

Supporting information

London Dispersion Dominating Diamantane Packing in Helium Nanodroplets

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1. Computations

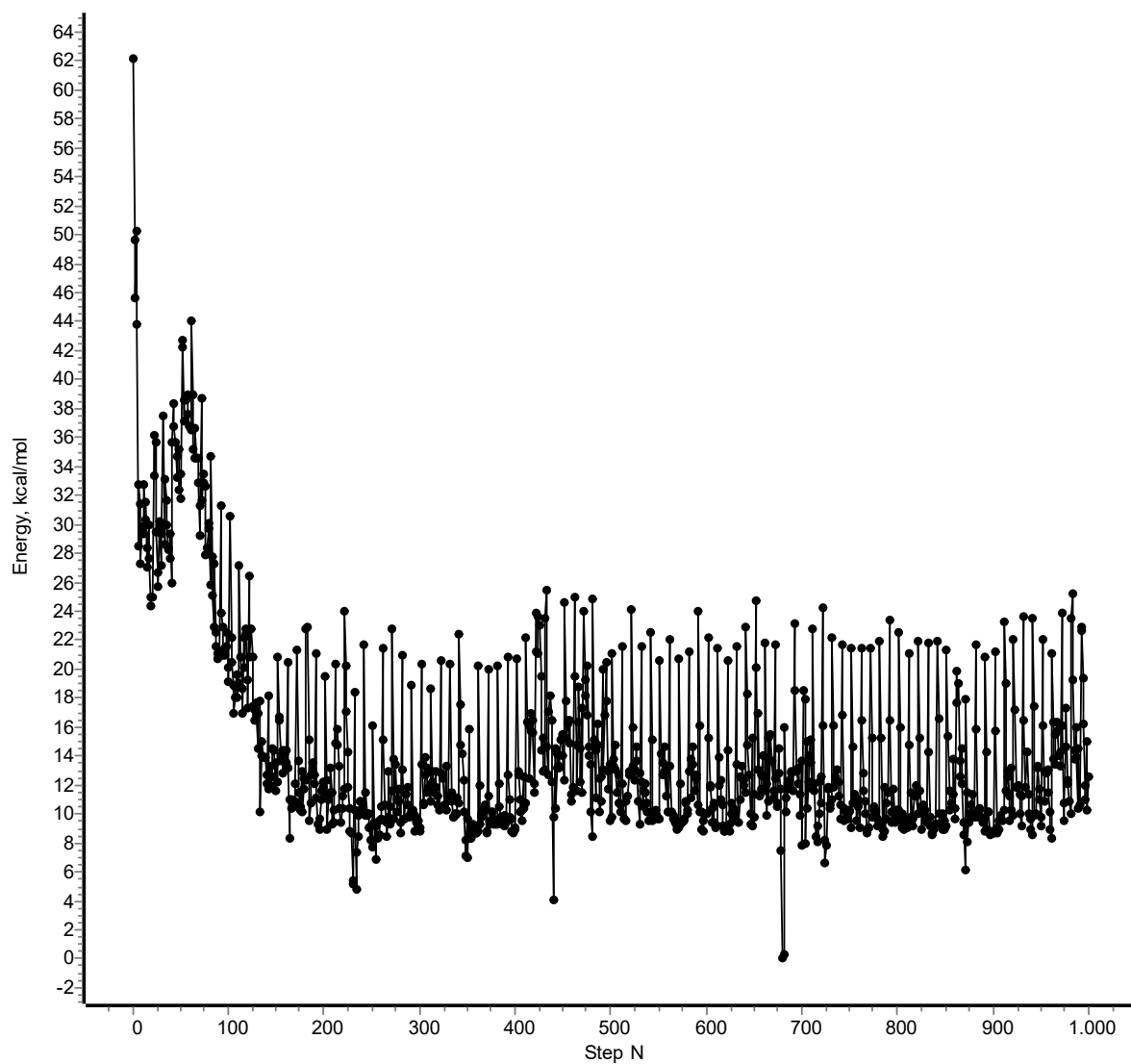


Figure S1. Trajectory from a constrained meta-dynamics (MTD) simulation of **CL2** using the GFN2-xTB method lasting for 100 ps with a timestep of 1 fs at a temperature of 0.4 K.

