Electronic Supplementary Information

Molecular Recognition of Upper Rim Functionalized Cavitand and Its Unique Dimeric Capsule in the Solid State

Mutsumi Kobayashi, Mei Takatsuka, Ryo Sekiya,
and Takeharu Haino*

Department of Chemistry, Graduate School of Science, Hiroshima University, 1-3-1 Kagamiyama, Higashi-Hiroshima, Hiroshima, 739-8526 Japan.

*To whom correspondence should be addressed.
Email: haino@hiroshima-u.ac.jp

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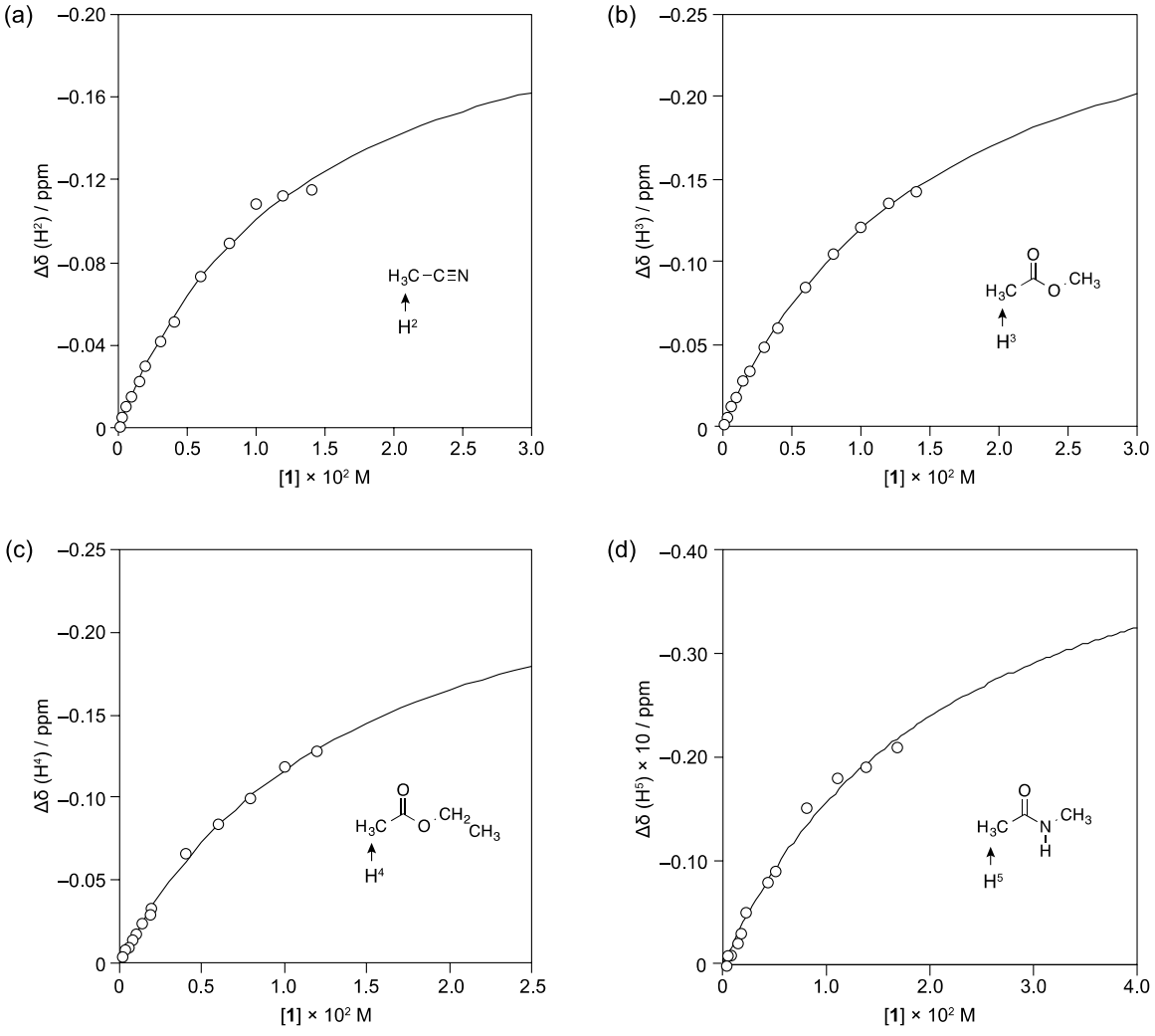

Figure S1. Non-linear least square fitting of the titration data of (a) **5**, (b) **6**, (c) **7**, and (d) **10** (chloroform-d_1, 293 K).

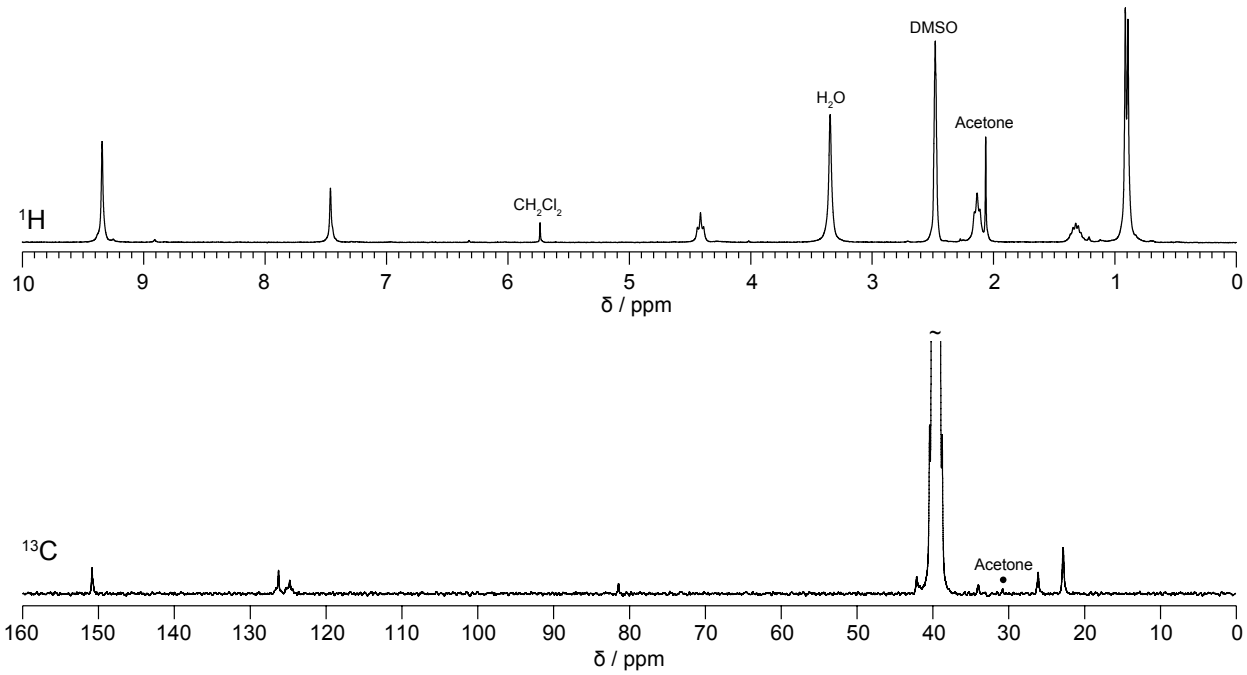

Figure S2. ^{1}H (300 MHz) and ^{13}C (75 MHz) NMR spectra of **14** in dimethylsulfoxide-d_6.

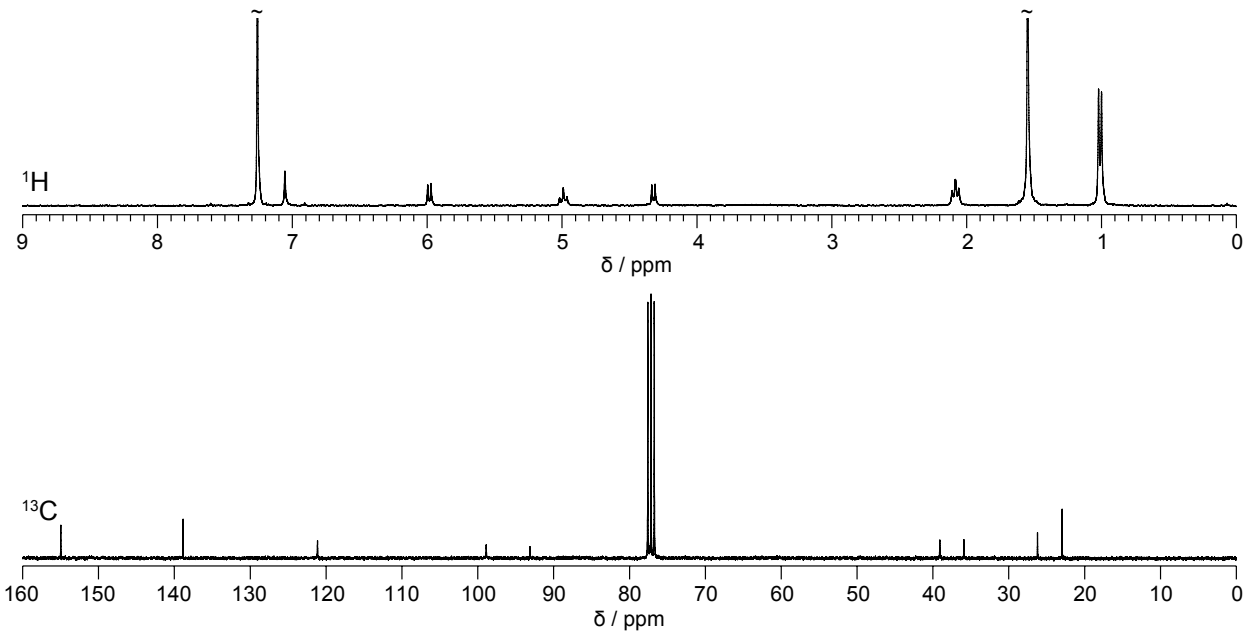

Figure S3. ^{1}H (300 MHz) and ^{13}C (75 MHz) NMR spectra of **4** in chloroform-d_1.

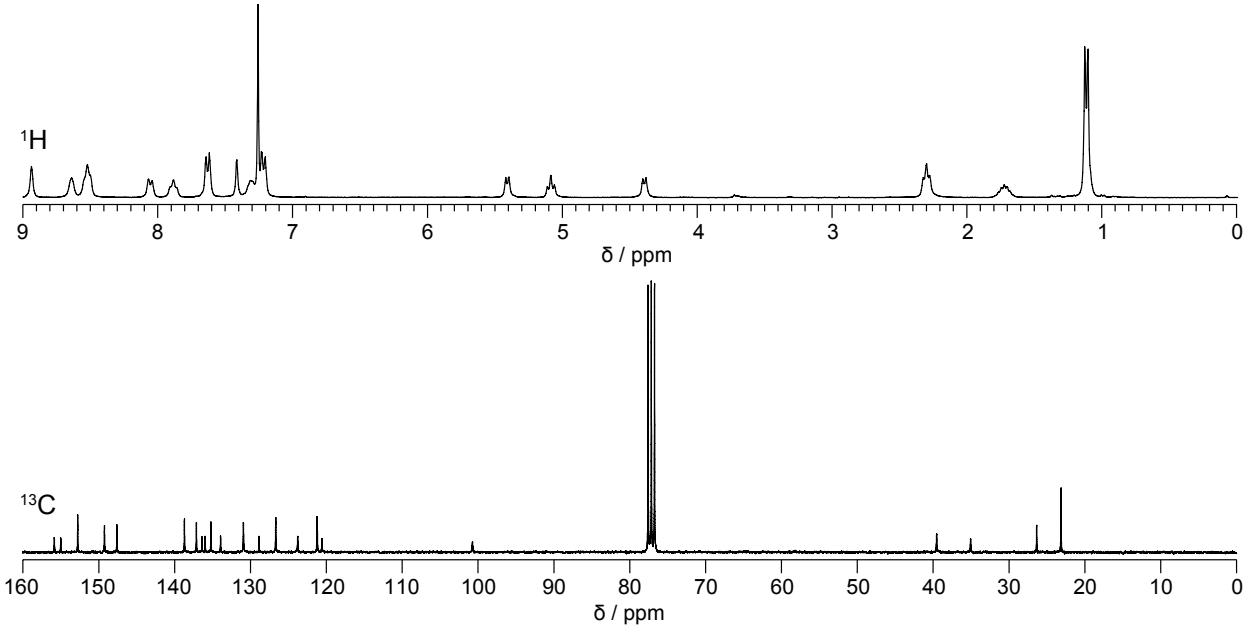

Figure S4. ^{1}H (300 MHz) and ^{13}C (75 MHz) NMR spectra of **2** in chloroform-d_1.

Computational Details

Geometry optimization for the host-guest complexes was carried out by Macromodel V. 9.1 using MMFF force field.[1] (guest = nitromethane (**5**), nitroethane (**6**), acetonitrile (**7**), methyl acetate (**8**), ethyl acetate (**9**), *N*,*N*-dimethylacetamide (**11**), *N*-methylacetamide (**12**)) Cartesian coordinates of the host-guest complexes were listed in Tables S1-S7. Optimized structures were shown in Figures S5–S15.

