

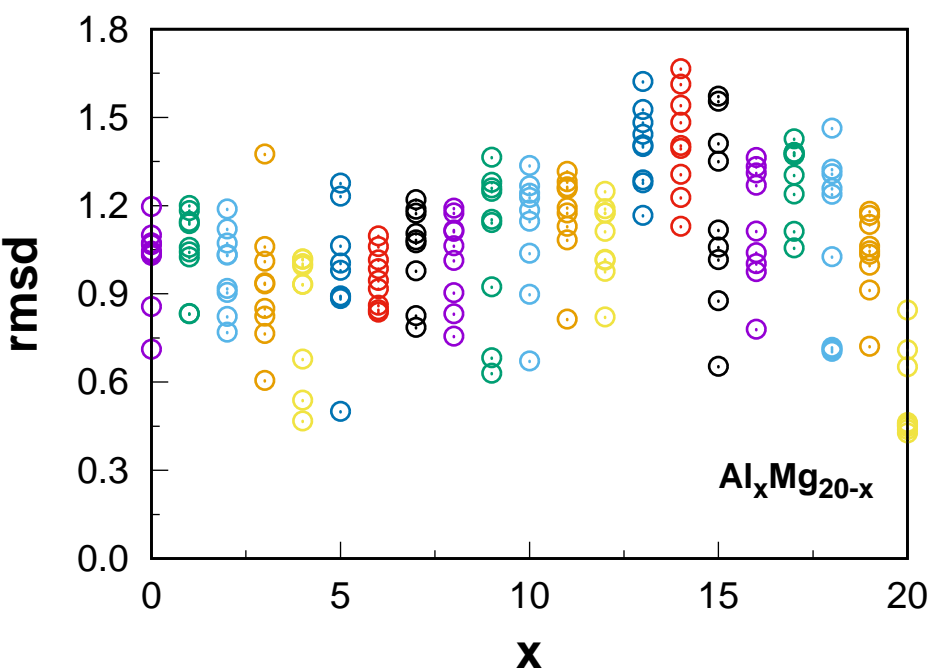
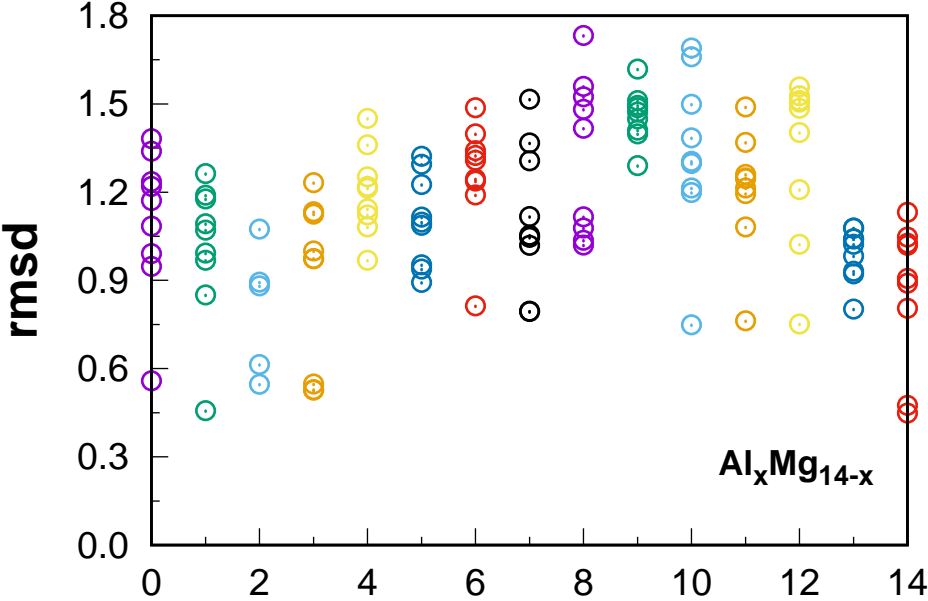
A Method for Predicting Basins in the Global Optimization of Nanoclusters With Applications to Al_xCu_y nanoclusters