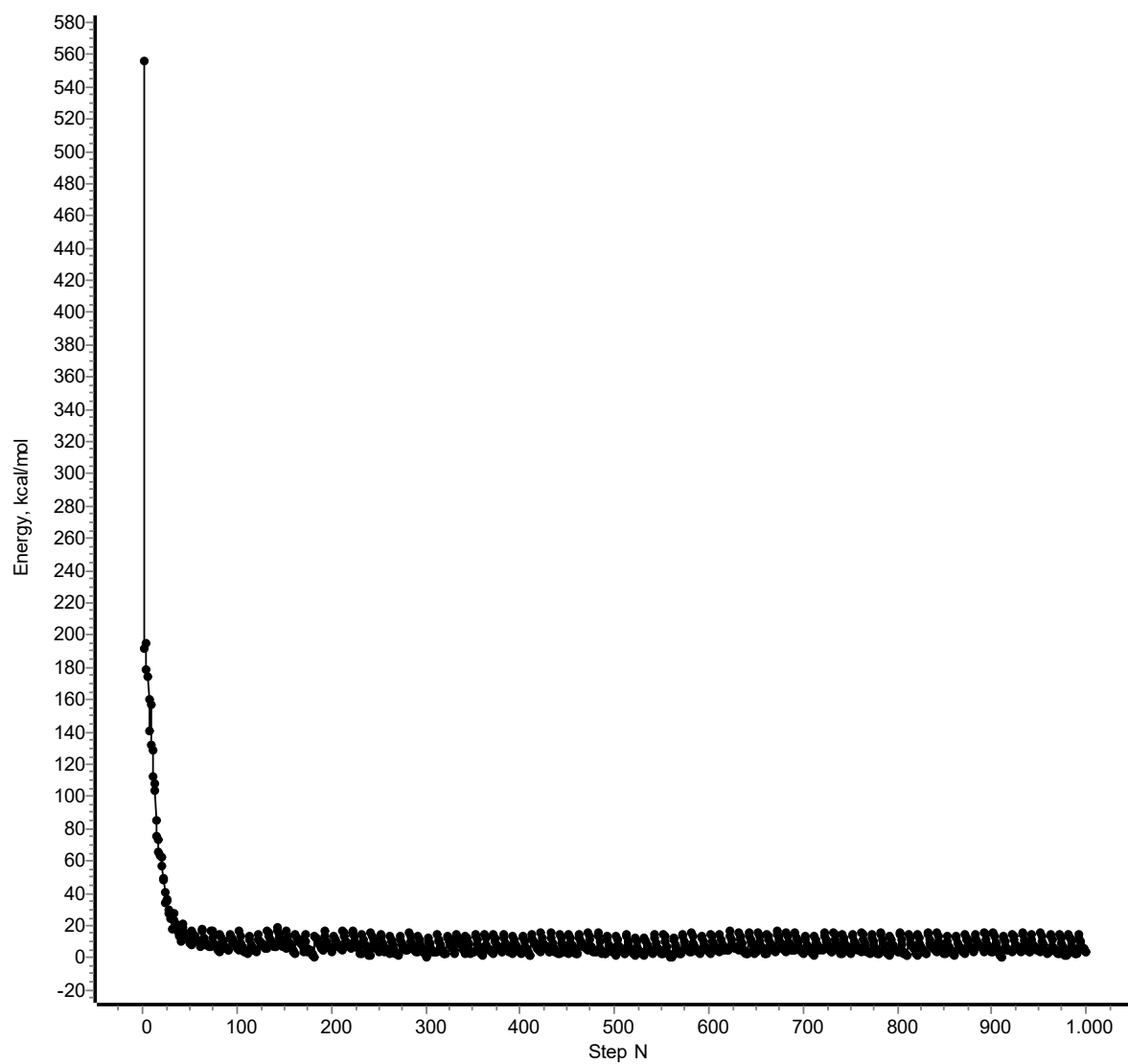


Figure S2. Trajectory from a constrained meta-dynamics (MTD) simulation of **CL13** using the GFN2-xTB method lasting for 100 ps with a timestep of 1 fs at 0.4 K.

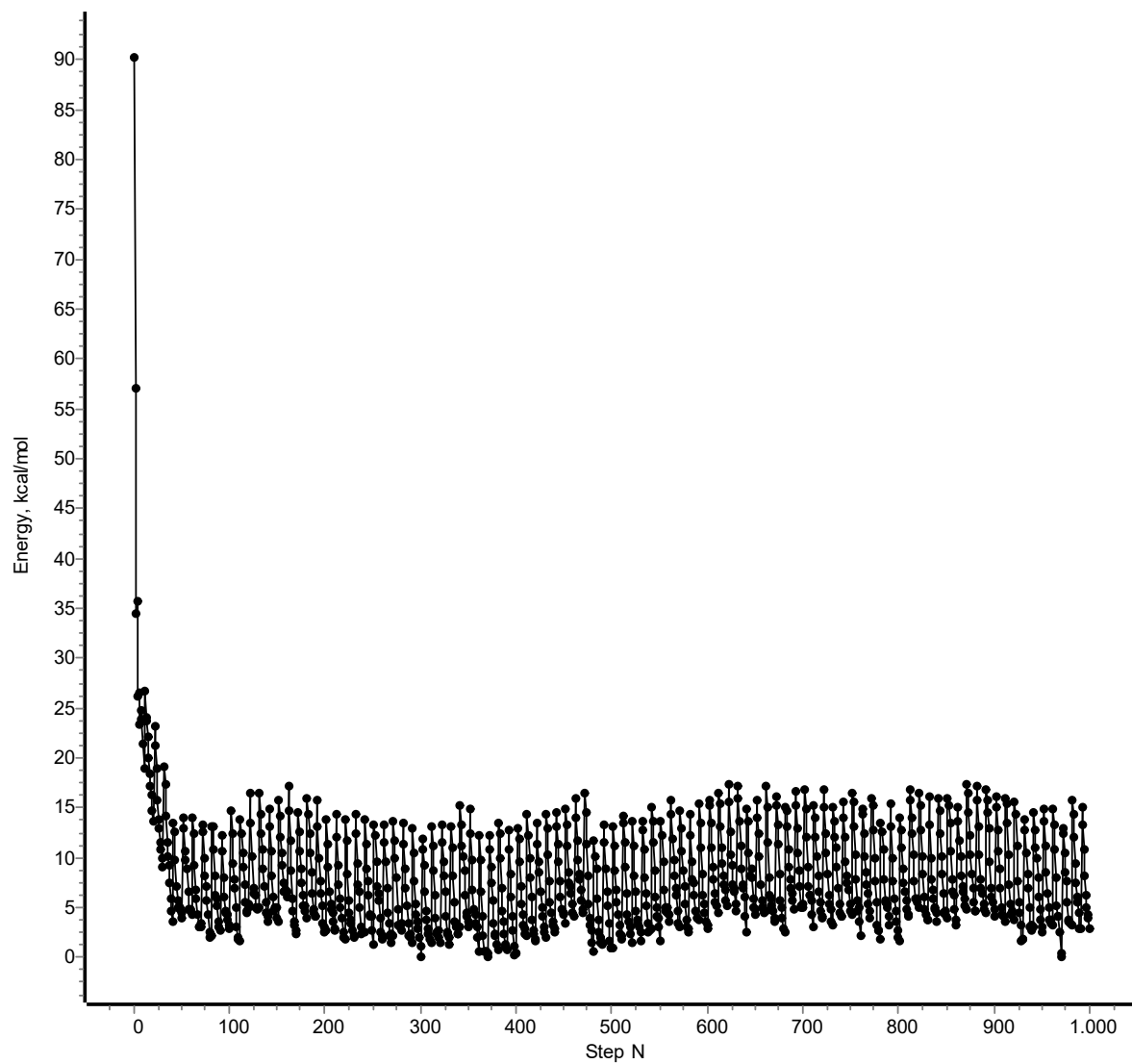
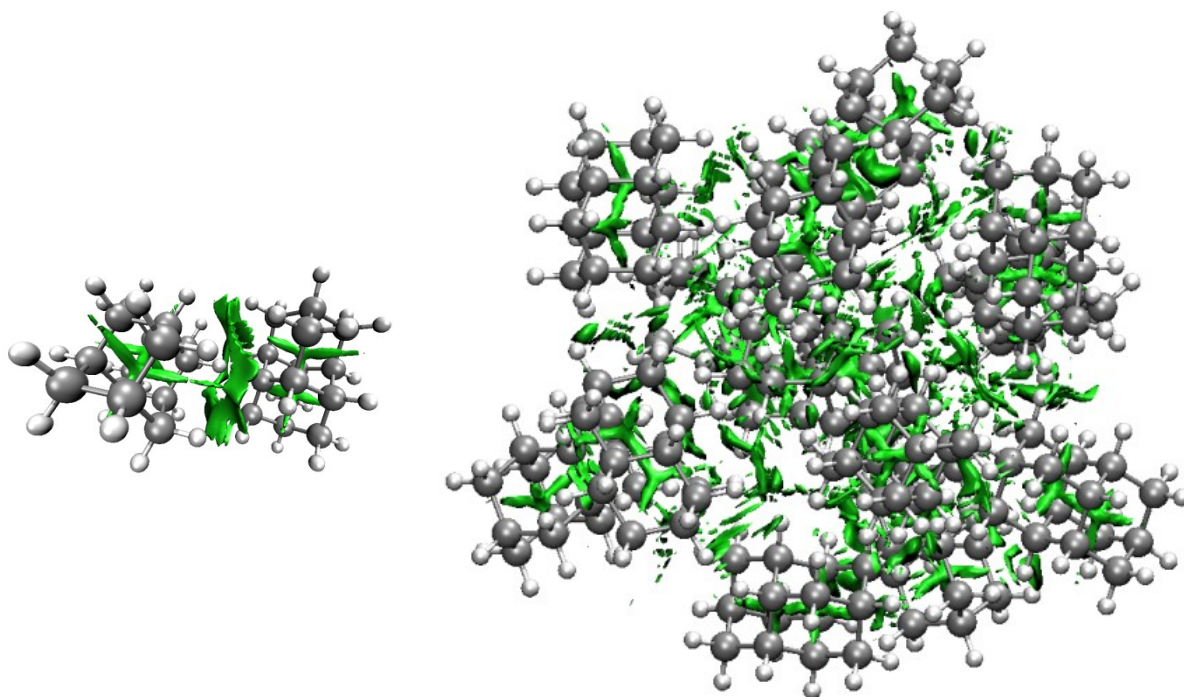
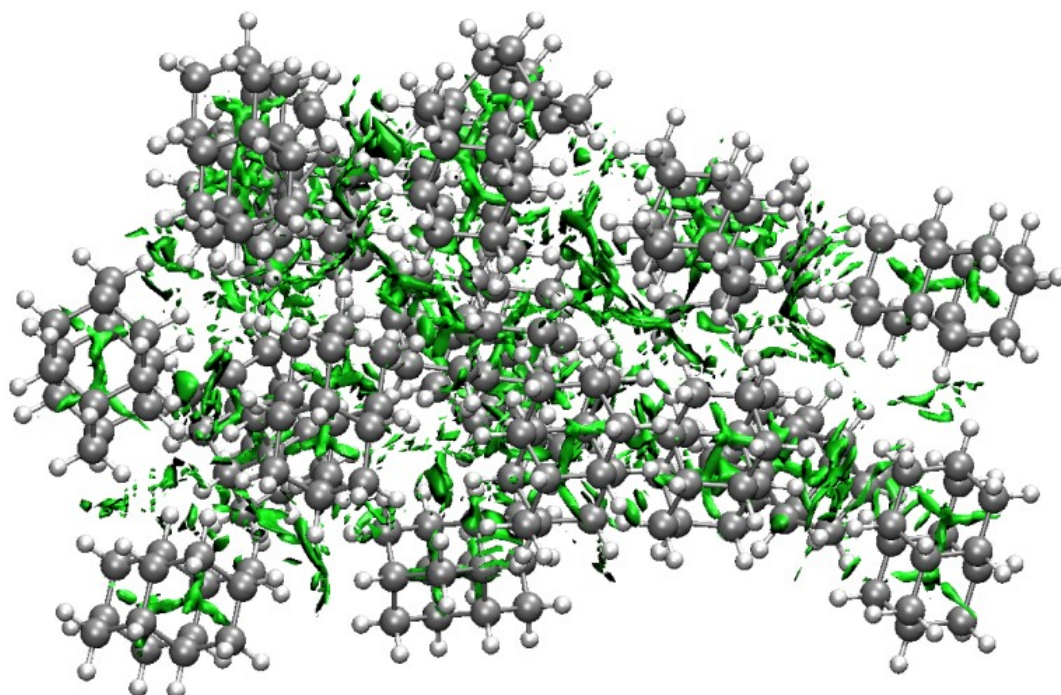