Table S1. Cartesian coordinates of **5**⊂**16**

Atom	*x* / Å	*y* / Å	*z* / Å
C	0.73640	2.48840	-0.86620
C	-0.47800	2.82470	-1.50140
C	-1.68150	2.48210	-0.84780
C	-1.69170	1.89190	0.43050
C	-0.45920	1.58890	1.03180
C	0.76410	1.89640	0.41200
C	-3.09020	-1.01080	1.33530
C	-3.46470	0.15190	0.64040
C	-4.20850	0.00950	-0.54710
C	-4.62970	-1.25310	-1.01440
C	-4.21130	-2.39340	-0.29670
C	-3.46590	-2.29060	0.89400
C	0.75430	-4.05380	1.02150
C	-0.46630	-3.62760	1.57130
C	-1.70130	-4.04720	1.04820
C	-1.69670	-4.89100	-0.08030
C	-0.49550	-5.36320	-0.65100
C	0.71970	-4.89860	-0.10440
C	3.63740	-1.25400	-1.11390
C	3.24440	0.00890	-0.62300
C	2.52650	0.14690	0.58030
C	2.15630	-1.01820	1.27260
C	2.51220	-2.29750	0.81390
C	3.22290	-2.39750	-0.39820
C	-3.01640	1.53640	1.10230
C	2.09790	1.53160	1.06040
C	2.09180	-3.55890	1.56590
O	1.92350	2.81650	-1.48200
O	-2.87700	2.79920	-1.45290
O	3.62580	1.13980	-1.30980
O	3.58830	-3.63960	-0.86630
O	-2.89510	-5.32000	-0.60540
O	-4.59140	-3.63810	-0.74610
O	-4.58110	1.13410	-1.24810
O	1.90420	-5.32540	-0.66140
C	2.49120	-4.31720	-1.49950
C	-3.50050	1.64800	-2.04340
C	-3.51150	-4.30720	-1.41760
H	-0.45140	1.09490	1.99930
H	-2.48020	-0.91840	2.22940
H	-0.45510	-2.94300	2.41470
H	1.56920	-0.92760	2.18220
C	-3.02320	-3.55230	1.63220
H	-3.76940	2.26460	0.77100
H	2.84940	2.25770	0.72140
H	2.84510	-4.33460	1.37150
H	1.74710	-3.62290	-1.91860
H	2.91900	-4.84890	-2.35660
H	-3.95310	1.99610	-2.97840
H	-2.77530	0.87230	-2.33230
H	-2.78070	-3.60650	-1.84380
H	-3.96060	-4.83120	-2.26840
H	-3.78060	-4.32940	1.45970
C	2.54660	1.67470	-2.09340
H	1.82090	0.90800	-2.39350
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C	-0.32620	-8.59490	-2.61120
C	-0.32650	-7.68320	-1.54910
C	-0.50350	-6.31190	-1.77710

C	-0.67750	-5.87810	-3.09750
C	-0.67840	-6.79080	-4.15950
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C	4.69370	-1.65170	-4.73350
C	3.89240	-1.54150	-3.59040
C	4.46650	-1.37320	-2.32430
C	5.86370	-1.31730	-2.23290
C	6.66430	-1.42680	-3.37590
H	4.20620	-1.76510	-5.70050
H	2.81310	-1.58220	-3.70440
H	6.34100	-1.18860	-1.26300
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C	-0.37640	3.50570	-5.23050
C	-0.35470	2.82870	-4.00490
C	-0.49480	3.52380	-2.79720
C	-0.66080	4.91430	-2.84960
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H	-0.80360	6.67260	-4.06950
C	-7.15130	-1.60910	-4.50030
C	-5.75330	-1.68150	-4.61000
C	-4.93120	-1.56620	-3.48230
C	-5.48140	-1.37480	-2.20870
C	-6.87590	-1.30070	-2.09390
C	-7.69720	-1.41730	-3.22130
H	-5.28550	-1.84600	-5.57940
H	-3.85500	-1.63420	-3.61250
H	-7.33460	-1.14960	-1.11830
H	-8.77540	-1.34420	-3.08880
C	-0.57560	-10.91310	-7.20180
N	-1.57440	-9.99860	-7.06460
C	-1.51440	-9.14460	-6.01050
C	-0.50380	-9.12480	-5.05080
C	0.50930	-10.07370	-5.21270
C	0.47600	-10.96800	-6.28620
H	-2.35040	-8.45070	-5.95470
H	1.34150	-10.12090	-4.51370
H	1.27160	-11.69880	-6.40260
C	8.49340	-1.99690	-8.15460
C	8.72840	-0.93190	-7.28420
C	7.94920	-0.79170	-6.13240
C	6.93610	-1.71120	-5.84750
C	6.77440	-2.74300	-6.77040
N	7.51330	-2.90590	-7.89810
H	9.51070	-0.20810	-7.49590
H	8.13610	0.05020	-5.46940
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C	0.42230	5.42510	-7.54190
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H	-2.39160	6.71170	-6.20910
H	1.25650	4.74950	-7.36540
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C	-9.89760	-2.70390	-6.86560
C	-9.09880	-2.61390	-5.72230
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C	-7.80660	-0.97510	-6.83540
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C	-12.22950	-2.89850	-10.34810
N	-11.47290	-2.83040	-9.22860
C	-10.42310	-1.95980	-9.21740

C	-10.13610	-1.16140	-10.32780
C	-10.93330	-1.25300	-11.46800
H	-12.64100	-2.23360	-12.35150
H	-13.05330	-3.60600	-10.30840
H	-9.29770	-0.47070	-10.30940
H	-10.71810	-0.63630	-12.33620
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C	11.00630	-1.44240	-10.77050
N	10.26740	-1.28410	-9.64820
C	9.28700	-2.19730	-9.39310
C	9.05140	-3.26500	-10.26330
C	9.82880	-3.40290	-11.41250
H	11.44880	-2.55310	-12.55810
H	11.77420	-0.69030	-10.92980
H	8.26820	-3.98750	-10.05160
H	9.65330	-4.22970	-12.09510
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C	0.56410	7.99110	-12.51270
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H	-2.26420	9.77170	-12.05870
H	1.35050	6.63730	-11.03690
H	1.36150	7.80320	-13.22640
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C	-1.75030	-12.67180	-10.34830
C	-1.71910	-11.77990	-9.27710
C	-0.66450	-11.83500	-8.36190
N	0.33870	-12.74880	-8.49790
C	0.28300	-13.60180	-9.54660
H	-0.72460	-14.30960	-11.30970
H	-2.56610	-12.63680	-11.06510
H	-2.51400	-11.04860	-9.16040
H	1.10430	-14.31040	-9.61180
C	2.13420	1.71230	2.58850
H	3.13860	1.50200	2.97410
H	1.88220	2.74470	2.85720
H	1.43930	1.05980	3.12480
C	-3.02610	1.72800	2.62950
H	-4.02480	1.52580	3.03370
H	-2.32550	1.07520	3.15840
H	-2.76400	2.76080	2.88690
C	-3.03090	-3.42360	3.16610
H	-2.77350	-4.38220	3.63140
H	-2.32610	-2.67930	3.54770
H	-4.02790	-3.13700	3.52050
C	2.14290	-3.43090	3.09900
H	3.14870	-3.14190	3.42520
H	1.44700	-2.68900	3.50110
H	1.90130	-4.39050	3.57080
C	-0.48390	-1.29720	-1.61460
H	0.25510	-0.54550	-1.34910
H	-1.48040	-0.98140	-1.31710
H	-0.22670	-2.26150	-1.18470
N	-0.49330	-1.46160	-3.08840
O	-1.31680	-2.25450	-3.55810
O	0.32110	-0.80060	-3.74140

Table S2. Cartesian coordinates of **6⊂16**

Atom	*x* / Å	*y* / Å	*z* / Å
C	0.753000	2.403000	-0.917000
C	-0.473000	2.764000	-1.519000
C	-1.664000	2.430000	-0.834000
C	-1.651000	1.831000	0.440000
C	-0.409000	1.515000	1.010000
C	0.802000	1.815000	0.364000
C	-2.961000	1.477000	1.138000
C	2.143000	1.461000	1.001000
C	2.145000	-3.620000	1.519000
O	1.931000	2.715000	-1.562000
O	-2.874000	2.754000	-1.407000
O	1.931000	-5.383000	-0.709000
C	2.532000	-4.366000	-1.529000
C	-3.511000	1.605000	-1.987000
C	-3.486000	-4.372000	-1.376000
C	-2.964000	-3.605000	1.655000
C	2.560000	1.555000	-2.138000
C	-0.637000	4.887000	-5.283000
C	-0.238000	3.543000	-5.229000
C	-0.183000	2.851000	-4.012000
C	-0.521000	3.481000	-2.807000
C	-0.921000	4.823000	-2.859000
C	-0.979000	5.515000	-4.075000
C	-0.730000	6.967000	-9.009000
C	-1.843000	7.019000	-8.170000
C	-1.824000	6.343000	-6.947000
C	-0.696000	5.614000	-6.560000
C	0.370000	5.620000	-7.458000
N	0.381000	6.266000	-8.653000
C	-0.731000	8.999000	-12.740000
C	-1.802000	9.007000	-11.865000
N	-1.808000	8.362000	-10.675000
C	-0.692000	7.664000	-10.319000
C	0.426000	7.615000	-11.156000
C	0.404000	8.289000	-12.377000
C	2.197000	1.653000	2.528000
C	-2.938000	1.662000	2.666000
C	-2.951000	-3.474000	3.189000
C	2.209000	-3.493000	3.052000
H	-0.383000	1.015000	1.974000
H	-3.719000	2.209000	0.827000
H	2.884000	2.192000	0.650000
H	2.890000	-4.403000	1.321000
H	1.796000	-3.653000	-1.927000
H	2.943000	-4.888000	-2.400000
H	-3.977000	1.954000	-2.915000
H	-2.793000	0.827000	-2.287000
H	-2.754000	-3.679000	-1.817000
H	-3.941000	-4.902000	-2.220000
H	-3.726000	-4.381000	1.495000
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H	-1.285000	6.560000	-4.065000
H	-2.728000	7.579000	-8.461000
H	-2.704000	6.383000	-6.309000
H	1.293000	5.092000	-7.232000
H	-0.780000	9.535000	-13.682000
H	-2.713000	9.548000	-12.104000
H	1.311000	7.056000	-10.864000
H	1.268000	8.256000	-13.034000
H	3.209000	1.457000	2.901000
H	1.936000	2.683000	2.793000
H	1.518000	0.994000	3.077000
H	-3.928000	1.461000	3.090000
H	-2.228000	1.005000	3.177000
H	-2.667000	2.693000	2.922000
H	-2.691000	-4.433000	3.652000
H	-2.237000	-2.733000	3.560000
H	-3.941000	-3.183000	3.556000
H	3.221000	-3.216000	3.371000
H	1.525000	-2.743000	3.461000

H	1.960000	-4.450000	3.526000
C	-3.032000	-1.069000	1.357000
C	-3.423000	0.097000	0.679000
C	-4.196000	-0.040000	-0.489000
C	-4.627000	-1.301000	-0.957000
C	-4.182000	-2.447000	-0.261000
C	-3.417000	-2.346000	0.918000
O	-4.564000	-3.690000	-0.713000
O	-4.580000	1.090000	-1.176000
C	-7.277000	-1.592000	-4.359000
C	-5.917000	-1.922000	-4.474000
C	-5.053000	-1.831000	-3.375000
C	-5.521000	-1.407000	-2.124000
C	-6.878000	-1.075000	-2.007000
C	-7.741000	-1.167000	-3.105000
C	-9.857000	-1.838000	-7.749000
C	-10.236000	-2.455000	-6.556000
C	-9.399000	-2.380000	-5.439000
C	-8.185000	-1.691000	-5.510000
C	-7.890000	-1.104000	-6.739000
N	-8.680000	-1.160000	-7.842000
C	-12.358000	-2.035000	-11.179000
C	-12.671000	-2.627000	-9.968000
N	-11.880000	-2.568000	-8.872000
C	-10.704000	-1.884000	-8.968000
C	-10.325000	-1.262000	-10.161000
C	-11.161000	-1.339000	-11.274000
H	-2.398000	-0.981000	2.235000
H	-5.518000	-2.273000	-5.425000
H	-4.012000	-2.102000	-3.507000
H	-7.274000	-0.737000	-1.051000
H	-8.786000	-0.891000	-2.970000
H	-11.176000	-2.997000	-6.489000
H	-9.702000	-2.876000	-4.520000
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H	-13.030000	-2.113000	-12.026000
H	-13.596000	-3.182000	-9.843000
H	-9.386000	-0.720000	-10.227000
H	-10.875000	-0.859000	-12.206000
C	0.801000	-4.103000	0.983000
C	-0.410000	-3.673000	1.550000
C	-1.651000	-4.101000	1.057000
C	-1.663000	-4.957000	-0.060000
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C	-0.611000	-8.272000	-3.904000
C	-0.839000	-8.669000	-2.578000
C	-0.794000	-7.745000	-1.527000
C	-0.516000	-6.393000	-1.768000
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C	-1.684000	-11.650000	-9.428000
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N	-0.202000	-13.125000	-8.241000
C	-0.283000	-13.978000	-9.289000
H	-0.384000	-2.978000	2.385000
H	-1.068000	-9.708000	-2.346000
H	-0.979000	-8.090000	-0.511000
H	-0.069000	-4.954000	-3.318000
H	-0.134000	-6.563000	-5.152000
H	-2.002000	-8.119000	-6.273000
H	0.672000	-10.695000	-4.104000
H	0.543000	-12.280000	-5.984000
H	-1.065000	-14.456000	-11.234000
H	-2.354000	-12.318000	-11.366000
H	-2.240000	-10.718000	-9.474000
H	0.293000	-14.893000	-9.187000

C	3.743000	-1.322000	-1.133000
C	3.319000	-0.062000	-0.657000
C	2.579000	0.078000	0.531000
C	2.203000	-1.085000	1.220000
C	2.571000	-2.362000	0.769000
C	3.303000	-2.465000	-0.431000
O	3.667000	1.072000	-1.358000
O	3.649000	-3.714000	-0.898000
C	6.398000	-1.591000	-4.536000
C	5.054000	-1.980000	-4.638000
C	4.190000	-1.897000	-3.538000
C	4.638000	-1.424000	-2.300000
C	5.981000	-1.033000	-2.197000
C	6.846000	-1.115000	-3.295000
C	9.006000	-1.920000	-7.899000
C	8.954000	-0.719000	-7.190000
C	8.104000	-0.600000	-6.087000
C	7.306000	-1.676000	-5.690000
C	7.425000	-2.836000	-6.454000
N	8.240000	-2.982000	-7.531000
C	11.569000	-2.341000	-11.262000
C	11.468000	-1.179000	-10.518000
N	10.655000	-1.038000	-9.446000
C	9.888000	-2.105000	-9.079000
C	9.941000	-3.309000	-9.787000
C	10.789000	-3.425000	-10.887000
H	1.596000	-0.995000	2.116000
H	4.653000	-2.338000	-5.585000
H	3.157000	-2.203000	-3.667000
H	6.367000	-0.660000	-1.249000
H	7.883000	-0.811000	-3.163000
H	9.567000	0.127000	-7.491000
H	8.065000	0.346000	-5.552000
H	6.851000	-3.727000	-6.209000
H	12.238000	-2.398000	-12.113000
H	12.058000	-0.303000	-10.771000
H	9.327000	-4.153000	-9.487000
H	10.836000	-4.357000	-11.444000
C	-0.947000	-1.424000	-3.554000
N	0.329000	-1.615000	-4.308000
O	0.696000	-2.779000	-4.510000
O	0.942000	-0.596000	-4.649000
C	-0.630000	-1.427000	-2.074000
H	-1.386000	-0.477000	-3.880000
H	-1.613000	-2.247000	-3.830000
H	-0.191000	-2.378000	-1.763000
H	0.075000	-0.634000	-1.812000
H	-1.540000	-1.273000	-1.493000