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Supporting Information

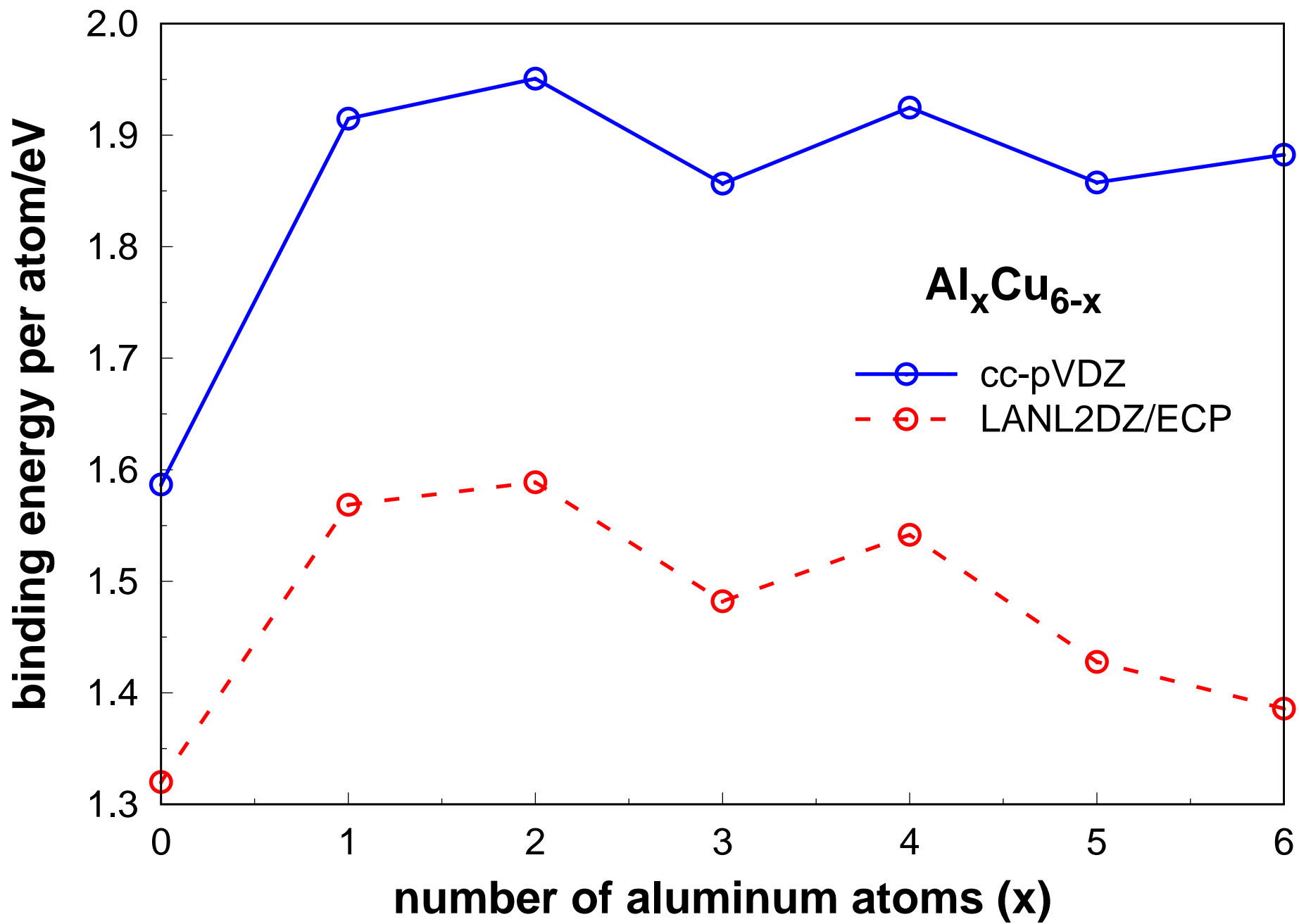
Part I

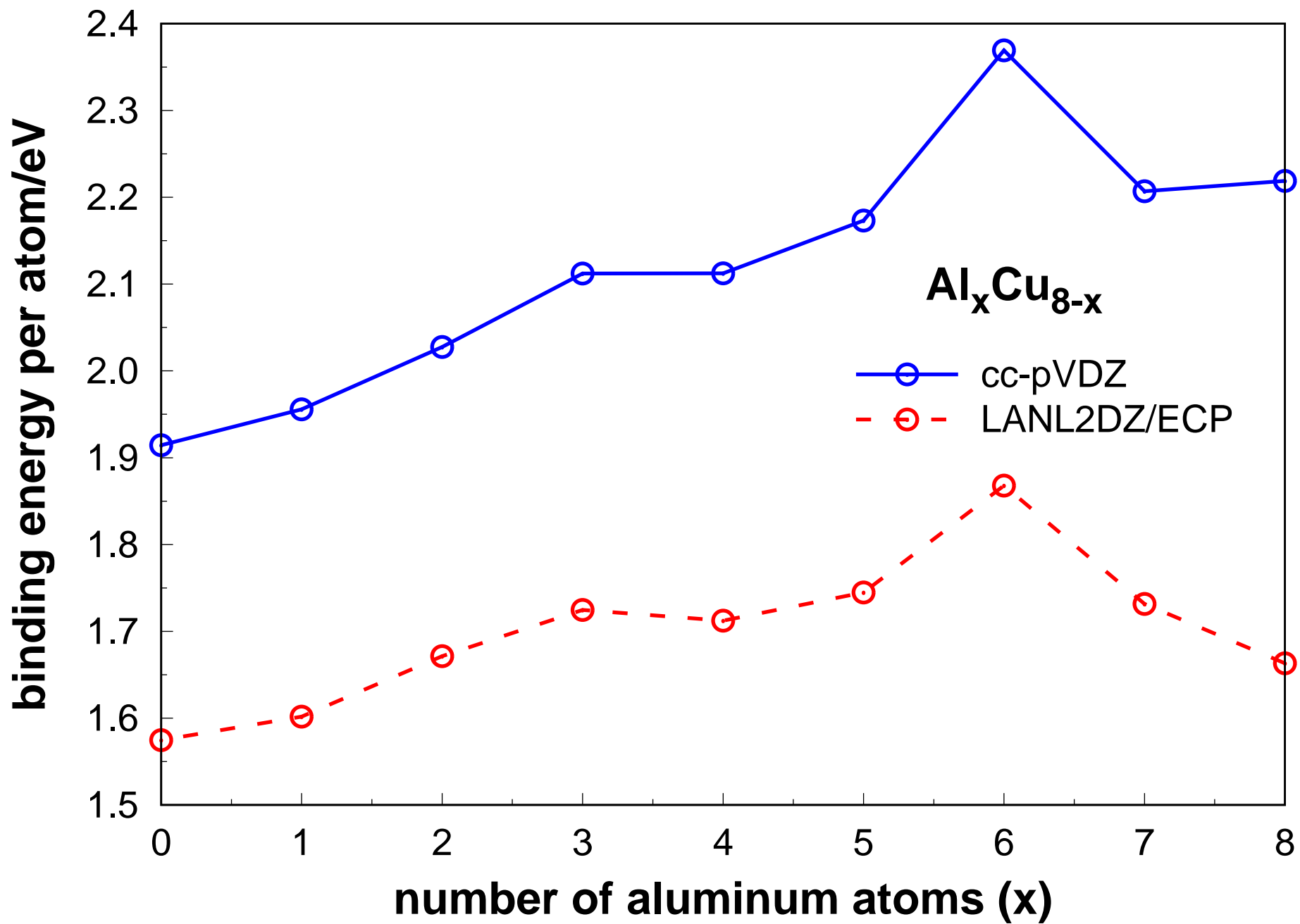
Dissimilarity between the structure of the global minima of for several Al_xMg_y clusters with the nine lowest energy isomers using the Gupta potential.