Figure S3. Trajectory from a constrained meta-dynamics (MTD) simulation of **CL19** using the GFN2-xTB method lasting for 100 ps with a timestep of 1 fs at 0.4 K.



a)

b)



c)

Figure S4. NCI plots of **CL2** (a), **CL13** (b) and **CL19** (c). Non-covalent interactions are depicted in green.

Table S1. Electronic energies, zero-point vibrational energies, enthalpies and Gibbs energies of diamantane (**D**), 1-diamantyl cation (**Dp**) and clusters **CL2**, **CL13** and **CL19** in Hartree computed using the GFN2-xTB method at 0.4 K.

compound	<i>E</i>	<i>ZPVE</i>	<i>H</i>	<i>G</i>
D	-40.292908	0.312047	-39.980856	-39.980866
Dp	-39.689966	0.298400	-39.391561	-39.391573
CL2	-79.991445	0.609472	-79.381968	-79.381981
CL13	-523.327286	4.049740	-519.277541	-519.277484
CL19	-765.155096	5.925712	-759.229379	-759.229283

Table S2. Electronic energies of diamantane (**D**), 1-diamantyl cation (**Dp**) and clusters **CL2**, **CL13** and **CL19** in Hartree computed at various levels of theory at 0.4 K.^a

level of theory	D	Dp	CL2	CL13 s.p.	CL19 s.p.
HF-3c	-538.455970	-537.596438	-1076.065555	-6999.239776	-10230.072868
PBEh-3c	-544.416185	-543.524277	-1087.954447	-7076.701972	-10343.290096
B3LYP-gCP-D3(BJ)/def2-TZVPP	-545.439573	-544.561400	-1090.015310	-7090.011461	-10362.742886
B3LYP-gCP-D3(BJ)-ABC/def2-TZVPP	-545.439079	-544.560961	-1090.013829	-7089.990531	-10362.711159
B3LYP-gCP/def2-TZVPP	-545.359585	-544.483153	-1089.844172	n.d.	n.d.
ω B97X-gCP-D3(BJ)/def2-TZVPP	-546.087719	-545.193132	-1091.292373	-7098.415323	-10375.033228
TightPNO-DLPNO-CCSD(T)/cc-pVTZ	-544.570843	-543.679302	-1088.261099	n.d.	n.d.

