98598797	10.05385521		

H	4.06451622	6.28191970	9.49936311
H	6.58379424	5.80931708	11.13614677
H	4.61150703	4.21877587	12.21868175
H	7.22250813	3.65469385	10.23680423
H	4.30936652	5.95580408	11.99776502
H	6.64637499	4.55705056	8.83952168
H	1.27930822	5.16620069	7.24101843
H	5.15823289	6.85777858	8.52881628
H	5.39478367	2.79584203	8.62880798
C	5.82548151	5.13360007	10.73604912
C	4.52788842	5.02546621	11.45760436
C	6.29832396	4.10378451	9.80459468
O	4.90243623	6.80932461	9.48527855
O	3.41909715	4.77757984	10.58272815
O	5.32141834	3.09348512	9.56802666
Cu	0.00000000	0.00000000	0.00000000
Cu	2.55597888	0.00000000	0.00000000
Cu	5.11195776	0.00000000	0.00000000
Cu	7.66793665	0.00000000	0.00000000
Cu	8.94591056	2.21354264	0.00000000
Cu	1.27798944	2.21354264	0.00000000
Cu	3.83396832	2.21354264	0.00000000
Cu	6.38994721	2.21354264	0.00000000
Cu	-2.55597888	4.42708529	0.00000000
Cu	0.00000000	4.42708529	0.00000000
Cu	2.55597888	4.42708529	0.00000000
Cu	5.11195776	4.42708529	0.00000000
Cu	6.38993168	6.64062793	0.00000000
Cu	-1.27798944	6.64062793	0.00000000
Cu	1.27798944	6.64062793	0.00000000
Cu	3.83396832	6.64062793	0.00000000
Cu	-0.00000000	1.47569510	2.08694802
Cu	2.55597888	1.47569510	2.08694802
Cu	5.11195776	1.47569510	2.08694802
Cu	7.66793665	1.47569510	2.08694802
Cu	-1.27798944	3.68923774	2.08694802
Cu	1.27798944	3.68923774	2.08694802
Cu	3.83396832	3.68923774	2.08694802
Cu	6.38994721	3.68923774	2.08694802
Cu	-2.55597888	5.90278038	2.08694802
Cu	0.00000000	5.90278038	2.08694802
Cu	2.55597888	5.90278038	2.08694802
Cu	5.11195776	5.90278038	2.08694802
Cu	-3.83396832	8.11632302	2.08694802

Cu	-1.27798944	8.11632302	2.08694802
Cu	1.27798944	8.11632302	2.08694802
Cu	3.83396832	8.11632302	2.08694802
Cu	1.27798944	0.73784755	4.17389604
Cu	3.83396832	0.73784755	4.17389604
Cu	6.38994721	0.73784755	4.17389604
Cu	8.94592609	0.73784755	4.17389604
Cu	0.00000000	2.95139019	4.17389604
Cu	2.55597888	2.95139019	4.17389604
Cu	5.11195776	2.95139019	4.17389604
Cu	7.66793665	2.95139019	4.17389604
Cu	-1.27798944	5.16493283	4.17389604
Cu	1.27798944	5.16493283	4.17389604
Cu	3.83396832	5.16493283	4.17389604
Cu	6.38994721	5.16493283	4.17389604
Cu	-2.55597888	7.37847548	4.17389604
Cu	0.00000000	7.37847548	4.17389604
Cu	2.55597888	7.37847548	4.17389604
Cu	5.11195776	7.37847548	4.17389604
Cu	-1.27757298	2.21677396	6.24798018
Cu	3.85537545	6.65304657	6.23726667
Cu	5.11368553	8.85110234	6.26835830
Cu	1.28042749	2.19287199	6.24241543
Cu	7.66657817	0.00194929	6.25091372
Cu	-3.83121834	6.63802518	6.25426519
Cu	2.55515266	4.43078895	6.30050649
Cu	5.11646999	0.00276984	6.25440320
Cu	-1.29491713	6.65142468	6.24386375
Cu	6.38962850	2.21515160	6.25815119
Cu	1.28009453	6.63821333	6.29879008
Cu	7.66770779	4.42461357	6.26261490
Cu	2.55939917	0.00151676	6.25971132
Cu	5.11438250	4.42318887	6.25582693
Cu	0.00365578	4.42955107	6.29971284
Cu	3.83999652	2.21904381	6.25493424

Str 5

Free energy from VASP is -328.14228800 eV

PBC	10.223900	10.223900	20.000000	90.000000	90.000000
120.000000					
H	4.62509881	0.34002366	9.10968468		
H	5.96708112	0.99346867	8.76151844		
H	3.88596560	7.99729836	8.65962667		

