

**Study of host-guest interactions in  
benzodiazacoronands by means of solid state NMR  
spectroscopy, X-Ray diffraction and quantum  
mechanical computations.**

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Włodzimierz Ciesielski, Grzegorz D. Bujacz, Janusz Jurczak\* and Marek J. Potrzebowski†

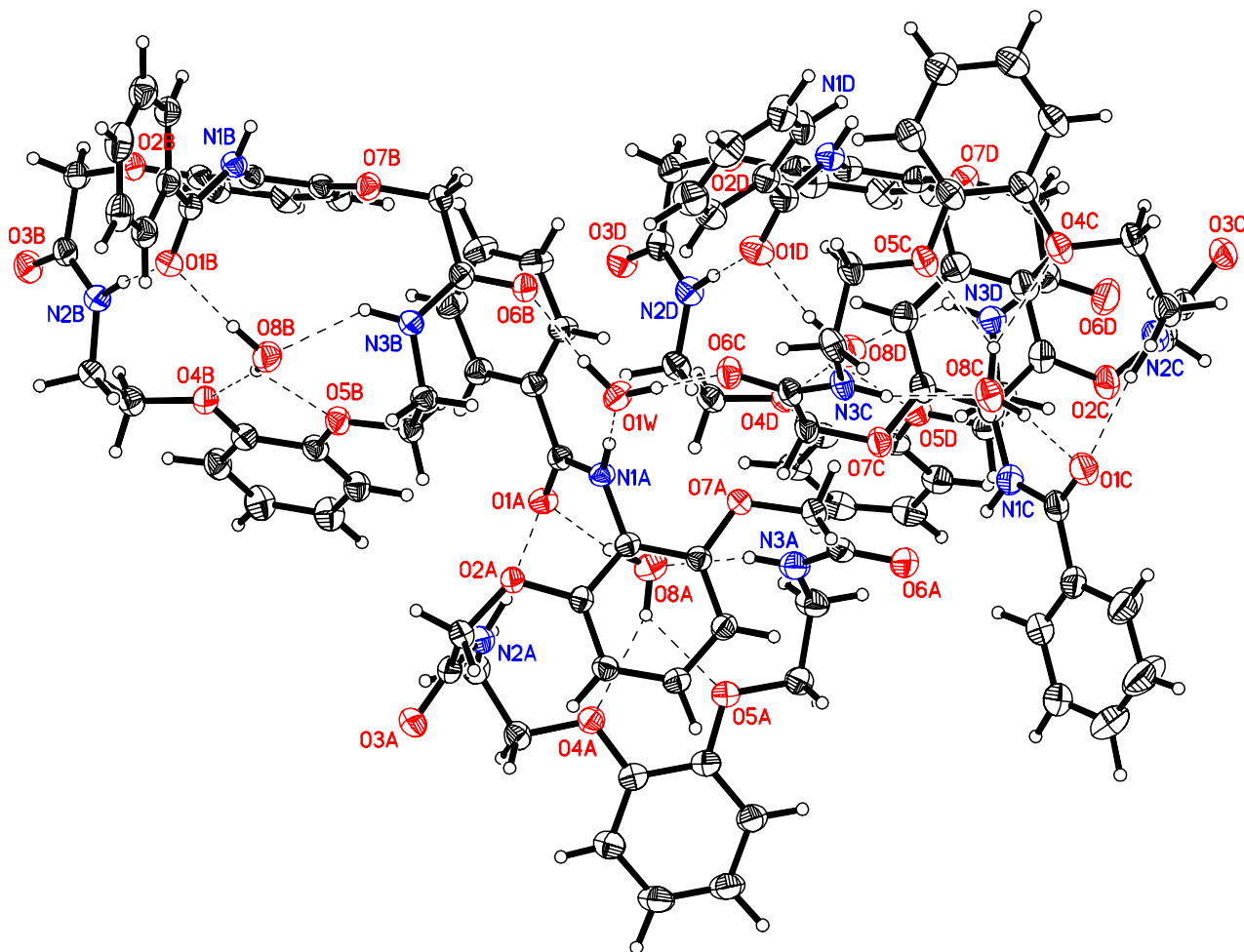
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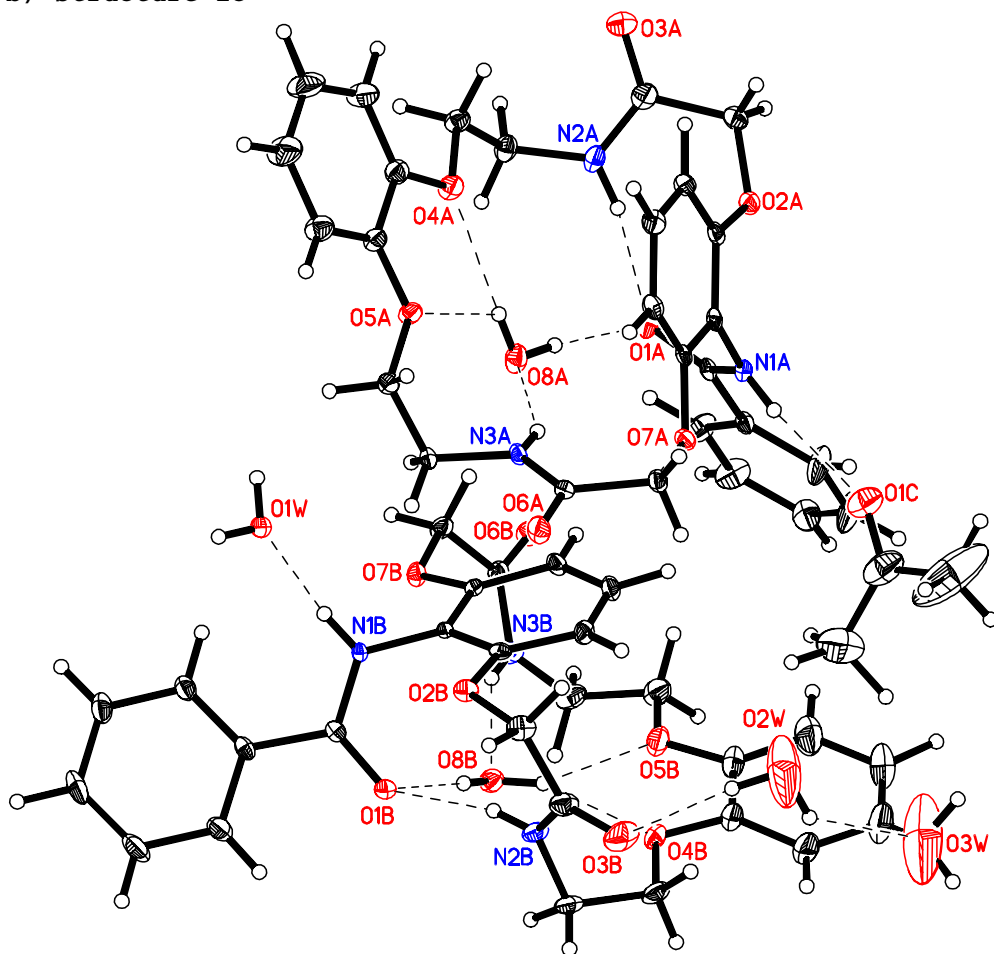
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1) X-ray structure of complexes 1 with full numbering system