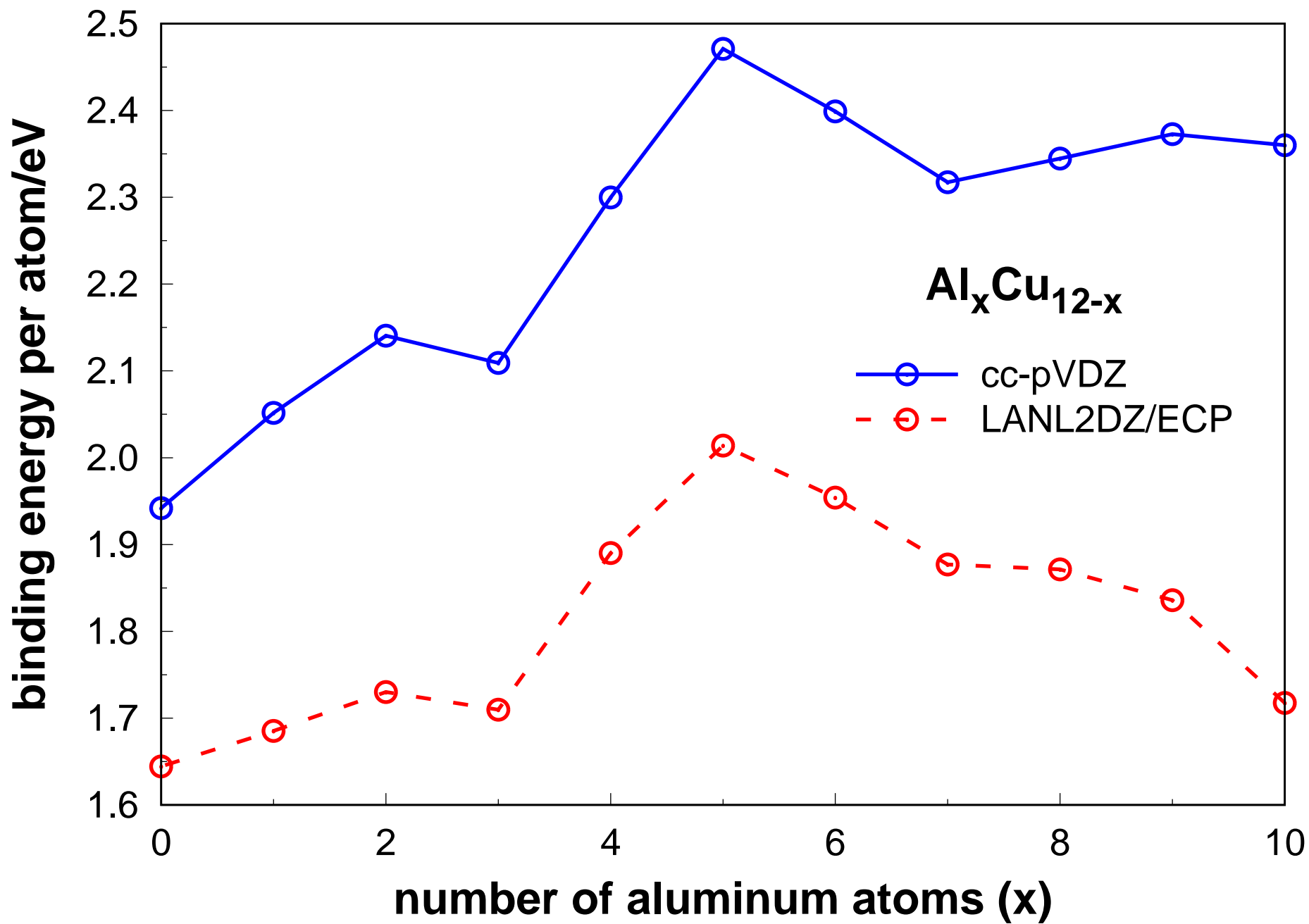


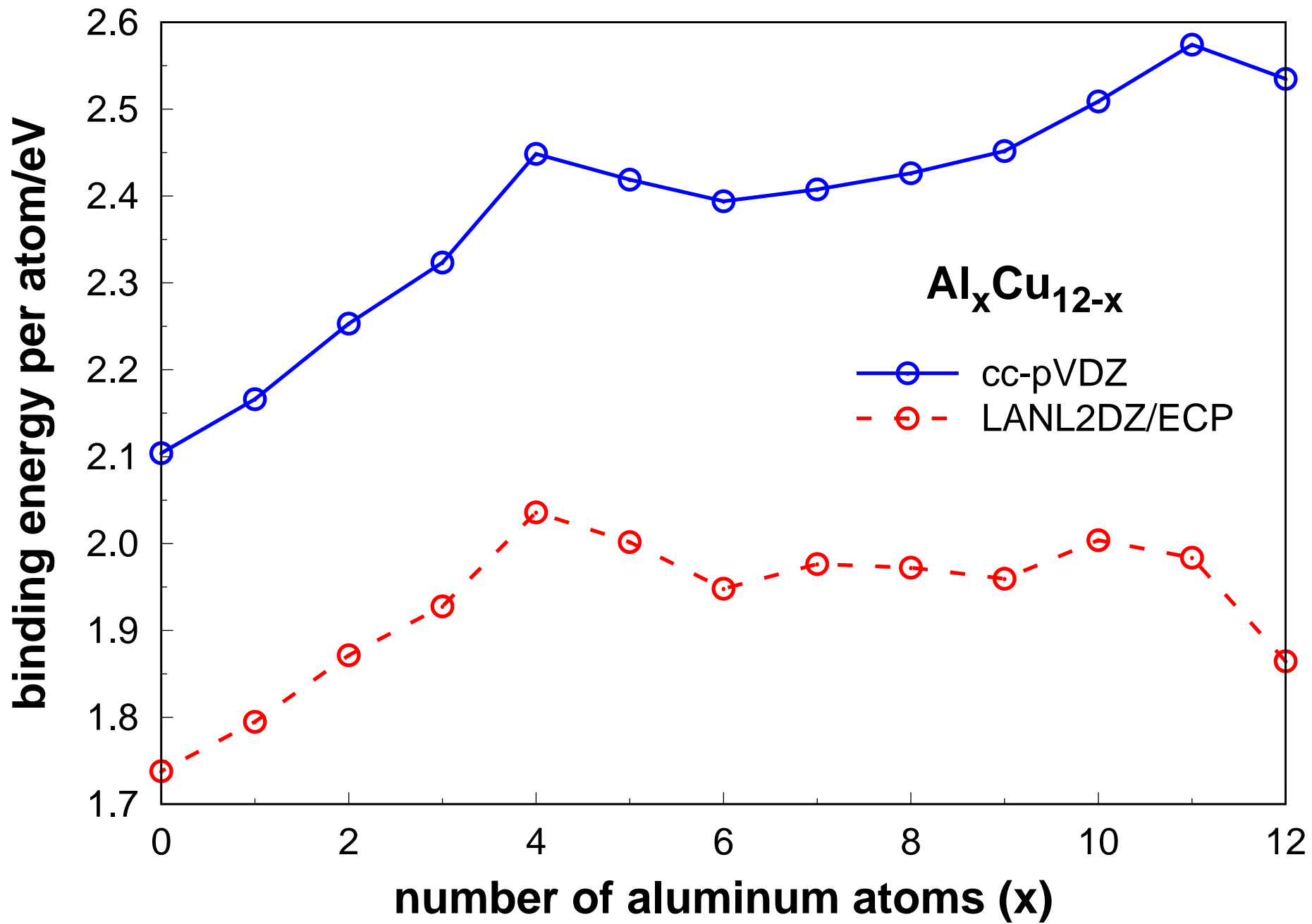
Part II

Comparisons between cc-pVDZ and LANL2DZ/ECP results









Part III

Cartesian coordinates for the putative global minimum
for each composition at the MP2/cc-pVDZ level

6

Cu	0.26608086	2.30009151	1.48789632
Cu	0.75391382	1.07416248	-0.49732512
Cu	-1.47927356	-2.10622978	0.97495830
Cu	1.21188128	-0.19325106	-2.46353674
Cu	-0.62377721	0.10121373	1.25306940
Cu	-0.12882532	-1.17598689	-0.75506216

6

Al	-0.92638677	-1.15556276	-0.52872384
Cu	0.92931980	1.15922177	0.53040832
Cu	-0.65469038	-0.23898987	1.66568542
Cu	-1.30504131	1.20042777	-0.34070742
Cu	0.65321314	0.23714833	-1.66651833
Cu	1.30358553	-1.20224535	0.33985576

6

Al	-1.17059100	-1.39822185	-0.65315461
Al	1.17054987	1.39813590	0.65301806
Cu	-0.60396910	-0.22101256	1.55564988
Cu	-1.19717407	1.14352131	-0.30231619
Cu	0.60394228	0.22101052	-1.55558121
Cu	1.19724202	-1.14343333	0.30238414

6

Al	-1.20528626	-1.72209847	0.11609134
Al	1.20116186	1.60852623	0.63951606
Al	0.01417178	0.36284417	-2.40393233
Cu	-0.98936152	0.72263551	-0.04401124
Cu	0.99215722	-0.67767614	-0.24367431
Cu	-0.01284293	-0.29423138	1.93601048