^a Geometries for **CL13** and **CL19** single point computations from the GFN2-xTB level of theory optimization at 0.4 K.

Table S3. Electronic energies of diamantane (**D**), 1-diamantyl cation (**Dp**) and cluster **CL2** and interaction energies, $\Delta H(0\text{ K})$, for **CL2** computed at various levels of theory with or without the geometrical counterpoise (gCP) correction.^{a,b}

Level of theory	$E(\mathbf{D})$ / Hartree	$E(\mathbf{Dp})$ / Hartree	$E(\mathbf{CL2})$ / Hartree	$\Delta H_{0\text{K}}(\mathbf{CL2})^c$ / kcal mol ⁻¹
B3LYP-gCP-D3(BJ)/def2-TZVPP	-545.439573	-544.561400	-1090.015310	-8.4
B3LYP-D3(BJ)/def2-TZVPP	-545.463886	-544.584505	-1090.064070	-9.5
ωB97X-gCP-D3(BJ)/cc-pVDZ	-545.875011	-544.983341	-1090.867050	-4.8
ωB97X-D3(BJ)/cc-pVDZ	-545.965977	-545.070619	-1091.049375	-7.7
B3LYP-gCP-D3(BJ)/6-31G(d)	-545.173000	-544.302869	-1089.488033	-7.0
B3LYP-gCP-D3(BJ)/6-31+G(d,p)	-545.209420	-544.334072	-1089.554587	-6.3
B3LYP-gCP-D3(BJ)/aug-cc-pVDZ	-545.299474	-544.421622	-1089.739607	-11.0
B3LYP-gCP-D3(BJ)/cc-pVDZ	-545.269196	-544.392380	-1089.677294	-9.2
B3LYP-gCP-D3(BJ)/def2-TZVP	-545.432167	-544.554168	-1090.000545	-8.3
ω B97X-gCP-D3(BJ)/aug-cc-pVDZ	-545.899884	-545.008649	-1090.919261	-6.1
ω B97X-gCP-D3(BJ)/def2-TZVP	-546.081411	-545.186981	-1091.279850	-6.6
ω B97X-gCP-D3(BJ)/def2-TZVPP	-546.087719	-545.193132	-1091.292373	-6.6

^a Interaction energies are defined as a difference between the energy of the cluster and the energy of the corresponding number of diamantane moieties. ^b Single point computations done on optimized geometries obtained by using the B3LYP-D3(BJ)/def2-TZVPP level of theory. ^c *ZPVE* taken from GFN2-xTB computations.

Table S4. Geometries of diamantane (**D**), 1-diamantyl cation (**Dp**) and clusters **CL2**, **CL13** and **CL19** in Cartesian coordinates in Å computed using the GFN2-xTB method at 0.4 K.

D			
1	-6.922650380	-0.687599871	4.116590698
6	-6.677725611	-0.933747254	5.157024171
1	-6.653967466	-3.058765143	4.791389859
6	-7.157481778	-2.354242769	5.464592076
1	-7.540260243	0.407161785	8.209362171
6	-7.036746086	-0.297360114	7.536159587
1	-7.271577855	-1.964002593	8.884161842
6	-7.516502511	-1.717855609	7.843728469
1	-7.124065008	-3.716549219	7.135804875
6	-6.794808065	-2.694480854	6.912099365
1	-7.070163953	1.064946675	5.864947186
6	-7.399420753	0.042878205	6.088652860
1	-9.164020666	0.202731758	4.855624949
6	-8.910339477	-0.055135796	5.886885386
1	-4.775378396	-3.306040713	6.456414908
6	-5.283891506	-2.596462489	7.113880905
1	-9.418857445	0.654440295	6.544351379
1	-5.030205842	-2.854328128	8.145141508
1	-9.002014744	-3.475582663	5.469132712
6	-8.668036277	-2.455852196	5.261876024
1	-4.828486243	0.179249390	5.121288754
6	-5.166631194	-0.833094929	5.356161183
1	-9.365745558	-2.830864648	7.879455369
6	-9.027595453	-1.818520522	7.644586006
1	-5.192206834	0.823987343	7.531609570
6	-5.526190947	-0.195742079	7.738867030
1	-9.537468441	-1.129373558	8.322416745
1	-5.275315220	-0.425788764	8.777369361
1	-8.918916936	-2.225804527	4.223374088
1	-4.656753837	-1.522241971	4.678332269
6	-4.819601035	-1.174909935	6.803686912
6	-9.374627389	-1.476692530	6.197063984
1	-3.735442411	-1.103081688	6.948071898
1	-10.458785986	-1.548520698	6.052678883

Dp			
1	-0.098069070	2.149599953	1.179912168
1	-0.098095734	-2.149541254	1.180016655
1	0.109104533	2.119139261	-1.289351102
1	0.089545733	0.000059807	2.446001576
1	0.109079661	-2.119204746	-1.289246192
1	-2.191033955	-1.274088608	-1.765294424
1	-2.155990224	2.145522986	-0.236064710
1	-2.155356981	-0.880184950	1.947203806
1	2.161974022	2.147860601	0.150652112
1	2.198176185	-1.289318428	1.680727889
1	2.095944644	-0.892843494	-2.026946755
1	-2.156017184	-2.145509570	-0.235961711
1	-2.191020931	1.274030080	-1.765356148
1	-2.155348555	0.880304366	1.947162614
1	2.198193908	1.289374830	1.680665724

1	2.161948506	-2.147879807	0.150756788
1	2.095955785	0.892718027	-2.026991875
6	1.745215842	-0.000047554	-1.512935617
6	1.804663274	1.253112699	0.663329528
6	1.804647307	-1.253102308	0.663389409
6	-1.809630130	1.244727147	-0.743499851
6	-1.790624880	0.000045521	1.416503255
6	-1.809644806	-1.244742090	-0.743438839
6	2.311578637	-0.000014710	-0.037252102
6	-2.313257004	0.000013294	-0.019393731
6	0.282959237	-1.240417601	0.708047202
6	0.319396781	-0.000032443	-1.238334120
6	0.282974901	1.240449016	0.707986337
6	-0.259763066	0.000036289	1.408619555
6	-0.283565287	-1.236938358	-0.780078239
6	-0.283550610	1.236903129	-0.780138546
1	3.401385173	-0.000022981	-0.104005386
1	-3.405472077	0.000020130	-0.008525328