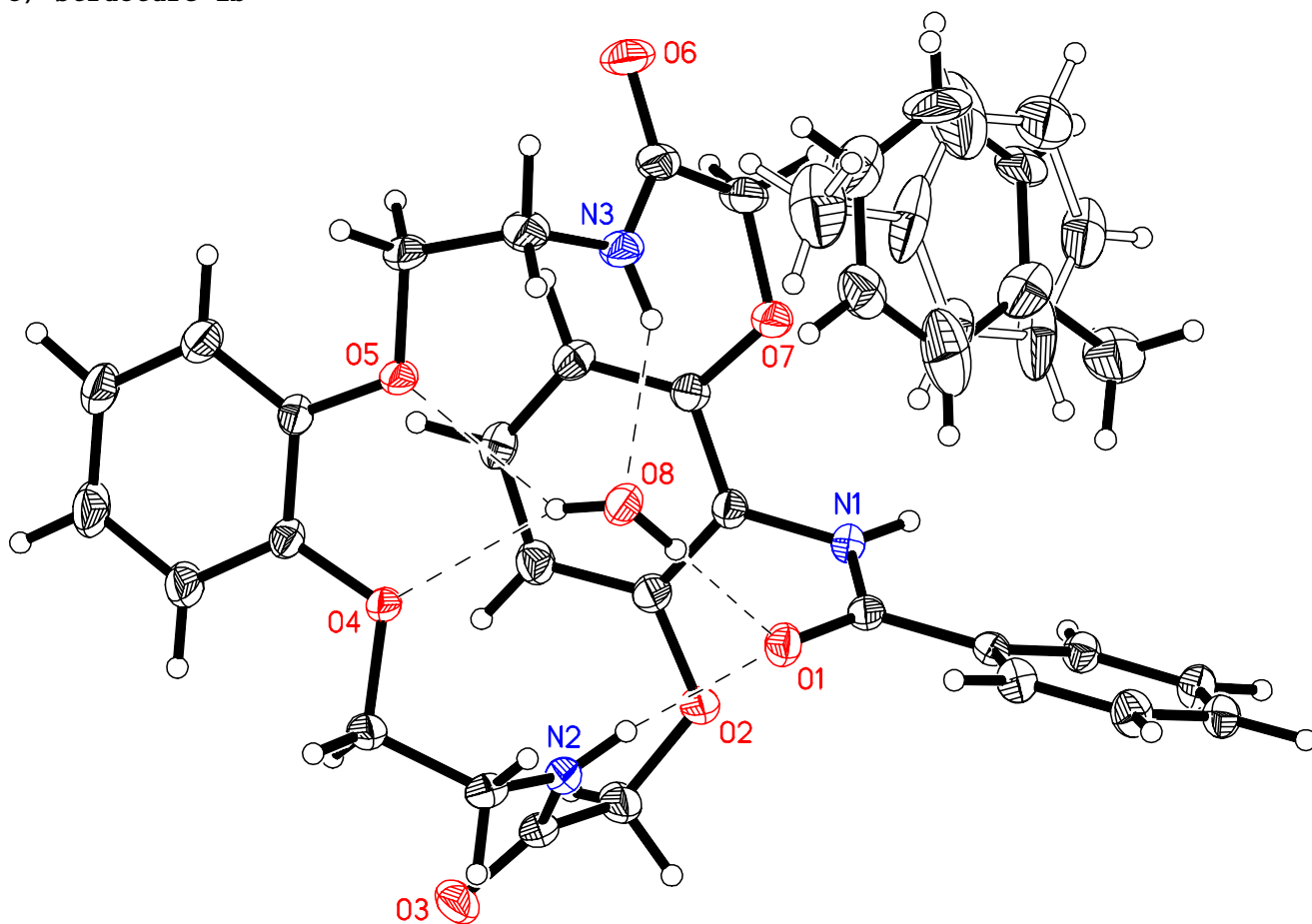
a) Structure 1d



b) Structure 1c

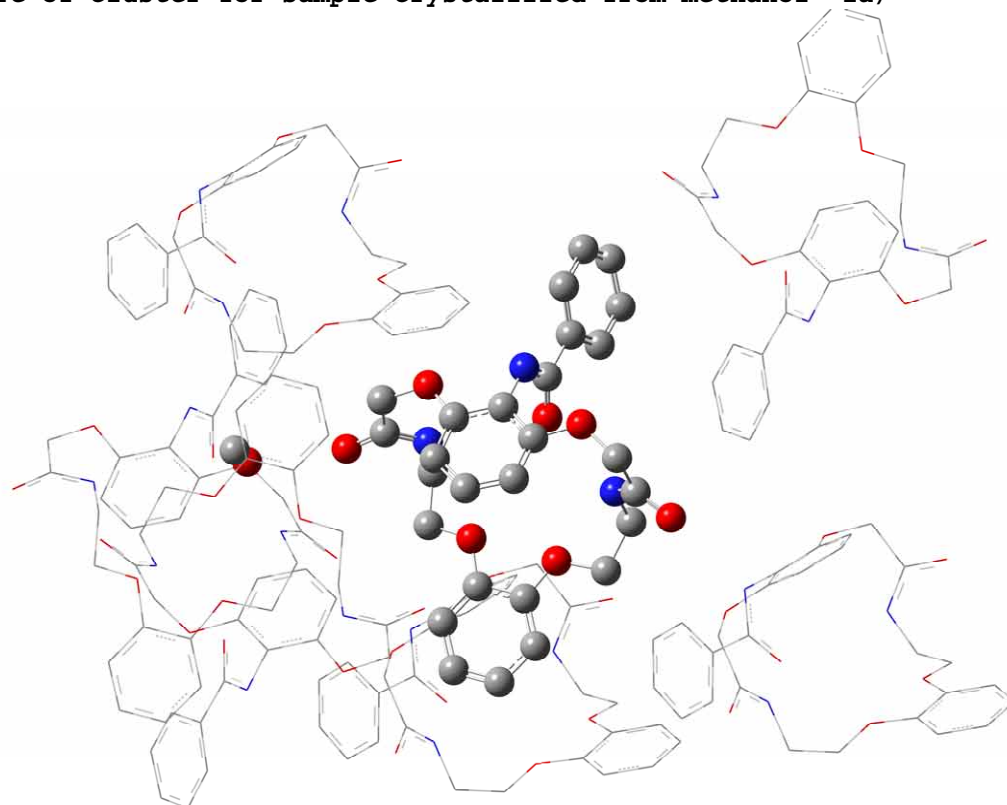


c) Structure 1b

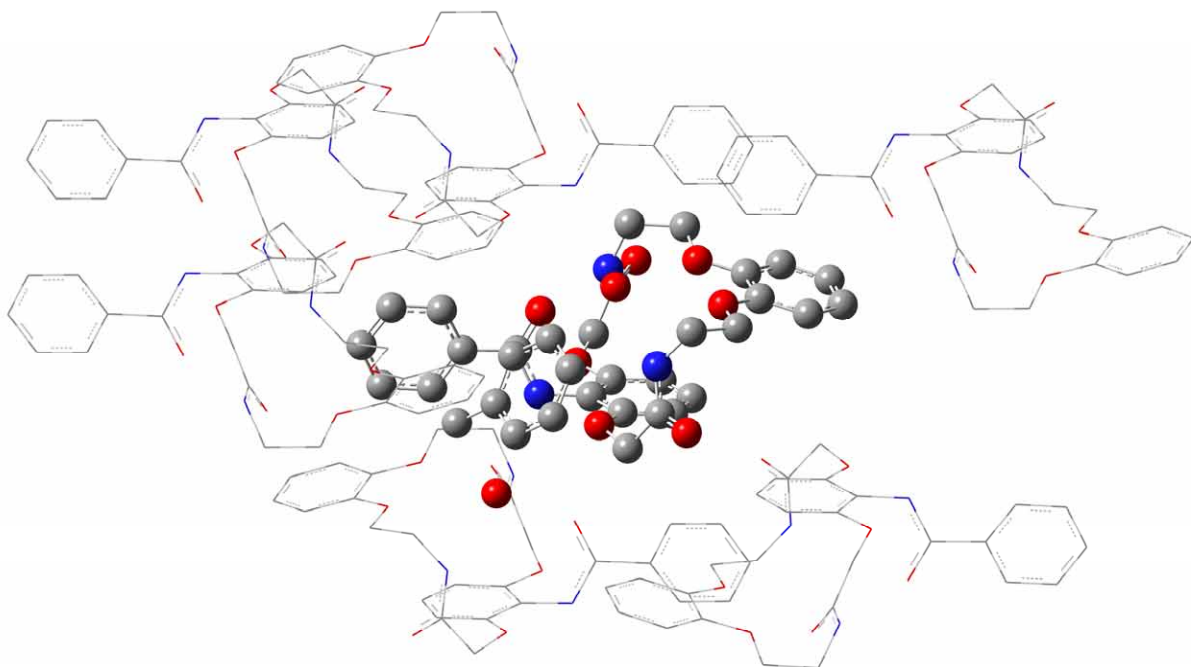


2) Input files with structure of clusters used for DFT GIAO calculations.

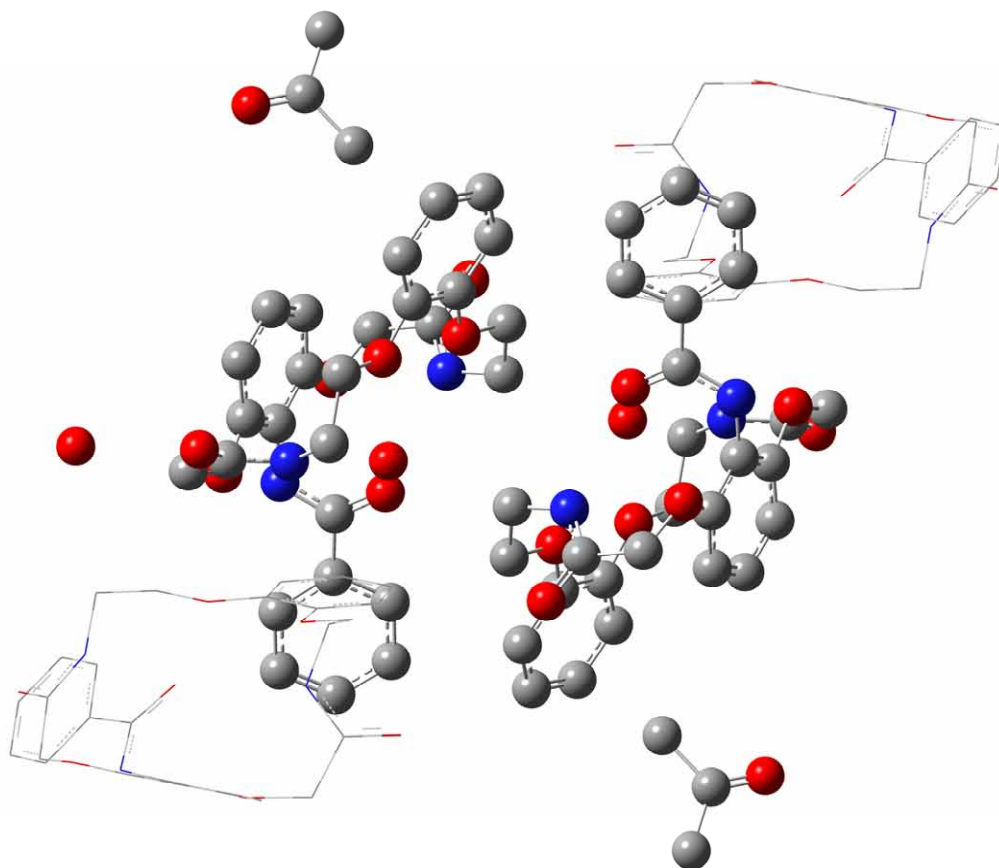
a) Structure of cluster for Sample crystallized from methanol 1a)



b) Structure of cluster for Sample crystallized from toluene 1b)



c) Structure of cluster for Sample crystallized from acetone 1c)



d) Gaussian input files for Sample crystallized from methanol 1a)

```
%chk=koron_219_metanol.chk  
%mem=4048MB  
%nproc=4  
# NMR oniom(b3lyp/6-311++g(d,p):uff)
```

Sample crystallized from methanol 1a)

```
0 1 0 1 0 1  
O-O_3      0    2.115574    1.681644    0.867345 H  
O-O_3      0   -0.965419    3.042701    2.399130 H  
O-O_3      0   -3.476127    1.254929    0.569543 H  
O-O_3      0   -0.295298   -1.516482    0.481810 H  
O-O_3      0    2.030355   -2.240930    1.219610 H  
O-O_3      0    5.436022   -1.008142    3.796802 H  
O-O_3      0    3.230358    1.792551    3.939725 H  
N-N_3      0    1.710739    3.300333    2.355188 H  
N-N_3      0   -1.244211    1.238525    0.369449 H  
N-N_3      0    3.869963   -0.332971    2.330585 H  
C-C_3      0    3.629840    3.372824   -0.768327 H  
C-C_3      0    4.239712    4.258479   -1.640900 H  
C-C_3      0    4.092510    5.614926   -1.488300 H  
C-C_3      0    3.451037    6.086244   -0.405412 H  
C-C_3      0    2.882523    5.212615    0.504085 H  
C-C_3      0    2.934427    3.846401    0.323543 H  
C-C_3      0    2.232605    2.857839    1.194587 H  
C-C_3      0    1.093109    2.364157    3.239646 H  
C-C_3      0    1.882336    1.542887    4.042771 H  
C-C_3      0    1.301040    0.567503    4.827215 H  
C-C_3      0   -0.057359    0.410192    4.795460 H  
C-C_3      0   -0.862360    1.205620    4.011743 H  
C-C_3      0   -0.284992    2.193789    3.234975 H  
C-C_3      0   -2.292121    2.694196    2.013496 H  
C-C_3      0   -2.365270    1.662069    0.920971 H  
C-C_3      0   -1.255690    0.255389   -0.698740 H  
C-C_3      0   -1.476953   -1.136973   -0.208208 H  
C-C_3      0   -0.210617   -2.797170    0.959121 H  
C-C_3      0   -1.257640   -3.684582    1.046846 H  
C-C_3      0   -1.044599   -4.966548    1.521901 H  
C-C_3      0    0.196195   -5.362287    1.891634 H  
C-C_3      0    1.266283   -4.473438    1.806509 H  
C-C_3      0    1.070390   -3.192397    1.344146 H  
C-C_3      0    3.378607   -2.588730    1.502593 H  
C-C_3      0    4.180218   -1.340965    1.330071 H  
C-C_3      0    4.513969   -0.250729    3.475831 H  
C-C_3      0    4.153120    0.839273    4.451487 H  
O-O_3      0   -6.196229    1.194158    1.110062 H  
C-C_3      0   -6.425785    1.697781    2.393275 H  
O-O_3      0   -7.528003    0.605910   -5.267548 L  
O-O_3      0  -10.608996    1.966966   -3.735763 L  
O-O_3      0  -13.119704    0.179195   -5.565350 L  
O-O_3      0   -9.938876   -2.592217   -5.653083 L  
O-O_3      0   -7.613222   -3.316664   -4.915283 L  
O-O_3      0   -4.207555   -2.083876   -2.338091 L  
O-O_3      0   -6.413219    0.716817   -2.195168 L  
N-N_3      0   -7.932838    2.224599   -3.779705 L  
N-N_3      0  -10.887788    0.162791   -5.765444 L  
N-N_3      0   -5.773614   -1.408705   -3.804307 L
```