6

Al	-1.08678794	-1.34830952	-0.36861148
Al	0.77966577	2.05712485	-0.75445426
Al	0.14880264	-0.06962460	-2.31988740
Al	-0.37987086	1.03483200	1.38555408
Cu	1.12817371	-0.39326575	0.07965862
Cu	-0.58998322	-1.28075695	1.97774053

6

Al	-0.55830479	-1.93511868	0.80409855
Al	0.76067066	1.46685123	-0.22486196
Al	1.02976549	-0.07045092	1.90722299

Al	-1.78103030	1.98804116	-0.79645747
Al	-0.86578637	-0.44287574	-1.35464227
Cu	1.41468525	-1.00644708	-0.33535981

6

Al	-0.17298934	-1.52394736	-1.56574869
Al	-1.05833459	1.01654136	-1.46588767
Al	1.32516527	0.63106656	-0.64857018
Al	1.09225941	-1.70185506	0.84535927
Al	0.65892559	0.77491367	1.80765355
Al	-1.84502637	0.80328077	1.02719378

8

Cu	-0.01948599	-1.34093034	-1.82295299
Cu	0.23887071	-1.52130282	0.55526662
Cu	-0.14206044	1.56229639	0.46771640
Cu	-1.08516681	-0.07772847	1.98428261
Cu	1.43706369	0.22673857	1.73338962
Cu	-1.58344471	-0.20580836	-0.35871598
Cu	-0.33240321	1.19192672	-1.89486134
Cu	1.48662686	0.16480826	-0.66412497

8

Al	0.42755231	0.31573814	1.54249895
Cu	1.61455727	0.35833770	-0.57820195
Cu	-1.50710928	1.65164042	2.08441973
Cu	-0.41968000	-0.33359617	-1.57849967
Cu	-0.47388500	1.70613420	-0.20586360
Cu	-1.66731644	-0.32496071	0.54067022
Cu	0.40830061	-1.69458485	0.17639220
Cu	1.61758053	-1.67870879	-1.98141587

8

Al	0.52045238	0.62582356	1.76885343
Al	-0.52044320	-0.62575012	-1.76889372
Cu	-1.05898750	1.31670451	-0.14708464
Cu	1.87403095	-1.00506330	-2.14272714
Cu	-1.27588952	-0.87849492	0.69337589
Cu	-1.87402189	1.00499046	2.14276528
Cu	1.05905092	-1.31665444	0.14722653
Cu	1.27580798	0.87844414	-0.69351566

8

Al	-1.39061511	0.14568684	-1.96189606
Al	-0.56399518	-1.54022825	1.76459479

Al	1.95461142	1.39447689	0.19729219
Cu	-0.64467949	0.83005100	0.51842731
Cu	0.64469421	-0.82996595	-0.51839304
Cu	0.54178840	1.47952127	-1.69510484
Cu	1.33581185	-0.13995296	1.88461959
Cu	-1.87761617	-1.33958876	-0.18954006

8

Al	-1.36244869	0.18581317	-1.19237518
Al	1.49775290	1.16422260	1.60715818
Al	0.98118740	-1.41876602	0.58055907
Al	-0.38013247	2.44999671	0.18642920
Cu	0.29828674	-1.50821590	-1.75927174
Cu	-1.35324192	-1.90334368	0.06626628
Cu	-0.82390845	0.27979085	1.34225905
Cu	1.14250457	0.75050241	-0.83102494

8

Al	-1.46914160	-0.63508999	-1.12778509
Al	2.05751181	-0.66977203	0.76157522
Al	0.83281916	1.65726078	1.10182631
Al	-0.58627439	1.98000681	-1.20679224
Al	-0.66035444	-1.26950216	1.43200278
Cu	0.95580834	0.17451216	-1.23682380
Cu	-1.56761885	0.93987954	0.79455179
Cu	0.43724987	-2.17729521	-0.51855499

8

Al	-1.54993629	-0.65375817	-0.96593595
Al	2.04308057	-0.52923107	0.55851877
Al	0.63802207	1.53328001	1.41713560
Al	-0.32428467	1.89684582	-1.03102851
Al	-0.56237930	-1.02695596	1.54656446
Al	1.08076262	-0.16566017	-1.88963187
Cu	-1.70953190	1.00947332	0.82193261
Cu	0.38426694	-2.06399369	-0.45755500

8

Al	1.01655746	0.23709741	1.72683692
Al	-0.20303346	2.00351167	0.14635752
Al	-0.88925701	-0.21002720	-1.79950130
Al	1.33400917	1.22889948	-1.86782062
Al	2.53359699	-0.51030374	-0.31216621
Al	0.33016258	-1.97750962	-0.21986325
Al	-3.05998707	-0.57529718	1.72731304

Cu -1.06204867 -0.19637081 0.59884393
8

Al -1.16380835 -1.38004684 -2.02961588
Al 1.87084901 -0.03983984 -0.20877476
Al 1.16412699 1.37975538 2.02964854
Al -0.07369684 1.84388351 -0.37396467
Al -0.62691981 -0.41751444 2.61028218
Al 0.62658787 0.41785905 -2.61031079
Al -1.87087846 0.03974741 0.20847578
Al 0.07373958 -1.84384429 0.37425971