Table S3. Cartesian coordinates of **7⊂16**

Atom	*x* / Å	*y* / Å	*z* / Å
C	0.722000	2.463000	-0.712000
C	-0.500000	2.796000	-1.334000
C	-1.693000	2.480000	-0.652000
C	-1.687000	1.896000	0.630000
C	-0.445000	1.590000	1.215000
C	0.770000	1.885000	0.572000
C	-3.005000	1.524000	1.307000
C	2.115000	1.527000	1.204000
C	2.128000	-3.567000	1.725000
O	1.896000	2.779000	-1.357000
O	-2.895000	2.800000	-1.239000
O	1.910000	-5.308000	-0.533000
C	2.511000	-4.298000	-1.357000
C	-3.509000	1.655000	-1.849000
C	-3.520000	-4.357000	-1.219000
C	-2.992000	-3.568000	1.841000
C	2.499000	1.624000	-1.960000
C	-0.610000	4.704000	-5.204000
C	-0.501000	3.309000	-5.088000
C	-0.463000	2.686000	-3.835000
C	-0.532000	3.441000	-2.656000
C	-0.642000	4.834000	-2.765000
C	-0.681000	5.454000	-4.019000
C	-0.663000	6.557000	-9.048000
C	-1.646000	6.890000	-8.116000
C	-1.638000	6.290000	-6.854000
C	-0.651000	5.358000	-6.520000
C	0.291000	5.089000	-7.511000
N	0.309000	5.653000	-8.746000
C	-0.636000	8.345000	-12.903000
C	-1.581000	8.629000	-11.934000
N	-1.596000	8.064000	-10.705000
C	-0.620000	7.160000	-10.404000
C	0.366000	6.826000	-11.336000
C	0.356000	7.425000	-12.596000
C	2.171000	1.720000	2.730000
C	-3.006000	1.710000	2.834000
C	-2.985000	-3.435000	3.374000
C	2.186000	-3.449000	3.258000
H	-0.425000	1.100000	2.184000
H	-3.768000	2.244000	0.982000
H	2.858000	2.254000	0.849000
H	2.872000	-4.349000	1.521000
H	1.775000	-3.588000	-1.765000
H	2.933000	-4.822000	-2.221000
H	-3.981000	2.019000	-2.768000
H	-2.779000	0.896000	-2.168000
H	-2.805000	-3.680000	-1.709000
H	-4.004000	-4.914000	-2.029000
H	-3.750000	-4.345000	1.675000
H	1.764000	0.845000	-2.215000
H	2.920000	1.964000	-2.913000
H	-0.459000	2.685000	-5.980000
H	-0.384000	1.603000	-3.793000
H	-0.697000	5.448000	-1.868000
H	-0.756000	6.540000	-4.059000
H	-2.421000	7.611000	-8.364000
H	-2.418000	6.551000	-6.142000
H	1.103000	4.387000	-7.333000
H	-0.672000	8.828000	-13.873000
H	-2.378000	9.342000	-12.126000
H	1.140000	6.105000	-11.088000
H	1.119000	7.172000	-13.327000
H	3.181000	1.519000	3.104000
H	1.917000	2.754000	2.994000
H	1.486000	1.068000	3.280000
H	-3.999000	1.494000	3.245000
H	-2.293000	1.065000	3.356000
H	-2.756000	2.746000	3.093000
H	-2.724000	-4.392000	3.839000
H	-2.276000	-2.690000	3.747000
H	-3.978000	-3.146000	3.737000
H	3.196000	-3.174000	3.582000
H	1.500000	-2.702000	3.667000

H	1.935000	-4.409000	3.725000
C	-3.069000	-1.026000	1.539000
C	-3.441000	0.136000	0.839000
C	-4.166000	-0.013000	-0.359000
C	-4.561000	-1.280000	-0.838000
C	-4.167000	-2.417000	-0.101000
C	-3.439000	-2.308000	1.099000
O	-4.570000	-3.659000	-0.536000
O	-4.568000	1.107000	-1.050000
C	-6.882000	-1.680000	-4.454000
C	-5.479000	-1.641000	-4.496000
C	-4.723000	-1.511000	-3.325000
C	-5.349000	-1.414000	-2.074000
C	-6.748000	-1.452000	-2.026000
C	-7.502000	-1.584000	-3.198000
C	-9.143000	-2.019000	-8.058000
C	-9.416000	-2.883000	-6.996000
C	-8.682000	-2.780000	-5.811000
C	-7.677000	-1.818000	-5.683000
C	-7.475000	-0.998000	-6.792000
N	-8.169000	-1.074000	-7.957000
C	-11.338000	-2.285000	-11.686000
C	-11.557000	-3.109000	-10.597000
N	-10.862000	-3.030000	-9.439000
C	-9.888000	-2.081000	-9.341000
C	-9.614000	-1.215000	-10.403000
C	-10.346000	-1.320000	-11.584000
H	-2.467000	-0.929000	2.438000
H	-4.955000	-1.727000	-5.447000
H	-3.638000	-1.490000	-3.402000
H	-7.262000	-1.378000	-1.070000
H	-8.588000	-1.599000	-3.118000
H	-10.194000	-3.637000	-7.084000
H	-8.899000	-3.468000	-4.997000
H	-6.723000	-0.213000	-6.776000
H	-11.926000	-2.392000	-12.591000
H	-12.322000	-3.880000	-10.628000
H	-8.836000	-0.462000	-10.314000
H	-10.141000	-0.651000	-12.416000
C	0.783000	-4.048000	1.179000
C	-0.432000	-3.636000	1.752000
C	-1.673000	-4.060000	1.245000
C	-1.680000	-4.890000	0.107000
C	-0.486000	-5.327000	-0.503000
C	0.735000	-4.871000	0.037000
O	-2.881000	-5.340000	-0.391000
C	-0.575000	-7.962000	-3.920000
C	-0.614000	-8.466000	-2.610000
C	-0.586000	-7.610000	-1.503000
C	-0.515000	-6.221000	-1.671000
C	-0.476000	-5.711000	-2.976000
C	-0.506000	-6.569000	-4.083000
C	-0.719000	-10.532000	-7.324000
N	-1.572000	-9.474000	-7.239000
C	-1.494000	-8.683000	-6.138000
C	-0.604000	-8.864000	-5.081000
C	0.260000	-9.957000	-5.192000
C	0.204000	-10.792000	-6.311000
C	-0.934000	-13.032000	-10.754000
C	-1.804000	-11.954000	-10.667000
C	-1.751000	-11.121000	-9.551000
C	-0.825000	-11.382000	-8.537000
N	0.031000	-12.441000	-8.620000
C	-0.043000	-13.232000	-9.715000
H	-0.413000	-2.961000	2.603000
H	-0.679000	-9.539000	-2.436000
H	-0.621000	-8.036000	-0.502000
H	-0.419000	-4.639000	-3.148000
H	-0.458000	-6.134000	-5.080000
H	-2.212000	-7.866000	-6.129000
H	0.993000	-10.165000	-4.416000
H	0.884000	-11.636000	-6.387000
H	-0.950000	-13.699000	-11.609000
H	-2.520000	-11.760000	-11.461000
H	-2.428000	-10.276000	-9.475000
H	0.659000	-14.062000	-9.736000

C	3.643000	-1.265000	-0.972000
C	3.249000	-0.004000	-0.483000
C	2.551000	0.141000	0.732000
C	2.205000	-1.022000	1.442000
C	2.559000	-2.303000	0.983000
C	3.256000	-2.404000	-0.237000
O	3.603000	1.120000	-1.194000
O	3.614000	-3.647000	-0.708000
C	5.954000	-1.629000	-4.600000
C	4.550000	-1.629000	-4.634000
C	3.797000	-1.511000	-3.460000
C	4.425000	-1.390000	-2.213000
C	5.825000	-1.390000	-2.173000
C	6.577000	-1.506000	-3.348000
C	8.205000	-2.049000	-8.203000
C	8.515000	-1.014000	-7.320000
C	7.785000	-0.867000	-6.138000
C	6.746000	-1.751000	-5.833000
C	6.508000	-2.755000	-6.770000
N	7.198000	-2.923000	-7.928000
C	10.385000	-2.544000	-11.815000
C	10.641000	-1.541000	-10.899000
N	9.951000	-1.377000	-9.747000
C	8.943000	-2.254000	-9.474000
C	8.631000	-3.292000	-10.356000
C	9.360000	-3.437000	-11.536000
H	1.628000	-0.930000	2.357000
H	4.023000	-1.705000	-5.584000
H	2.713000	-1.512000	-3.534000
H	6.343000	-1.300000	-1.220000
H	7.663000	-1.512000	-3.271000
H	9.318000	-0.318000	-7.547000
H	8.030000	-0.048000	-5.465000
H	5.728000	-3.495000	-6.609000
H	10.971000	-2.629000	-12.724000
H	11.433000	-0.817000	-11.072000
H	7.827000	-3.987000	-10.130000
H	9.125000	-4.240000	-12.229000
C	-0.567000	-1.338000	-1.370000
H	0.368000	-1.387000	-0.816000
H	-1.063000	-0.402000	-1.120000
H	-1.201000	-2.158000	-1.040000
N	-0.128000	-1.489000	-3.945000
C	-0.325000	-1.423000	-2.804000

Table S4-1. Cartesian coordinates of **8⊂16**

Atom	*x* / Å	*y* / Å	*z* / Å
C	0.728000	2.522000	-0.743000
C	-0.481000	2.860000	-1.385000
C	-1.686000	2.511000	-0.741000
C	-1.699000	1.914000	0.535000
C	-0.469000	1.608000	1.141000
C	0.755000	1.920000	0.529000
C	-3.026000	1.544000	1.193000
C	2.089000	1.554000	1.176000
C	2.101000	-3.535000	1.694000
O	1.917000	2.839000	-1.361000
O	-2.880000	2.818000	-1.353000
O	1.925000	-5.298000	-0.542000
C	2.506000	-4.278000	-1.370000
C	-3.480000	1.656000	-1.950000
C	-3.492000	-4.302000	-1.315000
C	-3.013000	-3.541000	1.737000
C	2.510000	1.685000	-1.975000
C	-0.473000	4.926000	-5.177000
C	-0.649000	3.534000	-5.112000
C	-0.652000	2.861000	-3.885000
C	-0.481000	3.557000	-2.682000
C	-0.302000	4.946000	-2.741000
C	-0.300000	5.619000	-3.969000
C	-0.413000	6.923000	-8.948000
C	-1.239000	7.406000	-7.933000
C	-1.266000	6.760000	-6.693000
C	-0.471000	5.634000	-6.466000
C	0.323000	5.224000	-7.535000
N	0.371000	5.828000	-8.750000
C	-0.291000	8.841000	-12.738000
C	-1.088000	9.265000	-11.691000
N	-1.132000	8.660000	-10.482000
C	-0.343000	7.565000	-10.285000
C	0.488000	7.083000	-11.300000
C	0.512000	7.727000	-12.536000
C	2.123000	1.736000	2.704000
C	-3.049000	1.735000	2.721000
C	-3.026000	-3.407000	3.270000
C	2.141000	-3.407000	3.228000
H	-0.466000	1.102000	2.102000
H	-3.783000	2.266000	0.857000
H	2.841000	2.279000	0.837000
H	2.855000	-4.311000	1.505000
H	1.760000	-3.575000	-1.768000
H	2.926000	-4.795000	-2.240000
H	-3.921000	1.995000	-2.894000
H	-2.742000	0.889000	-2.221000
H	-2.767000	-3.601000	-1.754000
H	-3.944000	-4.832000	-2.162000
H	-3.768000	-4.321000	1.564000
H	1.769000	0.919000	-2.250000
H	2.941000	2.034000	-2.920000
H	-0.804000	2.956000	-6.022000
H	-0.798000	1.784000	-3.879000
H	-0.162000	5.516000	-1.825000
H	-0.149000	6.697000	-3.970000
H	-1.864000	8.279000	-8.098000
H	-1.923000	7.141000	-5.915000
H	0.984000	4.364000	-7.442000
H	-0.295000	9.365000	-13.687000
H	-1.735000	10.132000	-11.799000
H	1.113000	6.210000	-11.134000
H	1.155000	7.360000	-13.331000
H	3.126000	1.525000	3.092000
H	1.872000	2.770000	2.971000
H	1.425000	1.086000	3.240000
H	-4.049000	1.522000	3.117000
H	-2.346000	1.090000	3.255000
H	-2.801000	2.771000	2.981000
H	-2.768000	-4.363000	3.740000
H	-2.325000	-2.659000	3.651000
H	-4.026000	-3.122000	3.620000
H	3.145000	-3.118000	3.561000
H	1.443000	-2.664000	3.625000

H	1.896000	-4.366000	3.698000
C	-3.082000	-1.002000	1.428000
C	-3.458000	0.157000	0.726000
C	-4.190000	0.008000	-0.468000
C	-4.604000	-1.258000	-0.932000
C	-4.194000	-2.392000	-0.200000
C	-3.455000	-2.283000	0.993000
O	-4.573000	-3.639000	-0.642000
O	-4.568000	1.130000	-1.171000
C	-7.072000	-1.684000	-4.451000
C	-5.689000	-1.468000	-4.560000
C	-4.886000	-1.328000	-3.422000
C	-5.440000	-1.398000	-2.137000
C	-6.819000	-1.616000	-2.023000
C	-7.622000	-1.757000	-3.161000
C	-9.486000	-2.042000	-7.952000
C	-9.592000	-3.006000	-6.948000
C	-8.807000	-2.898000	-5.797000
C	-7.917000	-1.832000	-5.645000
C	-7.880000	-0.916000	-6.696000
N	-8.627000	-0.994000	-7.827000
C	-11.844000	-2.318000	-11.476000
C	-11.896000	-3.240000	-10.447000
N	-11.148000	-3.159000	-9.322000
C	-10.293000	-2.104000	-9.197000
C	-10.190000	-1.135000	-10.199000
C	-10.973000	-1.245000	-11.347000
H	-2.474000	-0.904000	2.322000
H	-5.216000	-1.418000	-5.539000
H	-3.819000	-1.166000	-3.551000
H	-7.281000	-1.676000	-1.039000
H	-8.691000	-1.914000	-3.027000
H	-10.278000	-3.842000	-7.055000
H	-8.892000	-3.663000	-5.028000
H	-7.226000	-0.047000	-6.656000
H	-12.467000	-2.432000	-12.357000
H	-12.561000	-4.097000	-10.500000
H	-9.506000	-0.298000	-10.090000
H	-10.900000	-0.497000	-12.132000
C	0.767000	-4.032000	1.141000
C	-0.457000	-3.610000	1.685000
C	-1.689000	-4.036000	1.158000
C	-1.678000	-4.877000	0.028000
C	-0.473000	-5.341000	-0.541000
C	0.738000	-4.876000	0.014000
O	-2.871000	-5.312000	-0.504000
C	-0.455000	-8.083000	-3.876000
C	-0.221000	-8.529000	-2.566000
C	-0.230000	-7.638000	-1.486000
C	-0.472000	-6.272000	-1.682000
C	-0.703000	-5.822000	-2.988000
C	-0.696000	-6.713000	-4.068000
C	-0.495000	-10.765000	-7.196000
N	-1.536000	-9.909000	-7.004000
C	-1.486000	-9.075000	-5.934000
C	-0.444000	-9.019000	-5.010000
C	0.612000	-9.908000	-5.226000
C	0.589000	-10.781000	-6.318000
C	-0.619000	-13.390000	-10.534000
C	-1.685000	-12.524000	-10.336000
C	-1.665000	-11.655000	-9.246000
C	-0.575000	-11.666000	-8.372000
N	0.474000	-12.516000	-8.566000
C	0.428000	-13.349000	-9.632000
H	-0.452000	-2.921000	2.524000
H	-0.039000	-9.584000	-2.368000
H	-0.046000	-8.020000	-0.483000
H	-0.886000	-4.769000	-3.178000
H	-0.867000	-6.322000	-5.069000
H	-2.356000	-8.430000	-5.834000
H	1.470000	-9.924000	-4.557000
H	1.418000	-11.465000	-6.477000
H	-0.603000	-14.078000	-11.372000
H	-2.529000	-12.523000	-11.021000
H	-2.496000	-10.975000	-9.083000
H	1.286000	-14.006000	-9.744000