C-C_3	0	-6.013737	2.297089	-6.903220	L
C-C_3	0	-5.403865	3.182744	-7.775793	L
C-C_3	0	-5.551068	4.539191	-7.623193	L
C-C_3	0	-6.192540	5.010509	-6.540305	L
C-C_3	0	-6.761054	4.136880	-5.630808	L
C-C_3	0	-6.709150	2.770667	-5.811350	L
C-C_3	0	-7.410972	1.782105	-4.940306	L
C-C_3	0	-8.550468	1.288422	-2.895247	L
C-C_3	0	-7.761241	0.467153	-2.092122	L
C-C_3	0	-8.342537	-0.508232	-1.307678	L
C-C_3	0	-9.700936	-0.665542	-1.339433	L
C-C_3	0	-10.505937	0.129886	-2.123150	L
C-C_3	0	-9.928569	1.118054	-2.899918	L
C-C_3	0	-11.935698	1.618461	-4.121397	L
C-C_3	0	-12.008847	0.586335	-5.213922	L
C-C_3	0	-10.899267	-0.820345	-6.833633	L
C-C_3	0	-11.120531	-2.212707	-6.343101	L
C-C_3	0	-9.854195	-3.872905	-5.175772	L
C-C_3	0	-10.901217	-4.760317	-5.088047	L
C-C_3	0	-10.688177	-6.042283	-4.612992	L
C-C_3	0	-9.447382	-6.438021	-4.243259	L
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C-C_3	0	-8.573187	-4.268131	-4.790746	L
C-C_3	0	-6.264971	-3.664464	-4.632300	L
C-C_3	0	-5.463359	-2.416699	-4.804822	L
C-C_3	0	-5.129608	-1.326464	-2.659062	L
C-C_3	0	-5.490457	-0.236462	-1.683406	L
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O-O_3	0	-6.853691	0.928335	6.081291	L
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O-O_3	0	-8.053694	-3.105146	3.361176	L
N-N_3	0	-6.534075	-4.612928	4.945713	L
N-N_3	0	-3.579125	-2.551120	6.931452	L
N-N_3	0	-8.693299	-0.979624	4.970316	L
C-C_3	0	-8.453176	-4.685419	8.069228	L
C-C_3	0	-9.063048	-5.571074	8.941801	L
C-C_3	0	-8.915845	-6.927521	8.789201	L
C-C_3	0	-8.274373	-7.398839	7.706313	L
C-C_3	0	-7.705859	-6.525210	6.796816	L
C-C_3	0	-7.757763	-5.158996	6.977358	L
C-C_3	0	-7.055941	-4.170434	6.106314	L
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C-C_3	0	-2.531215	-4.006791	5.287405	L
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C-C_3	0	-3.346382	-0.175622	7.509109	L
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C-C_3	0	-3.778736	3.653953	5.779000	L
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C-C_3	0	-8.201942	1.276135	5.798308	L

C-C_3	0	-9.003554	0.028370	5.970830	L
C-C_3	0	-9.337305	-1.061866	3.825070	L
C-C_3	0	-8.976456	-2.151868	2.849414	L
O-O_3	0	-1.591669	-6.372940	-2.792265	L
O-O_3	0	-0.085133	-2.995281	-2.680044	L
O-O_3	0	3.283109	-3.788469	-1.745871	L
O-O_3	0	2.185664	-7.287512	-3.833550	L
O-O_3	0	0.530153	-8.580023	-5.271094	L
O-O_3	0	-3.412923	-8.195350	-7.287139	L
O-O_3	0	-3.141824	-5.173492	-5.410042	L
N-N_3	0	-2.412084	-4.303938	-3.000734	L
N-N_3	0	1.497960	-5.116542	-2.012310	L
N-N_3	0	-2.217664	-7.754506	-5.433744	L
C-C_3	0	-3.440976	-7.055731	-0.806752	L
C-C_3	0	-4.256125	-7.323291	0.280308	L
C-C_3	0	-4.896370	-6.309984	0.949797	L
C-C_3	0	-4.827256	-5.058648	0.464550	L
C-C_3	0	-4.059431	-4.784896	-0.653062	L
C-C_3	0	-3.330530	-5.768706	-1.287815	L
C-C_3	0	-2.384024	-5.516583	-2.414352	L
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C-C_3	0	2.718264	-7.864687	-4.955410	L
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C-C_3	0	4.468481	-8.452942	-6.474897	L
C-C_3	0	3.594797	-9.161853	-7.227816	L
C-C_3	0	2.252597	-9.231975	-6.858701	L
C-C_3	0	1.808342	-8.586155	-5.727944	L
C-C_3	0	-0.441459	-9.365816	-5.947355	L
C-C_3	0	-1.740645	-9.116005	-5.255278	L
C-C_3	0	-3.005066	-7.405160	-6.429258	L
C-C_3	0	-3.480248	-5.978922	-6.531954	L
O-O_3	0	-5.960981	6.777581	1.770052	L
O-O_3	0	-4.454445	10.155241	1.882273	L
O-O_3	0	-1.086203	9.362052	2.816445	L
O-O_3	0	-2.183648	5.863009	0.728767	L
O-O_3	0	-3.839159	4.570498	-0.708778	L
O-O_3	0	-7.782234	4.955171	-2.724822	L
O-O_3	0	-7.511136	7.977030	-0.847725	L
N-N_3	0	-6.781396	8.846584	1.561582	L
N-N_3	0	-2.871351	8.033980	2.550007	L
N-N_3	0	-6.586976	5.396016	-0.871427	L
C-C_3	0	-7.810288	6.094791	3.755565	L
C-C_3	0	-8.625437	5.827231	4.842625	L
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C-C_3	0	-4.227162	9.370657	-1.699551	L

C-C_3	0	-3.849236	9.860616	-0.469894	L
C-C_3	0	-4.711032	9.728501	0.603865	L
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C-C_3	0	-2.283403	9.214784	2.555175	L
C-C_3	0	-2.131046	6.823352	2.857206	L
C-C_3	0	-1.289511	6.349117	1.719144	L
C-C_3	0	-1.651047	5.285835	-0.393093	L
C-C_3	0	-0.329182	5.346038	-0.767802	L
C-C_3	0	0.099169	4.697579	-1.912580	L
C-C_3	0	-0.774515	3.988669	-2.665500	L
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C-C_3	0	-2.560970	4.564367	-1.165627	L
C-C_3	0	-4.810771	3.784706	-1.385039	L
C-C_3	0	-6.109957	4.034516	-0.692962	L
C-C_3	0	-7.374378	5.745361	-1.866942	L
C-C_3	0	-7.849560	7.171599	-1.969637	L
O-O_3	0	8.051908	-5.297206	3.342628	L
O-O_3	0	9.558444	-1.919546	3.454849	L
O-O_3	0	12.926686	-2.712735	4.389022	L
O-O_3	0	11.829241	-6.211778	2.301343	L
O-O_3	0	10.173730	-7.504289	0.863798	L
O-O_3	0	6.230654	-7.119616	-1.152246	L
O-O_3	0	6.501753	-4.097757	0.724851	L
N-N_3	0	7.231493	-3.228204	3.134159	L
N-N_3	0	11.141537	-4.040807	4.122583	L
N-N_3	0	7.425913	-6.678772	0.701149	L
C-C_3	0	6.202601	-5.979997	5.328141	L
C-C_3	0	5.387452	-6.247556	6.415201	L
C-C_3	0	4.747207	-5.234249	7.084690	L
C-C_3	0	4.816321	-3.982914	6.599443	L
C-C_3	0	5.584146	-3.709162	5.481831	L
C-C_3	0	6.313047	-4.692972	4.847078	L
C-C_3	0	7.259553	-4.440848	3.720541	L
C-C_3	0	8.078130	-2.981100	2.010546	L
C-C_3	0	7.723419	-3.467795	0.753742	L
C-C_3	0	8.580158	-3.321422	-0.318311	L
C-C_3	0	9.785727	-2.704131	-0.126975	L
C-C_3	0	10.163653	-2.214171	1.102682	L
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C-C_3	0	10.907602	-1.638366	3.817176	L
C-C_3	0	11.729486	-2.860003	4.127751	L
C-C_3	0	11.881843	-5.251435	4.429782	L
C-C_3	0	12.723378	-5.725670	3.291720	L
C-C_3	0	12.361842	-6.788952	1.179483	L
C-C_3	0	13.683707	-6.728749	0.804774	L
C-C_3	0	14.112058	-7.377208	-0.340004	L
C-C_3	0	13.238374	-8.086118	-1.092923	L
C-C_3	0	11.896174	-8.156240	-0.723808	L
C-C_3	0	11.451919	-7.510420	0.406949	L
C-C_3	0	9.202118	-8.290082	0.187538	L
C-C_3	0	7.902932	-8.040271	0.879614	L
C-C_3	0	6.638511	-6.329426	-0.294365	L
C-C_3	0	6.163329	-4.903188	-0.397061	L
O-O_3	0	8.887549	4.902867	-1.172302	L
O-O_3	0	11.968542	3.541810	-2.704086	L
O-O_3	0	14.479250	5.329582	-0.874500	L
O-O_3	0	11.298421	8.100993	-0.786767	L
O-O_3	0	8.972768	8.825441	-1.524567	L
O-O_3	0	5.567100	7.592653	-4.101758	L
O-O_3	0	7.772765	4.791960	-4.244681	L
N-N_3	0	9.292429	3.284220	-2.660222	L

