

“Quantum chemical studies of the adsorption of single acetone molecules on hexagonal ice I_h and cubic ice I_c ”

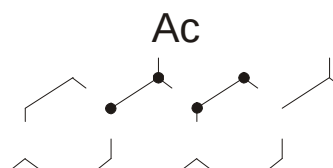
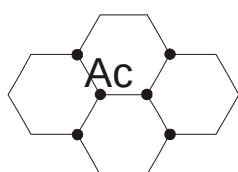
Author: Dr. Holger Somnitz

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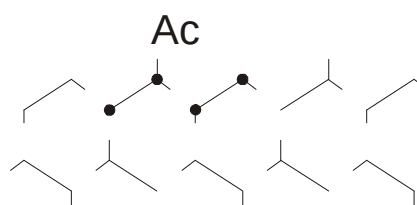
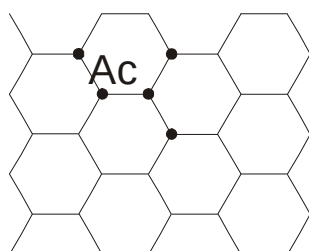
I. Relevant cluster representations considered for ice I_h :

Schematic top/side views:

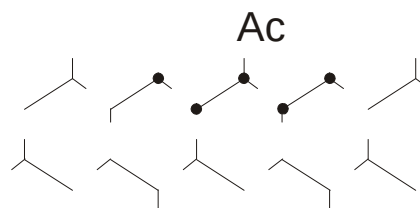
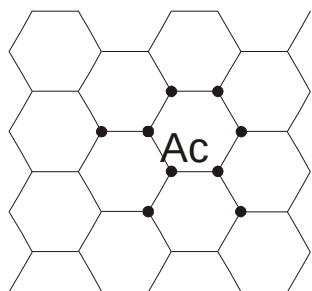
Ih-CL3: 24 x H_2O (6 unconstrained) + acetone (unconstrained)



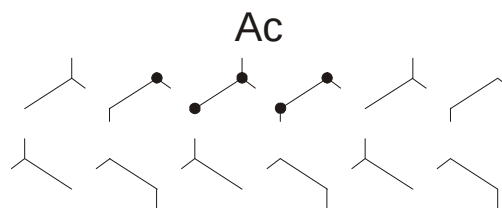
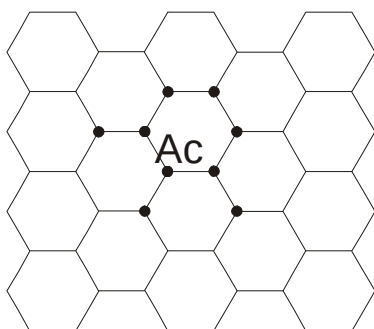
Ih-CL4: 70 x H_2O (5 unconstrained) + acetone (unconstrained)



Ih-CL6: 80 x H₂O (9 unconstrained) + acetone (unconstrained)



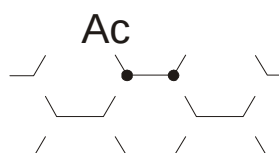
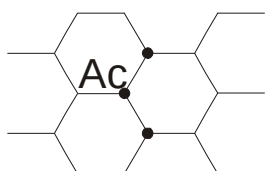
Ih-CL7: 108 x H₂O (9 unconstrained) + acetone (unconstrained)



II. Relevant cluster representations considered for ice Ic:

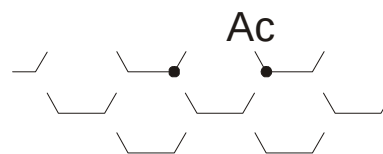
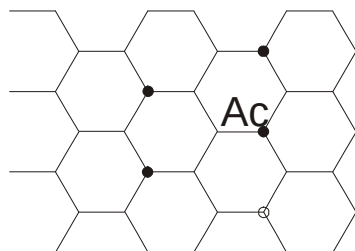
Schematic top/side views:

Ic-CL1: 30 x H₂O (3 unconstrained) + acetone (unconstrained)

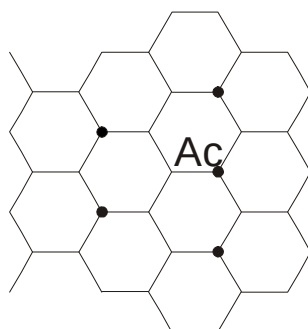


Ic-CL2: 57 x H₂O (4 unconstrained) + acetone (unconstrained)

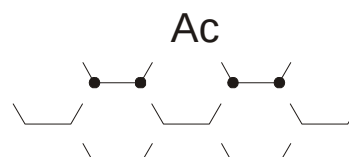
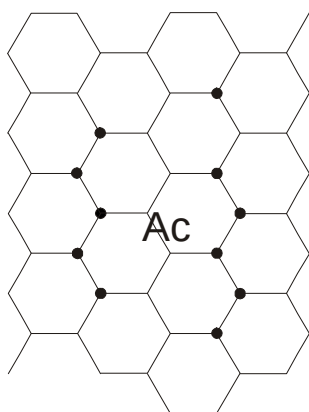
Ic-CL3: 39 x H₂O (5 unconstrained) + acetone (unconstrained)



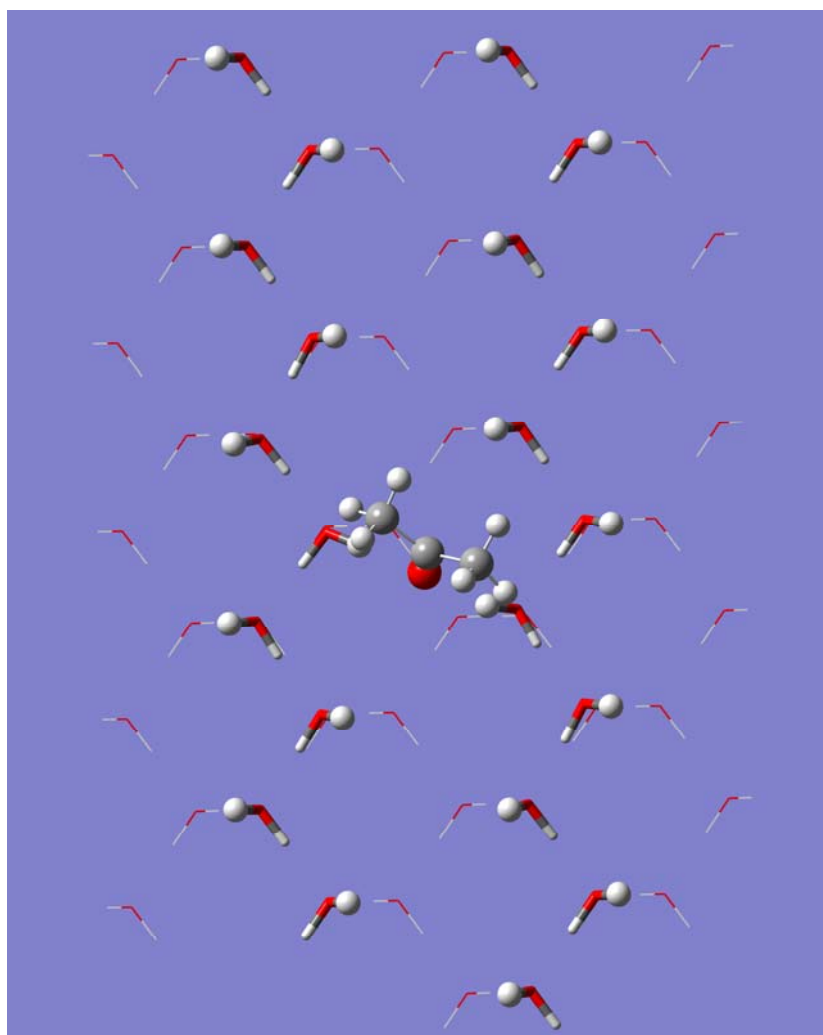
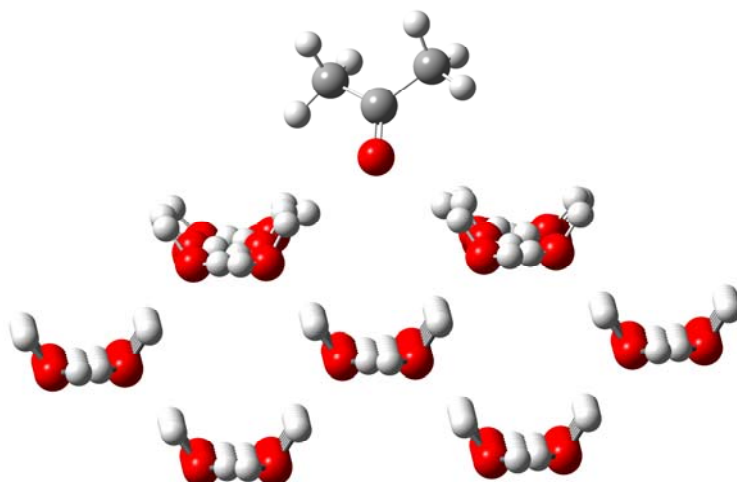
Ic-CL4: 39 x H₂O (5 unconstrained) + acetone (unconstrained)