10

Cu 0.5843291862 -3.0066086526 -0.3591883539
Cu -1.0197060520 -0.1526192492 1.8765705011
Cu 0.3603985295 1.1923789007 -1.5688363055
Cu -0.5093097916 -0.8340443713 -0.3991215616
Cu -0.0238029393 3.2265224578 -0.0785957629
Cu -2.7760411735 -0.6685817419 0.1261628287
Cu 1.0342244744 -1.3811315258 1.3631242639
Cu 1.7166611319 -0.7856652524 -0.9256788609
Cu -1.4718525112 1.3699882819 -0.0097119659
Cu 0.8278701456 0.9923483629 0.7517823970

10

Al -2.09473538 0.39971626 -0.97495836
Cu -1.41736984 0.53449738 1.37180805
Cu 0.34134200 1.01429868 -0.18418658
Cu 0.53718865 1.92977726 2.06015754
Cu 2.58451557 0.92315394 0.97039998
Cu 0.00719866 -0.32417354 -2.17738724
Cu 0.78396553 -0.45653853 1.68315220
Cu -0.60076940 -1.40821505 -0.11765883
Cu -1.95406044 -1.74926400 -2.14157033
Cu 1.81272471 -0.86325246 -0.48975646

10

Al 1.55353856 0.57427377 1.17113698
Al -1.55286312 -0.57598269 -1.16976833
Cu 0.23839350 -1.52936709 0.90187138
Cu -0.24077478 1.52880371 -0.90414524
Cu 0.40372458 2.65323091 1.10739315
Cu -2.13338470 -1.81127954 0.77590162
Cu 2.13044405 1.81339788 -0.77320451
Cu 1.05889106 -0.51341259 -1.14987731

Cu	-1.05672288	0.51448107	1.15076864
Cu	-0.40124607	-2.65414548	-1.11007619

Al	1.32010090	1.94978023	0.52286470
Al	0.50261283	-0.28524470	-1.00262713
Al	-1.23979974	1.92682230	-0.75391692
Cu	-0.58748436	0.07010382	1.17671120
Cu	1.67470503	0.10598356	2.11316800
Cu	-2.69666767	0.06666246	-0.06708702
Cu	-1.54605234	-0.07193798	-2.21129227
Cu	-1.19063115	-1.87438262	-0.40419886
Cu	2.69725561	-0.03376692	-0.09494465
Cu	1.06596088	-1.85402000	0.72132319

Al	1.85022664	0.74620253	-0.91184449
Al	-1.60225201	1.17961264	0.92360693
Al	1.12454414	0.82485211	1.92052162
Al	-0.50609761	-1.82235181	-0.52170891
Cu	-0.66365266	-0.90700638	1.74939871
Cu	-2.54830384	-0.64754182	-0.23203312
Cu	1.06185400	-1.10074854	-2.15127969
Cu	-0.68146718	0.57611787	-1.41782677
Cu	0.34932062	2.34400463	0.10361192
Cu	1.61582792	-1.19314122	0.53755391

Al	2.04637170	-0.75428504	-0.55378109
Al	-0.17942883	1.17980850	2.23270178
Al	-1.90675259	-0.16373211	-1.18353021
Al	-0.33736023	-2.22447705	0.03159187
Al	0.47696894	1.30647802	-1.76885581
Cu	1.44103491	1.37228024	0.46613586
Cu	0.92582250	-0.86187148	1.60530865
Cu	-1.06024361	1.74591827	0.06767239
Cu	0.16909310	-1.11191082	-2.10411811
Cu	-1.57550609	-0.48820883	1.20687473

Al	1.35178065	-1.39413095	-1.46010280
Al	-1.24807537	-0.22290690	-1.58993518
Al	-0.05117832	-0.26727343	2.05020618
Al	1.91881740	0.67861074	0.37049171
Al	-0.61707747	-2.33940935	0.21922195

Al	-1.30737078	3.42112827	0.39785111
Cu	-2.09838486	-0.42200527	0.69604945
Cu	-0.44712132	1.24725914	0.17726319
Cu	1.63905311	-1.69900537	0.96495277
Cu	0.85955703	0.99773324	-1.82599843
10			

Al	-2.10819912	-1.55826735	0.78562593
Al	0.62384278	-1.65696228	0.97041893
Al	2.39325094	1.71474862	-1.32783592
Al	-1.78697240	1.37124622	0.93742830
Al	1.27341425	-2.23201394	-2.09630942
Al	-1.32615101	-0.20386021	-1.38081884
Al	0.90520096	1.06891549	1.33156526
Cu	0.97916973	-0.15681922	-0.85407627
Cu	-0.74048036	-0.28046095	2.47079396
Cu	-0.21307592	1.93347359	-0.83679181
10			

Al	-1.18802464	-1.14823246	0.10120154
Al	1.34040475	1.10417712	1.65763879
Al	-0.05261181	2.41267896	-0.20009081
Al	-2.33188272	1.33194005	0.49568018
Al	1.54917610	-2.28570580	-0.56704432
Al	-0.95684236	0.61292517	-2.23007846
Al	-1.02115893	0.21562909	2.51955175
Al	1.09328604	-1.03907621	-2.85987592
Cu	0.76136696	-1.28126061	1.59765434
Cu	0.80628657	0.07692467	-0.51463711
10			