CL2

1	1.370489985	-0.650040867	-6.404975478
1	1.635387689	1.782585310	-6.004025242
1	0.175768379	-1.204258134	-2.338796875
1	0.425318758	1.256181763	-1.934559012
1	1.426666223	2.663458347	-3.697990180
1	0.359143062	-2.075817725	-4.648926779
1	2.821540772	-1.982236356	-4.809876471
1	-0.553921786	2.775320994	-5.186636109
1	2.318202127	-2.196923974	-3.133711563
1	-1.034986814	2.561295139	-3.504809982
1	3.604210929	1.658308760	-4.505279877
1	-1.092928392	-0.752340959	-6.251779255
1	2.884017518	1.343388708	-2.106523562
1	-1.771645359	-1.133228672	-3.899758509
1	2.359781371	-0.244034167	-1.543093920
1	-1.893009762	0.195359851	-2.712535769
1	3.577626503	0.292347841	-5.620029243
1	-0.575908244	0.850907902	-6.778855373
6	-0.564622122	0.151554294	-5.941840882
6	3.065727852	0.746874926	-4.770235069
6	-1.249740259	-0.214373868	-3.620847297
6	2.357193840	0.434087946	-2.399746464
6	-0.538902734	2.076199942	-4.349406360
6	2.320747048	-1.496090201	-3.971181665
6	-1.278726732	0.797945058	-4.742169645
6	3.062795477	-0.218550660	-3.586419636
6	0.164280467	-0.496471129	-3.175219794
6	0.920302559	0.778310543	-2.788779626
6	0.871192771	-0.181980453	-5.550879209
6	1.627711382	1.089344780	-5.156757637
6	0.904497896	1.742756085	-3.976163350
6	0.887404501	-1.156024346	-4.373485625
1	-2.308406942	1.030609991	-5.031285298
1	4.091732513	-0.463844306	-3.309733865
6	-5.137073329	1.667221367	-1.884344105

6	-5.833085207	0.364841568	-1.507172305
6	-4.879785748	-0.508069423	-0.699198363
1	-5.803815329	2.297790396	-2.477374329
1	-6.722243646	0.580620271	-0.913434976
1	-6.160034665	-0.163158937	-2.405065671
1	-5.368197203	-1.450524888	-0.436491159
6	-4.678104267	2.406768698	-0.633155489
6	-3.890778572	1.331617811	-2.743751473
6	-3.620560153	-0.849777961	-1.550915409
6	-4.419665099	0.212487649	0.566990854
6	-3.733910946	1.518602509	0.168973551
1	-4.179723931	3.338914723	-0.906486384
1	-5.542596829	2.666306868	-0.020798412
6	-3.027435260	0.479898411	-1.878430426
1	-4.212349618	0.801883165	-3.641183602
1	-3.396145513	2.259190858	-3.032534527
6	-2.680600043	-1.737943023	-0.736828663
1	-3.949222486	-1.369853890	-2.456077361
6	-3.471210008	-0.673082539	1.374088142
1	-5.295188015	0.445481463	1.180428188
6	-2.471670437	1.174138094	-0.681277668
1	-3.392048880	2.048589771	1.062408737
6	-2.243384438	-1.001784927	0.528070502
1	-3.197813305	-2.660367698	-0.470081761
1	-1.811421123	-2.011073729	-1.337801383
1	-3.168831688	-0.157068378	2.286435560
1	-3.981851567	-1.591747165	1.665988574
6	-1.533729746	0.294600179	0.144736405
1	-1.976573323	2.110454785	-0.957120716
1	-1.561317253	-1.634541939	1.101796781
1	-0.628190921	0.074094290	-0.421495838
1	-1.234565601	0.835281761	1.043718097

CL13

1	-0.274923490	0.474360982	5.393782943
1	-3.405945235	-0.752859755	-7.737089844
1	2.638521151	-3.129784741	-0.820424186
1	4.651346118	-1.432576192	-4.196491617
1	6.117585550	-0.703422513	-0.238979258
1	1.103372244	2.395373106	6.131839500
1	-1.774840325	-0.478774357	-9.584742008
1	2.939631900	-2.970431446	-3.279571385
1	6.412114203	-0.537822195	-2.695537873
1	4.402799647	-2.243630225	0.679000107
1	-3.785483184	2.418546993	6.887041803
1	-0.608997492	0.998037324	-5.008881666
1	-2.410428260	4.338295325	7.621265157
1	1.021600621	1.270335112	-6.855746936
1	0.061829154	4.184370553	7.498009190
1	0.534622668	0.261305897	-9.066652737
1	-2.749029495	0.627176245	5.508588023
1	-2.922852925	0.264800599	-5.531035975
1	-1.542477773	-0.527864597	7.336681946
1	-2.430286124	-2.140959194	-5.880306811
1	2.417852391	-0.844363993	0.209260178

1	2.379331673	-0.568811930	-3.515918560
1	5.029580462	1.166220318	-1.545089030
1	0.292591637	4.537225140	5.056478556
1	-1.114481286	1.940899797	-9.841205401
1	5.202706216	-3.836679965	-3.961091757
1	7.502503048	-2.404485526	-1.394052527
1	4.626454439	-4.536810546	-0.339291717
1	3.852907333	0.161452583	0.444392273
1	1.553121366	-1.280239389	-2.121220825
1	4.424960826	0.860486512	-3.177657640
1	-2.989145003	0.280278753	7.947417830
1	-1.272387285	-1.424616044	-4.751760840
1	-1.158079765	5.334182996	5.672463764
1	0.037508112	2.664679927	-8.716369105
1	6.638274223	-2.836558530	-3.722685544
1	6.676408875	-3.105758729	-0.000305392
1	4.024060778	-4.841188204	-1.971996960
1	0.870930982	2.040432826	8.573471286
1	-0.126646581	-2.163691550	-8.814877394
1	-1.488357390	1.611188286	3.567387429
1	-3.912907185	1.649407940	-7.389534307
1	-1.196756546	3.186600622	9.451210003
1	1.519553847	-1.133612407	-7.205628968
1	-3.569691414	2.761830464	4.443835525
1	-2.261804852	2.684060651	-5.777610043
1	-2.785515237	2.461245573	9.193527979
1	1.045656953	-0.830634366	-5.531745893
1	-3.420796360	4.292197316	5.312158093
1	-0.634580415	3.096789379	-6.334885308
1	0.731811852	0.513519268	7.698306298
1	-1.753042312	-2.579568495	-8.268520912
1	0.100793076	2.351103915	3.818838991
1	-3.434969169	1.342628749	-9.060443551
6	-0.886641308	2.202902328	4.266018688
6	-3.076806721	1.355332386	-8.029169916
6	4.499542628	-4.094813477	-1.330768067
6	5.669024142	-3.104966931	-3.297150717
6	6.524050938	-2.679439639	-0.994666225
6	0.245148310	1.474938199	7.880104516
6	-0.941169840	-1.857084709	-8.155398766
6	2.531103108	-0.998165414	-2.521658055
6	4.553219624	0.419574244	-2.185461647
6	3.386442468	-0.571889242	-0.218295576
6	-2.936004430	3.330621189	5.132612924
6	-1.448332004	2.375849008	-6.440801459
6	-1.798719866	2.607132917	8.748250249
6	0.686003279	-0.839087146	-6.564874627
6	-0.694935026	4.361734531	5.491028039
6	-0.781046635	1.945821862	-8.801475411
6	-1.998581557	0.448614462	7.518748828
6	-1.608463099	-1.425949024	-5.793197715
6	-1.553952650	3.552894505	4.521351804
6	-1.933975363	2.358084849	-7.888626982
6	5.860019294	-3.708538578	-1.907100855
6	-1.138149962	1.254490701	8.489369618