Ic-CL5: 73 x H₂O (11 unconstrained) + acetone (unconstrained)



II. Pictorial side/top views of **Ic-CL5** (lying)



III. Selected coordinate files (XYZ-files, coordinates in Angstroms)

Ih-CL6 + acetone:

2 Layer- ONIOM (B3LYP/6-31+G(d):HF/3-21+G*) constrained optimisation:

```
250
2 bi-layer/250 atoms/80*H2O + acetone
O      0.091783      8.247383      6.775861
O      0.091783     15.864523      6.775861
O      0.091783     23.481664      6.775861
H      0.893836      7.773369      7.113885
H      0.893836     15.390509      7.113885
H      0.893836     23.007650      7.113885
H     -0.711012      7.776872      7.117785
H     -0.711012     15.394012      7.117785
H     -0.711012     23.011153      7.117785
O      2.308006     12.066389      6.764232
O      2.308006     19.683530      6.764232
H      2.305878     12.062275      5.773128
H      2.305878     19.679415      5.773128
H      3.124070     11.597401      7.075893
H      3.124070     19.214541      7.075893
O      4.491913      8.247383      6.775861
O      4.491913     15.864523      6.775861
O      4.491913     23.481664      6.775861
O      8.892044      8.247383      6.775861
O      8.892044     15.864523      6.775861
O      8.892044     23.481664      6.775861
O     13.292174      8.247383      6.775861
O     13.292174     15.864523      6.775861
O     13.292174     23.481664      6.775861
H      5.293966      7.773369      7.113885
H      5.293966     15.390509      7.113885
H      5.293966     23.007650      7.113885
H      9.694097      7.773369      7.113885
H      9.694097     15.390509      7.113885
H      9.694097     23.007650      7.113885
H     14.094227      7.773369      7.113885
H     14.094227     15.390509      7.113885
H     14.094227     23.007650      7.113885
H      3.689118      7.776872      7.117785
H      3.689118     15.394012      7.117785
H      3.689118     23.011153      7.117785
H      8.089249      7.776872      7.117785
H      8.089249     15.394012      7.117785
H      8.089249     23.011153      7.117785
H     12.489379      7.776872      7.117785
H     12.489379     15.394012      7.117785
H     12.489379     23.011153      7.117785
O      6.708137     12.066389      6.764232
O      6.708137     19.683530      6.764232
O     11.108267     12.066389      6.764232
O     11.108267     19.683530      6.764232
O     15.508397     12.066389      6.764232
O     15.508397     19.683530      6.764232
H      6.706009     12.062275      5.773128
H      6.706009     19.679415      5.773128
H     11.106139     12.062275      5.773128
H     11.106139     19.679415      5.773128
H     15.506269     12.062275      5.773128
H     15.506269     19.679415      5.773128
H      7.524201     11.597401      7.075893
H      7.524201     19.214541      7.075893
H     11.924331     11.597401      7.075893
H     11.924331     19.214541      7.075893
```

H	16.324461	11.597401	7.075893
H	16.324461	19.214541	7.075893
O	2.294837	6.987584	7.685708
H	2.308896	6.977377	8.677245
H	2.301130	6.050142	7.362925
O	2.343533	6.986899	10.387226
H	3.145586	7.460913	10.725250
H	1.540738	7.457410	10.729150
O	6.694968	6.987584	7.685708
O	11.095098	6.987584	7.685708
O	15.495228	6.987584	7.685708
H	6.709027	6.977377	8.677245
H	11.109157	6.977377	8.677245
H	15.509287	6.977377	8.677245
H	6.701261	6.050142	7.362925
H	11.101391	6.050142	7.362925
H	15.501521	6.050142	7.362925
O	6.743664	6.986899	10.387226
O	11.143794	6.986899	10.387226
O	15.543924	6.986899	10.387226
H	7.545717	7.460913	10.725250
H	11.945847	7.460913	10.725250
H	16.345977	7.460913	10.725250
H	5.940868	7.457410	10.729150
H	10.340999	7.457410	10.729150
H	14.741129	7.457410	10.729150
O	2.294837	14.604724	7.685708
O	2.294837	22.221865	7.685708
O	2.360800	12.058238	11.277067
O	2.360800	19.675379	11.277067
O	0.159626	10.785033	10.375598
O	0.159626	18.402173	10.375598
H	2.308896	14.594517	8.677245
H	2.308896	22.211658	8.677245
H	2.301130	13.667283	7.362925
H	2.301130	21.284424	7.362925
H	2.367124	12.993547	10.947204
H	2.367124	20.610688	10.947204
H	3.173290	11.604561	10.936226
H	3.173290	19.221701	10.936226
H	0.157498	10.789147	9.384495
H	0.157498	18.406287	9.384495
H	0.975690	11.254021	10.687258
H	0.975690	18.871161	10.687258
O	0.146457	8.246698	11.297074
O	0.146457	15.863838	11.297074
O	0.146457	23.480979	11.297074
O	0.109050	10.793184	7.665701
O	0.109050	18.410324	7.665701
O	2.343533	14.604039	10.387226
O	2.343533	22.221180	10.387226
H	0.160516	8.256905	12.288610
H	0.160516	15.874045	12.288610
H	0.160516	23.491186	12.288610
H	0.152750	9.184139	10.974290
H	0.152750	16.801279	10.974290
H	0.152750	24.418420	10.974290
H	0.115373	9.857875	7.335839
H	0.115373	17.475015	7.335839
H	0.921540	11.246861	7.324861
H	0.921540	18.864001	7.324861
H	3.145586	15.078053	10.725250
H	3.145586	22.695194	10.725250
H	1.540738	15.074550	10.729150
H	1.540738	22.691691	10.729150
O	6.694968	14.604724	7.685708
O	6.694968	22.221865	7.685708
O	11.095098	14.604724	7.685708
O	11.095098	22.221865	7.685708
O	15.495228	14.604724	7.685708