N-N_3	0	12.247379	5.346028	-0.674484	L			
N-N_3	0	7.133244	6.917491	-2.635488	L			
C-C_3	0	7.373367	3.211696	0.463424	L			
C-C_3	0	6.763495	2.326042	1.335997	L			
C-C_3	0	6.910613	0.969585	1.183343	L			
C-C_3	0	7.552085	0.498267	0.100455	L			
C-C_3	0	8.120600	1.371896	-0.809041	L			
C-C_3	0	8.068696	2.738110	-0.628499	L			
C-C_3	0	8.770518	3.726672	-1.499544	L			
C-C_3	0	9.910059	4.220397	-3.544681	L			
C-C_3	0	9.120832	5.041666	-4.347806	L			
C-C_3	0	9.702128	6.017050	-5.132249	L			
C-C_3	0	11.060482	6.174319	-5.100416	L			
C-C_3	0	11.865483	5.378891	-4.316699	L			
C-C_3	0	11.288115	4.390722	-3.539931	L			
C-C_3	0	13.295328	3.890325	-2.318399	L			
C-C_3	0	13.368477	4.922451	-1.225874	L			
C-C_3	0	12.258813	6.329122	0.393784	L			
C-C_3	0	12.480160	7.721493	-0.096695	L			
C-C_3	0	11.213824	9.381690	-1.264024	L			
C-C_3	0	12.260808	10.269136	-1.351881	L			
C-C_3	0	12.047768	11.551102	-1.826936	L			
C-C_3	0	10.807012	11.946807	-2.196537	L			
C-C_3	0	9.736840	11.057949	-2.111466	L			
C-C_3	0	9.932778	9.776950	-1.649181	L			
C-C_3	0	7.624516	9.173241	-1.807550	L			
C-C_3	0	6.822905	7.925476	-1.635027	L			
C-C_3	0	6.489154	6.835240	-3.780787	L			
C-C_3	0	6.850003	5.745238	-4.756443	L			
H-H_	0	7.952738	6.470645	-2.533883	L			
H-H_	0	3.693380	2.306357	-0.927863	H			
H-H_	0	4.785195	3.868092	-2.490531	H			
H-H_	0	4.463183	6.289107	-2.234871	H			
H-H_	0	3.341011	7.151036	-0.247005	H			
H-H_	0	2.349959	5.641972	1.344091	H			
H-H_	0	1.897692	-0.089565	5.439197	H			
H-H_	0	-0.512936	-0.366318	5.392394	H			
H-H_	0	-1.926817	1.033488	4.006710	H			
H-H_	0	-2.249873	-3.365441	0.775560	H			
H-H_	0	-1.882458	-5.646904	1.593828	L	H-H_	30	0.0000
H-H_	0	0.372777	-6.365378	2.255512	H			
H-H_	0	2.251561	-4.803966	2.099327	H			
H-H_	0	-2.760978	3.605095	1.659915	H			
H-H_	0	-0.299873	0.312053	-1.215709	H			
H-H_	0	-1.667552	-1.811817	-1.048402	H			
H-H_	0	3.723435	-3.369353	0.819165	H			
H-H_	0	3.975343	-0.913593	0.349240	H			
H-H_	0	5.065167	1.393851	4.659820	H			
H-H_	0	-2.892835	2.349994	2.855665	H			
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H-H_	0	1.825658	4.253529	2.651426	H			
H-H_	0	-0.342579	1.537667	0.711684	H			
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H-H_	0	-4.904513	2.836085	-8.548330	L
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H-H_	0	-11.471623	-0.030979	-2.106216	L
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H-H_	0	-11.275032	-2.825068	-7.132433	L
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H-H_	0	-4.352311	-1.023591	1.952452	L
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H-H_	0	-7.052971	3.492563	5.158506	L
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H-H_	0	-8.557840	2.051862	6.512744	L
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H-H_	0	-1.883577	-3.747787	4.424905	L
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H-H_	0	-8.303119	1.604591	4.850063	L
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H-H_	0	-8.701471	-1.747256	1.855295	L
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H-H_	0	-4.332959	-8.244769	0.613744	L
H-H_	0	-5.490222	-6.521833	1.830506	L
H-H_	0	-5.352388	-4.257863	0.966742	L
H-H_	0	-3.968286	-3.854840	-0.915595	L
H-H_	0	-1.274994	-4.733103	-7.347922	L
H-H_	0	0.757434	-3.684225	-7.023449	L

H-H_	0	1.396515	-2.860300	-4.956783	L
H-H_	0	4.772902	-7.253630	-4.756628	L
H-H_	0	5.413769	-8.403945	-6.739386	L
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H-H_	0	1.588097	-9.808260	-7.487117	L
H-H_	0	1.241220	-2.107639	-1.395552	L
H-H_	0	1.589920	-7.056898	-1.442888	L
H-H_	0	3.684279	-7.546046	-2.524146	L
H-H_	0	-0.181431	-10.445739	-5.877043	L
H-H_	0	-1.639070	-9.303044	-4.267952	L
H-H_	0	-4.588520	-6.031349	-6.551412	L
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H-H_	0	2.825399	-6.169068	-0.897741	L
H-H_	0	3.634769	-6.038423	-3.201517	L
H-H_	0	-0.522899	-9.087384	-6.914654	L
H-H_	0	-2.494530	-9.843185	-5.631745	L
H-H_	0	-3.222770	-5.521611	-7.507400	L
H-H_	0	-3.373429	-3.949435	-3.120954	L
H-H_	0	0.576006	-5.208625	-2.195697	L
H-H_	0	-1.766137	-7.089782	-4.947837	L
H-H_	0	-7.331616	5.350628	3.325829	L
H-H_	0	-8.738528	4.906786	5.161152	L
H-H_	0	-9.868151	6.625835	6.386132	L
H-H_	0	-9.727610	8.892305	5.527640	L
H-H_	0	-8.376393	9.302918	3.633993	L
H-H_	0	-5.643949	8.416888	-2.785556	L
H-H_	0	-3.611718	9.465994	-2.461050	L
H-H_	0	-2.972805	10.290417	-0.393056	L
H-H_	0	0.389658	5.920961	-0.207320	L
H-H_	0	1.043522	4.749999	-2.179291	L
H-H_	0	-0.432444	3.477288	-3.556713	L
H-H_	0	-2.780813	3.339361	-2.922731	L
H-H_	0	-3.145346	11.024648	3.185188	L
H-H_	0	-2.778860	6.092556	3.119148	L
H-H_	0	-0.678843	5.609969	2.036217	L
H-H_	0	-4.550678	2.708382	-1.321795	L
H-H_	0	-5.998782	3.857198	0.293930	L
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H-H_	0	-2.595630	11.110656	1.526879	L
H-H_	0	-1.542790	6.980883	3.663793	L
H-H_	0	-0.738197	7.113997	1.359700	L
H-H_	0	-4.893565	4.064179	-2.351874	L
H-H_	0	-6.868638	3.304839	-1.047540	L
H-H_	0	-7.591584	7.627670	-2.945688	L
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H-H_	0	-6.134337	6.060856	-0.386645	L
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H-H_	0	5.309566	-7.169344	6.747730	L
H-H_	0	4.152642	-5.447548	7.964382	L
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H-H_	0	5.682704	-2.778092	5.224577	L
H-H_	0	8.366663	-3.656391	-1.213070	L
H-H_	0	10.400115	-2.606705	-0.888974	L
H-H_	0	11.039142	-1.782501	1.179027	L
H-H_	0	14.416404	-6.177525	1.377819	L
H-H_	0	15.057309	-7.328117	-0.604607	L
H-H_	0	13.580084	-8.596081	-1.985197	L
H-H_	0	11.231654	-8.732480	-1.352255	L
H-H_	0	10.867442	-1.049985	4.757653	L
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H-H_	0	13.328592	-6.470031	3.610377	L
H-H_	0	9.462120	-9.370010	0.257796	L
H-H_	0	8.004401	-8.227385	1.866923	L
H-H_	0	5.058610	-4.968178	-0.399572	L
H-H_	0	11.417033	-0.964018	3.099374	L
H-H_	0	12.470197	-5.093282	5.236232	L
H-H_	0	13.277415	-4.962484	2.932482	L
H-H_	0	9.120623	-8.011619	-0.779760	L
H-H_	0	7.149000	-8.767352	0.502976	L
H-H_	0	6.410819	-4.443040	-1.374088	L
H-H_	0	6.269999	-2.874223	3.013438	L
H-H_	0	10.221980	-4.134653	3.928504	L
H-H_	0	7.877420	-6.014016	1.187006	L
H-H_	0	7.290166	4.177215	0.631646	L
H-H_	0	6.270206	2.672036	2.112919	L
H-H_	0	6.529004	0.289781	1.918072	L
H-H_	0	7.651609	-0.569245	-0.040909	L
H-H_	0	8.620463	0.969198	-1.547328	L
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H-H_	0	11.474409	6.876145	-5.651634	L
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H-H_	0	13.267027	9.997172	-1.064421	L
H-H_	0	12.800362	12.179987	-1.890427	L
H-H_	0	10.644913	12.953077	-2.562770	L
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H-H_	0	13.756232	2.970732	-1.900948	L
H-H_	0	11.381816	6.287760	0.894690	L
H-H_	0	12.634636	8.333832	0.692660	L
H-H_	0	7.268174	9.949090	-1.093435	L
H-H_	0	6.986262	7.540142	-0.715865	L
H-H_	0	5.909896	5.185960	-4.948616	L
H-H_	0	13.943167	4.148662	-3.180393	L
H-H_	0	12.978062	6.093258	1.063550	L
H-H_	0	13.279567	7.746170	-0.712161	L
H-H_	0	7.526914	9.500566	-2.757914	L
H-H_	0	5.744608	8.195488	-1.671312	L
H-H_	0	7.124715	6.148548	-5.750894	L
H-H_	0	9.137700	2.327876	-3.041097	L
H-H_	0	11.405769	5.017451	-0.949778	L

e) Gaussian input files for Sample crystallized from toluene 1b)

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%chk=koron_219_toluen.chk  
%mem=4GB  
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# NMR oniom(b3lyp/6-311++g(d,p):uff)
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Sample crystallized from toluene 1b)

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O-O_3      0    0.865778   -2.266966    2.908392 H  
O-O_3      0    2.334935   -5.190454    1.405416 H  
O-O_3      0    3.514280   -2.172916   -1.138766 H  
O-O_3      0    4.084807    0.316276   -1.602202 H  
O-O_3      0    3.185200    4.507643   -0.305794 H  
O-O_3      0    1.145734    2.175867    1.563702 H  
N-N_3      0   -0.325139    0.054889    2.352154 H  
N-N_3      0    1.351213   -3.383864    0.446556 H  
N-N_3      0    2.320006    2.500990   -0.912796 H  
C-C_3      0   -3.327946   -0.606121    0.388637 H  
C-C_3      0   -4.715374   -0.508548    0.440049 H  
C-C_3      0   -5.341348   -0.274939    1.653557 H  
C-C_3      0   -4.592441   -0.128179    2.813632 H  
C-C_3      0   -3.204291   -0.207571    2.762211 H  
C-C_3      0   -2.568261   -0.445330    1.550007 H  
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C-C_3      0    7.502228   -1.001543   -1.089300 H  
C-C_3      0    6.486183   -0.082660   -1.341208 H  
C-C_3      0    5.157151   -0.499323   -1.349575 H  
C-C_3      0    4.387124    1.680065   -1.930982 H  
C-C_3      0    3.069359    2.394267   -2.149228 H  
C-C_3      0    2.515204    3.501844   -0.065199 H  
C-C_3      0    1.856150    3.391796    1.302226 H  
O-O_3      0    1.156400   -0.155791   -1.425248 H  
C-C_3      0   -1.979478    3.559640    0.189525 H  
C-C_3      0   -1.467432    4.851000    0.163999 H  
C-C_3      0   -0.620253    5.244206   -0.865219 H  
C-C_3      0   -0.285224    4.344091   -1.870871 H  
C-C_3      0   -0.795401    3.052855   -1.845665 H  
C-C_3      0   -1.642580    2.659649   -0.816447 H  
C-C_3      0   -2.849343    3.132553    1.318976 H  
O-O_3      0    9.032351   -5.403901   -0.895458 L  
O-O_3      0    9.423042   -4.157993   -3.673362 L  
O-O_3      0   10.918366   -1.037638   -2.677632 L  
O-O_3      0   13.251108   -3.821903   -0.734645 L  
O-O_3      0   14.257822   -6.206192   -0.541095 L
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N-N_3	0	10.548498	-2.934052	-1.487137	L
N-N_3	0	12.660614	-8.614243	-0.655088	L
C-C_3	0	6.550675	-6.288330	0.055798	L
C-C_3	0	5.249245	-6.564396	0.464650	L
C-C_3	0	4.292286	-6.903253	-0.477903	L
C-C_3	0	4.627068	-6.978024	-1.823452	L
C-C_3	0	5.931516	-6.719764	-2.232873	L
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C-C_3	0	11.777706	-4.747044	-4.033534	L
C-C_3	0	10.469687	-5.046369	-3.672203	L
C-C_3	0	9.728462	-2.764933	-3.777806	L
C-C_3	0	10.463252	-2.180828	-2.597589	L
C-C_3	0	11.294997	-2.493611	-0.338824	L
C-C_3	0	12.784720	-2.468156	-0.593683	L
C-C_3	0	14.537318	-3.971586	-1.212333	L
C-C_3	0	15.302842	-2.945891	-1.747826	L
C-C_3	0	16.599657	-3.203497	-2.211978	L
C-C_3	0	17.113175	-4.471770	-2.127557	L
C-C_3	0	16.364894	-5.507889	-1.573778	L
C-C_3	0	15.071753	-5.265289	-1.116560	L
C-C_3	0	14.824592	-7.512343	-0.361027	L
C-C_3	0	13.756828	-8.385015	0.265507	L
C-C_3	0	12.691056	-9.600202	-1.541269	L
C-C_3	0	11.608014	-9.605786	-2.610566	L
O-O_3	0	9.317399	8.837083	0.536379	L
O-O_3	0	7.872174	9.961031	-1.927305	L
O-O_3	0	6.403018	12.884519	-0.424329	L
O-O_3	0	5.223672	9.866981	2.119853	L
O-O_3	0	4.653145	7.377789	2.583288	L
O-O_3	0	5.552752	3.186422	1.286881	L
O-O_3	0	7.592218	5.518198	-0.582616	L
N-N_3	0	9.063091	7.639176	-1.371067	L
N-N_3	0	7.386739	11.077929	0.534531	L
N-N_3	0	6.417946	5.193075	1.893883	L
C-C_3	0	12.065898	8.300186	0.592449	L
C-C_3	0	13.453326	8.202613	0.541037	L
C-C_3	0	14.079300	7.969004	-0.672470	L
C-C_3	0	13.330393	7.822244	-1.832545	L
C-C_3	0	11.942243	7.901636	-1.781124	L
C-C_3	0	11.306213	8.139395	-0.568921	L
C-C_3	0	9.813297	8.236828	-0.430564	L
C-C_3	0	7.633959	7.733875	-1.307221	L
C-C_3	0	6.866004	6.633035	-0.916086	L
C-C_3	0	5.482734	6.740463	-0.825269	L
C-C_3	0	4.885515	7.952193	-1.130787	L
C-C_3	0	5.627493	9.066415	-1.500387	L
C-C_3	0	7.008335	8.945710	-1.599259	L
C-C_3	0	7.373027	11.300612	-1.894141	L
C-C_3	0	7.001900	11.811251	-0.524644	L
C-C_3	0	7.012582	11.443958	1.874742	L
C-C_3	0	5.532329	11.272086	2.128103	L
C-C_3	0	3.882394	9.542628	2.091803	L
C-C_3	0	2.857653	10.449428	1.862811	L