Al	1.06548798	0.02454537	-2.73237062
Al	2.37379813	-1.01354945	-0.62659454
Al	-2.07216239	-0.47560957	0.35260269
Al	-1.91087174	2.06846619	0.49921396
Al	0.23400435	-1.74285960	1.24130893
Al	-1.33706546	1.02159452	-2.05382538
Al	-0.57682168	0.66951114	2.45867896
Al	0.50653470	0.88787335	-0.04724691
Al	2.02980089	-0.09808662	2.01461005
Cu	-0.31270453	-1.34188545	-1.10637736
10			

Al	2.50787807	-0.71856976	-1.26997077
Al	-2.50734019	0.71771777	1.27144051

Al	2.50828195	1.45319855	0.12428950
Al	-0.00043772	-1.11654210	-0.71792471
Al	-2.50870752	-1.45220840	-0.12571999
Al	-0.71115303	-1.38044858	2.14643717
Al	-1.90347803	0.99783945	-1.54907274
Al	1.90337455	-0.99622691	1.55005431
Al	0.71107751	1.37924838	-2.14709258
Al	0.00050433	1.11599159	0.71755922

12

Cu	-1.1503812542	0.6661041703	-0.6591392420
Cu	0.8185298224	-0.4867369751	0.4768961917
Cu	2.4094264419	-1.2829070220	-1.0812467157
Cu	-1.4474277927	-1.4425102438	0.5134183234
Cu	1.6160682651	0.7322245852	2.3398493054
Cu	-3.1469424551	0.2470119426	0.6504433144
Cu	-2.6409279471	-1.0362781205	-1.5291641050
Cu	1.1366327140	0.7216319619	-1.6015052357
Cu	2.8706664475	0.7659277121	0.2148917593
Cu	0.6594012690	1.9328589145	0.4552511416
Cu	-0.1744091796	-1.3933434965	-1.5619949825
Cu	-0.9506362910	0.5760163013	1.7823003950

12

Al	1.0546110422	-1.8828805248	-0.8917190086
Cu	-0.5537705830	0.9961138415	1.7994487146
Cu	2.7656858857	-1.3618869356	0.7859574336
Cu	2.8149102031	-0.2719075032	-1.4573026310
Cu	-0.9734040667	-0.3332929489	-0.1833268322
Cu	0.3836890652	-1.3634394534	1.4986821104
Cu	1.3965067130	0.5807503521	0.3128605230
Cu	-0.5066814617	2.0394177768	-0.3478322847
Cu	0.4601314700	0.3284237160	-1.9830765133
Cu	-2.1421776435	-0.8825163325	1.7879864372
Cu	-2.0619051838	0.8965628231	-1.8734406535
Cu	-2.6375953505	1.2546551188	0.5517628446

12

Al	-0.93894398	-0.05279230	-2.09053516
Al	1.26508296	1.59206247	1.05809486
Cu	1.56355417	-0.46810037	2.27471662
Cu	-0.91228801	1.49056101	-0.14007160
Cu	1.26923430	-1.32079208	-2.04667926
Cu	2.73694515	-0.22534722	0.04999693
Cu	-2.85294938	1.37054992	1.28101158

Cu	-2.06739378	-0.59472942	0.05042849
Cu	-0.71139240	0.41705033	1.98739874
Cu	0.40575776	-0.87555933	0.17341229
Cu	-0.91794246	-2.31983471	-1.26993179
Cu	1.16033578	0.98693156	-1.32784152

12

AL	0.4312429879	1.8267478784	-1.5653408402
AL	-2.1101176159	-0.6972921063	-0.1159101954
AL	1.6346923634	0.6940960214	0.7398552514
CU	-1.7663724722	1.7146325214	-0.4524255547
CU	-1.1816004149	0.0278626132	-2.2461365107
CU	0.2023358804	2.7105964367	0.6608882499
CU	-0.7200439519	0.5973234972	1.5137780116
CU	1.0785677404	-0.6586195070	2.6749954693
CU	-0.0633118058	-1.6396456414	0.8202769141
CU	2.2979759101	-1.6527971717	0.5743771844
CU	0.9541137897	-0.6167388627	-1.2052519643
CU	-0.7574824112	-2.3061656792	-1.3991060153

12

Al	-0.93107051	0.10576822	-2.26094460
Al	-0.50430763	-2.20577002	0.93290913
Al	2.73895407	-0.23176104	-0.53376293
Al	-0.31907171	1.66728091	1.24928105
Cu	0.81705260	1.18081331	-0.98679245
Cu	-1.63131893	-2.06738281	-1.27830005
Cu	2.17096853	1.70333481	0.94269359
Cu	-1.63172591	-0.10212774	0.14419250
Cu	0.66670734	-1.32293880	-1.04652178
Cu	-1.02065086	-0.36527815	2.48032427
Cu	-1.47284508	2.08362269	-0.90344673
Cu	1.11730814	-0.44556141	1.26036799

12

Al	-1.92659342	1.77290475	0.37705854
Al	-2.21427226	-2.05678415	-1.57525885
Al	0.03561469	-1.68593359	1.57119405
Al	0.53430396	-0.11216693	-2.11647367
Al	2.19937325	1.69883776	1.15928900
Cu	2.52535653	1.18718171	-1.30407548
Cu	0.30581552	1.78310061	-0.54086071
Cu	-1.11675763	-0.33237213	-0.39455312
Cu	-0.03235823	0.80079091	1.70406902
Cu	-2.14200234	-0.35920253	1.75132084