O	15.495228	22.221865	7.685708
O	6.723991	12.040245	11.383486
O	6.757806	19.620376	11.449021
O	11.161061	12.058238	11.277067
O	11.077196	19.621955	11.399673
O	15.561191	12.058238	11.277067
O	15.561191	19.675379	11.277067
O	4.559756	10.785033	10.375598
O	4.585734	18.329049	10.337841
O	8.959887	10.785033	10.375598
O	8.902869	18.324397	10.350018
O	13.360017	10.785033	10.375598
O	13.360017	18.402173	10.375598
H	6.709027	14.594517	8.677245
H	6.709027	22.211658	8.677245
H	11.109157	14.594517	8.677245
H	11.109157	22.211658	8.677245
H	15.509287	14.594517	8.677245
H	15.509287	22.211658	8.677245
H	6.701261	13.667283	7.362925
H	6.701261	21.284424	7.362925
H	11.101391	13.667283	7.362925
H	11.101391	21.284424	7.362925
H	15.501521	13.667283	7.362925
H	15.501521	21.284424	7.362925
H	6.721677	12.967214	11.057819
H	6.748817	20.524279	11.066986
H	11.167385	12.993547	10.947204
H	11.095670	20.529483	11.027877
H	15.567515	12.993547	10.947204
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H	7.541737	11.629457	11.022206
H	7.528319	19.163534	11.028818
H	11.973551	11.604561	10.936226
H	11.872533	19.175833	11.033427
H	16.373681	11.604561	10.936226
H	16.373681	19.221701	10.936226
H	4.557628	10.789147	9.384495
H	4.533423	18.378033	9.340901
H	8.957759	10.789147	9.384495
H	8.880389	18.377618	9.355204
H	13.357889	10.789147	9.384495
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H	5.384729	18.825231	10.645331
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H	9.703015	18.816683	10.667956
H	14.176081	11.254021	10.687258
H	14.176081	18.871161	10.687258
O	4.546587	8.246698	11.297074
O	4.555250	15.939789	11.424390
O	4.546587	23.480979	11.297074
O	8.946718	8.246698	11.297074
O	8.969881	15.862666	11.411042
O	8.946718	23.480979	11.297074
O	13.346848	8.246698	11.297074
O	13.346848	15.863838	11.297074
O	13.346848	23.480979	11.297074
O	4.509180	10.793184	7.665701
O	4.509180	18.410324	7.665701
O	8.909311	10.793184	7.665701
O	8.909311	18.410324	7.665701
O	13.309441	10.793184	7.665701
O	13.309441	18.410324	7.665701
O	6.731384	14.664352	10.359132
O	6.743664	22.221180	10.387226
O	11.079762	14.664161	10.311199
O	11.143794	22.221180	10.387226
O	15.543924	14.604039	10.387226
O	15.543924	22.221180	10.387226

H	4.560646	8.256905	12.288610
H	4.262023	16.051502	12.340796
H	4.560646	23.491186	12.288610
H	8.960777	8.256905	12.288610
H	8.983395	16.012767	12.385127
H	8.960777	23.491186	12.288610
H	13.360907	8.256905	12.288610
H	13.360907	15.874045	12.288610
H	13.360907	23.491186	12.288610
H	4.552880	9.184139	10.974290
H	4.540519	16.856991	11.005890
H	4.552880	24.418420	10.974290
H	8.953011	9.184139	10.974290
H	8.936585	16.771960	10.999483
H	8.953011	24.418420	10.974290
H	13.353141	9.184139	10.974290
H	13.353141	16.801279	10.974290
H	13.353141	24.418420	10.974290
H	4.515503	9.857875	7.335839
H	4.515503	17.475015	7.335839
H	8.915634	9.857875	7.335839
H	8.915634	17.475015	7.335839
H	13.315764	9.857875	7.335839
H	13.315764	17.475015	7.335839
H	5.321670	11.246861	7.324861
H	5.321670	18.864001	7.324861
H	9.721801	11.246861	7.324861
H	9.721801	18.864001	7.324861
H	14.121931	11.246861	7.324861
H	14.121931	18.864001	7.324861
H	7.512995	15.076640	10.799649
H	7.545717	22.695194	10.725250
H	11.841842	15.110688	10.735173
H	11.945847	22.695194	10.725250
H	16.345977	15.078053	10.725250
H	16.345977	22.695194	10.725250
H	5.945437	15.068340	10.800716
H	5.940868	22.691691	10.729150
H	10.272186	15.058679	10.751153
H	10.340999	22.691691	10.729150
H	14.741129	15.074550	10.729150
H	14.741129	22.691691	10.729150
H	6.802165	18.291732	13.462983
C	6.801526	17.360010	14.049477
H	6.009341	17.441840	14.801708
H	6.584448	16.540968	13.359581
C	8.156287	17.172309	14.686385
O	9.055433	16.547261	14.130059
C	8.382810	17.798734	16.044637
H	9.437518	17.743049	16.322782
H	8.042673	18.841772	16.048469
H	7.781057	17.267115	16.794119

Ih-CL7 + acetone:

2 Layer- ONIOM (B3LYP/6-31G(d):HF/3-21+G*) constrained optimisation:

```

334
2 bi-layer/334 atoms/108*H2O + acetone
O      0.09178300    8.24738300    6.77586100
O      0.09178300    15.86452300    6.77586100
O      0.09178300    23.48166400    6.77586100
H      0.89383600     7.77336900    7.11388500
H      0.89383600    15.39050900    7.11388500
H      0.89383600    23.00765000    7.11388500

```


H	-0.71101200	7.77687200	7.11778500
H	-0.71101200	15.39401200	7.11778500
H	-0.71101200	23.01115300	7.11778500
O	2.30800600	12.06638900	6.76423200
O	2.30800600	19.68353000	6.76423200
H	2.30587800	12.06227500	5.77312800
H	2.30587800	19.67941500	5.77312800
H	3.12407000	11.59740100	7.07589300
H	3.12407000	19.21454100	7.07589300
O	4.49191300	8.24738300	6.77586100
O	4.49191300	15.86452300	6.77586100
O	4.49191300	23.48166400	6.77586100
O	8.89204400	8.24738300	6.77586100
O	8.89204400	15.86452300	6.77586100
O	8.89204400	23.48166400	6.77586100
O	13.29217400	8.24738300	6.77586100
O	13.29217400	15.86452300	6.77586100
O	13.29217400	23.48166400	6.77586100
H	5.29396600	7.77336900	7.11388500
H	5.29396600	15.39050900	7.11388500
H	5.29396600	23.00765000	7.11388500
H	9.69409700	7.77336900	7.11388500
H	9.69409700	15.39050900	7.11388500
H	9.69409700	23.00765000	7.11388500
H	14.09422700	7.77336900	7.11388500
H	14.09422700	15.39050900	7.11388500
H	14.09422700	23.00765000	7.11388500
H	3.68911800	7.77687200	7.11778500
H	3.68911800	15.39401200	7.11778500
H	3.68911800	23.01115300	7.11778500
H	8.08924900	7.77687200	7.11778500
H	8.08924900	15.39401200	7.11778500
H	8.08924900	23.01115300	7.11778500
H	12.48937900	7.77687200	7.11778500
H	12.48937900	15.39401200	7.11778500
H	12.48937900	23.01115300	7.11778500
O	6.70813700	12.06638900	6.76423200
O	6.70813700	19.68353000	6.76423200
O	11.10826700	12.06638900	6.76423200
O	11.10826700	19.68353000	6.76423200
O	15.50839700	12.06638900	6.76423200
O	15.50839700	19.68353000	6.76423200
H	6.70600900	12.06227500	5.77312800
H	6.70600900	19.67941500	5.77312800
H	11.10613900	12.06227500	5.77312800
H	11.10613900	19.67941500	5.77312800
H	15.50626900	12.06227500	5.77312800
H	15.50626900	19.67941500	5.77312800
H	7.52420100	11.59740100	7.07589300
H	7.52420100	19.21454100	7.07589300
H	11.92433100	11.59740100	7.07589300
H	11.92433100	19.21454100	7.07589300
H	16.32446100	11.59740100	7.07589300
H	16.32446100	19.21454100	7.07589300
O	2.29483700	6.98758400	7.68570800
H	2.30889600	6.97737700	8.67724500
H	2.30113000	6.05014200	7.36292500
O	2.34353300	6.98689900	10.38722600
H	3.14558600	7.46091300	10.72525000
H	1.54073800	7.45741000	10.72915000
O	6.69496800	6.98758400	7.68570800
O	11.09509800	6.98758400	7.68570800
O	15.49522800	6.98758400	7.68570800
H	6.70902700	6.97737700	8.67724500
H	11.10915700	6.97737700	8.67724500
H	15.50928700	6.97737700	8.67724500
H	6.70126100	6.05014200	7.36292500
H	11.10139100	6.05014200	7.36292500
H	15.50152100	6.05014200	7.36292500
O	6.74366400	6.98689900	10.38722600