C-C_3	0	1.524817	10.017136	1.848727	L
C-C_3	0	1.235724	8.695608	2.070387	L
C-C_3	0	2.251770	7.776725	2.322294	L
C-C_3	0	3.580802	8.193388	2.330662	L
C-C_3	0	4.350828	6.014000	2.912068	L
C-C_3	0	5.668594	5.299798	3.130315	L
C-C_3	0	6.222748	4.192221	1.046286	L
C-C_3	0	6.881802	4.302269	-0.321139	L
O-O_3	0	-9.460573	-6.632377	2.269634	L
O-O_3	0	-9.069882	-5.386469	-0.508270	L
O-O_3	0	-7.574558	-2.266114	0.487460	L
O-O_3	0	-5.241816	-5.050379	2.430447	L
O-O_3	0	-4.235102	-7.434668	2.623997	L
O-O_3	0	-4.966633	-11.734391	1.606761	L
O-O_3	0	-7.791851	-9.725868	0.569897	L
N-N_3	0	-9.700507	-7.829296	0.359823	L
N-N_3	0	-7.944426	-4.162528	1.677955	L
N-N_3	0	-5.832311	-9.842719	2.510004	L
C-C_3	0	-11.942249	-7.516807	3.220890	L
C-C_3	0	-13.243680	-7.792872	3.629742	L
C-C_3	0	-14.200638	-8.131729	2.687189	L
C-C_3	0	-13.865856	-8.206500	1.341640	L
C-C_3	0	-12.561409	-7.948240	0.932219	L
C-C_3	0	-11.596029	-7.604038	1.870209	L
C-C_3	0	-10.167166	-7.312608	1.508533	L
C-C_3	0	-8.355591	-7.550413	-0.051080	L
C-C_3	0	-7.366734	-8.534487	0.039244	L
C-C_3	0	-6.057392	-8.248158	-0.330688	L
C-C_3	0	-5.756017	-6.976829	-0.789967	L
C-C_3	0	-6.715219	-5.975520	-0.868442	L
C-C_3	0	-8.023237	-6.274845	-0.507111	L
C-C_3	0	-8.764462	-3.993409	-0.612714	L
C-C_3	0	-8.029672	-3.409304	0.567503	L
C-C_3	0	-7.197927	-3.722087	2.826268	L
C-C_3	0	-5.708204	-3.696632	2.571409	L
C-C_3	0	-3.955606	-5.200062	1.952760	L
C-C_3	0	-3.190082	-4.174368	1.417266	L
C-C_3	0	-1.893267	-4.431973	0.953114	L
C-C_3	0	-1.379749	-5.700246	1.037535	L
C-C_3	0	-2.128030	-6.736366	1.591314	L
C-C_3	0	-3.421171	-6.493765	2.048532	L
C-C_3	0	-3.668332	-8.740819	2.804066	L
C-C_3	0	-4.736097	-9.613491	3.430599	L
C-C_3	0	-5.801868	-10.828678	1.623823	L
C-C_3	0	-6.884910	-10.834262	0.554526	L
O-O_3	0	-11.042756	6.024664	-2.062092	L
O-O_3	0	-10.652065	7.270572	-4.839996	L
O-O_3	0	-9.156741	10.390927	-3.844266	L
O-O_3	0	-6.823999	7.606662	-1.901278	L
O-O_3	0	-5.817284	5.222373	-1.707729	L
O-O_3	0	-6.548816	0.922650	-2.724964	L
O-O_3	0	-9.374034	2.931173	-3.761829	L
N-N_3	0	-11.282690	4.827745	-3.971903	L
N-N_3	0	-9.526608	8.494513	-2.653771	L
N-N_3	0	-7.414493	2.814322	-1.821721	L
C-C_3	0	-13.524431	5.140235	-1.110835	L
C-C_3	0	-14.825862	4.864169	-0.701984	L
C-C_3	0	-15.782821	4.525313	-1.644536	L
C-C_3	0	-15.448039	4.450541	-2.990086	L
C-C_3	0	-14.143591	4.708801	-3.399507	L
C-C_3	0	-13.178212	5.053003	-2.461517	L

C-C_3	0	-11.749349	5.344434	-2.823193	L
C-C_3	0	-9.937774	5.106628	-4.382806	L
C-C_3	0	-8.948916	4.122554	-4.292481	L
C-C_3	0	-7.639574	4.408884	-4.662413	L
C-C_3	0	-7.338200	5.680212	-5.121692	L
C-C_3	0	-8.297401	6.681521	-5.200168	L
C-C_3	0	-9.605420	6.382196	-4.838837	L
C-C_3	0	-10.346645	8.663632	-4.944439	L
C-C_3	0	-9.611855	9.247737	-3.764222	L
C-C_3	0	-8.780110	8.934954	-1.505458	L
C-C_3	0	-7.290387	8.960409	-1.760317	L
C-C_3	0	-5.537788	7.456979	-2.378966	L
C-C_3	0	-4.772265	8.482674	-2.914460	L
C-C_3	0	-3.475450	8.225068	-3.378612	L
C-C_3	0	-2.961932	6.956795	-3.294191	L
C-C_3	0	-3.710213	5.920676	-2.740412	L
C-C_3	0	-5.003354	6.163276	-2.283194	L
C-C_3	0	-5.250514	3.916222	-1.527660	L
C-C_3	0	-6.318279	3.043550	-0.901126	L
C-C_3	0	-7.384051	1.828363	-2.707903	L
C-C_3	0	-8.467093	1.822779	-3.777200	L
O-O_3	0	-0.538936	-2.600292	-5.645239	L
O-O_3	0	-0.929627	-3.846199	-2.867335	L
O-O_3	0	-2.424950	-6.966554	-3.863065	L
O-O_3	0	-4.757693	-4.182289	-5.806053	L
O-O_3	0	-5.764393	-1.797967	-5.999509	L
O-O_3	0	-5.032862	2.501756	-4.982273	L
O-O_3	0	-2.207644	0.493233	-3.945409	L
N-N_3	0	-0.299001	-1.403372	-3.735428	L
N-N_3	0	-2.055069	-5.070107	-5.053467	L
N-N_3	0	-4.167198	0.610051	-5.885609	L
C-C_3	0	1.942740	-1.715862	-6.596496	L
C-C_3	0	3.244185	-1.439763	-7.005254	L
C-C_3	0	4.201129	-1.100940	-6.062795	L
C-C_3	0	3.866348	-1.026168	-4.717245	L
C-C_3	0	2.561900	-1.284429	-4.307824	L
C-C_3	0	1.596520	-1.628631	-5.245814	L
C-C_3	0	0.167657	-1.920061	-4.884138	L
C-C_3	0	-1.643918	-1.682255	-3.324525	L
C-C_3	0	-2.632775	-0.698181	-3.414849	L
C-C_3	0	-3.942103	-0.984477	-3.044825	L
C-C_3	0	-4.243491	-2.255840	-2.585639	L
C-C_3	0	-3.284290	-3.257148	-2.507163	L
C-C_3	0	-1.976258	-2.957790	-2.868401	L
C-C_3	0	-1.235046	-5.239259	-2.762892	L
C-C_3	0	-1.969837	-5.823364	-3.943109	L
C-C_3	0	-2.801582	-5.510581	-6.201873	L
C-C_3	0	-4.291305	-5.536036	-5.947014	L
C-C_3	0	-6.043903	-4.032607	-5.328365	L
C-C_3	0	-6.809427	-5.058301	-4.792871	L
C-C_3	0	-8.106241	-4.800695	-4.328719	L
C-C_3	0	-8.619746	-3.532388	-4.413047	L
C-C_3	0	-7.871479	-2.496303	-4.966919	L
C-C_3	0	-6.578336	-2.738776	-5.424076	L
C-C_3	0	-6.331177	-0.491849	-6.179671	L
C-C_3	0	-5.263412	0.380822	-6.806205	L
C-C_3	0	-4.197627	1.596043	-4.999335	L
C-C_3	0	-3.114599	1.601594	-3.930131	L
O-O_3	0	-1.080982	1.155451	5.040730	H
O-O_3	0	1.287784	0.440924	6.208271	L
O-O_3	0	0.897093	-0.804983	8.986175	L