H	2.59610873	5.23419346	9.03350500
H	4.98122835	5.17059155	9.09131645
H	2.50175966	6.61457762	10.16007755
H	5.14742164	6.58200881	10.19256831
H	1.06934053	7.64111425	8.81858687
H	-3.18771479	6.16821028	8.81601346
H	1.27033473	3.69658800	7.22906109
C	3.85521402	6.91008112	8.47028491
C	2.58827411	6.33388947	9.09329444
C	5.05914967	6.27282783	9.13313314
O	5.56835502	0.33071100	9.36898684
O	1.35730507	6.75561663	8.45829925
O	6.29179593	6.70287927	8.47926226
Cu	0.00131675	-0.00631136	-0.00343018
Cu	2.55727590	-0.00418161	0.00013694
Cu	5.10986926	0.00058301	0.00017630
Cu	7.66399152	-0.00074911	-0.00529097
Cu	8.94222705	2.21678250	-0.01156311
Cu	1.27798108	2.21762492	-0.00047550
Cu	3.83594278	2.21122692	-0.00472789
Cu	6.38823538	2.21416761	-0.01039540
Cu	-2.55840522	4.43206758	-0.01131651
Cu	-0.00126779	4.42742981	0.00057837
Cu	2.55395356	4.42589578	0.00196874
Cu	5.11492801	4.43039433	-0.01092355
Cu	6.38951673	6.64098653	0.01197542
Cu	-1.28303241	6.64206219	-0.00253299
Cu	1.27624679	6.64486499	0.00318377
Cu	3.83777656	6.64242748	0.00813240
Cu	-0.00206185	1.47357402	2.05986565
Cu	2.55003587	1.47319582	2.06617908
Cu	5.10995378	1.47893270	2.07173291
Cu	7.66713866	1.47864981	2.06296022
Cu	-1.28433481	3.69423503	2.06325003
Cu	1.27546710	3.70526354	2.08623637
Cu	3.83552228	3.70159131	2.07102224
Cu	6.38618567	3.70139586	2.07464460
Cu	-2.55515897	5.90339475	2.09131783
Cu	-0.00232692	5.90725217	2.08168195
Cu	2.55448603	5.90711222	2.09019349
Cu	5.10373683	5.90349327	2.09573203
Cu	-3.84500527	8.12053340	2.10033667
Cu	-1.27788401	8.10640533	2.09726743
Cu	1.28417381	8.11186987	2.08799611

Cu	3.82740455	8.10853149	2.09676866
Cu	1.26834314	0.77212409	4.17082010
Cu	3.82248209	0.74220288	4.12510769
Cu	6.38820405	0.74230434	4.13604334
Cu	8.94142181	0.73858324	4.12910706
Cu	-0.00556103	2.95811329	4.12870582
Cu	2.55275899	2.96210392	4.12863045
Cu	5.10370444	2.96387310	4.13422523
Cu	7.65748255	2.96034690	4.12928167
Cu	-1.26074776	5.15601116	4.16380439
Cu	1.27304804	5.19324524	4.18883204
Cu	3.80451825	5.18533391	4.21535211
Cu	6.37783680	5.19001811	4.16709471
Cu	-2.58814609	7.37737488	4.17015289
Cu	0.01908255	7.37698957	4.17850957
Cu	2.56102111	7.36143085	4.22808132
Cu	5.09094403	7.36035909	4.20594841
Cu	6.38347068	2.22670525	6.22754359
Cu	8.92123654	2.21977417	6.20443426
Cu	-0.00845966	0.04011790	6.19216900
Cu	3.84325708	2.20639436	6.20858225
Cu	7.65817404	0.05051350	6.19802456
Cu	-1.28545882	6.64238265	6.19213286
Cu	5.09280664	0.03637284	6.19472112
Cu	7.67332179	4.41735575	6.20052588
Cu	3.83961766	6.64958712	6.43292641
Cu	2.56005612	0.02359455	6.20552486
Cu	-0.01540183	4.40955422	6.27667771
Cu	-3.82469830	6.64042470	6.30872459
Cu	5.10878275	4.40073880	6.20074551
Cu	1.25211597	6.67509869	6.34365649
Cu	2.54634765	4.39205164	6.25756673
Cu	1.27123131	2.22207077	6.29071472