6	-0.457910211	-1.840867033	-6.707454425
6	3.194406261	0.030060994	-1.608194074
6	-2.792561468	2.570898905	6.449205831
6	-0.957785989	0.983103497	-6.050640329
6	5.638516341	-1.439194577	-0.896078403
6	3.617305503	-2.852259168	-1.234350305
6	4.786426251	-1.862852159	-3.196830952
6	-1.933631548	3.369561460	7.431827442
6	0.197160699	0.553932484	-6.958388547
6	5.437955589	-0.822140041	-2.282701248
6	4.270556307	-1.812818501	-0.320550230
6	3.418904447	-2.236519934	-2.621546873
6	-0.751290535	1.442669971	5.583733824
6	-2.583285598	-0.035653351	-7.637106453
6	0.107950817	2.240864215	6.566128180
6	-1.428378262	-0.463114868	-8.545471550
6	-0.555228293	3.599165750	6.807809989
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CL19

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1	-11.123497123	5.684378526	-1.553555084
1	-12.571797987	10.624841087	2.882526120
6	-12.350916572	2.287818731	4.292565230
1	-11.525938755	1.617612613	4.017699740
6	-12.655117749	2.127289844	5.783884216
1	-11.761618387	2.388185745	6.365627525
6	-14.736654691	2.858786567	3.869969379
1	-15.629711560	2.600431164	3.288831099
1	-15.864875999	3.363642503	5.636698722
6	-15.040492886	2.695876277	5.361035222
1	-14.006349599	2.976476473	7.232551070
6	-13.793284723	3.077624975	6.161906399
1	-13.385514561	2.012979467	2.420837646
6	-13.598542478	1.908574105	3.491513527
6	-13.995774215	0.464788550	3.789557545

1	-13.183710166	-0.209386475	3.505171022
6	-13.394303102	4.521206858	5.861859722
1	-12.512270611	4.791900412	6.448193973
1	-14.877402928	0.192934173	3.204071294
1	-14.204777444	5.196214840	6.145683198
1	-13.249159467	0.568032929	7.153169903
6	-13.049958514	0.683452549	6.085251550
6	-11.950896757	3.730158171	3.991521317
1	-11.721940207	3.837375079	2.927116385
6	-15.439350528	1.252412226	5.662347248
1	-15.668048556	1.145188525	6.725240245
1	-14.135450712	4.409054360	2.496106289
6	-14.338011621	4.301196049	3.564873203
1	-16.337937960	0.990855267	5.098659828
1	-15.159139908	4.974834539	3.820616202
1	-12.225026306	0.015545813	5.824857282
1	-11.052294328	3.988297974	4.557991744
6	-13.094230664	4.667498796	4.371783042
6	-14.294726985	0.316873538	5.279769481
1	-12.805746676	5.702562438	4.156131712
1	-14.580766541	-0.719165146	5.495944496

Table S5. Geometries of diamantane (**D**), 1-diamantyl cation (**Dp**) and cluster **CL2** in Cartesian coordinates in Å computed at the B3LYP-D3(BJ)/def2-TZVPP level of theory at 0.4 K.

D			
1	-6.919405000	-0.684186000	4.112531000
6	-6.672461000	-0.929893000	5.150127000
1	-6.649210000	-3.060076000	4.789943000
6	-7.160817000	-2.360836000	5.457925000
1	-7.545116000	0.408312000	8.210649000
6	-7.033480000	-0.290910000	7.542642000
1	-7.274893000	-1.967487000	8.888117000
6	-7.521811000	-1.721773000	7.850513000
1	-7.120843000	-3.721523000	7.137945000
6	-6.788402000	-2.702670000	6.915427000
1	-7.073275000	1.069765000	5.862804000
6	-7.405775000	0.050895000	6.085162000
1	-9.182921000	0.223808000	4.859005000
6	-8.920786000	-0.049895000	5.885330000
1	-4.764508000	-3.308742000	6.454409000
6	-5.273450000	-2.601713000	7.115411000
1	-9.429453000	0.657097000	6.546556000
1	-5.011430000	-2.875362000	8.141775000
1	-9.011449000	-3.483198000	5.458955000
6	-8.675658000	-2.462211000	5.255161000
1	-4.809216000	0.173792000	5.105482000
6	-5.157656000	-0.833076000	5.353750000
1	-9.385017000	-2.825508000	7.895116000
6	-9.036572000	-1.818639000	7.646854000
1	-5.182849000	0.831509000	7.541898000
6	-5.518700000	-0.189522000	7.745506000
1	-9.545687000	-1.126426000	8.323200000
1	-5.263433000	-0.411230000	8.785941000
1	-8.931043000	-2.240631000	4.214730000

1	-4.648547000	-1.525322000	4.677467000
6	-4.804717000	-1.171873000	6.808941000
6	-9.389542000	-1.479740000	6.191702000
1	-3.724204000	-1.097992000	6.954890000
1	-10.470087000	-1.553640000	6.046003000