C	3.643000	-1.233000	-0.989000
C	3.239000	0.030000	-0.508000
C	2.524000	0.170000	0.697000
C	2.163000	-0.994000	1.398000
C	2.529000	-2.273000	0.947000
C	3.245000	-2.374000	-0.261000
O	3.606000	1.154000	-1.213000
O	3.609000	-3.616000	-0.729000
C	6.007000	-1.612000	-4.581000
C	4.611000	-1.470000	-4.646000
C	3.842000	-1.346000	-3.483000
C	4.444000	-1.361000	-2.218000
C	5.836000	-1.505000	-2.148000
C	6.605000	-1.627000	-3.311000
C	8.301000	-2.040000	-8.153000
C	8.675000	-1.079000	-7.212000
C	7.931000	-0.931000	-6.038000
C	6.816000	-1.739000	-5.801000
C	6.519000	-2.673000	-6.792000
N	7.220000	-2.840000	-7.944000
C	10.519000	-2.533000	-11.743000
C	10.831000	-1.597000	-10.774000
N	10.129000	-1.435000	-9.628000
C	9.051000	-2.242000	-9.418000
C	8.680000	-3.209000	-10.357000
C	9.422000	-3.354000	-11.528000
H	1.569000	-0.903000	2.303000
H	4.108000	-1.438000	-5.611000
H	2.766000	-1.235000	-3.573000
H	6.333000	-1.525000	-1.179000
H	7.683000	-1.746000	-3.212000
H	9.538000	-0.443000	-7.386000
H	8.227000	-0.170000	-5.319000
H	5.677000	-3.353000	-6.684000
H	11.117000	-2.620000	-12.644000
H	11.681000	-0.931000	-10.895000
H	7.819000	-3.848000	-10.180000
H	9.141000	-4.103000	-12.263000
C	-0.440000	-1.361000	-1.692000
C	-0.561000	-1.420000	-3.180000
O	-1.318000	-0.720000	-3.838000
O	0.285000	-2.357000	-3.683000
C	0.239000	-2.488000	-5.107000
H	0.579000	-1.091000	-1.418000
H	-1.117000	-0.601000	-1.300000
H	-0.712000	-2.323000	-1.263000
H	0.954000	-3.263000	-5.398000
H	-0.760000	-2.796000	-5.430000
H	0.531000	-1.548000	-5.586000

Table S4-2. Cartesian coordinates of **8⊂16**

Atom	*x* / Å	*y* / Å	*z* / Å
C	0.798000	2.452000	-0.709000
C	-0.419000	2.793000	-1.335000
C	-1.617000	2.465000	-0.667000
C	-1.621000	1.868000	0.608000
C	-0.385000	1.554000	1.197000
C	0.835000	1.858000	0.568000
C	-2.943000	1.498000	1.276000
C	2.172000	1.487000	1.206000
C	2.168000	-3.608000	1.634000
O	1.978000	2.781000	-1.338000
O	-2.816000	2.788000	-1.262000
O	1.949000	-5.334000	-0.626000
C	2.520000	-4.294000	-1.438000
C	-3.424000	1.638000	-1.868000
C	-3.449000	-4.339000	-1.291000
C	-2.943000	-3.594000	1.765000
C	2.596000	1.637000	-1.948000
C	-0.498000	4.744000	-5.182000
C	-0.333000	3.354000	-5.080000
C	-0.308000	2.719000	-3.832000
C	-0.443000	3.456000	-2.648000
C	-0.609000	4.843000	-2.745000
C	-0.637000	5.477000	-3.993000
C	-0.516000	6.638000	-9.007000
C	-1.549000	6.905000	-8.107000
C	-1.553000	6.292000	-6.852000
C	-0.528000	5.412000	-6.492000
C	0.463000	5.207000	-7.450000
N	0.493000	5.786000	-8.678000
C	-0.454000	8.468000	-12.841000
C	-1.450000	8.684000	-11.906000
N	-1.477000	8.104000	-10.684000
C	-0.459000	7.258000	-10.354000
C	0.580000	6.995000	-11.251000
C	0.580000	7.607000	-12.504000
C	2.217000	1.650000	2.736000
C	-2.951000	1.673000	2.805000
C	-2.933000	-3.474000	3.299000
C	2.235000	-3.508000	3.169000
H	-0.373000	1.050000	2.159000
H	-3.701000	2.225000	0.954000
H	2.919000	2.221000	0.871000
H	2.915000	-4.385000	1.420000
H	1.769000	-3.575000	-1.798000
H	2.915000	-4.790000	-2.332000
H	-3.873000	1.991000	-2.803000
H	-2.692000	0.871000	-2.159000
H	-2.715000	-3.647000	-1.732000
H	-3.909000	-4.863000	-2.136000
H	-3.706000	-4.366000	1.596000
H	1.869000	0.860000	-2.231000
H	3.031000	1.994000	-2.888000
H	-0.237000	2.746000	-5.978000
H	-0.185000	1.640000	-3.791000
H	-0.717000	5.443000	-1.843000
H	-0.758000	6.559000	-4.024000
H	-2.353000	7.585000	-8.376000
H	-2.370000	6.501000	-6.165000
H	1.306000	4.551000	-7.249000
H	-0.483000	8.960000	-13.807000
H	-2.282000	9.350000	-12.121000
H	1.386000	6.320000	-10.980000
H	1.384000	7.409000	-13.208000
H	3.225000	1.441000	3.113000
H	1.961000	2.678000	3.018000
H	1.529000	0.987000	3.268000
H	-3.947000	1.460000	3.210000
H	-2.244000	1.020000	3.326000
H	-2.695000	2.705000	3.073000
H	-2.677000	-4.437000	3.756000
H	-2.219000	-2.737000	3.677000
H	-3.924000	-3.182000	3.666000
H	3.246000	-3.232000	3.491000
H	1.548000	-2.769000	3.591000

H	1.991000	-4.475000	3.626000
C	-3.012000	-1.051000	1.485000
C	-3.386000	0.116000	0.799000
C	-4.122000	-0.020000	-0.395000
C	-4.535000	-1.279000	-0.875000
C	-4.127000	-2.423000	-0.158000
C	-3.387000	-2.328000	1.035000
O	-4.519000	-3.662000	-0.614000
O	-4.505000	1.109000	-1.085000
C	-6.956000	-1.648000	-4.429000
C	-5.561000	-1.505000	-4.515000
C	-4.774000	-1.385000	-3.364000
C	-5.357000	-1.402000	-2.090000
C	-6.747000	-1.546000	-1.998000
C	-7.534000	-1.668000	-3.149000
C	-9.316000	-1.955000	-7.971000
C	-9.478000	-2.901000	-6.958000
C	-8.711000	-2.809000	-5.793000
C	-7.783000	-1.776000	-5.637000
C	-7.691000	-0.876000	-6.696000
N	-8.419000	-0.939000	-7.841000
C	-11.614000	-2.184000	-11.537000
C	-11.720000	-3.091000	-10.499000
N	-10.992000	-3.024000	-9.361000
C	-10.100000	-2.001000	-9.230000
C	-9.942000	-1.049000	-10.241000
C	-10.706000	-1.143000	-11.403000
H	-2.401000	-0.965000	2.379000
H	-5.070000	-1.500000	-5.487000
H	-3.698000	-1.281000	-3.468000
H	-7.230000	-1.563000	-1.022000
H	-8.612000	-1.767000	-3.035000
H	-10.194000	-3.711000	-7.069000
H	-8.840000	-3.561000	-5.017000
H	-7.006000	-0.032000	-6.653000
H	-12.224000	-2.285000	-12.428000
H	-12.416000	-3.923000	-10.555000
H	-9.229000	-0.237000	-10.128000
H	-10.591000	-0.407000	-12.194000
C	0.824000	-4.088000	1.095000
C	-0.388000	-3.666000	1.667000
C	-1.629000	-4.090000	1.166000
C	-1.639000	-4.933000	0.038000
C	-0.448000	-5.395000	-0.560000
C	0.774000	-4.922000	-0.039000
O	-2.844000	-5.355000	-0.477000
C	-0.566000	-8.175000	-3.863000
C	-0.738000	-8.609000	-2.539000
C	-0.700000	-7.705000	-1.471000
C	-0.486000	-6.337000	-1.692000
C	-0.316000	-5.900000	-3.011000
C	-0.355000	-6.804000	-4.079000
C	-0.731000	-10.884000	-7.157000
N	-1.485000	-9.750000	-7.174000
C	-1.405000	-8.917000	-6.105000
C	-0.604000	-9.126000	-4.984000
C	0.159000	-10.296000	-4.989000
C	0.098000	-11.176000	-6.074000
C	-0.958000	-13.517000	-10.484000
C	-1.730000	-12.364000	-10.502000
C	-1.671000	-11.486000	-9.420000
C	-0.837000	-11.778000	-8.337000
N	-0.078000	-12.911000	-8.318000
C	-0.155000	-13.745000	-9.381000
H	-0.364000	-2.981000	2.509000
H	-0.915000	-9.661000	-2.323000
H	-0.840000	-8.076000	-0.457000
H	-0.145000	-4.848000	-3.220000
H	-0.198000	-6.424000	-5.087000
H	-2.043000	-8.039000	-6.180000
H	0.819000	-10.531000	-4.157000
H	0.700000	-12.081000	-6.067000
H	-0.981000	-14.220000	-11.309000
H	-2.375000	-12.146000	-11.348000
H	-2.272000	-10.581000	-9.426000
H	0.468000	-14.633000	-9.319000

C	3.723000	-1.266000	-1.004000
C	3.328000	-0.013000	-0.491000
C	2.606000	0.110000	0.710000
C	2.235000	-1.064000	1.384000
C	2.592000	-2.336000	0.905000
C	3.302000	-2.419000	-0.309000
O	3.692000	1.126000	-1.174000
O	3.644000	-3.656000	-0.808000
C	6.142000	-1.516000	-4.573000
C	4.761000	-1.765000	-4.617000
C	3.974000	-1.686000	-3.462000
C	4.542000	-1.359000	-2.224000
C	5.920000	-1.107000	-2.176000
C	6.706000	-1.184000	-3.332000
C	8.505000	-1.830000	-8.114000
C	8.610000	-0.686000	-7.321000
C	7.842000	-0.573000	-6.160000
C	6.969000	-1.598000	-5.786000
C	6.931000	-2.704000	-6.635000
N	7.662000	-2.843000	-7.770000
C	10.811000	-2.230000	-11.660000
C	10.863000	-1.122000	-10.834000
N	10.132000	-0.988000	-9.704000
C	9.294000	-2.007000	-9.359000
C	9.192000	-3.155000	-10.148000
C	9.957000	-3.266000	-11.308000
H	1.641000	-0.989000	2.290000
H	4.275000	-2.013000	-5.559000
H	2.908000	-1.882000	-3.539000
H	6.393000	-0.849000	-1.231000
H	7.775000	-0.992000	-3.247000
H	9.283000	0.120000	-7.602000
H	7.926000	0.330000	-5.558000
H	6.290000	-3.555000	-6.414000
H	11.420000	-2.285000	-12.555000
H	11.516000	-0.284000	-11.066000
H	8.521000	-3.962000	-9.865000
H	9.885000	-4.155000	-11.928000
C	-0.463000	-1.346000	-1.780000
O	-0.995000	-1.016000	-3.065000
C	-1.038000	-1.296000	-5.396000
H	0.602000	-1.109000	-1.735000
H	-0.984000	-0.750000	-1.030000
H	-0.630000	-2.403000	-1.562000
H	-1.092000	-0.207000	-5.478000
H	-2.035000	-1.735000	-5.467000
H	-0.423000	-1.667000	-6.221000
C	-0.406000	-1.684000	-4.094000
O	0.496000	-2.501000	-3.979000

Table S5-1. Cartesian coordinates of **9⊂16**

Atom	*x* / Å	*y* / Å	*z* / Å
C	0.72000	2.54320	-0.70960
C	-0.48950	2.87380	-1.35640
C	-1.69410	2.51600	-0.71650
C	-1.70730	1.91610	0.55810
C	-0.47730	1.60980	1.16450
C	0.74700	1.93150	0.55780
C	-3.08350	-1.00220	1.44820
C	-3.46400	0.15620	0.74960
C	-4.19890	0.00750	-0.44320
C	-4.61450	-1.25790	-0.90630
C	-4.20550	-2.39130	-0.17250
C	-3.45900	-2.28380	1.01570
C	0.76830	-4.02630	1.12250
C	-0.45220	-3.60620	1.67610
C	-1.68760	-4.03320	1.15990
C	-1.68380	-4.87320	0.02830
C	-0.48240	-5.33440	-0.55170
C	0.73240	-4.86550	-0.00730
C	3.63700	-1.20500	-0.99680
C	3.23160	0.05320	-0.50240
C	2.51730	0.18160	0.70530
C	2.15820	-0.98970	1.39360
C	2.52630	-2.26420	0.93200
C	3.23880	-2.35300	-0.27910
C	-3.03320	1.54400	1.21590
C	2.08140	1.55950	1.19920
C	2.10500	-3.53240	1.66990
O	1.91000	2.87210	-1.31930
O	-2.88900	2.81970	-1.32960
O	3.59940	1.18580	-1.19370
O	3.59720	-3.59170	-0.76260
O	-2.88110	-5.30960	-0.49370
O	-4.58750	-3.63940	-0.61100
O	-4.57620	1.12990	-1.14600
O	1.91570	-5.27790	-0.57860
C	2.48870	-4.24740	-1.40010
C	-3.48820	1.65610	-1.92410
C	-3.51330	-4.29920	-1.29630
H	-0.47390	1.09480	2.12030
H	-2.46740	-0.90410	2.33680
H	-0.44070	-2.91690	2.51500
H	1.56280	-0.90850	2.29810
C	-3.00760	-3.54280	1.75150
H	-3.79180	2.26480	0.88120
H	2.83300	2.28970	0.86920
H	2.85900	-4.30610	1.46990
H	1.73860	-3.54100	-1.78380
H	2.90080	-4.75430	-2.27960
H	-3.92860	1.99320	-2.86890
H	-2.74920	0.88880	-2.19380
H	-2.79350	-3.59520	-1.74080
H	-3.97260	-4.82750	-2.13920
H	-3.76240	-4.32370	1.58510
C	2.50440	1.72820	-1.94960
H	1.76440	0.96570	-2.23640
H	2.93690	2.09170	-2.88840
C	-0.49950	-8.08660	-3.87820
C	-0.19150	-8.51720	-2.57910
C	-0.18850	-7.62250	-1.50310
C	-0.49030	-6.26740	-1.69160
C	-0.79100	-5.83180	-2.98850
C	-0.80010	-6.72820	-4.06360
H	0.03810	-9.56370	-2.38650
H	0.05070	-7.99230	-0.50750
H	-1.01610	-4.78570	-3.17510
H	-1.02920	-6.34910	-5.05790
C	6.01240	-1.54560	-4.58440
C	4.63290	-1.29630	-4.65310
C	3.85860	-1.18910	-3.49200
C	4.44110	-1.32120	-2.22510
C	5.81770	-1.57070	-2.15250
C	6.59110	-1.68030	-3.31360
H	4.14700	-1.16920	-5.61870
H	2.79330	-0.99890	-3.58630