O-O_3	0	-0.598231	-3.925338	7.990444	L
O-O_3	0	-2.930973	-1.141073	6.047457	L
O-O_3	0	-3.937687	1.243216	5.853908	L
O-O_3	0	-3.206156	5.542939	6.871143	L
O-O_3	0	-0.380938	3.534416	7.908008	L
N-N_3	0	1.527718	1.637844	8.118082	L
N-N_3	0	-0.228363	-2.028925	6.799950	L
N-N_3	0	-2.340478	3.651267	5.967900	L
C-C_3	0	3.769460	1.325354	5.257014	L
C-C_3	0	5.070891	1.601419	4.848163	L
C-C_3	0	6.027849	1.940276	5.790715	L
C-C_3	0	5.693067	2.015048	7.136265	L
C-C_3	0	4.388619	1.756787	7.545686	L
C-C_3	0	3.423240	1.412585	6.607696	L
C-C_3	0	1.994377	1.121155	6.969372	L
C-C_3	0	0.182802	1.358961	8.528984	L
C-C_3	0	-0.806055	2.343035	8.438660	L
C-C_3	0	-2.115397	2.056705	8.808592	L
C-C_3	0	-2.416772	0.785376	9.267871	L
C-C_3	0	-1.457571	-0.215932	9.346347	L
C-C_3	0	-0.149552	0.083393	8.985016	L
C-C_3	0	0.591673	-2.198043	9.090618	L
C-C_3	0	-0.143117	-2.782148	7.910401	L
C-C_3	0	-0.974862	-2.469365	5.651636	L
C-C_3	0	-2.464585	-2.494820	5.906496	L
C-C_3	0	-4.217183	-0.991391	6.525145	L
C-C_3	0	-4.982707	-2.017085	7.060638	L
C-C_3	0	-6.279522	-1.759479	7.524791	L
C-C_3	0	-6.793040	-0.491206	7.440369	L
C-C_3	0	-6.044759	0.544913	6.886591	L
C-C_3	0	-4.751618	0.302313	6.429373	L
C-C_3	0	-4.504457	2.549367	5.673839	L
C-C_3	0	-3.436693	3.422038	5.047305	L
C-C_3	0	-2.370921	4.637226	6.854082	L
C-C_3	0	-1.287879	4.642810	7.923379	L
H-H_	0	-0.684483	5.560035	7.759556	L
H-H_	0	-0.761562	0.490125	3.158961	H
H-H_	0	0.775607	-2.554346	0.580513	H
H-H_	0	1.717129	1.705996	-0.699658	H
H-H_	0	-2.801912	-0.811522	-0.534701	H
H-H_	0	-5.307240	-0.613425	-0.464052	H
H-H_	0	-6.424042	-0.192711	1.702711	H
H-H_	0	-5.102203	0.043066	3.754137	H
H-H_	0	-2.631558	-0.081140	3.673230	H
H-H_	0	3.819526	1.768102	1.414097	H
H-H_	0	4.930651	-0.353267	2.017491	H
H-H_	0	3.613854	-2.310834	2.680959	H
H-H_	0	0.546098	-4.220619	3.260681	H
H-H_	0	2.220407	-3.737451	3.546548	H
H-H_	0	1.156216	-3.122409	-1.583062	H
H-H_	0	1.470076	-4.800379	-1.079069	H
H-H_	0	3.753344	-4.092150	-0.356527	H
H-H_	0	3.487970	-4.003016	-2.120256	H
H-H_	0	5.661349	-3.799642	-0.720005	H
H-H_	0	7.997588	-3.041433	-0.662700	H
H-H_	0	8.530202	-0.649881	-1.071043	H
H-H_	0	6.741676	0.953164	-1.528714	H
H-H_	0	5.001797	1.712449	-2.841607	H
H-H_	0	4.937922	2.142093	-1.107954	H
H-H_	0	3.269631	3.400208	-2.530048	H
H-H_	0	2.463278	1.845586	-2.875235	H

H-H_	0	2.618372	3.552464	2.071231	H
H-H_	0	1.107119	4.182756	1.380253	H
H-H_	0	0.536292	-0.508456	-0.757299	H
H-H_	0	2.016545	-0.574682	-1.243694	H
H-H_	0	-1.739559	5.555550	0.947755	H
H-H_	0	-0.217587	6.254409	-0.886212	H
H-H_	0	0.382363	4.652795	-2.671356	H
H-H_	0	-0.509187	2.338328	-2.612762	H
H-H_	0	-2.039949	1.648602	-0.793978	H
H-H_	0	-3.663064	2.473196	0.997000	H
H-H_	0	-3.292956	3.988673	1.839482	H
H-H_	0	-2.261660	2.563588	2.048936	H
H-H_	0	8.317321	-7.274011	-3.271933	L
H-H_	0	10.430693	-3.855534	-1.538461	L
H-H_	0	11.967138	-7.969811	-0.655635	L
H-H_	0	7.219371	-6.046647	0.734976	L
H-H_	0	5.008107	-6.510470	1.416122	L
H-H_	0	3.371058	-7.094765	-0.194338	L
H-H_	0	3.940563	-7.211072	-2.487448	L
H-H_	0	6.143664	-6.755587	-3.190878	L
H-H_	0	13.155277	-7.682936	-3.431121	L
H-H_	0	13.663680	-5.541299	-4.210829	L
H-H_	0	12.044385	-3.857316	-4.348169	L
H-H_	0	8.766166	-2.218018	-3.862831	L
H-H_	0	10.274421	-2.554504	-4.722698	L
H-H_	0	11.080452	-3.161814	0.524884	L
H-H_	0	10.956773	-1.474976	-0.045819	L
H-H_	0	12.931758	-1.876889	-1.517737	L
H-H_	0	13.306293	-1.975083	0.255786	L
H-H_	0	14.990017	-2.021353	-1.810187	L
H-H_	0	17.141381	-2.476620	-2.593048	L
H-H_	0	18.024212	-4.649448	-2.452211	L
H-H_	0	16.778467	-6.395694	-1.522814	L
H-H_	0	15.696966	-7.463806	0.328440	L
H-H_	0	15.123214	-7.957218	-1.336926	L
H-H_	0	14.209607	-9.350170	0.584095	L
H-H_	0	13.370526	-7.895385	1.186827	L
H-H_	0	12.061384	-9.725985	-3.619689	L
H-H_	0	11.004675	-10.523108	-2.447047	L
H-H_	0	9.439070	7.021805	-1.982784	L
H-H_	0	7.597984	10.178187	0.426951	L
H-H_	0	6.982984	5.921184	1.677828	L
H-H_	0	11.634486	8.465656	1.460496	L
H-H_	0	13.986882	8.306117	1.360275	L
H-H_	0	15.059654	7.907653	-0.712739	L
H-H_	0	13.781840	7.662410	-2.691162	L
H-H_	0	11.431116	7.815856	-2.615143	L
H-H_	0	4.931699	6.002997	-0.518191	L
H-H_	0	3.908323	8.033844	-1.055131	L
H-H_	0	5.159635	9.907592	-1.688087	L
H-H_	0	8.172978	11.964799	-2.282442	L
H-H_	0	6.522078	11.417594	-2.599532	L
H-H_	0	7.584327	10.827642	2.604063	L
H-H_	0	7.294327	12.503900	2.061814	L
H-H_	0	5.012819	11.818985	1.318093	L
H-H_	0	5.262512	11.712588	3.112964	L
H-H_	0	3.010570	11.404888	1.720650	L
H-H_	0	0.798804	10.659634	1.684067	L
H-H_	0	0.299596	8.394453	2.059970	L
H-H_	0	1.996178	6.843678	2.484917	L
H-H_	0	3.752797	5.961671	3.849239	L

H-H_	0	3.813701	5.523395	2.075347	L
H-H_	0	5.472778	4.291754	3.557659	L
H-H_	0	6.271846	5.853248	3.883480	L
H-H_	0	6.139607	4.114723	-1.126539	L
H-H_	0	7.614122	3.470988	-0.391684	L
H-H_	0	-10.175360	-8.502768	-0.106693	L
H-H_	0	-8.061553	-5.084127	1.626544	L
H-H_	0	-6.525682	-9.198180	2.509348	L
H-H_	0	-11.272777	-7.278171	3.900498	L
H-H_	0	-13.484440	-7.740730	4.581510	L
H-H_	0	-15.122515	-8.319407	2.972494	L
H-H_	0	-14.551649	-8.441852	0.677659	L
H-H_	0	-12.348818	-7.985863	-0.025691	L
H-H_	0	-5.337673	-8.911485	-0.266693	L
H-H_	0	-4.829653	-6.769741	-1.048164	L
H-H_	0	-6.448421	-5.086726	-1.186531	L
H-H_	0	-9.725111	-3.445227	-0.703718	L
H-H_	0	-8.212089	-3.783150	-1.552535	L
H-H_	0	-7.411833	-4.389349	3.690823	L
H-H_	0	-7.533785	-2.702188	3.118258	L
H-H_	0	-5.563652	-3.113585	1.643224	L
H-H_	0	-5.184295	-3.199443	3.417518	L
H-H_	0	-3.505954	-3.252859	1.351429	L
H-H_	0	-1.362904	-3.709288	0.554709	L
H-H_	0	-0.473608	-5.881057	0.702303	L
H-H_	0	-1.715241	-7.624609	1.639731	L
H-H_	0	-2.795854	-8.692143	3.493407	L
H-H_	0	-3.369751	-9.185631	1.828122	L
H-H_	0	-4.283299	-10.578626	3.749199	L
H-H_	0	-5.122368	-9.123789	4.351896	L
H-H_	0	-6.431507	-10.954400	-0.454597	L
H-H_	0	-7.488235	-11.751597	0.717998	L
H-H_	0	-11.757366	4.153891	-4.438063	L
H-H_	0	-9.644084	7.572939	-2.705095	L
H-H_	0	-8.107806	3.458826	-1.822315	L
H-H_	0	-12.854945	5.378800	-0.431218	L
H-H_	0	-15.066612	4.916265	0.249789	L
H-H_	0	-16.704689	4.337599	-1.359226	L
H-H_	0	-16.133822	4.215139	-3.654059	L
H-H_	0	-13.930974	4.671079	-4.357404	L
H-H_	0	-6.927955	3.755407	-4.571007	L
H-H_	0	-6.410147	5.888537	-5.371811	L
H-H_	0	-8.030298	7.571540	-5.513573	L
H-H_	0	-11.308378	9.210794	-5.031218	L
H-H_	0	-9.799807	8.873508	-5.889052	L
H-H_	0	-8.993831	8.266448	-0.641698	L
H-H_	0	-9.117778	9.953732	-1.212332	L
H-H_	0	-7.143200	9.551646	-2.684370	L
H-H_	0	-6.768678	9.453392	-0.910852	L
H-H_	0	-5.084938	9.407261	-2.976554	L
H-H_	0	-2.933345	8.951990	-3.758981	L
H-H_	0	-2.050148	6.778786	-3.616804	L
H-H_	0	-3.296769	5.032541	-2.689578	L
H-H_	0	-4.384558	3.972257	-0.844173	L
H-H_	0	-4.958428	3.480508	-2.504051	L
H-H_	0	-5.863442	2.078847	-0.585407	L
H-H_	0	-6.703283	3.530843	0.021791	L
H-H_	0	-8.016518	1.715400	-4.786990	L
H-H_	0	-9.068011	0.902754	-3.619735	L
H-H_	0	0.101607	-0.613140	-3.413181	L
H-H_	0	-1.937628	-4.148532	-5.001962	L