O	11.14379400	6.98689900	10.38722600
O	15.54392400	6.98689900	10.38722600
H	7.54571700	7.46091300	10.72525000
H	11.94584700	7.46091300	10.72525000
H	16.34597700	7.46091300	10.72525000
H	5.94086800	7.45741000	10.72915000
H	10.34099900	7.45741000	10.72915000
H	14.74112900	7.45741000	10.72915000
O	2.29483700	14.60472400	7.68570800
O	2.29483700	22.22186500	7.68570800
O	2.36080000	12.05823800	11.27706700
O	2.36080000	19.67537900	11.27706700
O	0.15962600	10.78503300	10.37559800
O	0.15962600	18.40217300	10.37559800
H	2.30889600	14.59451700	8.67724500
H	2.30889600	22.21165800	8.67724500
H	2.30113000	13.66728300	7.36292500
H	2.30113000	21.28442400	7.36292500
H	2.36712400	12.99354700	10.94720400
H	2.36712400	20.61068800	10.94720400
H	3.17329000	11.60456100	10.93622600
H	3.17329000	19.22170100	10.93622600
H	0.15749800	10.78914700	9.38449500
H	0.15749800	18.40628700	9.38449500
H	0.97569000	11.25402100	10.68725800
H	0.97569000	18.87116100	10.68725800
O	0.14645700	8.24669800	11.29707400
O	0.14645700	15.86383800	11.29707400
O	0.14645700	23.48097900	11.29707400
O	0.10905000	10.79318400	7.66570100
O	0.10905000	18.41032400	7.66570100
O	2.34353300	14.60403900	10.38722600
O	2.34353300	22.22118000	10.38722600
H	0.16051600	8.25690500	12.28861000
H	0.16051600	15.87404500	12.28861000
H	0.16051600	23.49118600	12.28861000
H	0.15275000	9.18413900	10.97429000
H	0.15275000	16.80127900	10.97429000
H	0.15275000	24.41842000	10.97429000
H	0.11537300	9.85787500	7.33583900
H	0.11537300	17.47501500	7.33583900
H	0.92154000	11.24686100	7.32486100
H	0.92154000	18.86400100	7.32486100
H	3.14558600	15.07805300	10.72525000
H	3.14558600	22.69519400	10.72525000
H	1.54073800	15.07455000	10.72915000
H	1.54073800	22.69169100	10.72915000
O	6.69496800	14.60472400	7.68570800
O	6.69496800	22.22186500	7.68570800
O	11.09509800	14.60472400	7.68570800
O	11.09509800	22.22186500	7.68570800
O	15.49522800	14.60472400	7.68570800
O	15.49522800	22.22186500	7.68570800
O	6.71810100	11.99539200	11.43462700
O	6.74464600	19.59684100	11.40186700
O	11.16106100	12.05823800	11.27706700
O	11.04898500	19.58210300	11.40066800
O	15.56119100	12.05823800	11.27706700
O	15.56119100	19.67537900	11.27706700
O	4.55975600	10.78503300	10.37559800
O	4.60425400	18.28994000	10.30129200
O	8.95988700	10.78503300	10.37559800
O	8.90462900	18.30919900	10.31725900
O	13.36001700	10.78503300	10.37559800
O	13.36001700	18.40217300	10.37559800
H	6.70902700	14.59451700	8.67724500
H	6.70902700	22.21165800	8.67724500
H	11.10915700	14.59451700	8.67724500
H	11.10915700	22.21165800	8.67724500
H	15.50928700	14.59451700	8.67724500

H	15.50928700	22.21165800	8.67724500
H	6.70126100	13.66728300	7.36292500
H	6.70126100	21.28442400	7.36292500
H	11.10139100	13.66728300	7.36292500
H	11.10139100	21.28442400	7.36292500
H	15.50152100	13.66728300	7.36292500
H	15.50152100	21.28442400	7.36292500
H	6.71196000	12.91547000	11.08741200
H	6.73187200	20.52880400	11.08221900
H	11.16738500	12.99354700	10.94720400
H	11.06683600	20.50482300	11.06424200
H	15.56751500	12.99354700	10.94720400
H	15.56751500	20.61068800	10.94720400
H	7.52868500	11.59140600	11.04744200
H	7.52503800	19.17286300	10.96656900
H	11.97355100	11.60456100	10.93622600
H	11.86272600	19.16783300	11.03458300
H	16.37368100	11.60456100	10.93622600
H	16.37368100	19.22170100	10.93622600
H	4.55762800	10.78914700	9.38449500
H	4.52522800	18.36431200	9.30660600
H	8.95775900	10.78914700	9.38449500
H	8.88275000	18.37319400	9.32284100
H	13.35788900	10.78914700	9.38449500
H	13.35788900	18.40628700	9.38449500
H	5.37582000	11.25402100	10.68725800
H	5.39026900	18.81214200	10.60774000
H	9.77595100	11.25402100	10.68725800
H	9.70423100	18.80197900	10.65014000
H	14.17608100	11.25402100	10.68725800
H	14.17608100	18.87116100	10.68725800
O	4.54658700	8.24669800	11.29707400
O	4.61341000	15.92043800	11.31003900
O	4.54658700	23.48097900	11.29707400
O	8.94671800	8.24669800	11.29707400
O	8.96803000	15.85441600	11.28007000
O	8.94671800	23.48097900	11.29707400
O	13.34684800	8.24669800	11.29707400
O	13.34684800	15.86383800	11.29707400
O	13.34684800	23.48097900	11.29707400
O	4.50918000	10.79318400	7.66570100
O	4.50918000	18.41032400	7.66570100
O	8.90931100	10.79318400	7.66570100
O	8.90931100	18.41032400	7.66570100
O	13.30944100	10.79318400	7.66570100
O	13.30944100	18.41032400	7.66570100
O	6.74848700	14.59811000	10.31404300
O	6.74366400	22.22118000	10.38722600
O	11.10129200	14.66382600	10.27698400
O	11.14379400	22.22118000	10.38722600
O	15.54392400	14.60403900	10.38722600
O	15.54392400	22.22118000	10.38722600
H	4.56064600	8.25690500	12.28861000
H	4.39523800	16.05236300	12.24449300
H	4.56064600	23.49118600	12.28861000
H	8.96077700	8.25690500	12.28861000
H	8.97944500	16.00014000	12.25553600
H	8.96077700	23.49118600	12.28861000
H	13.36090700	8.25690500	12.28861000
H	13.36090700	15.87404500	12.28861000
H	13.36090700	23.49118600	12.28861000
H	4.55288000	9.18413900	10.97429000
H	4.59402500	16.85231700	10.89169900
H	4.55288000	24.41842000	10.97429000
H	8.95301100	9.18413900	10.97429000
H	8.93352300	16.77982300	10.88576100
H	8.95301100	24.41842000	10.97429000
H	13.35314100	9.18413900	10.97429000
H	13.35314100	16.80127900	10.97429000
H	13.35314100	24.41842000	10.97429000