Cu	0.27820918	-2.26270151	-0.82796252
Cu	1.55331087	-0.43365490	0.19625273

12

Al	2.88715410	0.24966444	1.82898903
Al	-1.80333853	1.49062681	1.08265007
Al	-0.94526625	-1.01347089	1.33944249
Al	0.11939318	2.09595633	-0.72899163
Al	-1.27928221	-0.09030364	-2.27394986
Al	1.21142411	-0.24945965	-1.00796735
Cu	3.47356749	-1.19399023	-0.08656589
Cu	-2.65167356	-0.44745702	-0.29078096
Cu	-0.61418927	-1.94601429	-0.85698700
Cu	-2.34304738	1.82207704	-1.23349202
Cu	0.60514551	0.89833397	1.30819416
Cu	1.34011292	-1.61596286	0.91945904

12

Al	-1.63053024	-0.94827944	1.89862835
Al	-0.01446132	3.44555640	-0.29067397
Al	2.49902415	-0.90690744	0.55241132
Al	-0.58748811	1.91909242	1.81875896
Al	-0.85144877	-1.28946590	-2.18496132
Al	0.23204952	-2.39505887	0.24448363
Al	0.17696458	1.58403945	-2.18976188
Cu	-2.07812476	-2.07569051	-0.22296779
Cu	1.29189610	-0.55441546	-1.51441753
Cu	-0.89099115	0.21615385	-0.18789099
Cu	0.63098937	-0.26504388	1.94947171
Cu	1.22212064	1.27001941	0.12691955

12

Al	-1.0929578870	-0.3331804679	1.5012980868
Al	2.6291232426	-1.5512271499	-0.3495952177
Al	-0.3978748304	-2.5106980717	-2.2556882405
Al	0.3830220824	1.7691382939	2.6098444531
Al	2.3475649446	-0.0666498337	2.1375559920
Al	-1.8864004460	-0.5073701423	-1.4888158814
Al	-2.9903291477	1.1190869315	0.3186318563
Al	-0.1213831380	1.7275884162	-1.5345938660
Cu	0.9481799026	-0.4438275261	-1.9525663241
Cu	0.0940445953	-1.7456934503	-0.0112229039
Cu	-0.8531233978	2.1059333147	0.6907277229
Cu	0.9401339095	0.4368997358	0.3344243225

12

Al	0.13036361	-2.64910293	0.55582952
Al	-1.37859535	1.25795734	1.27342272
Al	0.75509238	0.74881369	2.96093273
Al	-0.49884087	2.72439456	-1.07868826
Al	2.12185836	-1.25884640	1.62726605
Al	1.28785706	1.11061978	0.21469857
Al	0.76922232	0.93064684	-2.65306020
Al	-0.89774621	-1.13256836	-2.46631384
Al	-2.34120703	0.85023743	-1.44848919
Cu	-0.65820122	-1.03983414	2.21648526
Cu	1.44546688	-1.00753212	-1.02829421
Cu	-0.73526990	-0.53478563	-0.17378893
12			

Al	2.20932198	-1.82121277	-0.87652600
Al	0.34425956	-1.85269260	1.26309776
Al	-2.38246846	-1.74941254	0.48051241
Al	-2.72576857	0.46673596	-0.90783447
Al	1.96557379	1.95245016	-0.10872941
Al	2.66216564	-0.19317047	1.17060113
Al	-1.65129423	2.00931787	0.96109134
Al	1.80632961	0.39538094	-2.24816751
Al	-1.60256600	-0.12669224	2.43111539
Al	-0.43956321	-1.04077542	-1.43166769
Cu	0.19421153	0.43533039	0.63386440
Cu	-0.38020152	1.52474082	-1.36735725
12			

Al	2.24537802	-0.83073509	-1.29069293
Al	-2.29705596	0.83522904	1.42967415
Al	1.06104958	1.48952210	-2.16254711
Al	2.19724512	1.56750405	0.33723441
Al	0.23470843	1.18532658	2.43686414
Al	0.31426117	-2.69477820	-0.19697559
Al	-0.17086944	-1.29676521	-2.51150584
Al	-2.24535060	-1.70033288	-0.29187492
Al	-0.25375471	2.80740666	0.27423117
Al	-0.94884604	0.51944005	-0.79299903
Al	-0.92921859	-1.44856286	2.10648489
Cu	0.79245299	-0.43325421	0.66210639
12			

Al	-2.47760868	-0.54993868	0.56802613
Al	0.41023988	2.48721480	-0.63934612

AI	1.99583852	-1.34245622	1.39669490
AI	-1.99583745	1.34245944	-1.39669788
AI	2.47761035	0.54993612	-0.56801927
AI	-0.41023827	-2.48721480	0.63934976
AI	0.41260475	0.54534894	-2.50916338
AI	1.37615466	-1.81044030	-1.26260304
AI	1.37236643	1.33184671	1.76307285
AI	-1.37615585	1.81044161	1.26259983
AI	-0.41260877	-0.54534954	2.50916100
AI	-1.37236547	-1.33184814	-1.76307464