H	6.29880	-1.68400	-1.18260
H	7.65550	-1.88500	-3.21290
C	-0.46300	4.91280	-5.16150
C	-0.68840	3.52970	-5.08480
C	-0.69850	2.86570	-3.85260
C	-0.48590	3.56410	-2.65720
C	-0.25800	4.94430	-2.72960
C	-0.24800	5.60810	-3.96170
H	-0.87780	2.95220	-5.98800
H	-0.88160	1.79480	-3.83690
H	-0.08330	5.51440	-1.81890
H	-0.05770	6.67970	-3.97380
C	-7.05020	-1.70050	-4.44320
C	-5.66850	-1.47360	-4.54100
C	-4.87640	-1.32770	-3.39620
C	-5.44090	-1.40070	-2.11650
C	-6.81920	-1.62880	-2.01410
C	-7.61070	-1.77670	-3.15890
H	-5.18720	-1.41960	-5.51590
H	-3.81000	-1.15700	-3.51610
H	-7.28800	-1.69110	-1.03380
H	-8.67970	-1.93970	-3.03420
C	-0.58580	-10.77940	-7.18410
N	-1.65610	-9.97490	-6.93850
C	-1.58920	-9.13690	-5.87330
C	-0.50320	-9.02590	-5.00760
C	0.58270	-9.86140	-5.27940
C	0.54380	-10.73850	-6.36620
H	-2.48390	-8.53610	-5.72630
H	1.47430	-9.83190	-4.65730
H	1.39490	-11.38220	-6.57040
C	8.30750	-1.94140	-8.15660
C	8.73240	-1.05410	-7.16710
C	7.98940	-0.91680	-5.99200
C	6.82380	-1.66280	-5.80320
C	6.47730	-2.52540	-6.84100
N	7.17500	-2.67950	-7.99450
H	9.63600	-0.46670	-7.30540
H	8.32560	-0.21260	-5.23430
H	5.59360	-3.15530	-6.77120
C	-0.38320	6.87780	-8.94650
C	-1.19040	7.38800	-7.92920
C	-1.22390	6.75320	-6.68510
C	-0.45400	5.61080	-6.45440
C	0.32310	5.17400	-7.52520
N	0.37620	5.76600	-8.74520
H	-1.79570	8.27420	-8.09870
H	-1.86710	7.15490	-5.90540
H	0.96450	4.30090	-7.42920
C	-9.42770	-2.07730	-7.96520
C	-9.53180	-3.04400	-6.96460
C	-8.75850	-2.93040	-5.80650
C	-7.88240	-1.85440	-5.64470
C	-7.84630	-0.93630	-6.69220
N	-8.58100	-1.02020	-7.83030
H	-10.20800	-3.88630	-7.08110
H	-8.84140	-3.69790	-5.04040
H	-7.20450	-0.05940	-6.64390
C	-11.74790	-2.37140	-11.51060
C	-11.79530	-3.29890	-10.48600
N	-11.06040	-3.21240	-9.35450
C	-10.22210	-2.14590	-9.21650
C	-10.12460	-1.17140	-10.21290
C	-10.89470	-1.28670	-11.36880
H	-12.36050	-2.49140	-12.39680
H	-12.44670	-4.16610	-10.54790
H	-9.45360	-0.32570	-10.09180
H	-10.82500	-0.53350	-12.14820
C	10.52160	-2.39730	-11.75250
C	10.87890	-1.52700	-10.73900
N	10.18000	-1.37630	-9.59160
C	9.05480	-2.12810	-9.42480
C	8.63580	-3.02740	-10.40850
C	9.37670	-3.16180	-11.58140
H	11.12040	-2.47730	-12.65250
H	11.76630	-0.90600	-10.82370

H	7.73810	-3.62180	-10.26460
H	9.05800	-3.85880	-12.35100
C	-0.24290	8.76160	-12.75070
C	-1.02670	9.20990	-11.70330
N	-1.07690	8.61630	-10.48970
C	-0.30780	7.50850	-10.28740
C	0.50770	7.00150	-11.30220
C	0.53920	7.63470	-12.54350
H	-0.24190	9.27780	-13.70390
H	-1.65710	10.08760	-11.81390
H	1.11640	6.11860	-11.12960
H	1.17050	7.24710	-13.33770
C	-0.75900	-13.41830	-10.50770
C	-1.86000	-12.61660	-10.24400
C	-1.82370	-11.74380	-9.15790
C	-0.68340	-11.68860	-8.35260
N	0.39940	-12.47620	-8.61050
C	0.33660	-13.31300	-9.67040
H	-0.75430	-14.10760	-11.34420
H	-2.74270	-12.66580	-10.87500
H	-2.68080	-11.11210	-8.94260
H	1.22380	-13.91840	-9.83360
C	2.11410	1.72430	2.72920
H	3.11700	1.50880	3.11550
H	1.86270	2.75430	3.00780
H	1.41630	1.06780	3.25700
C	-3.05590	1.73270	2.74350
H	-4.05510	1.51830	3.14020
H	-2.35160	1.08760	3.27670
H	-2.80770	2.76800	3.00440
C	-3.00570	-3.41070	3.28490
H	-2.74000	-4.36680	3.75070
H	-2.30270	-2.66170	3.66070
H	-4.00180	-3.12870	3.64530
C	2.15470	-3.41620	3.20400
H	3.16010	-3.12920	3.53320
H	1.45820	-2.67760	3.61140
H	1.91320	-4.37940	3.66830
C	-0.43010	-1.37510	-1.76770
H	0.58260	-1.08530	-1.49190
H	-1.12420	-0.63640	-1.36460
H	-0.68010	-2.34890	-1.34940
C	-0.55340	-1.41980	-3.25680
O	-1.32060	-0.72310	-3.90560
O	0.30550	-2.33970	-3.77350
C	0.25700	-2.45360	-5.20220
H	-0.74880	-2.75800	-5.51260
H	0.50890	-1.48920	-5.65740
C	1.26460	-3.50120	-5.63360
H	1.25960	-3.62260	-6.72040
H	2.27340	-3.22390	-5.31450
H	1.04340	-4.46670	-5.16970

Table S5-2. Cartesian coordinates of **9⊂16**

Atom	*x* / Å	*y* / Å	*z* / Å
C	0.702000	2.544000	-0.704000
C	-0.514000	2.874000	-1.340000
C	-1.712000	2.509000	-0.693000
C	-1.714000	1.905000	0.580000
C	-0.479000	1.602000	1.176000
C	0.740000	1.929000	0.561000
C	-3.034000	1.523000	1.245000
C	2.080000	1.558000	1.190000
C	2.121000	-3.529000	1.675000
O	1.887000	2.874000	-1.323000
O	-2.912000	2.809000	-1.299000
O	1.927000	-5.283000	-0.568000
C	2.498000	-4.254000	-1.391000
C	-3.506000	1.646000	-1.897000
C	-3.514000	-4.351000	-1.264000
C	-2.990000	-3.561000	1.779000
C	2.476000	1.728000	-1.954000
C	-0.539000	4.939000	-5.131000
C	-0.671000	3.543000	-5.069000
C	-0.665000	2.869000	-3.841000
C	-0.526000	3.571000	-2.636000
C	-0.393000	4.965000	-2.694000
C	-0.402000	5.637000	-3.921000
C	-0.504000	6.940000	-8.901000
C	-1.351000	7.400000	-7.892000
C	-1.370000	6.752000	-6.654000
C	-0.546000	5.648000	-6.420000
C	0.268000	5.261000	-7.483000
N	0.309000	5.867000	-8.697000
C	-0.402000	8.864000	-12.688000
C	-1.220000	9.266000	-11.648000
N	-1.257000	8.659000	-10.439000
C	-0.440000	7.586000	-10.237000
C	0.411000	7.126000	-11.245000
C	0.429000	7.772000	-12.481000
C	2.127000	1.726000	2.720000
C	-3.050000	1.710000	2.773000
C	-2.986000	-3.427000	3.312000
C	2.178000	-3.410000	3.208000
H	-0.466000	1.086000	2.132000
H	-3.799000	2.239000	0.915000
H	2.828000	2.289000	0.853000
H	2.876000	-4.302000	1.474000
H	1.746000	-3.552000	-1.778000
H	2.911000	-4.764000	-2.269000
H	-3.959000	1.989000	-2.833000
H	-2.764000	0.887000	-2.186000
H	-2.803000	-3.664000	-1.743000
H	-3.988000	-4.902000	-2.084000
H	-3.744000	-4.343000	1.616000
H	1.732000	0.964000	-2.222000
H	2.893000	2.086000	-2.902000
H	-0.794000	2.961000	-5.981000
H	-0.774000	1.789000	-3.837000
H	-0.279000	5.539000	-1.776000
H	-0.285000	6.720000	-3.921000
H	-1.999000	8.255000	-8.062000
H	-2.045000	7.114000	-5.881000
H	0.951000	4.420000	-7.385000
H	-0.413000	9.389000	-13.637000
H	-1.888000	10.115000	-11.760000
H	1.059000	6.271000	-11.075000
H	1.087000	7.423000	-13.271000
H	3.134000	1.512000	3.097000
H	1.878000	2.757000	2.998000
H	1.434000	1.071000	3.255000
H	-4.045000	1.487000	3.175000
H	-2.337000	1.069000	3.301000
H	-2.808000	2.746000	3.034000
H	-2.719000	-4.383000	3.778000
H	-2.282000	-2.678000	3.686000
H	-3.981000	-3.145000	3.674000
H	3.184000	-3.120000	3.533000
H	1.482000	-2.671000	3.617000

H	1.940000	-4.372000	3.676000
C	-3.075000	-1.023000	1.473000
C	-3.458000	0.134000	0.776000
C	-4.189000	-0.017000	-0.418000
C	-4.590000	-1.285000	-0.888000
C	-4.183000	-2.419000	-0.155000
C	-3.444000	-2.306000	1.038000
O	-4.577000	-3.666000	-0.585000
O	-4.582000	1.103000	-1.115000
C	-6.981000	-1.693000	-4.457000
C	-5.579000	-1.657000	-4.526000
C	-4.801000	-1.525000	-3.370000
C	-5.402000	-1.422000	-2.108000
C	-6.800000	-1.457000	-2.033000
C	-7.577000	-1.591000	-3.189000
C	-9.311000	-2.044000	-8.015000
C	-9.561000	-2.906000	-6.947000
C	-8.805000	-2.800000	-5.777000
C	-7.800000	-1.835000	-5.670000
C	-7.623000	-1.015000	-6.783000
N	-8.339000	-1.095000	-7.934000
C	-11.574000	-2.322000	-11.601000
C	-11.767000	-3.148000	-10.508000
N	-11.050000	-3.065000	-9.364000
C	-10.080000	-2.110000	-9.283000
C	-9.832000	-1.242000	-10.350000
C	-10.587000	-1.351000	-11.518000
H	-2.463000	-0.924000	2.365000
H	-5.075000	-1.748000	-5.487000
H	-3.719000	-1.508000	-3.463000
H	-7.295000	-1.378000	-1.067000
H	-8.661000	-1.604000	-3.088000
H	-10.338000	-3.663000	-7.019000
H	-9.003000	-3.487000	-4.957000
H	-6.873000	-0.227000	-6.782000
H	-12.178000	-2.433000	-12.494000
H	-12.527000	-3.924000	-10.524000
H	-9.058000	-0.484000	-10.277000
H	-10.401000	-0.680000	-12.352000
C	0.784000	-4.027000	1.132000
C	-0.435000	-3.611000	1.692000
C	-1.671000	-4.047000	1.184000
C	-1.670000	-4.890000	0.055000
C	-0.471000	-5.343000	-0.532000
C	0.745000	-4.868000	0.004000
O	-2.870000	-5.342000	-0.447000
C	-0.512000	-8.117000	-3.842000
C	-0.236000	-8.546000	-2.534000
C	-0.223000	-7.644000	-1.464000
C	-0.482000	-6.282000	-1.667000
C	-0.749000	-5.847000	-2.971000
C	-0.768000	-6.750000	-4.041000
C	-0.637000	-10.837000	-7.129000
N	-1.670000	-9.975000	-6.924000
C	-1.592000	-9.129000	-5.865000
C	-0.530000	-9.066000	-4.965000
C	0.518000	-9.962000	-5.195000
C	0.467000	-10.847000	-6.275000
C	-0.845000	-13.498000	-10.434000
C	-1.904000	-12.627000	-10.221000
C	-1.856000	-11.745000	-9.142000
C	-0.746000	-11.751000	-8.293000
N	0.295000	-12.606000	-8.501000
C	0.222000	-13.451000	-9.556000
H	-0.423000	-2.921000	2.530000
H	-0.042000	-9.598000	-2.330000
H	-0.011000	-8.014000	-0.463000
H	-0.945000	-4.796000	-3.166000
H	-0.974000	-6.372000	-5.040000
H	-2.458000	-8.480000	-5.752000
H	1.390000	-9.974000	-4.545000
H	1.290000	-11.536000	-6.445000
H	-0.851000	-14.197000	-11.264000
H	-2.762000	-12.631000	-10.887000
H	-2.681000	-11.060000	-8.969000
H	1.076000	-14.113000	-9.679000

C	3.634000	-1.207000	-1.013000
C	3.222000	0.051000	-0.521000
C	2.515000	0.181000	0.693000
C	2.167000	-0.988000	1.389000
C	2.538000	-2.262000	0.931000
C	3.245000	-2.353000	-0.283000
O	3.581000	1.186000	-1.213000
O	3.606000	-3.595000	-0.759000
C	6.015000	-1.587000	-4.604000
C	4.669000	-1.192000	-4.668000
C	3.896000	-1.069000	-3.507000
C	4.440000	-1.332000	-2.242000
C	5.782000	-1.730000	-2.177000
C	6.557000	-1.854000	-3.337000
C	8.323000	-1.999000	-8.171000
C	8.836000	-1.254000	-7.107000
C	8.088000	-1.114000	-5.935000
C	6.831000	-1.713000	-5.820000
C	6.401000	-2.439000	-6.930000
N	7.102000	-2.594000	-8.083000
C	10.546000	-2.461000	-11.762000
C	10.996000	-1.738000	-10.672000
N	10.293000	-1.587000	-9.525000
C	9.070000	-2.183000	-9.441000
C	8.555000	-2.928000	-10.505000
C	9.301000	-3.067000	-11.675000
H	1.578000	-0.906000	2.298000
H	4.210000	-0.956000	-5.627000
H	2.861000	-0.757000	-3.602000
H	6.238000	-1.948000	-1.212000
H	7.593000	-2.174000	-3.238000
H	9.810000	-0.780000	-7.185000
H	8.496000	-0.520000	-5.119000
H	5.441000	-2.950000	-6.924000
H	11.152000	-2.549000	-12.657000
H	11.964000	-1.245000	-10.691000
H	7.579000	-3.400000	-10.428000
H	8.910000	-3.644000	-12.508000
C	-0.467000	-1.397000	-1.848000
C	-0.286000	-1.276000	-3.346000
O	0.378000	-2.452000	-3.824000
C	0.853000	-2.346000	-5.097000
O	0.748000	-1.355000	-5.806000
C	1.515000	-3.622000	-5.514000
H	0.501000	-1.465000	-1.350000
H	-1.004000	-0.537000	-1.446000
H	-1.016000	-2.307000	-1.598000
H	2.096000	-3.447000	-6.424000
H	2.203000	-3.960000	-4.734000
H	0.757000	-4.383000	-5.712000
H	-1.262000	-1.195000	-3.836000
H	0.307000	-0.383000	-3.567000