Dp

1	4.616992000	-0.805307000	-3.878954000
1	6.457157000	-0.880542000	0.023944000
1	3.600035000	-3.008865000	-3.391293000
1	6.311593000	0.151226000	-2.276359000
1	5.406887000	-3.089614000	0.425784000
1	3.038739000	-2.226588000	0.648351000
1	2.360740000	-0.903762000	-2.806440000
1	4.729754000	0.907218000	-0.535416000
1	5.871620000	-2.856135000	-4.507830000
1	8.112632000	-1.651888000	-1.719150000
1	6.033747000	-4.732299000	-1.245392000
1	4.197527000	-0.991054000	1.091856000
1	1.940510000	-2.174939000	-1.676817000
1	3.971995000	0.943105000	-2.115749000
1	7.006583000	-1.601684000	-4.064194000
1	7.702601000	-2.937051000	-0.606422000
1	5.265316000	-4.704433000	-2.864122000
6	5.632767000	-4.103468000	-2.036314000
6	6.225303000	-2.254413000	-3.670056000
6	7.297569000	-2.301151000	-1.394577000
6	2.754068000	-1.524890000	-2.001274000
6	4.368277000	0.274752000	-1.348819000
6	3.819101000	-1.574828000	0.252474000
6	6.808920000	-3.139841000	-2.573007000
6	3.263761000	-0.661321000	-0.843679000
6	6.154209000	-1.448077000	-0.856460000
6	4.686232000	-3.100977000	-1.570016000
6	5.093424000	-1.404979000	-3.103294000
6	5.538953000	-0.536804000	-1.922879000
6	4.960525000	-2.425552000	-0.311676000
6	3.898811000	-2.379562000	-2.555342000
1	7.587780000	-3.798369000	-2.953981000
1	2.440484000	-0.071582000	-0.440365000

CL2

1	-0.996108000	0.145457000	-1.994674000
1	0.776530000	1.889518000	-2.001402000
1	2.004285000	-2.875165000	-1.418604000
1	3.768082000	-1.125488000	-1.410082000
1	3.158916000	1.214310000	-2.001774000
1	-0.380542000	-2.204357000	-1.424296000
1	-0.520726000	-1.591488000	-3.846303000
1	2.111276000	1.828198000	0.171535000
1	0.704863000	-2.818351000	-3.579555000
1	3.333072000	0.587019000	0.400407000
1	1.847248000	1.286219000	-4.161328000
1	-0.832300000	-0.481406000	0.407016000
1	3.627962000	-0.492257000	-3.810973000

1	0.928353000	-2.270359000	0.743377000
1	3.163440000	-2.170295000	-3.581411000
1	2.632175000	-1.847769000	0.754287000
1	0.149617000	0.847005000	-4.182008000
1	-0.344449000	1.194970000	0.164065000
6	-0.066793000	0.157779000	-0.043029000
6	1.113175000	0.611646000	-3.716615000
6	1.670929000	-1.604040000	0.296343000
6	2.866090000	-1.139857000	-3.370952000
6	2.353936000	0.783625000	-0.042154000
6	0.449945000	-1.774947000	-3.380195000
6	1.303979000	-0.142722000	0.581882000
6	1.499253000	-0.846949000	-4.000152000
6	1.739427000	-1.833989000	-1.215800000
6	2.794381000	-0.911278000	-1.858413000
6	0.001119000	-0.079240000	-1.553133000
6	1.042435000	0.847140000	-2.204668000
6	2.414329000	0.551163000	-1.554218000
6	0.368719000	-1.540355000	-1.867186000
1	1.254993000	0.027062000	1.658990000
1	1.545004000	-1.014892000	-5.077956000
6	-4.690910000	-0.913296000	-3.807075000
6	-5.615556000	-0.717173000	-2.609384000
6	-5.252860000	0.575511000	-1.885009000
1	-4.895717000	-1.849796000	-4.324507000
1	-6.651929000	-0.669036000	-2.949440000
1	-5.549458000	-1.565653000	-1.926480000
1	-5.859332000	0.716619000	-0.989975000
6	-4.769022000	0.282171000	-4.755887000
6	-3.189836000	-1.010948000	-3.266891000
6	-3.725902000	0.480859000	-1.333176000
6	-5.329750000	1.805848000	-2.799052000
6	-4.418085000	1.564670000	-4.007304000
1	-4.097861000	0.140998000	-5.604393000
1	-5.778619000	0.363326000	-5.163228000
6	-3.047093000	0.287444000	-2.611884000
1	-3.103433000	-1.850896000	-2.581998000
1	-2.523231000	-1.140087000	-4.113433000
6	-3.383706000	1.773453000	-0.588793000
1	-3.662414000	-0.402351000	-0.700144000
6	-4.935538000	3.085389000	-2.049710000
1	-6.356622000	1.903758000	-3.160069000
6	-2.894823000	1.469562000	-3.455075000
1	-4.418179000	2.425718000	-4.676928000
6	-3.495316000	2.970896000	-1.537158000
1	-4.069641000	1.886333000	0.251628000
1	-2.379803000	1.695738000	-0.174683000
1	-5.040464000	3.945215000	-2.714455000
1	-5.618129000	3.246240000	-1.213466000
6	-2.540505000	2.763478000	-2.716394000
1	-2.252852000	1.277872000	-4.312206000
1	-3.221156000	3.881485000	-1.003592000
1	-1.505718000	2.715159000	-2.375076000
1	-2.607028000	3.594260000	-3.419838000

Table S6. Geometries of diamantane (**D**), 1-diamantyl cation (**Dp**) and cluster **CL2** in Cartesian coordinates in Å computed at the B3LYP/def2-TZVPP level of theory at 0.4 K.