H-H_	0	-3.474076	-0.034703	-5.884508	L
H-H_	0	1.273288	-1.954541	-7.276066	L
H-H_	0	3.485075	-1.492239	-7.956946	L
H-H_	0	5.123406	-0.914645	-6.347746	L
H-H_	0	4.555409	-0.796489	-4.057349	L
H-H_	0	2.346582	-1.261716	-3.356625	L
H-H_	0	-4.652974	-0.329967	-3.132865	L
H-H_	0	-5.170809	-2.464257	-2.332310	L
H-H_	0	-3.550833	-4.145675	-2.188462	L
H-H_	0	-0.274527	-5.787606	-2.673734	L
H-H_	0	-1.785802	-5.449179	-1.822138	L
H-H_	0	-2.587798	-4.842084	-7.065597	L
H-H_	0	-2.463924	-6.529388	-6.494880	L
H-H_	0	-4.438303	-6.127039	-5.022656	L
H-H_	0	-4.813149	-6.029250	-6.796225	L
H-H_	0	-6.495424	-5.982156	-4.726456	L
H-H_	0	-8.645723	-5.526348	-3.941922	L
H-H_	0	-9.529201	-3.353961	-4.084374	L
H-H_	0	-8.283866	-1.607600	-5.014757	L
H-H_	0	-7.207647	-0.537668	-6.863939	L
H-H_	0	-6.617779	-0.056747	-5.201103	L
H-H_	0	-5.717291	1.346262	-7.122690	L
H-H_	0	-4.877529	-0.107790	-7.728125	L
H-H_	0	-3.566123	1.709291	-2.921072	L
H-H_	0	-2.517364	2.521885	-4.094807	L
H-H_	0	-0.287713	1.707388	4.959765	H
H-H_	0	-1.139083	0.860321	5.960311	H
H-H_	0	2.002197	2.312130	8.583771	L
H-H_	0	-0.100285	-1.109952	6.850313	L
H-H_	0	-1.570092	3.130662	5.911987	L
H-H_	0	3.095801	1.091612	4.582782	L
H-H_	0	5.312424	1.556510	3.896818	L
H-H_	0	6.948883	2.130932	5.504673	L
H-H_	0	6.378674	2.251327	7.800065	L
H-H_	0	4.175912	1.794742	8.503529	L
H-H_	0	-2.835227	2.719745	8.743146	L
H-H_	0	-3.343651	0.578186	9.523083	L
H-H_	0	-1.724436	-1.105720	9.660575	L
H-H_	0	1.553435	-2.745172	9.177180	L
H-H_	0	0.044906	-2.407981	10.035234	L
H-H_	0	-0.772428	-1.791148	4.795320	L
H-H_	0	-0.636001	-3.485816	5.354416	L
H-H_	0	-2.612535	-3.087369	6.829371	L
H-H_	0	-2.984885	-2.985786	5.054459	L
H-H_	0	-4.670565	-2.941950	7.121091	L
H-H_	0	-6.821626	-2.486631	7.904734	L
H-H_	0	-7.704346	-0.313695	7.764281	L
H-H_	0	-6.458551	1.432507	6.834597	L
H-H_	0	-5.375790	2.500358	4.983044	L
H-H_	0	-4.803723	2.994395	6.649281	L
H-H_	0	-3.884169	4.385625	4.717266	L
H-H_	0	-3.051047	2.916347	4.141895	L
H-H_	0	-1.741204	4.763060	8.932484	L

f) Gaussian input files for Sample crystallized from acetone 1c)

```
%chk=koron_219_aceton.chk
%mem=4096MB
%nproc=4
# nmr oniom (b3lyp/6-311++g(d,p):uff)

Sample crystallized from acetone 1c)

0 1 0 1 0 1
O-O_3      0      8.670271      0.457323      -1.854762 L
O-O_3      0      8.896580      3.143410      -0.878332 L
O-O_3      0      5.464012      3.834671      -0.066479 L
O-O_3      0      5.958612      0.190170      1.839238 L
O-O_3      0      7.415911      -1.592798      3.081962 L
O-O_3      0     11.863214      -2.536650      3.701098 L
O-O_3      0     11.632218      -0.109932      1.063883 L
N-N_3      0     10.713233      1.106306      -1.113593 L
N-N_3      0      6.493315      1.896091      -0.620806 L
N-N_3      0     10.146840      -2.067033      2.279700 L
C-C_3      0     11.762366      0.579549      -3.786331 L
C-C_3      0     12.193955      0.249152      -5.064829 L
C-C_3      0     11.351014      -0.389097      -5.955480 L
C-C_3      0     10.065721      -0.715461      -5.566169 L
C-C_3      0      9.625964      -0.395150      -4.288824 L
C-C_3      0     10.461837      0.260945      -3.393260 L
C-C_3      0      9.883874      0.609866      -2.056048 L
C-C_3      0     10.236775      1.514391      0.168870 L
C-C_3      0     10.711200      0.878639      1.309358 L
C-C_3      0     10.241443      1.222637      2.577104 L
C-C_3      0      9.283685      2.227192      2.673161 L
C-C_3      0      8.805545      2.887889      1.560673 L
C-C_3      0      9.289614      2.542288      0.292327 L
C-C_3      0      7.734082      3.971515      -0.830483 L
C-C_3      0      6.453014      3.216540      -0.462571 L
C-C_3      0      5.346468      1.028433      -0.345655 L
C-C_3      0      4.976273      0.950200      1.120214 L
C-C_3      0      5.587366      -0.105369      3.126820 L
C-C_3      0      4.489876      0.463974      3.774591 L
C-C_3      0      4.153547      0.070049      5.069781 L
C-C_3      0      4.917084      -0.862461      5.726413 L
C-C_3      0      6.031423      -1.430417      5.089809 L
C-C_3      0      6.369364      -1.066691      3.789207 L
C-C_3      0      8.225407      -2.577322      3.746802 L
C-C_3      0      9.232758      -3.098228      2.747532 L
C-C_3      0     11.357186      -1.883401      2.785548 L
C-C_3      0     12.209484      -0.777503      2.176360 L
O-O_3      0     -8.669870      -0.457275      1.855022 L
O-O_3      0     -8.896096      -3.143393      0.878547 L
O-O_3      0     -5.463575      -3.834530      0.066742 L
O-O_3      0     -5.958127      -0.190153      -1.839023 L
O-O_3      0     -7.415426      1.592814      -3.081747 L
O-O_3      0    -11.862729      2.536667      -3.700883 L
O-O_3      0    -11.631817      0.109980      -1.063623 L
N-N_3      0    -10.712832      -1.106258      1.113853 L
N-N_3      0     -6.492830      -1.896074      0.621021 L
N-N_3      0    -10.146355      2.067049      -2.279485 L
C-C_3      0    -11.762006      -0.579482      3.786500 L
C-C_3      0    -12.193470      -0.249136      5.065044 L
C-C_3      0    -11.350613      0.389145      5.955739 L
```



C-C_3	0	-10.065320	0.715509	5.566428	L
C-C_3	0	-9.625479	0.395167	4.289039	L
C-C_3	0	-10.461436	-0.260897	3.393520	L
C-C_3	0	-9.883473	-0.609818	2.056307	L
C-C_3	0	-10.236374	-1.514343	-0.168611	L
C-C_3	0	-10.710799	-0.878591	-1.309099	L
C-C_3	0	-10.241043	-1.222589	-2.576845	L
C-C_3	0	-9.283200	-2.227175	-2.672946	L
C-C_3	0	-8.805144	-2.887841	-1.560413	L
C-C_3	0	-9.289213	-2.542240	-0.292068	L
C-C_3	0	-7.733597	-3.971499	0.830698	L
C-C_3	0	-6.452613	-3.216491	0.462830	L
C-C_3	0	-5.346067	-1.028385	0.345914	L
C-C_3	0	-4.975872	-0.950152	-1.119955	L
C-C_3	0	-5.586881	0.105386	-3.126605	L
C-C_3	0	-4.489475	-0.463926	-3.774332	L
C-C_3	0	-4.153146	-0.070001	-5.069522	L
C-C_3	0	-4.916599	0.862478	-5.726198	L
C-C_3	0	-6.030938	1.430434	-5.089594	L
C-C_3	0	-6.368880	1.066707	-3.788992	L
C-C_3	0	-8.225006	2.577370	-3.746543	L
C-C_3	0	-9.232357	3.098276	-2.747273	L
C-C_3	0	-11.356785	1.883449	-2.785289	L
C-C_3	0	-12.209084	0.777551	-2.176100	L
O-O_3	0	-2.615106	0.125432	2.483075	L
O-O_3	0	-2.021836	2.414089	4.367312	L
O-O_3	0	1.569408	2.487039	4.067912	L
O-O_3	0	0.466765	2.417982	0.091869	L
O-O_3	0	-1.290669	3.364034	-1.583079	L
O-O_3	0	-5.639713	4.215170	-2.252617	L
O-O_3	0	-5.311297	2.808737	1.063505	L
N-N_3	0	-4.285099	1.495945	3.191127	L
N-N_3	0	-0.042128	1.406667	2.868920	L
N-N_3	0	-4.160861	2.702208	-1.454162	L
C-C_3	0	-5.859859	-0.865358	3.780465	L
C-C_3	0	-6.521600	-2.007542	4.218666	L
C-C_3	0	-5.823017	-3.190033	4.403359	L
C-C_3	0	-4.459637	-3.240075	4.133604	L
C-C_3	0	-3.791108	-2.106031	3.689649	L
C-C_3	0	-4.487420	-0.904471	3.529488	L
C-C_3	0	-3.721791	0.284365	3.032725	L
C-C_3	0	-3.651184	2.682500	2.709020	L
C-C_3	0	-4.200926	3.383586	1.634915	L
C-C_3	0	-3.601697	4.555426	1.168773	L
C-C_3	0	-2.405095	4.967829	1.742807	L
C-C_3	0	-1.818676	4.270007	2.778233	L
C-C_3	0	-2.465656	3.143640	3.297158	L
C-C_3	0	-0.692900	2.668002	4.831294	L
C-C_3	0	0.385953	2.174745	3.874953	L
C-C_3	0	0.858710	0.840044	1.870691	L
C-C_3	0	1.470066	1.875254	0.954846	L
C-C_3	0	0.889712	3.439834	-0.724192	L
C-C_3	0	2.196089	3.928655	-0.748160	L
C-C_3	0	2.522132	4.993063	-1.597726	L
C-C_3	0	1.567509	5.574640	-2.376573	L
C-C_3	0	0.257485	5.072348	-2.389394	L
C-C_3	0	-0.071425	3.988834	-1.577930	L
C-C_3	0	-2.248613	3.810603	-2.545153	L
C-C_3	0	-3.331629	2.750348	-2.649533	L
C-C_3	0	-5.221860	3.500873	-1.336182	L
C-C_3	0	-5.954544	3.513798	0.000132	L