Table S6-1. Cartesian coordinates of **11⊂16**

Atom	*x* / Å	*y* / Å	*z* / Å
C	0.692000	2.432000	-0.714000
C	-0.522000	2.777000	-1.348000
C	-1.724000	2.425000	-0.694000
C	-1.728000	1.831000	0.584000
C	-0.494000	1.521000	1.179000
C	0.726000	1.830000	0.558000
C	-3.046000	1.478000	1.271000
C	2.061000	1.461000	1.200000
C	2.055000	-3.618000	1.737000
O	1.879000	2.740000	-1.343000
O	-2.922000	2.744000	-1.294000
O	1.887000	-5.415000	-0.452000
C	2.450000	-4.412000	-1.309000
C	-3.561000	1.586000	-1.857000
C	-3.490000	-4.305000	-1.299000
C	-3.060000	-3.613000	1.760000
C	2.471000	1.578000	-1.944000
C	-0.528000	4.905000	-5.113000
C	-0.934000	3.563000	-5.043000
C	-0.932000	2.868000	-3.827000
C	-0.526000	3.492000	-2.639000
C	-0.118000	4.832000	-2.708000
C	-0.119000	5.526000	-3.924000
C	-0.510000	6.968000	-8.850000
C	-1.145000	7.549000	-7.752000
C	-1.157000	6.882000	-6.523000
C	-0.536000	5.638000	-6.388000
C	0.076000	5.136000	-7.535000
N	0.103000	5.757000	-8.742000
C	-0.446000	8.943000	-12.611000
C	-1.060000	9.461000	-11.485000
N	-1.084000	8.837000	-10.284000
C	-0.466000	7.627000	-10.179000
C	0.175000	7.046000	-11.277000
C	0.184000	7.711000	-12.502000
C	2.104000	1.647000	2.727000
C	-3.040000	1.664000	2.799000
C	-3.083000	-3.501000	3.296000
C	2.099000	-3.473000	3.269000
H	-0.483000	1.016000	2.140000
H	-3.798000	2.213000	0.950000
H	2.813000	2.185000	0.856000
H	2.812000	-4.393000	1.555000
H	1.694000	-3.726000	-1.721000
H	2.866000	-4.949000	-2.169000
H	-4.015000	1.919000	-2.797000
H	-2.844000	0.797000	-2.132000
H	-2.745000	-3.582000	-1.662000
H	-3.901000	-4.792000	-2.190000
H	-3.815000	-4.389000	1.573000
H	1.730000	0.807000	-2.200000
H	2.895000	1.913000	-2.897000
H	-1.277000	3.047000	-5.938000
H	-1.259000	1.832000	-3.818000
H	0.208000	5.348000	-1.807000
H	0.213000	6.563000	-3.931000
H	-1.635000	8.514000	-7.844000
H	-1.666000	7.342000	-5.679000
H	0.596000	4.180000	-7.518000
H	-0.457000	9.487000	-13.549000
H	-1.566000	10.422000	-11.518000
H	0.665000	6.081000	-11.184000
H	0.679000	7.268000	-13.361000
H	3.110000	1.434000	3.109000
H	1.857000	2.681000	2.994000
H	1.409000	0.999000	3.269000
H	-4.036000	1.469000	3.211000
H	-2.341000	1.003000	3.319000
H	-2.766000	2.693000	3.058000
H	-2.829000	-4.464000	3.753000
H	-2.383000	-2.760000	3.692000
H	-4.083000	-3.219000	3.643000
H	3.101000	-3.174000	3.596000
H	1.396000	-2.732000	3.660000

H	1.862000	-4.429000	3.750000
C	-3.121000	-1.071000	1.488000
C	-3.505000	0.098000	0.812000
C	-4.269000	-0.033000	-0.363000
C	-4.690000	-1.288000	-0.844000
C	-4.251000	-2.435000	-0.153000
C	-3.500000	-2.345000	1.035000
O	-4.603000	-3.675000	-0.638000
O	-4.643000	1.101000	-1.047000
C	-7.230000	-1.599000	-4.319000
C	-5.832000	-1.657000	-4.436000
C	-5.007000	-1.555000	-3.311000
C	-5.552000	-1.395000	-2.032000
C	-6.946000	-1.335000	-1.908000
C	-7.772000	-1.437000	-3.034000
C	-9.702000	-1.857000	-7.788000
C	-9.973000	-2.680000	-6.694000
C	-9.170000	-2.604000	-5.553000
C	-8.099000	-1.708000	-5.500000
C	-7.905000	-0.925000	-6.636000
N	-8.665000	-0.976000	-7.760000
C	-12.105000	-2.045000	-11.288000
C	-12.315000	-2.835000	-10.172000
N	-11.555000	-2.780000	-9.054000
C	-10.519000	-1.894000	-9.028000
C	-10.249000	-1.066000	-10.121000
C	-11.050000	-1.144000	-11.259000
H	-2.495000	-0.989000	2.372000
H	-5.366000	-1.804000	-5.409000
H	-3.930000	-1.612000	-3.439000
H	-7.400000	-1.208000	-0.927000
H	-8.850000	-1.377000	-2.895000
H	-10.801000	-3.383000	-6.724000
H	-9.385000	-3.260000	-4.712000
H	-7.103000	-0.191000	-6.677000
H	-12.747000	-2.131000	-12.158000
H	-13.128000	-3.556000	-10.145000
H	-9.422000	-0.362000	-10.090000
H	-10.849000	-0.504000	-12.114000
C	0.720000	-4.121000	1.195000
C	-0.504000	-3.684000	1.724000
C	-1.733000	-4.105000	1.188000
C	-1.717000	-4.950000	0.060000
C	-0.512000	-5.443000	-0.480000
C	0.694000	-4.983000	0.085000
O	-2.908000	-5.353000	-0.502000
C	-0.473000	-8.242000	-3.767000
C	-0.291000	-8.672000	-2.443000
C	-0.308000	-7.764000	-1.378000
C	-0.505000	-6.395000	-1.603000
C	-0.680000	-5.961000	-2.922000
C	-0.667000	-6.869000	-3.987000
C	-0.508000	-10.977000	-7.043000
N	-1.518000	-10.076000	-6.904000
C	-1.470000	-9.225000	-5.846000
C	-0.460000	-9.197000	-4.885000
C	0.564000	-10.133000	-5.049000
C	0.543000	-11.023000	-6.126000
C	-0.626000	-13.655000	-10.340000
C	-1.661000	-12.742000	-10.194000
C	-1.642000	-11.854000	-9.119000
C	-0.584000	-11.896000	-8.207000
N	0.433000	-12.792000	-8.349000
C	0.389000	-13.642000	-9.401000
H	-0.502000	-2.986000	2.556000
H	-0.148000	-9.729000	-2.223000
H	-0.167000	-8.133000	-0.364000
H	-0.830000	-4.905000	-3.132000
H	-0.801000	-6.485000	-4.997000
H	-2.314000	-8.542000	-5.788000
H	1.396000	-10.173000	-4.349000
H	1.347000	-11.744000	-6.244000
H	-0.611000	-14.358000	-11.165000
H	-2.479000	-12.717000	-10.909000
H	-2.448000	-11.136000	-8.998000
H	1.222000	-14.337000	-9.471000

C	3.604000	-1.334000	-0.967000
C	3.205000	-0.070000	-0.479000
C	2.487000	0.076000	0.722000
C	2.117000	-1.085000	1.419000
C	2.476000	-2.366000	0.969000
C	3.188000	-2.474000	-0.244000
O	3.571000	1.058000	-1.181000
O	3.555000	-3.720000	-0.703000
C	6.061000	-1.642000	-4.514000
C	4.728000	-2.080000	-4.520000
C	3.928000	-1.982000	-3.374000
C	4.435000	-1.448000	-2.182000
C	5.767000	-1.009000	-2.175000
C	6.565000	-1.102000	-3.321000
C	8.470000	-2.012000	-8.017000
C	8.405000	-0.783000	-7.360000
C	7.620000	-0.650000	-6.211000
C	6.900000	-1.742000	-5.717000
C	7.027000	-2.929000	-6.435000
N	7.779000	-3.089000	-7.555000
C	10.834000	-2.474000	-11.518000
C	10.718000	-1.283000	-10.824000
N	9.967000	-1.128000	-9.709000
C	9.285000	-2.212000	-9.242000
C	9.357000	-3.446000	-9.894000
C	10.139000	-3.576000	-11.041000
H	1.523000	-0.990000	2.323000
H	4.291000	-2.495000	-5.427000
H	2.900000	-2.329000	-3.425000
H	6.196000	-0.588000	-1.267000
H	7.597000	-0.759000	-3.266000
H	8.958000	0.074000	-7.735000
H	7.571000	0.317000	-5.715000
H	6.515000	-3.833000	-6.113000
H	11.451000	-2.541000	-12.407000
H	11.243000	-0.391000	-11.157000
H	8.810000	-4.305000	-9.514000
H	10.201000	-4.531000	-11.555000
C	-0.297000	-1.285000	-2.804000
N	-0.353000	-1.366000	-4.256000
C	0.587000	-0.539000	-4.998000
C	-1.207000	-2.283000	-4.852000
O	-1.987000	-2.981000	-4.204000
C	-1.154000	-2.405000	-6.355000
H	-0.532000	-0.262000	-2.500000
H	-1.002000	-1.964000	-2.321000
H	0.714000	-1.539000	-2.477000
H	0.200000	-0.285000	-5.987000
H	0.779000	0.388000	-4.453000
H	1.520000	-1.095000	-5.114000
H	-1.757000	-3.262000	-6.670000
H	-1.566000	-1.503000	-6.816000
H	-0.128000	-2.569000	-6.692000

Table S6-2. Cartesian coordinates of **11⊂16**

Atom	*x* / Å	*y* / Å	*z* / Å
C	0.724000	2.501000	-0.749000
C	-0.495000	2.872000	-1.352000
C	-1.685000	2.522000	-0.682000
C	-1.681000	1.903000	0.581000
C	-0.442000	1.585000	1.159000
C	0.771000	1.894000	0.522000
C	-2.999000	1.522000	1.247000
C	2.113000	1.523000	1.147000
C	2.111000	-3.561000	1.695000
O	1.903000	2.785000	-1.404000
O	-2.893000	2.818000	-1.274000
O	1.899000	-5.316000	-0.560000
C	2.512000	-4.291000	-1.361000
C	-3.458000	1.647000	-1.884000
C	-3.525000	-4.354000	-1.209000
C	-2.994000	-3.553000	1.818000
C	2.465000	1.596000	-1.990000
C	-0.645000	5.012000	-5.101000
C	-0.377000	3.634000	-5.065000
C	-0.326000	2.938000	-3.852000
C	-0.536000	3.596000	-2.634000
C	-0.807000	4.971000	-2.665000
C	-0.861000	5.667000	-3.879000
C	-0.728000	7.098000	-8.824000
C	-1.787000	7.255000	-7.929000
C	-1.770000	6.578000	-6.707000
C	-0.699000	5.744000	-6.376000
C	0.315000	5.649000	-7.327000
N	0.327000	6.292000	-8.523000
C	-0.725000	9.127000	-12.557000
C	-1.746000	9.233000	-11.629000
N	-1.753000	8.590000	-10.439000
C	-0.691000	7.790000	-10.137000
C	0.374000	7.638000	-11.029000
C	0.355000	8.313000	-12.248000
C	2.175000	1.720000	2.674000
C	-3.008000	1.709000	2.775000
C	-2.980000	-3.403000	3.350000
C	2.163000	-3.433000	3.228000
H	-0.422000	1.067000	2.114000
H	-3.766000	2.238000	0.921000
H	2.862000	2.245000	0.791000
H	2.855000	-4.346000	1.502000
H	1.781000	-3.568000	-1.756000
H	2.929000	-4.802000	-2.236000
H	-3.889000	1.982000	-2.835000
H	-2.701000	0.892000	-2.148000
H	-2.800000	-3.664000	-1.660000
H	-3.988000	-4.892000	-2.044000
H	-3.755000	-4.331000	1.667000
H	1.710000	0.819000	-2.176000
H	2.847000	1.893000	-2.973000
H	-0.216000	3.079000	-5.988000
H	-0.120000	1.871000	-3.869000
H	-0.977000	5.512000	-1.737000
H	-1.062000	6.737000	-3.856000
H	-2.628000	7.898000	-8.176000
H	-2.608000	6.701000	-6.025000
H	1.194000	5.034000	-7.146000
H	-0.771000	9.666000	-13.497000
H	-2.613000	9.859000	-11.824000
H	1.216000	6.998000	-10.779000
H	1.178000	8.201000	-12.948000
H	3.184000	1.510000	3.046000
H	1.930000	2.756000	2.936000
H	1.486000	1.076000	3.227000
H	-4.000000	1.483000	3.182000
H	-2.290000	1.071000	3.299000
H	-2.768000	2.747000	3.034000
H	-2.718000	-4.356000	3.825000
H	-2.268000	-2.656000	3.712000
H	-3.971000	-3.109000	3.715000
H	3.174000	-3.161000	3.554000
H	1.481000	-2.679000	3.630000

H	1.905000	-4.389000	3.700000
C	-3.055000	-1.019000	1.483000
C	-3.430000	0.135000	0.775000
C	-4.170000	-0.020000	-0.416000
C	-4.605000	-1.288000	-0.860000
C	-4.198000	-2.417000	-0.115000
C	-3.443000	-2.302000	1.067000
O	-4.592000	-3.669000	-0.536000
O	-4.549000	1.097000	-1.127000
C	-7.134000	-1.754000	-4.339000
C	-5.800000	-1.339000	-4.468000
C	-4.976000	-1.187000	-3.345000
C	-5.461000	-1.439000	-2.054000
C	-6.794000	-1.854000	-1.924000
C	-7.616000	-2.010000	-3.047000
C	-9.614000	-2.152000	-7.790000
C	-9.542000	-3.204000	-6.876000
C	-8.734000	-3.084000	-5.742000
C	-7.998000	-1.917000	-5.518000
C	-8.134000	-0.918000	-6.480000
N	-8.908000	-1.005000	-7.593000
C	-12.048000	-2.459000	-11.259000
C	-11.924000	-3.467000	-10.319000
N	-11.151000	-3.376000	-9.213000
C	-10.453000	-2.221000	-9.013000
C	-10.533000	-1.163000	-9.922000
C	-11.338000	-1.285000	-11.054000
H	-2.436000	-0.917000	2.370000
H	-5.380000	-1.140000	-5.453000
H	-3.949000	-0.870000	-3.494000
H	-7.206000	-2.058000	-0.937000
H	-8.648000	-2.324000	-2.896000
H	-10.107000	-4.117000	-7.040000
H	-8.679000	-3.917000	-5.044000
H	-7.610000	0.030000	-6.378000
H	-12.683000	-2.586000	-12.129000
H	-12.460000	-4.405000	-10.435000
H	-9.973000	-0.247000	-9.754000
H	-11.406000	-0.468000	-11.766000
C	0.771000	-4.044000	1.144000
C	-0.441000	-3.620000	1.713000
C	-1.682000	-4.054000	1.221000
C	-1.691000	-4.911000	0.104000
C	-0.500000	-5.370000	-0.500000
C	0.723000	-4.886000	0.014000
O	-2.900000	-5.352000	-0.389000
C	-0.640000	-8.203000	-3.765000
C	-0.981000	-8.579000	-2.457000
C	-0.934000	-7.657000	-1.404000
C	-0.542000	-6.329000	-1.622000
C	-0.203000	-5.950000	-2.928000
C	-0.249000	-6.872000	-3.982000
C	-0.817000	-10.960000	-7.019000
N	-1.434000	-9.751000	-7.122000
C	-1.356000	-8.905000	-6.063000
C	-0.686000	-9.172000	-4.870000
C	-0.061000	-10.420000	-4.788000
C	-0.125000	-11.314000	-5.860000
C	-1.041000	-13.636000	-10.311000
C	-1.675000	-12.406000	-10.417000
C	-1.614000	-11.513000	-9.348000
C	-0.918000	-11.867000	-8.189000
N	-0.295000	-13.076000	-8.084000
C	-0.370000	-13.923000	-9.136000
H	-0.418000	-2.926000	2.548000
H	-1.300000	-9.598000	-2.243000
H	-1.209000	-7.986000	-0.403000
H	0.110000	-4.933000	-3.141000
H	0.043000	-6.542000	-4.977000
H	-1.883000	-7.965000	-6.208000
H	0.492000	-10.705000	-3.896000
H	0.368000	-12.280000	-5.785000
H	-1.070000	-14.354000	-11.124000
H	-2.213000	-12.140000	-11.322000
H	-2.107000	-10.548000	-9.422000
H	0.141000	-14.873000	-9.004000