H	4.51550300	9.85787500	7.33583900
H	4.51550300	17.47501500	7.33583900
H	8.91563400	9.85787500	7.33583900
H	8.91563400	17.47501500	7.33583900
H	13.31576400	9.85787500	7.33583900
H	13.31576400	17.47501500	7.33583900
H	5.32167000	11.24686100	7.32486100
H	5.32167000	18.86400100	7.32486100
H	9.72180100	11.24686100	7.32486100
H	9.72180100	18.86400100	7.32486100
H	14.12193100	11.24686100	7.32486100
H	14.12193100	18.86400100	7.32486100
H	7.53820800	15.04024900	10.71347300
H	7.54571700	22.69519400	10.72525000
H	11.86476200	15.11219700	10.70057900
H	11.94584700	22.69519400	10.72525000
H	16.34597700	15.07805300	10.72525000
H	16.34597700	22.69519400	10.72525000
H	5.96049800	15.03262500	10.72990100
H	5.94086800	22.69169100	10.72915000
H	10.28147700	15.07620400	10.68611400
H	10.34099900	22.69169100	10.72915000
H	14.74112900	15.07455000	10.72915000
H	14.74112900	22.69169100	10.72915000
H	6.79652500	18.29554100	13.15024100
C	6.79012400	17.35476200	13.72596500
H	5.95125500	17.40830800	14.42849800
H	6.63529300	16.54080400	13.01437100
C	8.10404100	17.19835300	14.44525300
O	9.04556800	16.56800100	13.97403100
C	8.24051200	17.88041800	15.79061300
H	9.27070800	17.81658900	16.14648700
H	7.92906700	18.92942500	15.71884400
H	7.57135800	17.40104400	16.51661800
O	13.36001700	26.01931300	10.37559800
H	14.17608100	26.48830100	10.68725800
H	13.35788900	26.02342700	9.38449500
H	13.31576400	25.09215500	7.33583900
O	13.30944100	26.02746400	7.66570100
H	14.12193100	26.48114100	7.32486100
O	8.95988700	26.01931300	10.37559800
H	9.77595100	26.48830100	10.68725800
H	8.95775900	26.02342700	9.38449500
H	8.91563400	25.09215500	7.33583900
O	8.90931100	26.02746400	7.66570100
H	9.72180100	26.48114100	7.32486100
O	4.55975700	26.01931300	10.37559800
H	5.37582100	26.48830100	10.68725800
H	4.55762900	26.02342700	9.38449500
H	4.51550400	25.09215500	7.33583900
O	4.50918100	26.02746400	7.66570100
H	5.32167100	26.48114100	7.32486100
O	0.15962700	26.01931300	10.37559800
H	0.97569100	26.48830100	10.68725800
H	0.15749900	26.02342700	9.38449500
H	0.11537400	25.09215500	7.33583900
O	0.10905100	26.02746400	7.66570100
H	0.92154100	26.48114100	7.32486100
O	11.16106100	27.29251900	11.27706700
H	11.97355100	26.83884100	10.93622600
H	11.16738500	28.22782800	10.94720400
O	11.10826700	27.30067000	6.76423200
H	11.92433100	26.83168100	7.07589300
H	11.10613900	27.29655500	5.77312800
O	6.76093100	27.29251900	11.27706700
H	7.57342100	26.83884100	10.93622600
H	6.76725500	28.22782800	10.94720400
O	6.70813700	27.30067000	6.76423200
H	7.52420100	26.83168100	7.07589300
H	6.70600900	27.29655500	5.77312800

O	2.36080100	27.29251900	11.27706700
H	3.17329100	26.83884100	10.93622600
H	2.36712500	28.22782800	10.94720400
O	2.30800700	27.30067000	6.76423200
H	3.12407100	26.83168100	7.07589300
H	2.30587900	27.29655500	5.77312800
O	15.56119100	27.29251900	11.27706700
H	16.37368100	26.83884100	10.93622600
H	15.56751500	28.22782800	10.94720400
O	15.50839700	27.30067000	6.76423200
H	16.32446100	26.83168100	7.07589300
H	15.50626900	27.29655500	5.77312800
O	17.76014700	26.01931300	10.37559800
H	18.57621100	26.48830100	10.68725800
H	17.75801900	26.02342700	9.38449500
H	17.71589400	25.09215500	7.33583900
O	17.70957100	26.02746400	7.66570100
H	18.52206100	26.48114100	7.32486100
O	17.76014700	18.40217300	10.37559800
H	18.57621100	18.87116100	10.68725800
H	17.75801900	18.40628700	9.38449500
H	17.71589400	17.47501500	7.33583900
O	17.70957100	18.41032400	7.66570100
H	18.52206100	18.86400100	7.32486100
O	17.76014700	10.78503300	10.37559800
H	18.57621100	11.25402100	10.68725800
H	17.75801900	10.78914700	9.38449500
H	17.71589400	9.85787500	7.33583900
O	17.70957100	10.79318400	7.66570100
H	18.52206100	11.24686100	7.32486100
H	17.76103700	23.49118600	12.28861000
O	17.74697800	23.48097900	11.29707400
H	17.75327100	24.41842000	10.97429000
H	16.88950900	23.01115300	7.11778500
O	17.69230400	23.48166400	6.77586100
H	18.49435700	23.00765000	7.11388500
H	17.76103700	15.87404600	12.28861000
O	17.74697800	15.86383900	11.29707400
H	17.75327100	16.80128000	10.97429000
H	16.88950900	15.39401300	7.11778500
O	17.69230400	15.86452400	6.77586100
H	18.49435700	15.39051000	7.11388500
H	17.76103700	8.25690600	12.28861000
O	17.74697800	8.24669900	11.29707400
H	17.75327100	9.18414000	10.97429000
H	16.88950900	7.77687300	7.11778500
O	17.69230400	8.24738400	6.77586100
H	18.49435700	7.77337000	7.11388500

Ic-CL4 + acetone (lying):

B3LYP/6-31G(d) constrained optimisation:

127

2 layer/127 atoms/39*H2O + acetone (lying)

O	-6.48670896	-0.00270900	-0.07776302
H	-5.90725992	0.57396109	0.49710908
H	-7.06126406	-0.58202609	0.50135208
O	-6.50051895	-3.24107550	-3.32536152
H	-5.92106394	-2.66440742	-2.74948942
H	-7.07506907	-3.81939459	-2.74524442
O	-7.03384484	6.39582457	0.36463244
H	-6.21909381	6.86572068	0.67790270
H	-6.74035224	5.53773344	0.01905424
O	-8.11734124	1.61921525	-1.68814326