Str 6

Free energy from VASP is -328.11066000 eV

PBC	10.223900	10.223900	20.000000	90.000000	90.000000
120.000000					
H	-2.07345270	8.20375820	8.69199961		
H	-3.57537336	7.92828834	8.68693330		
H	3.03641587	5.17032736	9.27982242		
H	0.75080270	4.73369081	10.31761737		
H	2.50453965	3.02133743	10.31755628		

H	0.71064929	6.01211896	9.06909143
H	3.61604715	2.79506930	8.93222817
H	0.05345948	3.27983478	8.62814844
H	1.85157117	1.22932349	8.90959769
H	2.51288714	5.64373659	7.48178230
C	2.28315997	4.52245991	8.80789038
C	0.89369875	4.94241137	9.23858601
C	2.59101532	3.09016557	9.21160765
O	-2.89129674	8.42334123	9.19150062
O	-0.15588489	4.23878962	8.52255328
O	1.61866732	2.17246487	8.65180888
Cu	0.00371059	0.02104433	19.98645617
Cu	2.55978352	0.02014226	19.98796465
Cu	5.11805698	0.02039945	19.97085119
Cu	7.67088411	0.02022887	19.97346835
Cu	-1.27293873	2.23357115	19.97667034
Cu	1.28278296	2.23587839	0.00369692
Cu	3.83600749	2.23392819	-0.01134287
Cu	6.39542005	2.23233536	19.96018383
Cu	-2.54900543	4.44356285	-0.02128855
Cu	0.00742053	4.44333997	0.00800237
Cu	2.55724176	4.44476108	0.01946918
Cu	5.11399964	4.44477903	-0.00911519
Cu	-3.83038214	6.65903951	-0.00961457
Cu	-1.27199510	6.65772569	19.98268953
Cu	1.28416154	6.65568516	20.00065972
Cu	3.83423916	6.65545426	19.99911747
Cu	0.00150643	1.50139602	2.07840448
Cu	2.55925300	1.50532834	2.08772630
Cu	5.12002405	1.49202682	2.04933085
Cu	7.67103818	1.49122663	2.04813478
Cu	-1.26543598	3.70150931	2.08093278
Cu	1.28242368	3.70363445	2.11829846
Cu	3.82919484	3.70280078	2.09484713
Cu	6.39387638	3.70186060	2.05121117
Cu	-2.54394495	5.90895929	2.05932203
Cu	0.01068773	5.91306938	2.08988416
Cu	2.55134545	5.91377717	2.10672562
Cu	5.10507558	5.91194511	2.07630602
Cu	-3.83558349	8.13875413	2.06528364
Cu	-1.26918196	8.13081868	2.05314975
Cu	1.28204886	8.13097516	2.06414895
Cu	3.83440746	8.12935396	2.06228872
Cu	1.27759408	0.76098284	4.15534451

Cu	3.84345615	0.74507972	4.11760977
Cu	6.39447005	0.74689706	4.13129447
Cu	8.94581720	0.74106976	4.12550936
Cu	0.01611989	2.96464814	4.21499844
Cu	2.54906449	2.98609885	4.24474681
Cu	5.11887099	2.96196274	4.12840000
Cu	7.67063641	2.95960115	4.12982380
Cu	-1.26122829	5.16279635	4.17140739
Cu	1.27651726	5.15966570	4.24329041
Cu	3.81206888	5.16413973	4.20359142
Cu	6.39091651	5.17303253	4.12189530
Cu	-2.55570373	7.38115356	4.10479571
Cu	0.01488153	7.38060269	4.14924205
Cu	2.55814031	7.38165211	4.15820708
Cu	5.09863105	7.37617682	4.14279939
Cu	3.87895865	2.19419234	6.19090154
Cu	-3.84232517	6.63809687	6.19836107
Cu	3.82080899	6.63878074	6.28893292
Cu	5.11793064	-0.00327163	6.21989798
Cu	8.91748755	2.17754609	6.19177868
Cu	7.66585564	0.00485177	6.22065697
Cu	-0.01201676	-0.02231824	6.20284080
Cu	6.39495748	2.20603478	6.21610165
Cu	2.57186384	-0.02216995	6.16308632
Cu	7.63722752	4.42536142	6.20360778
Cu	5.13537352	4.41478354	6.20951471
Cu	-0.06110666	4.41827623	6.33505877
Cu	1.29621487	2.17461467	6.32486201
Cu	-1.28445405	6.65957329	6.20030347
Cu	1.29340565	6.66829290	6.26821157
Cu	2.55262089	4.40042482	6.48434394