D			
1	-6.914927000	-0.682410000	4.108622000
6	-6.670493000	-0.929030000	5.147510000
1	-6.652446000	-3.063477000	4.785970000
6	-7.162046000	-2.363009000	5.455612000
1	-7.541825000	0.411779000	8.214712000
6	-7.032220000	-0.288692000	7.545079000
1	-7.279316000	-1.969308000	8.892068000
6	-7.523765000	-1.722669000	7.853188000
1	-7.117076000	-3.725771000	7.139546000
6	-6.786774000	-2.705436000	6.916437000
1	-7.077180000	1.074071000	5.861158000
6	-7.407482000	0.053730000	6.084246000
1	-9.188732000	0.227013000	4.857421000
6	-8.925752000	-0.047948000	5.883931000
1	-4.758463000	-3.312096000	6.456912000
6	-5.268511000	-2.603748000	7.116759000
1	-9.435769000	0.660415000	6.543786000
1	-5.005535000	-2.878725000	8.143267000
1	-9.016769000	-3.485942000	5.455361000
6	-8.680215000	-2.464161000	5.252928000
1	-4.802802000	0.174842000	5.102603000
6	-5.152466000	-0.832003000	5.352198000
1	-9.391463000	-2.826543000	7.898094000
6	-9.041791000	-1.819700000	7.648502000
1	-5.177498000	0.834252000	7.545347000
6	-5.514053000	-0.187530000	7.747771000
1	-9.552036000	-1.128502000	8.326162000
1	-5.257473000	-0.407413000	8.788994000
1	-8.936795000	-2.244283000	4.211703000
1	-4.642219000	-1.523206000	4.674548000
6	-4.798727000	-1.171606000	6.809716000
6	-9.395534000	-1.480086000	6.190984000
1	-3.717451000	-1.097679000	6.955692000
1	-10.476811000	-1.554025000	6.045039000

Dp			
1	4.620582000	-0.805329000	-3.884785000
1	6.463976000	-0.880474000	0.024761000
1	3.595979000	-3.009718000	-3.391661000
1	6.311143000	0.158016000	-2.276142000
1	5.404683000	-3.090495000	0.429107000
1	3.035280000	-2.227826000	0.651555000
1	2.352207000	-0.904554000	-2.805915000
1	4.726508000	0.913435000	-0.534454000
1	5.876372000	-2.857142000	-4.513345000
1	8.119956000	-1.654804000	-1.719759000
1	6.032229000	-4.736808000	-1.245319000
1	4.191507000	-0.992381000	1.098364000
1	1.935640000	-2.175862000	-1.676425000
1	3.969015000	0.949080000	-2.113676000
1	7.011638000	-1.604444000	-4.069507000

1	7.709822000	-2.938137000	-0.606515000
1	5.264167000	-4.708886000	-2.863185000
6	5.633794000	-4.106150000	-2.036886000
6	6.229386000	-2.256198000	-3.673843000
6	7.303084000	-2.302977000	-1.395331000
6	2.749078000	-1.524389000	-2.000620000
6	4.365531000	0.279014000	-1.347429000
6	3.815434000	-1.574502000	0.255951000
6	6.812546000	-3.143601000	-2.574762000
6	3.259102000	-0.659018000	-0.841350000
6	6.157963000	-1.447452000	-0.856004000
6	4.688893000	-3.098685000	-1.571196000
6	5.095399000	-1.404391000	-3.106456000
6	5.539809000	-0.533027000	-1.923272000
6	4.960215000	-2.425018000	-0.309278000
6	3.896646000	-2.379066000	-2.556490000
1	7.591755000	-3.802880000	-2.955881000
1	2.435272000	-0.069005000	-0.437722000

CL2

1	-0.740306000	0.072392000	-1.856089000
1	1.020452000	1.823549000	-1.922110000
1	2.289267000	-2.945670000	-1.373349000
1	4.049298000	-1.190530000	-1.433828000
1	3.417055000	1.152830000	-1.993164000
1	-0.100863000	-2.280363000	-1.304651000
1	-0.341383000	-1.644220000	-3.713479000
1	2.443465000	1.763977000	0.216875000
1	0.887448000	-2.885557000	-3.510416000
1	3.668897000	0.519727000	0.403359000
1	2.038636000	1.220461000	-4.111111000
1	-0.491181000	-0.572621000	0.545399000
1	3.822889000	-0.565865000	-3.832903000
1	1.282136000	-2.342704000	0.822501000
1	3.366298000	-2.242345000	-3.581127000
1	2.983616000	-1.914120000	0.777742000
1	0.339551000	0.785798000	-4.087466000
1	-0.048391000	1.113093000	0.298322000
6	0.248014000	0.082828000	0.073417000
6	1.314778000	0.547051000	-3.645654000
6	2.006683000	-1.672268000	0.350918000
6	3.075717000	-1.210637000	-3.362707000
6	2.675277000	0.718302000	-0.007088000
6	0.650951000	-1.840941000	-3.290116000
6	1.643198000	-0.208968000	0.651148000
6	1.685186000	-0.914783000	-3.945840000
6	2.025422000	-1.903864000	-1.166422000
6	3.058358000	-0.977580000	-1.845892000
6	0.261551000	-0.147148000	-1.444912000
6	1.289701000	0.781097000	-2.127811000
6	2.685147000	0.488486000	-1.524691000
6	0.631185000	-1.612356000	-1.771265000
1	1.633987000	-0.042001000	1.730757000
1	1.694869000	-1.081583000	-5.025844000
6	-4.954392000	-0.838788000	-3.897318000

6	-5.906346000	-0.640272000	-2.718271000
6	-5.558093000	0.652208000	-1.980359000
1	-5.148618000	-1.774476000	-4.421297000
1	-6.935331000	-0.588995000	-3.081662000
1	-5.861182000	-1.490929000	-2.035564000
1	-6.181898000	0.789485000	-1.095930000
6	-5.002234000	0.361737000	-4.843243000
6	-3.461866000	-0.948269000	-3.307587000
6	-4.032955000	0.545130000	-1.383699000
6	-5.598637000	1.891083000	-2.887547000
6	-4.665392000	1.641710000	-4.080429000
1	-4.311474000	0.222313000	-5.676975000
1	-6.000504000	0.447277000	-5.278836000
6	-3.352108000	0.352115000	-2.655278000
1	-3.415371000	-1.786954000	-2.616585000
1	-2.762158000	-1.090391000	-4.127171000
6	-3.685373000	1.833503000	-0.628444000
1	-4.000243000	-0.342752000	-0.754638000
6	-5.203937000	3.164221000	-2.118525000
1	-6.617159000	2.008063000	-3.269072000
6	-3.144790000	1.530813000	-3.485593000
1	-4.635118000	2.504559000	-4.747955000
6	-3.772189000	3.036402000	-1.576248000
1	-4.375541000	1.950933000	0.208461000
1	-2.683031000	1.742534000	-0.205921000
1	-5.289604000	4.030708000	-2.778225000
1	-5.903636000	3.326674000	-1.296084000
6	-2.797125000	2.826873000	-2.740860000
1	-2.488699000	1.327283000	-4.330085000
1	-3.502633000	3.944505000	-1.034995000
1	-1.763017000	2.779526000	-2.393990000
1	-2.854122000	3.657375000	-3.446628000