H	-8.69287637	2.19489634	-1.10737418
H	-7.53691217	1.04088616	-1.11492518
O	-9.75172952	6.48313696	-3.29487750
H	-9.10066137	7.10030284	-2.90030711
H	-9.79094250	5.75443692	-2.65816650
O	-6.50602197	3.24391650	-3.31607651
H	-5.92656696	3.82058458	-2.74020442
H	-7.08057310	2.66559740	-2.73595942
O	-8.13665425	4.86584074	-4.92645676
H	-8.71218436	5.44151986	-4.34468767
H	-7.55622015	4.28851066	-4.35223666
O	-8.12284325	8.10320628	-1.67886226
H	-8.69837934	8.67988835	-1.09808916
H	-7.54241614	7.52587914	-1.10563716
O	-6.51152499	9.72890848	-3.30679150
H	-5.93206992	10.30557659	-2.73091942
H	-7.08607506	9.14958941	-2.72667542
O	-3.24200050	-3.24293050	-0.09895902
H	-2.66255041	-2.66626041	0.47591308
H	-3.81555659	-3.82124658	0.48015308
O	-4.87263274	-1.62100525	-1.70933926
H	-5.44716883	-1.04432416	-1.12857318
H	-4.29220366	-2.19833434	-1.13611918
O	-3.24750350	3.24206150	-0.08967402
H	-2.66805441	3.81873059	0.48519908
H	-3.82105958	2.66374441	0.48943808
O	-4.87813474	4.86398674	-1.70005426
H	-5.45267084	5.43966986	-1.11928917
H	-4.29770766	4.28665666	-1.12683418
O	-3.25300650	9.72705451	-0.08038902
H	-2.67355740	10.30372357	0.49448308
H	-3.82656158	9.14773840	0.49872308
O	-4.88363876	11.34897876	-1.69076926
H	-5.45817386	11.92465984	-1.11000518
H	-4.30320966	10.77164966	-1.11754918
O	0.03132100	-0.00641500	6.37403696
H	0.61077209	0.57025409	6.94890904
H	-0.54323308	-0.58573309	6.95315304
O	-3.22819350	-0.00456200	3.14763648
H	-2.64874941	0.57210808	3.72251358
H	-3.80175158	-0.58387809	3.72675058
O	0.01751300	-3.24478250	3.12643848
H	0.59696209	-2.66811240	3.70131157
H	-0.55704308	-3.82309958	3.70555556
O	-1.61411925	-1.62285824	1.51606324
H	-2.18865534	-1.04617616	2.09682932
H	-1.03269016	-2.20018634	2.08927832
O	-0.10909750	6.56874175	6.51424708
H	0.57528339	7.12534007	6.95344467
H	-0.55549778	6.08931695	7.22665613
O	-1.70407550	1.50482527	4.84455130
H	-2.18100635	2.02666375	5.50516205
H	-1.02787776	0.97718277	5.33134902
O	-3.60445622	6.37578383	3.18937662
H	-3.01199386	6.75386626	3.87573692
H	-4.02267823	5.54890051	3.49404771
O	0.01201000	3.24020950	3.13572348
H	0.59145909	3.81688059	3.71059556
H	-0.56254508	2.66189241	3.71484058
O	-5.01301070	1.59160632	1.75665215
H	-5.06731290	2.41693013	2.27515325
H	-4.30619428	1.04855196	2.17597477
O	-1.61961525	4.86213176	1.52535724
H	-2.19416934	5.43783885	2.10610132
H	-1.03819816	4.28480066	2.09856332
O	-1.89089214	7.85325269	4.81488691
H	-2.33474436	8.46528327	5.42029329
H	-1.20947953	7.39353096	5.35663142
O	0.00650700	9.72520250	3.14500848
H	0.58595609	10.30187160	3.71988058

H	-0.56804809	9.14588337	3.72412358
O	-5.03989527	7.90916222	1.48043367
H	-5.49077441	8.51387529	2.08812061
H	-4.43144215	7.37284785	2.04972353
O	-1.62512524	11.34712574	1.53463324
H	-2.19966034	11.92280782	2.11539732
H	-1.04369716	10.76979770	2.10784832
O	3.27603150	-3.24663650	6.35284198
H	3.85548059	-2.66996641	6.92771406
H	2.70247542	-3.82495259	6.93195309
O	1.64539426	-1.62471025	4.74146073
H	1.06986316	-1.04803116	5.32323181
H	2.22582734	-2.20204134	5.31568082
O	3.27052850	3.23835550	6.36212698
H	3.84997760	3.81502558	6.93699906
H	2.69697242	2.66003941	6.94123808
O	1.63989026	4.86028074	4.75074572
H	1.06436216	5.43596186	5.33251485
H	2.22032534	4.28295166	5.32496582
O	3.26502550	9.72334746	6.37141198
H	3.84447460	10.30001758	6.94628405
H	2.69147041	9.14403141	6.95052208
O	1.63438825	11.34527377	4.76003074
H	1.05885816	11.92095279	5.34179985
H	2.21482134	10.76794267	5.33425082
O	3.28433351	6.47572398	9.60872349
H	3.99204798	7.06100984	9.93242106
H	2.91174561	6.06864131	10.40851849
O	1.65920326	1.61365624	7.98905926
H	1.08366816	2.18933734	8.56982832
H	2.23963334	1.03532716	8.56227733
O	4.89840976	4.85842674	7.97714827
H	4.32387366	5.43410884	8.55791231
H	5.47883786	4.28109866	8.55036831
O	1.65370226	8.09764727	7.99834124
H	1.07816516	8.67432935	8.57911337
H	2.23412934	7.52031918	8.57156328
C	-6.59364552	4.47583962	3.25676888
C	-7.66925607	3.60131873	2.66018957
H	-8.49241901	3.46942889	3.37288751
H	-8.09073892	4.11350795	1.78611654
H	-7.27141272	2.62951764	2.36318544
C	-7.01281047	5.85016006	3.71760423
H	-7.34453497	6.40782197	2.83284252
H	-7.86289668	5.78819250	4.40655969
H	-6.17734077	6.37246488	4.18719903
O	-5.42359107	4.09997160	3.33454820

Ic-CL4 + acetone (up-right):

B3LYP/6-31+G(d) constrained optimisation:

127
 2 layer/127 atoms/39*H2O + acetone (up-right)

O	-6.48440800	-0.00702200	-0.07534800
H	-5.90501100	0.56969900	0.49952600
H	-7.05832100	-0.58698200	0.50376200
O	-6.49792900	-3.24372700	-3.32460300
H	-5.91852700	-2.66700800	-2.74872900
H	-7.07183900	-3.82268800	-2.74449200
O	-6.90899400	6.61510700	0.41433600
H	-6.06512600	7.04049800	0.69983800
H	-6.74228200	5.66657000	0.30964700
O	-8.11683200	1.61475100	-1.68406400
H	-8.69241600	2.18978800	-1.10270600
H	-7.53576400	1.03647600	-1.11143800

O	-9.75495300	6.47851700	-3.28746300
H	-9.17455200	7.05623800	-2.71159300
H	-10.32786100	5.89955600	-2.70735800
O	-6.50731400	3.24125400	-3.31198000
H	-5.92791300	3.81797300	-2.73610600
H	-7.08122400	2.66229300	-2.73186900
O	-8.13973900	4.86302800	-4.92069600
H	-8.71531800	5.43806300	-4.33833800
H	-7.55866700	4.28575000	-4.34706900
O	-8.12621500	8.09873300	-1.67144300
H	-8.70180100	8.67477000	-1.09008300
H	-7.54515100	7.52145900	-1.09881500
O	-6.51669900	9.72623600	-3.29935700
H	-5.93729800	10.30295500	-2.72348300
H	-7.09060800	9.14627400	-2.71924800
O	-3.23776800	-3.24528600	-0.09986100
H	-2.65837200	-2.66856400	0.47501300
H	-3.81068300	-3.82424400	0.47924500
O	-4.87019200	-1.62351200	-1.70857700
H	-5.44477800	-1.04747300	-1.12722300
H	-4.28912600	-2.20078700	-1.13594900
O	-3.24715400	3.23969500	-0.08723800
H	-2.66775700	3.81641700	0.48763600
H	-3.82006800	2.66073800	0.49186800
O	-4.87957800	4.86146900	-1.69595400
H	-5.45416000	5.43650600	-1.11460200
H	-4.29851100	4.28419400	-1.12332600
O	-3.25653900	9.72467700	-0.07461500
H	-2.67714300	10.30139800	0.50025900
H	-3.82945200	9.14471900	0.50448900
O	-4.88896200	11.34645100	-1.68333100
H	-5.46354700	11.92148900	-1.10197900
H	-4.30789600	10.76917500	-1.11070300
O	0.03691000	-0.01013900	6.37313300
H	0.61630500	0.56658500	6.94800500
H	-0.53700500	-0.59009600	6.95224100
O	-3.22424700	-0.00858000	3.14838800
H	-2.64486800	0.56814100	3.72327600
H	-3.79716400	-0.58853800	3.72749900
O	0.02338700	-3.24684100	3.12387600
H	0.60278300	-2.67012000	3.69874900
H	-0.55052800	-3.82580100	3.70298700
O	-1.61003700	-1.62506900	1.51516600
H	-2.18462300	-1.04903000	2.09652000
H	-1.02797100	-2.20234300	2.08778700
O	-0.08518000	6.54377000	6.49133400
H	0.56270900	7.08835300	6.99660200
H	-0.64121800	6.08406900	7.13750400
O	-1.71253500	1.53055500	4.84869900
H	-2.15544100	2.14861900	5.44853400
H	-1.05172400	1.01893600	5.37072900
O	-3.39278400	6.54319200	3.24743900
H	-2.72465900	7.07149200	3.73865400
H	-3.95057200	6.08745600	3.91039700
O	0.01400200	3.23814000	3.13649900
H	0.59339800	3.81486100	3.71137200
H	-0.55990900	2.65918300	3.71560800
O	-4.94024400	1.53667800	1.64626500
H	-5.30656400	2.16494800	2.28505900
H	-4.26291100	1.00237900	2.12739400
O	-1.61942000	4.85991100	1.52779100
H	-2.19400700	5.43495300	2.10913500
H	-1.03735600	4.28263700	2.10041000
O	-1.60590500	8.09561900	4.77604400
H	-2.18048400	8.67165800	5.35839500
H	-1.02383400	7.51834600	5.34966400
O	0.00461600	9.72312200	3.14912200
H	0.58401300	10.29984300	3.72399500
H	-0.56929600	9.14316100	3.72823100
O	-4.86606000	8.09717600	1.55230100