Str 7

Free energy from VASP is -329.56968300 eV

PBC	10.223900	10.223900	20.000000	90.000000	90.000000
120.000000					
H	6.25747729	2.12189376	8.49776367		
H	0.66700409	5.15485173	8.86149619		
H	6.23494419	1.74647777	10.22417389		
H	4.19774468	2.99963794	9.58108115		
H	8.48429008	2.48193202	9.44002223		
H	5.17573282	3.98403633	10.70108226		
H	7.83986771	3.54638426	10.72527046		

H	-0.12520029	6.46111332	8.81798965
H	-1.54797835	4.83587061	9.00836132
H	6.05186917	4.97237590	8.72696502
C	6.32591600	2.57943106	9.50731520
C	5.15137545	3.53227952	9.69327951
C	7.69483818	3.21476832	9.68245265
O	-0.05000860	5.63014387	9.33478302
O	5.13643670	4.60299892	8.71246973
O	-2.41325618	4.37166364	8.81357812
Cu	-5.11146824	8.85345592	19.99470598
Cu	2.55384040	0.00007768	19.99650122
Cu	5.11185002	0.00237968	19.99979659
Cu	7.66926840	0.00176614	19.99908633
Cu	8.94504204	2.21417733	0.00010223
Cu	1.27794870	2.21190502	19.99408096
Cu	3.83479246	2.21606654	0.00520495
Cu	6.38974416	2.21862320	0.01245909
Cu	7.66367195	4.42619973	0.01444242
Cu	-0.00238439	4.42497060	19.99788380
Cu	2.55962429	4.42593989	0.00170530
Cu	5.11461431	4.42706238	0.02025891
Cu	6.38819382	6.63629069	0.01448649
Cu	-1.28310754	6.63713461	0.00543438
Cu	1.27911500	6.63768833	0.00287734
Cu	3.83912655	6.63682209	0.00917289
Cu	0.00078265	1.47275644	2.07527069
Cu	2.55481741	1.47438659	2.07866645
Cu	5.11072043	1.48343453	2.09150777
Cu	7.66832404	1.48094448	2.08790271
Cu	-1.28167917	3.68649701	2.08764252
Cu	1.27826055	3.68635513	2.06890656
Cu	3.83609747	3.68970568	2.10017108
Cu	6.38857422	3.69122251	2.12015992
Cu	-2.56810062	5.89185073	2.11098742
Cu	-0.00933725	5.89525530	2.07790959
Cu	2.56801983	5.89519760	2.08708897
Cu	5.11929909	5.89223898	2.12167260
Cu	-3.83669964	8.11578293	2.07919611
Cu	-1.28055675	8.11463235	2.06981804
Cu	1.27983844	8.11366225	2.06985129
Cu	3.83639227	8.11288412	2.07466567
Cu	1.27741025	0.73316420	4.16061144
Cu	3.83171935	0.72881634	4.15088514
Cu	6.38771006	0.72764276	4.14746429

Cu	8.94650538	0.72770755	4.14848249
Cu	0.00379575	2.94470901	4.14599017
Cu	2.54790464	2.94699975	4.15506510
Cu	5.10280410	2.95956234	4.20057833
Cu	7.67144782	2.95406519	4.18788359
Cu	-1.29412755	5.15115344	4.18042822
Cu	1.27829299	5.16143493	4.13605071
Cu	3.84742075	5.14972162	4.21212254
Cu	6.38494184	5.13494219	4.26358761
Cu	-2.56030734	7.37597747	4.14916895
Cu	-0.00226404	7.37074811	4.13458061
Cu	2.55908658	7.36964350	4.14566278
Cu	5.11149958	7.37418071	4.16204972
Cu	-1.26065593	2.18525810	6.21485019
Cu	0.01237644	4.41576700	6.20905601
Cu	3.80682663	2.18502115	6.22205479
Cu	-2.53572084	4.39978689	6.36671014
Cu	2.52585927	4.41553289	6.23660549
Cu	3.82473201	6.64851370	6.23889449
Cu	5.07674249	4.40169845	6.41537159
Cu	-0.00540087	8.83439037	6.23095010
Cu	-3.83014654	6.65928741	6.22966147
Cu	-1.27667510	6.64587552	6.21132072
Cu	5.11097849	8.84651772	6.24515945
Cu	1.27413935	6.63497366	6.21318186
Cu	-2.55829939	8.84548176	6.24603999
Cu	2.55407145	8.84046758	6.22717588
Cu	6.38442212	2.17862385	6.20825519
Cu	1.27215608	2.20148085	6.24813154