C	3.683000	-1.280000	-0.983000
C	3.259000	-0.017000	-0.524000
C	2.539000	0.135000	0.678000
C	2.176000	-1.021000	1.388000
C	2.546000	-2.302000	0.951000
C	3.275000	-2.411000	-0.247000
O	3.597000	1.103000	-1.252000
O	3.623000	-3.663000	-0.704000
C	6.171000	-1.720000	-4.486000
C	4.791000	-1.490000	-4.604000
C	3.982000	-1.346000	-3.471000
C	4.525000	-1.424000	-2.183000
C	5.902000	-1.655000	-2.060000
C	6.712000	-1.799000	-3.193000
C	8.586000	-2.212000	-7.971000
C	8.988000	-1.312000	-6.984000
C	8.205000	-1.143000	-5.838000
C	7.022000	-1.870000	-5.676000
C	6.701000	-2.747000	-6.710000
N	7.439000	-2.933000	-7.835000
C	10.922000	-2.768000	-11.477000
C	11.261000	-1.891000	-10.462000
N	10.522000	-1.709000	-9.344000
C	9.375000	-2.434000	-9.209000
C	8.973000	-3.338000	-10.196000
C	9.755000	-3.505000	-11.338000
H	1.575000	-0.923000	2.288000
H	4.328000	-1.403000	-5.585000
H	2.919000	-1.166000	-3.606000
H	6.355000	-1.727000	-1.073000
H	7.775000	-1.987000	-3.052000
H	9.903000	-0.738000	-7.099000
H	8.524000	-0.429000	-5.082000
H	5.806000	-3.363000	-6.661000
H	11.552000	-2.874000	-12.353000
H	12.165000	-1.291000	-10.523000
H	8.058000	-3.911000	-10.080000
H	9.451000	-4.205000	-12.111000
C	-0.765000	-1.690000	-2.520000
C	-0.295000	-1.345000	-3.909000
N	-0.876000	-2.008000	-4.976000
C	-0.439000	-1.692000	-6.329000
O	0.583000	-0.493000	-4.054000
C	-1.914000	-3.023000	-4.876000
H	-0.220000	-1.085000	-1.788000
H	-1.829000	-1.471000	-2.418000
H	-0.569000	-2.741000	-2.307000
H	-0.048000	-2.603000	-6.793000
H	-1.300000	-1.333000	-6.901000
H	0.340000	-0.926000	-6.347000
H	-1.541000	-3.950000	-5.321000
H	-2.210000	-3.224000	-3.848000
H	-2.791000	-2.683000	-5.434000

Table S7-1. Cartesian coordinates of **12⊂16**

Atom	*x* / Å	*y* / Å	*z* / Å
C	0.688000	2.425000	-0.626000
C	-0.518000	2.738000	-1.290000
C	-1.729000	2.390000	-0.653000
C	-1.750000	1.803000	0.628000
C	-0.524000	1.504000	1.245000
C	0.705000	1.824000	0.647000
C	-3.078000	1.441000	1.290000
C	2.034000	1.450000	1.302000
C	2.038000	-3.644000	1.739000
O	1.881000	2.771000	-1.219000
O	-2.917000	2.717000	-1.269000
O	1.887000	-5.410000	-0.478000
C	2.445000	-4.393000	-1.324000
C	-3.559000	1.572000	-1.850000
C	-3.489000	-4.336000	-1.332000
C	-3.077000	-3.654000	1.733000
C	2.506000	1.645000	-1.849000
C	-0.460000	4.693000	-5.142000
C	-0.776000	3.330000	-5.028000
C	-0.797000	2.694000	-3.781000
C	-0.505000	3.401000	-2.606000
C	-0.187000	4.761000	-2.716000
C	-0.166000	5.397000	-3.963000
C	-0.358000	6.576000	-8.970000
C	-1.094000	7.163000	-7.940000
C	-1.133000	6.555000	-6.682000
C	-0.441000	5.364000	-6.450000
C	0.269000	4.852000	-7.535000
N	0.326000	5.417000	-8.768000
C	-0.204000	8.374000	-12.817000
C	-0.915000	8.900000	-11.754000
N	-0.969000	8.334000	-10.527000
C	-0.280000	7.174000	-10.327000
C	0.460000	6.587000	-11.357000
C	0.497000	7.194000	-12.612000
C	2.054000	1.607000	2.833000
C	-3.099000	1.612000	2.820000
C	-3.110000	-3.552000	3.269000
C	2.074000	-3.529000	3.274000
H	-0.526000	0.999000	2.207000
H	-3.826000	2.177000	0.964000
H	2.788000	2.181000	0.981000
H	2.801000	-4.410000	1.545000
H	1.685000	-3.713000	-1.738000
H	2.875000	-4.918000	-2.184000
H	-4.009000	1.922000	-2.786000
H	-2.845000	0.786000	-2.138000
H	-2.742000	-3.615000	-1.698000
H	-3.898000	-4.825000	-2.223000
H	-3.830000	-4.430000	1.535000
H	1.781000	0.885000	-2.174000
H	2.968000	2.027000	-2.766000
H	-1.029000	2.751000	-5.915000
H	-1.055000	1.640000	-3.736000
H	0.050000	5.339000	-1.824000
H	0.094000	6.453000	-4.004000
H	-1.640000	8.087000	-8.108000
H	-1.721000	7.018000	-5.892000
H	0.849000	3.937000	-7.440000
H	-0.196000	8.871000	-13.781000
H	-1.480000	9.822000	-11.864000
H	1.006000	5.664000	-11.188000
H	1.070000	6.746000	-13.419000
H	3.055000	1.390000	3.226000
H	1.800000	2.635000	3.115000
H	1.354000	0.947000	3.352000
H	-4.102000	1.412000	3.213000
H	-2.408000	0.947000	3.346000
H	-2.832000	2.639000	3.094000
H	-2.859000	-4.519000	3.721000
H	-2.413000	-2.814000	3.675000
H	-4.113000	-3.273000	3.611000
H	3.073000	-3.229000	3.612000
H	1.364000	-2.801000	3.677000

H	1.842000	-4.496000	3.735000
C	-3.143000	-1.110000	1.480000
C	-3.526000	0.063000	0.812000
C	-4.276000	-0.060000	-0.372000
C	-4.687000	-1.313000	-0.872000
C	-4.252000	-2.465000	-0.185000
C	-3.513000	-2.382000	1.012000
O	-4.602000	-3.702000	-0.678000
O	-4.645000	1.080000	-1.050000
C	-7.189000	-1.579000	-4.381000
C	-5.805000	-1.798000	-4.461000
C	-4.991000	-1.711000	-3.325000
C	-5.535000	-1.407000	-2.072000
C	-6.916000	-1.185000	-1.987000
C	-7.730000	-1.271000	-3.123000
C	-9.620000	-1.795000	-7.883000
C	-10.002000	-2.502000	-6.742000
C	-9.213000	-2.438000	-5.590000
C	-8.045000	-1.671000	-5.573000
C	-7.743000	-0.998000	-6.756000
N	-8.487000	-1.040000	-7.891000
C	-11.974000	-1.951000	-11.417000
C	-12.294000	-2.627000	-10.254000
N	-11.549000	-2.582000	-9.125000
C	-10.415000	-1.824000	-9.136000
C	-10.033000	-1.115000	-10.278000
C	-10.820000	-1.180000	-11.427000
H	-2.527000	-1.034000	2.372000
H	-5.341000	-2.058000	-5.412000
H	-3.924000	-1.892000	-3.429000
H	-7.369000	-0.940000	-1.028000
H	-8.796000	-1.082000	-3.013000
H	-10.906000	-3.104000	-6.743000
H	-9.517000	-3.004000	-4.712000
H	-6.860000	-0.367000	-6.828000
H	-12.608000	-2.022000	-12.294000
H	-13.187000	-3.243000	-10.196000
H	-9.128000	-0.514000	-10.276000
H	-10.530000	-0.632000	-12.319000
C	0.708000	-4.146000	1.184000
C	-0.521000	-3.718000	1.711000
C	-1.745000	-4.139000	1.166000
C	-1.721000	-4.977000	0.033000
C	-0.512000	-5.457000	-0.510000
C	0.691000	-4.995000	0.062000
O	-2.909000	-5.382000	-0.533000
C	-0.448000	-8.225000	-3.823000
C	-0.246000	-8.663000	-2.505000
C	-0.270000	-7.763000	-1.432000
C	-0.496000	-6.397000	-1.643000
C	-0.693000	-5.955000	-2.957000
C	-0.671000	-6.855000	-4.030000
C	-0.454000	-10.935000	-7.121000
N	-1.479000	-10.053000	-6.968000
C	-1.440000	-9.210000	-5.904000
C	-0.425000	-9.171000	-4.949000
C	0.616000	-10.086000	-5.128000
C	0.604000	-10.969000	-6.212000
C	-0.546000	-13.589000	-10.438000
C	-1.594000	-12.694000	-10.280000
C	-1.584000	-11.814000	-9.199000
C	-0.522000	-11.846000	-8.292000
N	0.510000	-12.725000	-8.445000
C	0.474000	-13.567000	-9.504000
H	-0.524000	-3.029000	2.550000
H	-0.079000	-9.718000	-2.295000
H	-0.112000	-8.139000	-0.423000
H	-0.866000	-4.901000	-3.159000
H	-0.821000	-6.465000	-5.035000
H	-2.296000	-8.542000	-5.835000
H	1.453000	-10.116000	-4.434000
H	1.420000	-11.673000	-6.341000
H	-0.523000	-14.286000	-11.268000
H	-2.416000	-12.677000	-10.991000
H	-2.401000	-11.111000	-9.067000
H	1.317000	-14.248000	-9.583000

C	3.554000	-1.305000	-0.931000
C	3.180000	-0.049000	-0.405000
C	2.468000	0.073000	0.803000
C	2.098000	-1.102000	1.476000
C	2.454000	-2.375000	0.998000
C	3.152000	-2.459000	-0.224000
O	3.574000	1.093000	-1.067000
O	3.535000	-3.692000	-0.703000
C	5.840000	-1.549000	-4.589000
C	4.479000	-1.892000	-4.563000
C	3.736000	-1.816000	-3.379000
C	4.331000	-1.398000	-2.180000
C	5.689000	-1.054000	-2.203000
C	6.431000	-1.127000	-3.388000
C	8.076000	-1.853000	-8.212000
C	8.124000	-0.668000	-7.477000
C	7.397000	-0.558000	-6.288000
C	6.622000	-1.627000	-5.832000
C	6.636000	-2.772000	-6.627000
N	7.329000	-2.908000	-7.787000
C	10.261000	-2.245000	-11.834000
C	10.259000	-1.098000	-11.063000
N	9.566000	-0.966000	-9.908000
C	8.825000	-2.028000	-9.481000
C	8.782000	-3.218000	-10.212000
C	9.507000	-3.326000	-11.399000
H	1.510000	-1.026000	2.386000
H	3.978000	-2.214000	-5.475000
H	2.685000	-2.088000	-3.403000
H	6.183000	-0.724000	-1.290000
H	7.487000	-0.861000	-3.358000
H	8.721000	0.172000	-7.822000
H	7.436000	0.376000	-5.732000
H	6.074000	-3.658000	-6.340000
H	10.836000	-2.297000	-12.752000
H	10.834000	-0.225000	-11.361000
H	8.189000	-4.059000	-9.864000
H	9.480000	-4.247000	-11.974000
C	-0.516000	-1.397000	-1.817000
N	-0.158000	-1.153000	-3.192000
C	-0.757000	-1.839000	-4.221000
O	-1.631000	-2.682000	-4.051000
C	-0.272000	-1.438000	-5.587000
H	-1.576000	-1.180000	-1.679000
H	-0.332000	-2.446000	-1.579000
H	0.085000	-0.755000	-1.174000
H	-0.385000	-2.280000	-6.275000
H	-0.864000	-0.591000	-5.944000
H	0.784000	-1.153000	-5.559000
H	0.546000	-0.459000	-3.404000

Table S7-2. Cartesian coordinates of **12⊂16**

Atom	*x* / Å	*y* / Å	*z* / Å
C	0.742000	2.484000	-0.742000
C	-0.477000	2.837000	-1.355000
C	-1.669000	2.504000	-0.679000
C	-1.666000	1.906000	0.594000
C	-0.428000	1.595000	1.177000
C	0.787000	1.895000	0.538000
C	-2.985000	1.539000	1.267000
C	2.129000	1.527000	1.166000
C	2.123000	-3.557000	1.723000
O	1.921000	2.778000	-1.392000
O	-2.876000	2.808000	-1.270000
O	1.899000	-5.311000	-0.530000
C	2.523000	-4.302000	-1.341000
C	-3.460000	1.642000	-1.868000
C	-3.539000	-4.347000	-1.170000
C	-2.986000	-3.538000	1.862000
C	2.500000	1.601000	-1.982000
C	-0.602000	4.861000	-5.168000
C	-0.378000	3.477000	-5.091000
C	-0.336000	2.818000	-3.857000
C	-0.514000	3.521000	-2.659000
C	-0.740000	4.902000	-2.730000
C	-0.783000	5.561000	-3.965000
C	-0.657000	6.834000	-8.952000
C	-1.701000	7.053000	-8.053000
C	-1.692000	6.413000	-6.810000
C	-0.646000	5.554000	-6.464000
C	0.354000	5.397000	-7.422000
N	0.374000	6.003000	-8.637000
C	-0.626000	8.750000	-12.745000
C	-1.632000	8.919000	-11.810000
N	-1.648000	8.312000	-10.601000
C	-0.611000	7.485000	-10.286000
C	0.438000	7.269000	-11.183000
C	0.428000	7.908000	-12.423000
C	2.189000	1.726000	2.692000
C	-2.989000	1.737000	2.794000
C	-2.966000	-3.385000	3.394000
C	2.183000	-3.426000	3.255000
H	-0.408000	1.092000	2.139000
H	-3.748000	2.257000	0.938000
H	2.877000	2.248000	0.809000
H	2.864000	-4.344000	1.527000
H	1.800000	-3.585000	-1.758000
H	2.948000	-4.829000	-2.203000
H	-3.900000	1.977000	-2.814000
H	-2.713000	0.880000	-2.139000
H	-2.824000	-3.662000	-1.647000
H	-4.017000	-4.896000	-1.989000
H	-3.746000	-4.318000	1.715000
H	1.753000	0.824000	-2.199000
H	2.903000	1.914000	-2.951000
H	-0.244000	2.889000	-5.997000
H	-0.163000	1.744000	-3.842000
H	-0.882000	5.478000	-1.818000
H	-0.950000	6.637000	-3.974000
H	-2.522000	7.716000	-8.311000
H	-2.519000	6.584000	-6.124000
H	1.214000	4.759000	-7.231000
H	-0.664000	9.262000	-13.700000
H	-2.479000	9.568000	-12.015000
H	1.261000	6.608000	-10.923000
H	1.240000	7.747000	-13.127000
H	3.198000	1.517000	3.065000
H	1.944000	2.762000	2.952000
H	1.500000	1.082000	3.246000
H	-3.983000	1.522000	3.205000
H	-2.276000	1.098000	3.322000
H	-2.741000	2.775000	3.045000
H	-2.699000	-4.336000	3.869000
H	-2.255000	-2.634000	3.751000
H	-3.956000	-3.093000	3.761000
H	3.196000	-3.155000	3.576000
H	1.504000	-2.669000	3.659000