H	-5.44064500	8.67321600	2.13365300
H	-4.28499300	7.51989900	2.12492900
O	-1.62880700	11.34489400	1.54041200
H	-2.20339100	11.91993300	2.12176400
H	-1.04674100	10.76762000	2.11303300
O	3.28354700	-3.24840000	6.34861800
H	3.86294400	-2.67167900	6.92349300
H	2.71063300	-3.82735800	6.92772500
O	1.65111900	-1.62662400	4.73890200
H	1.07553900	-1.05058800	5.32126200
H	2.23219000	-2.20390200	5.31253000
O	3.27416200	3.23658100	6.36124200
H	3.85355800	3.81330200	6.93611600
H	2.70124800	2.65762300	6.94034800
O	1.64173200	4.85835600	4.75152500
H	1.06615600	5.43339000	5.33388200
H	2.22806000	4.28108000	5.32515300
O	3.26477700	9.72156300	6.37386500
H	3.84417300	10.29828400	6.94873900
H	2.69186400	9.14160500	6.95296900
O	1.63234800	11.34333900	4.76414800
H	1.05676900	11.91837400	5.34650600
H	2.21342000	10.76606100	5.33777600
O	3.28768000	6.47228800	9.60949500
H	3.86707500	7.05001000	10.18437100
H	2.71476600	5.89333000	10.18860200
O	1.66464000	1.61008000	7.98815900
H	1.08905600	2.18511800	8.56951600
H	2.24570800	1.03180500	8.56078400
O	4.90189400	4.85679800	7.97626800
H	4.32731000	5.43183600	8.55762100
H	5.48296000	4.27952200	8.54889600
O	1.65525800	8.09406200	8.00078000
H	1.07967000	8.67009900	8.58213900
H	2.23632300	7.51678700	8.57340700
C	-6.40446900	5.31272700	5.21010600
C	-7.15497400	4.68761300	6.36620400
H	-7.90398400	5.38269000	6.76476500
H	-7.70571800	3.80559400	6.01283300
H	-6.46389600	4.38846400	7.15741600
C	-7.23202200	5.95651700	4.12356200
H	-8.08280000	5.32298200	3.84666600
H	-7.65960300	6.89345000	4.50770300
H	-6.63876900	6.17953900	3.23498700
O	-5.17643300	5.29474100	5.17568500

Ic-CL5 + acetone (lying):

2 Layer- ONIOM (B3LYP/6-31+G(d):HF/6-31+G*) constrained optimisation:

229

3 layer/229 atoms/73*H2O + acetone (lying)

O	-6.48683200	6.48406400	-6.59679500
H	-5.90952900	7.06206500	-6.02010000
H	-7.06493700	5.90747400	-6.01949100
O	-6.68052600	0.23742900	0.26648200
H	-6.12962700	0.83183200	0.82622300
H	-7.10617300	-0.39124500	0.86820100
O	-6.48971600	-3.24177900	-3.35132500
H	-5.91241300	-2.66477600	-2.77363000
H	-7.06782100	-3.81836800	-2.77302100
O	-6.65888200	6.57700400	0.03739400

H	-6.07914700	7.12473900	0.62329100
H	-7.16653700	5.98985800	0.61535000
O	-8.29863400	1.55854000	-1.54841900
H	-8.87085700	2.12127900	-1.00738500
H	-7.70734700	1.07124700	-0.92558200
O	-9.85441500	6.57467500	-3.20811200
H	-9.19053700	7.11334900	-2.71372700
H	-10.37480100	6.08348500	-2.55694300
O	-6.48742400	3.24322100	-3.35363800
H	-5.91012300	3.82022500	-2.77594400
H	-7.06552900	2.66662200	-2.77534000
O	-8.10812800	4.86421500	-4.97494100
H	-8.68583000	5.44163000	-4.39704300
H	-7.53123300	4.28721900	-4.39683200
O	-8.10643000	8.10737400	-1.73309900
H	-8.68413000	8.68577500	-1.15620300
H	-7.52952000	7.53036600	-1.15599500
O	-6.48513300	9.72822000	-3.35595200
H	-5.90783100	10.30522200	-2.77825700
H	-7.06323900	9.15063200	-2.77764600
O	-0.00301700	0.00008600	-0.11058800
H	0.57428600	0.57708800	0.46610700
H	-0.58112300	-0.57750400	0.46671600
O	-3.24716200	-3.24176800	-0.10887800
H	-2.66986000	-2.66476600	0.46781700
H	-3.82426800	-3.81835800	0.46842600
O	-4.86787300	-1.62077800	-1.73018200
H	-5.44455800	-1.04235700	-1.15328600
H	-4.29097100	-2.19777000	-1.15307300
O	-3.24657000	0.00007500	-3.35303500
H	-2.66926700	0.57707700	-2.77533900
H	-3.82367500	-0.57751500	-2.77473000
O	-0.00072600	6.48408500	-0.11290200
H	0.57657700	7.06208700	0.46379400
H	-0.57883000	5.90749600	0.46440400
O	-3.24487100	3.24323100	-0.11119200
H	-2.66756900	3.82023300	0.46550400
H	-3.82197700	2.66664100	0.46611300
O	-4.86557400	4.86422400	-1.73249200
H	-5.44228200	5.44164100	-1.15560100
H	-4.28867900	4.28722900	-1.15538600
O	-1.62472100	1.62108100	-1.73189000
H	-2.20141800	2.19849000	-1.15499800
H	-1.04682600	1.04308200	-1.15478200
O	-3.24427900	6.48407400	-3.35534800
H	-2.66697600	7.06207600	-2.77765300
H	-3.82138400	5.90748400	-2.77704500
O	-4.86727400	1.62106900	-4.97433700
H	-5.44397100	2.19847900	-4.39644400
H	-4.29037900	1.04307200	-4.39622900
O	-3.24258000	9.72823200	-0.11350500
H	-2.66527800	10.30523300	0.46319000
H	-3.81968300	9.15063600	0.46379900
O	-4.86328300	11.34922500	-1.73480700
H	-5.43998100	11.92663500	-1.15791500
H	-4.28638900	10.77222700	-1.15770000
O	-1.62242900	8.10508000	-1.73420300
H	-2.19912700	8.68348900	-1.15731200
H	-1.04453500	7.52808100	-1.15709600
O	-4.86498300	8.10506900	-4.97665000
H	-5.44168000	8.68347900	-4.39875800
H	-4.28808800	7.52807100	-4.39854300
O	-0.00191400	0.00239300	6.37440700
H	0.57539100	0.57940100	6.95110800
H	-0.58001400	-0.57518800	6.95172000
O	-3.44374700	0.02231300	3.32400100
H	-2.83065700	0.52339400	3.91008100
H	-3.91953500	-0.61189600	3.88150500
O	-0.00360900	-3.24175700	3.13256800
H	0.57369300	-2.66475600	3.70926400