O-O_3	0	2.615505	-0.125381	-2.482809	H
O-O_3	0	2.022323	-2.414072	-4.367097	H
O-O_3	0	-1.569050	-2.486973	-4.067741	H
O-O_3	0	-0.466362	-2.417927	-0.091616	H
O-O_3	0	1.291159	-3.364029	1.583296	H
O-O_3	0	5.640116	-4.215124	2.252875	H
O-O_3	0	5.311697	-2.808691	-1.063245	H
N-N_3	0	4.285583	-1.495926	-3.190911	H
N-N_3	0	0.042533	-1.406619	-2.868662	H
N-N_3	0	4.161303	-2.702169	1.454291	H
C-C_3	0	5.860222	0.865423	-3.780295	H
C-C_3	0	6.522001	2.007591	-4.218407	H
C-C_3	0	5.823502	3.190050	-4.403143	H
C-C_3	0	4.460036	3.240124	-4.133343	H
C-C_3	0	3.791592	2.106047	-3.689433	H
C-C_3	0	4.487821	0.904517	-3.529230	H
C-C_3	0	3.722275	-0.284344	-3.032513	H
C-C_3	0	3.651669	-2.682484	-2.708805	H
C-C_3	0	4.201328	-3.383540	-1.634656	H
C-C_3	0	3.602098	-4.555379	-1.168514	H
C-C_3	0	2.405496	-4.967782	-1.742549	H
C-C_3	0	1.819161	-4.269989	-2.778017	H
C-C_3	0	2.466140	-3.143623	-3.296944	H
C-C_3	0	0.693300	-2.667955	-4.831034	H
C-C_3	0	-0.385469	-2.174724	-3.874739	H
C-C_3	0	-0.858226	-0.840038	-1.870482	H
C-C_3	0	-1.469665	-1.875210	-0.954590	H
C-C_3	0	-0.889314	-3.439783	0.724453	H
C-C_3	0	-2.195607	-3.928634	0.748379	H
C-C_3	0	-2.521771	-4.992997	1.597896	H
C-C_3	0	-1.567024	-5.574624	2.376786	H
C-C_3	0	-0.257000	-5.072328	2.389608	H
C-C_3	0	0.071827	-3.988788	1.578188	H
C-C_3	0	2.249012	-3.810551	2.545416	H
C-C_3	0	3.332030	-2.750301	2.649790	H
C-C_3	0	5.222259	-3.500824	1.336442	H
C-C_3	0	5.954948	-3.513745	0.000127	H
O-O_3	0	8.247373	-1.209358	0.361931	L
O-O_3	0	-8.246889	1.209374	-0.361716	L
O-O_3	0	4.699151	5.600920	1.937738	L
O-O_3	0	-4.698790	-5.600855	-1.937567	H
O-O_3	0	-2.337065	1.164491	-0.029717	L
O-O_3	0	2.337550	-1.164470	0.029933	H
O-O_3	0	-7.765314	5.869360	-2.385192	L
O-O_3	0	7.765797	-5.869344	2.385407	H
O-O_3	0	2.822836	5.098926	3.914563	L
O-O_3	0	-2.822349	-5.098908	-3.914349	H
O-O_3	0	-0.281953	8.864561	1.473877	L
C-C_3	0	0.804337	8.336265	1.650533	L
C-C_3	0	1.001507	6.892334	1.244264	L
C-C_3	0	1.963011	9.084957	2.225067	L
O-O_3	0	0.282439	-8.864544	-1.473661	H
C-C_3	0	-0.803900	-8.336121	-1.650272	H
C-C_3	0	-1.001106	-6.892287	-1.244007	H
C-C_3	0	-1.962528	-9.084941	-2.224852	H
H-H_	0	-2.111498	-8.795168	-3.274434	H
H-H_	0	11.630415	1.254558	-1.293753	L
H-H_	0	6.945958	1.659857	-1.508491	L
H-H_	0	10.043266	-1.778358	1.397305	L
H-H_	0	12.424651	0.200098	-3.128056	L
H-H_	0	12.645988	1.036234	-5.503063	L

H-H_	0	11.809399	-1.184588	-6.371308	L
H-H_	0	9.397054	-0.412964	-6.256783	L
H-H_	0	9.181417	-1.301243	-3.822329	L
H-H_	0	9.894400	0.413973	3.064410	L
H-H_	0	9.456766	2.832482	3.462628	L
H-H_	0	8.909028	3.986751	1.705201	L
H-H_	0	7.877444	4.743714	-0.198031	L
H-H_	0	7.584584	4.413207	-1.837668	L
H-H_	0	5.557392	0.002305	-0.715962	L
H-H_	0	4.464507	1.413858	-0.897003	L
H-H_	0	4.882913	1.974274	1.539079	L
H-H_	0	3.998220	0.433118	1.186448	L
H-H_	0	4.577483	1.570714	3.772704	L
H-H_	0	3.065491	-0.152377	5.132483	L
H-H_	0	4.300073	-1.654168	6.205564	L
H-H_	0	6.827175	-1.330389	5.699418	L
H-H_	0	8.768998	-2.119168	4.602285	L
H-H_	0	7.598250	-3.423352	4.105963	L
H-H_	0	8.742165	-3.488740	1.957201	L
H-H_	0	9.798004	-3.933736	3.216594	L
H-H_	0	12.502622	-0.051760	2.967628	L
H-H_	0	13.067231	-1.199803	1.857771	L
H-H_	0	-11.630017	-1.254495	1.294004	L
H-H_	0	-6.945532	-1.659734	1.508632	L
H-H_	0	-10.051412	1.793251	-1.390681	L
H-H_	0	-12.424243	-0.199837	3.128287	L
H-H_	0	-12.645540	-1.036204	5.503263	L
H-H_	0	-11.809029	1.184673	6.371462	L
H-H_	0	-9.396656	0.413084	6.257076	L
H-H_	0	-9.180951	1.301263	3.822533	L
H-H_	0	-9.894654	-0.414009	-3.064760	L
H-H_	0	-9.456350	-2.832508	-3.462363	L
H-H_	0	-8.908549	-3.986711	-1.704937	L
H-H_	0	-7.876932	-4.743672	0.198209	L
H-H_	0	-7.584102	-4.413212	1.837873	L
H-H_	0	-5.553137	-0.002597	0.718435	L
H-H_	0	-4.464133	-1.415454	0.896228	L
H-H_	0	-4.882689	-1.974253	-1.538810	L
H-H_	0	-3.997800	-0.433287	-1.186472	L
H-H_	0	-4.577083	-1.570667	-3.772434	L
H-H_	0	-3.065063	0.152275	-5.132296	L
H-H_	0	-4.299537	1.654217	-6.205231	L
H-H_	0	-6.826695	1.330417	-5.699199	L
H-H_	0	-8.768517	2.119316	-4.602128	L
H-H_	0	-7.597960	3.423745	-4.105333	L
H-H_	0	-8.741353	3.489199	-1.957398	L
H-H_	0	-9.797615	3.933846	-3.216233	L
H-H_	0	-12.502227	0.051809	-2.967366	L
H-H_	0	-13.066826	1.199856	-1.857511	L
H-H_	0	-5.262509	1.548906	3.395954	L
H-H_	0	-0.989994	1.033102	2.839584	L
H-H_	0	-3.727297	2.209495	-0.674050	L
H-H_	0	-6.419650	0.069956	3.636434	L
H-H_	0	-7.599062	-1.969116	4.412055	L
H-H_	0	-6.346133	-4.087231	4.751181	L
H-H_	0	-3.908961	-4.180465	4.252736	L
H-H_	0	-2.718982	-2.161008	3.458957	L
H-H_	0	-4.037690	5.146860	0.353635	L
H-H_	0	-1.881815	5.856980	1.352620	L
H-H_	0	-0.864948	4.618671	3.199234	L
H-H_	0	-0.546900	3.740542	5.070800	L

H-H_	0	-0.687381	2.095836	5.775720	L
H-H_	0	1.685917	0.282818	2.364863	L
H-H_	0	0.280256	0.090007	1.285168	L
H-H_	0	2.205312	1.386528	0.288342	L
H-H_	0	1.989841	2.684392	1.510985	L
H-H_	0	2.961594	3.508699	-0.086175	L
H-H_	0	3.554422	5.359723	-1.613445	L
H-H_	0	1.812990	6.427998	-3.017930	L
H-H_	0	-0.485282	5.533986	-3.051403	L
H-H_	0	-1.769718	3.966675	-3.533642	L
H-H_	0	-2.651011	4.790445	-2.217094	L
H-H_	0	-3.945260	2.950433	-3.552545	L
H-H_	0	-2.882782	1.742279	-2.787730	L
H-H_	0	-6.958089	3.096829	-0.053064	L
H-H_	0	-6.108304	4.577166	0.297370	L
H-H_	0	5.257878	-1.552507	-3.417077	H
H-H_	0	0.989909	-1.032504	-2.840377	H
H-H_	0	3.721354	-2.219607	0.671239	H
H-H_	0	6.419529	-0.070792	-3.640774	H
H-H_	0	7.599279	1.968737	-4.413184	H
H-H_	0	6.346562	4.087047	-4.751689	H
H-H_	0	3.909245	4.180403	-4.252932	H
H-H_	0	2.719305	2.160759	-3.459140	H
H-H_	0	4.034530	-5.145931	-0.351182	H
H-H_	0	1.885071	-5.857273	-1.350101	H
H-H_	0	0.865453	-4.618383	-3.199278	H
H-H_	0	0.547416	-3.740571	-5.070329	H
H-H_	0	0.687873	-2.095994	-5.775573	H
H-H_	0	-1.685482	-0.282803	-2.364586	H
H-H_	0	-0.280016	-0.089907	-1.284794	H
H-H_	0	-2.205361	-1.386974	-0.288254	H
H-H_	0	-1.989356	-2.684434	-1.510666	H
H-H_	0	-2.961196	-3.508828	0.086287	H
H-H_	0	-3.554077	-5.359753	1.613287	H
H-H_	0	-1.812388	-6.428189	3.017861	H
H-H_	0	0.485799	-5.534144	3.051399	H
H-H_	0	1.770019	-3.966613	3.533787	H
H-H_	0	2.651468	-4.790374	2.217293	H
H-H_	0	3.945897	-2.950289	3.552632	H
H-H_	0	2.883209	-1.742249	2.787809	H
H-H_	0	6.910353	-2.959488	0.070376	H
H-H_	0	6.198749	-4.554312	-0.297039	H
H-H_	0	7.524268	-1.371223	-0.237215	L
H-H_	0	8.149518	-0.333189	0.713745	L
H-H_	0	-7.639976	1.062109	0.279293	L
H-H_	0	-8.246951	0.366325	-0.878096	L
H-H_	0	4.336891	6.463114	1.752369	L
H-H_	0	5.530478	5.719750	2.386201	L
H-H_	0	-4.419113	-6.501016	-1.796338	H
H-H_	0	-5.547608	-5.619350	-2.368359	H
H-H_	0	-1.470243	1.564837	-0.003040	L
H-H_	0	-2.495711	0.737117	0.816681	L
H-H_	0	1.472437	-1.569264	0.030724	H
H-H_	0	2.474907	-0.750399	-0.826265	H
H-H_	0	-7.014728	5.328424	-2.129864	L
H-H_	0	-7.748400	5.956116	-3.331110	L
H-H_	0	7.025945	-5.316408	2.125456	H
H-H_	0	7.773717	-5.911656	3.334443	H
H-H_	0	2.432130	4.226256	4.028435	L
H-H_	0	3.477661	5.040668	3.213791	L
H-H_	0	-2.434926	-4.224268	-4.024101	H

H-H_	0	-3.463421	-5.051296	-3.200306	H
H-H_	0	1.436880	6.828796	0.236253	L
H-H_	0	0.045410	6.338621	1.229026	L
H-H_	0	1.681008	6.370631	1.934099	L
H-H_	0	1.822865	10.173257	2.199946	L
H-H_	0	2.888082	8.848134	1.682664	L
H-H_	0	2.113885	8.791981	3.273515	L
H-H_	0	-1.591598	-6.820144	-0.319853	H
H-H_	0	-0.039152	-6.378572	-1.070479	H
H-H_	0	-1.533779	-6.336252	-2.029971	H
H-H_	0	-1.823343	-10.173340	-2.196210	H
H-H_	0	-2.888277	-8.845763	-1.684601	H