H	-0.58171500	-3.81834700	3.70987300
O	-1.62531300	-1.62076300	1.51126700
H	-2.20200900	-1.04235400	2.08815800
H	-1.04741900	-2.19776100	2.08837400
O	-0.18326900	6.52961200	6.59543600
H	0.47867800	7.10342300	7.04922300
H	-0.69521300	6.09443000	7.29400100
O	-1.78350100	1.54976800	4.92799500
H	-2.27277200	2.08210900	5.57291300
H	-1.12138000	1.01582700	5.42687600
O	-3.60771500	6.38477800	3.28577200
H	-3.07002800	6.83527600	3.97348700
H	-4.14094400	5.67267700	3.68867800
O	-0.00131800	3.24324200	3.13025500
H	0.57598400	3.82024400	3.70695000
H	-0.57942200	2.66665400	3.70755700
O	-5.10295600	1.80984900	1.97780800
H	-5.18009700	2.60279800	2.54051900
H	-4.47360900	1.20117900	2.42824500
O	-1.62300400	4.86424500	1.50896300
H	-2.19974300	5.44164600	2.08583100
H	-1.04513200	4.28723300	2.08606000
O	-1.96841000	7.94424300	4.95596700
H	-2.38909100	8.61813100	5.51172700
H	-1.31114500	7.47793200	5.51980000
O	0.00097400	9.72824000	3.12794200
H	0.57827100	10.30524800	3.70463600
H	-0.57712200	9.15064500	3.70524700
O	-5.08561900	8.06626800	1.71582100
H	-5.48655900	8.73287700	2.29306600
H	-4.51085000	7.49216100	2.28348100
O	-1.62073000	11.34923600	1.50664000
H	-2.19742800	11.92664500	2.08353200
H	-1.04283600	10.77223700	2.08374600
O	3.23894400	-3.24174600	6.37501500
H	3.81624600	-2.66474500	6.95171100
H	2.66183800	-3.81833700	6.95231900
O	1.61823900	-1.62075300	4.75271300
H	1.04054400	-1.04234000	5.33060500
H	2.19513500	-2.19774900	5.33082100
O	3.23953600	0.00009600	3.13085900
H	3.81683800	0.57709800	3.70755400
H	2.66243000	-0.57749400	3.70816300
O	6.48438000	6.48410700	6.37099200
H	7.06268300	7.06210800	6.94768700
H	5.90727500	5.90751600	6.94829600
O	3.24123500	3.24325300	6.37270200
H	3.81853700	3.82025500	6.94939700
H	2.66413000	2.66666300	6.95000600
O	1.62053400	4.86424600	4.75040300
H	1.04283300	5.44166300	5.32828900
H	2.19742500	4.28724800	5.32850700
O	4.86138500	1.62110200	4.75100400
H	4.28468800	2.19851200	5.32889600
H	5.43828000	1.04310400	5.32911100
O	3.24182700	6.48409600	3.12854500
H	3.81913000	7.06209700	3.70524100
H	2.66472100	5.90750500	3.70584900
O	1.61883200	1.62109100	1.50955700
H	1.04113500	2.19850100	2.08644900
H	2.19572700	1.04309300	2.08666500
O	3.24352700	9.72825200	6.37038800
H	3.82082800	10.30525400	6.94708400
H	2.66642100	9.15066300	6.94769400
O	1.62282300	11.34924600	4.74808600
H	1.04512500	11.92665600	5.32597900
H	2.19971700	10.77224800	5.32619300
O	4.86367700	8.10510100	4.74869000
H	4.28698000	8.68351100	5.32658300
H	5.44057100	7.52810300	5.32679800

O	1.62112400	8.10509000	1.50724300
H	1.04342600	8.68350000	2.08413500
H	2.19801800	7.52809200	2.08435100
O	3.24293500	6.48640900	9.61354400
H	3.82023600	7.06441000	10.19024100
H	2.71033900	5.97654500	10.25010000
O	1.61994000	1.62340400	7.99455600
H	1.05267200	2.10747300	8.61933600
H	2.19683300	1.04540600	8.57166400
O	4.86308500	4.86425800	7.99284700
H	4.28638700	5.44166800	8.56973900
H	5.43997900	4.28726000	8.56995400
O	1.62223100	8.10739500	7.99223100
H	1.04453600	8.68581400	8.56913800
H	2.19912100	7.53040800	8.56935700
C	-6.66917100	4.30531300	4.36254400
C	-7.72075200	3.24076600	4.15620900
H	-7.96470500	2.77555600	5.12065300
H	-8.65188000	3.68544800	3.78483800
H	-7.37165000	2.47282500	3.46306200
C	-7.06405300	5.51616700	5.17722100
H	-7.86659600	6.06248000	4.66519700
H	-7.46974200	5.20964100	6.14919400
H	-6.21246500	6.18407400	5.32409100
O	-5.53723300	4.19314100	3.88917700
O	-9.73267600	0.00005400	-9.83692900
H	-9.15537400	0.57705600	-9.25923300
H	-10.30978200	-0.57753600	-9.25862400
O	-8.11082700	1.62105900	-8.21578400
H	-8.68752400	2.19846900	-7.63889100
H	-7.53293200	1.04306100	-7.63867600
O	-6.48912300	0.00006400	-6.59448200
H	-5.91182100	0.57706600	-6.01778600
H	-7.06722900	-0.57752600	-6.01717700
O	-9.73038500	6.48405300	-9.83924200
H	-9.15308300	7.06105500	-9.26154600
H	-10.30749000	5.90646300	-9.26093700
O	-8.10853600	8.10505800	-8.21809700
H	-8.68523300	8.68246800	-7.64120400
H	-7.53064100	7.52706000	-7.64098900
O	-9.73156900	0.00236700	-3.35193000
H	-9.15426500	0.57937100	-2.77522900
H	-10.30867500	-0.57522300	-2.77462500
O	-11.35227300	1.62336100	-4.97323100
H	-11.90007700	2.16815000	-4.38936200
H	-10.77537900	1.04536300	-4.39612300
O	-12.97412200	0.00235600	-6.59337600
H	-12.39682000	0.57935800	-6.01668000
H	-13.55222800	-0.57523400	-6.01607200
O	-11.34998400	8.10736100	-4.97554200
H	-11.92668000	8.68477000	-4.39865200
H	-10.77308100	7.52936000	-4.39844100
O	-12.97183200	6.48635500	-6.59568900
H	-12.39452900	7.06335800	-6.01899400
H	-13.58876100	6.02282100	-6.01219900
O	-11.35168100	4.86420500	-8.21638800
H	-11.92837900	5.44161400	-7.63949500
H	-10.77478700	4.28720600	-7.63928000
O	-9.73097700	3.24321000	-6.59508600
H	-9.15367500	3.82021200	-6.01839000
H	-10.30808200	2.66662000	-6.01778200
O	-11.35397100	-1.62079300	-8.21407700
H	-11.93066800	-1.04238400	-7.63718500
H	-10.77707600	-2.19779100	-7.63697000
O	-9.73326700	-3.24178800	-6.59277500
H	-9.15596500	-2.66478600	-6.01608000
H	-10.31037200	-3.81837800	-6.01547100
O	-8.11141800	-1.62078200	-4.97263000
H	-8.68811500	-1.04237300	-4.39573800
H	-7.53352300	-2.19778100	-4.39552300

O	-11.34938900	11.34720500	-8.21870400
H	-11.92608600	11.92561500	-7.64181100
H	-10.77249400	10.77020700	-7.64159600
O	-9.72868500	9.72621100	-6.59740200
H	-9.15138300	10.30321300	-6.02070600
H	-10.30579000	9.14962100	-6.02009800
O	-8.10683600	11.34721600	-4.97725700
H	-8.68353300	11.92562600	-4.40036500
H	-7.52894100	10.77021700	-4.40015000