H	1.926000	-4.380000	3.731000
C	-3.051000	-1.003000	1.521000
C	-3.425000	0.149000	0.809000
C	-4.167000	-0.010000	-0.379000
C	-4.599000	-1.280000	-0.821000
C	-4.197000	-2.407000	-0.070000
C	-3.440000	-2.288000	1.111000
O	-4.595000	-3.658000	-0.485000
O	-4.546000	1.104000	-1.095000
C	-7.047000	-1.779000	-4.349000
C	-5.701000	-1.395000	-4.453000
C	-4.906000	-1.229000	-3.312000
C	-5.431000	-1.438000	-2.030000
C	-6.775000	-1.822000	-1.924000
C	-7.569000	-1.991000	-3.064000
C	-9.442000	-2.218000	-7.855000
C	-9.416000	-3.247000	-6.912000
C	-8.636000	-3.113000	-5.760000
C	-7.883000	-1.956000	-5.546000
C	-7.972000	-0.980000	-6.538000
N	-8.717000	-1.081000	-7.668000
C	-11.788000	-2.569000	-11.380000
C	-11.712000	-3.552000	-10.410000
N	-10.967000	-3.448000	-9.285000
C	-10.249000	-2.303000	-9.098000
C	-10.280000	-1.270000	-10.037000
C	-11.057000	-1.406000	-11.187000
H	-2.429000	-0.898000	2.406000
H	-5.251000	-1.231000	-5.431000
H	-3.869000	-0.933000	-3.441000
H	-7.216000	-1.993000	-0.943000
H	-8.611000	-2.279000	-2.934000
H	-9.995000	-4.153000	-7.068000
H	-8.618000	-3.928000	-5.039000
H	-7.431000	-0.041000	-6.447000
H	-12.402000	-2.706000	-12.263000
H	-12.266000	-4.481000	-10.514000
H	-9.705000	-0.362000	-9.879000
H	-11.087000	-0.607000	-11.924000
C	0.780000	-4.038000	1.179000
C	-0.431000	-3.614000	1.753000
C	-1.675000	-4.039000	1.260000
C	-1.689000	-4.883000	0.133000
C	-0.499000	-5.330000	-0.483000
C	0.727000	-4.868000	0.042000
O	-2.897000	-5.333000	-0.351000
C	-0.654000	-8.007000	-3.869000
C	-0.901000	-8.466000	-2.566000
C	-0.849000	-7.597000	-1.470000
C	-0.546000	-6.240000	-1.641000
C	-0.300000	-5.776000	-2.941000
C	-0.353000	-6.646000	-4.037000
C	-0.854000	-10.610000	-7.246000
N	-1.545000	-9.437000	-7.254000
C	-1.456000	-8.639000	-6.158000
C	-0.706000	-8.923000	-5.018000
C	-0.007000	-10.133000	-5.033000
C	-0.079000	-10.977000	-6.145000
C	-1.109000	-13.134000	-10.654000
C	-1.817000	-11.940000	-10.663000
C	-1.747000	-11.097000	-9.555000
C	-0.968000	-11.464000	-8.454000
N	-0.273000	-12.637000	-8.444000
C	-0.358000	-13.436000	-9.533000
H	-0.404000	-2.927000	2.594000
H	-1.148000	-9.512000	-2.388000
H	-1.049000	-7.989000	-0.474000
H	-0.056000	-4.732000	-3.114000
H	-0.137000	-6.251000	-5.028000
H	-2.043000	-7.726000	-6.227000
H	0.611000	-10.427000	-4.188000
H	0.472000	-11.913000	-6.146000
H	-1.142000	-13.812000	-11.500000
H	-2.420000	-11.663000	-11.523000
H	-2.298000	-10.160000	-9.553000
H	0.213000	-14.358000	-9.477000

C	3.680000	-1.282000	-0.969000
C	3.267000	-0.017000	-0.505000
C	2.552000	0.137000	0.699000
C	2.189000	-1.018000	1.411000
C	2.555000	-2.300000	0.973000
C	3.275000	-2.413000	-0.231000
O	3.618000	1.102000	-1.228000
O	3.628000	-3.664000	-0.684000
C	6.125000	-1.701000	-4.503000
C	4.732000	-1.554000	-4.601000
C	3.936000	-1.419000	-3.458000
C	4.506000	-1.423000	-2.179000
C	5.896000	-1.571000	-2.076000
C	6.692000	-1.706000	-3.219000
C	8.502000	-2.171000	-8.017000
C	8.870000	-1.218000	-7.066000
C	8.099000	-1.056000	-5.912000
C	6.962000	-1.842000	-5.704000
C	6.672000	-2.768000	-6.704000
N	7.399000	-2.949000	-7.837000
C	10.802000	-2.708000	-11.549000
C	11.110000	-1.782000	-10.569000
N	10.383000	-1.606000	-9.442000
C	9.279000	-2.388000	-9.263000
C	8.910000	-3.342000	-10.214000
C	9.679000	-3.502000	-11.366000
H	1.593000	-0.918000	2.313000
H	4.248000	-1.527000	-5.576000
H	2.862000	-1.302000	-3.578000
H	6.370000	-1.583000	-1.096000
H	7.767000	-1.828000	-3.093000
H	9.749000	-0.599000	-7.217000
H	8.391000	-0.302000	-5.185000
H	5.814000	-3.431000	-6.619000
H	11.421000	-2.807000	-12.434000
H	11.979000	-1.137000	-10.665000
H	8.030000	-3.961000	-10.063000
H	9.400000	-4.242000	-12.112000
C	-0.643000	-1.429000	-1.837000
C	-0.432000	-1.397000	-3.323000
N	-1.297000	-2.199000	-4.028000
C	-1.224000	-2.298000	-5.465000
O	0.452000	-0.729000	-3.845000
H	-0.191000	-0.546000	-1.381000
H	-1.708000	-1.432000	-1.605000
H	-0.180000	-2.325000	-1.424000
H	-0.289000	-2.794000	-5.740000
H	-2.076000	-2.884000	-5.819000
H	-1.249000	-1.297000	-5.904000
H	-1.993000	-2.748000	-3.543000

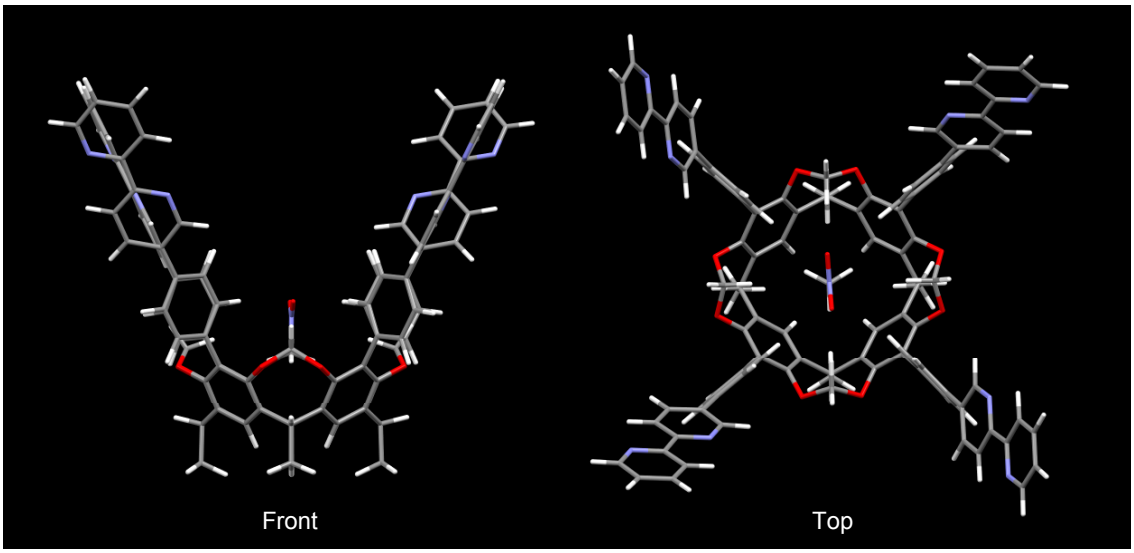

Figure S5. Front and top views of the energy minimized structure of **5⊂16** (Table S1). Color scheme: gray (carbon), white (hydrogen), light-blue (nitrogen), red (oxygen).

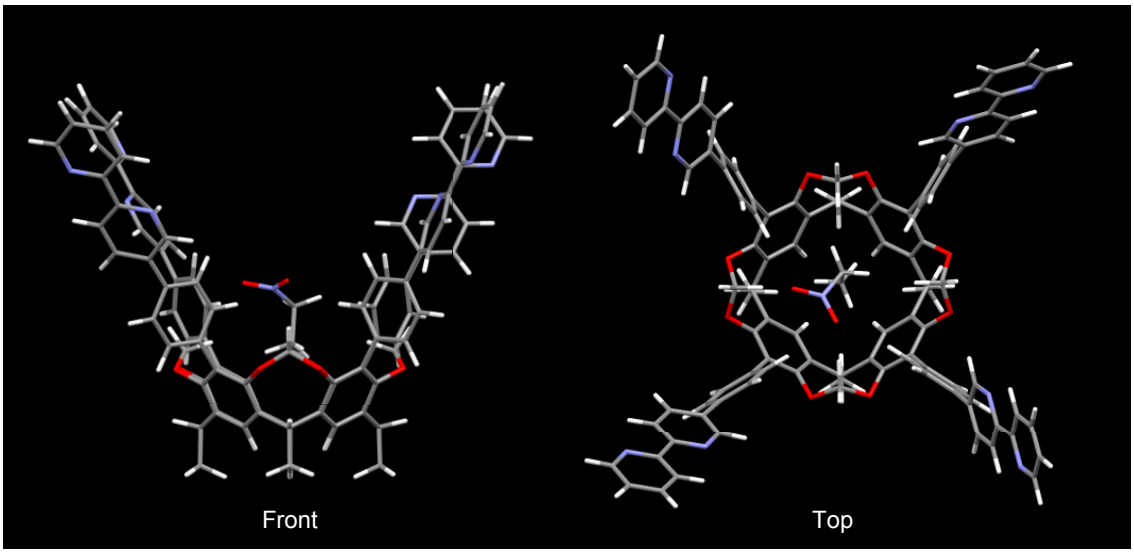

Figure S6. Front and top views of the energy minimized structure of **6⊂16** (Table S2). Color scheme: gray (carbon), white (hydrogen), light-blue (nitrogen), red (oxygen).

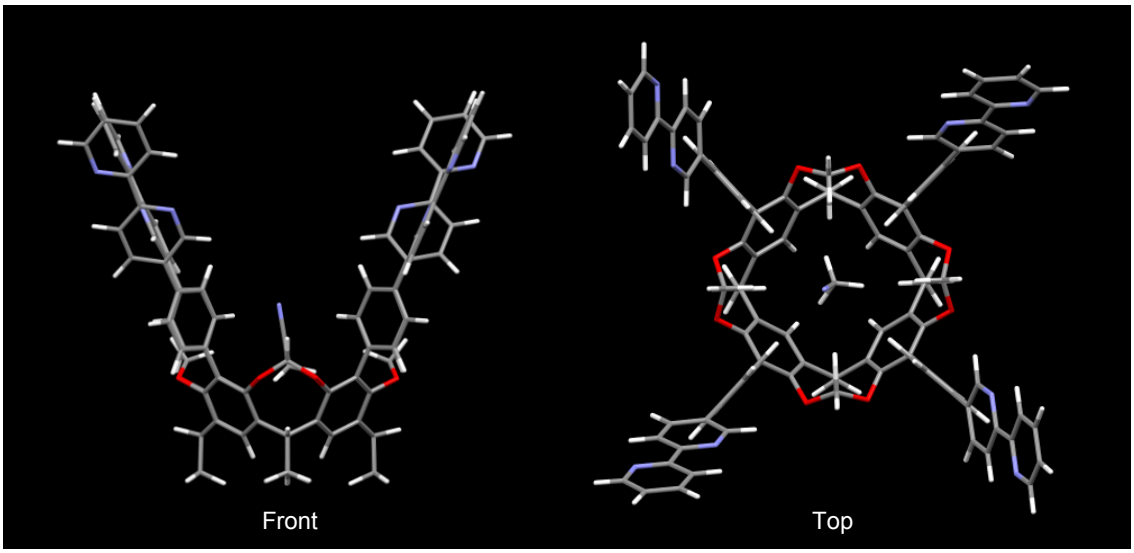

Figure S7. Front and top views of the energy minimized structure of **7⊂16** (Table S3). Color scheme: gray (carbon), white (hydrogen), light-blue (nitrogen), red (oxygen).

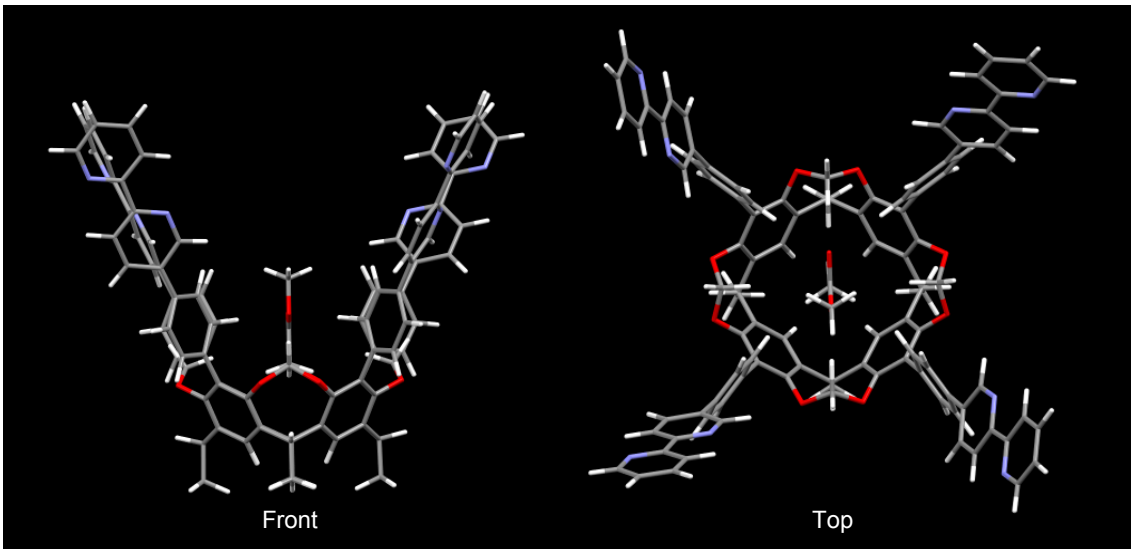

Figure S8. Front and top views of the energy minimized structure of **8⊂16** (Table S4-1). Color scheme: gray (carbon), white (hydrogen), light-blue (nitrogen), red (oxygen).

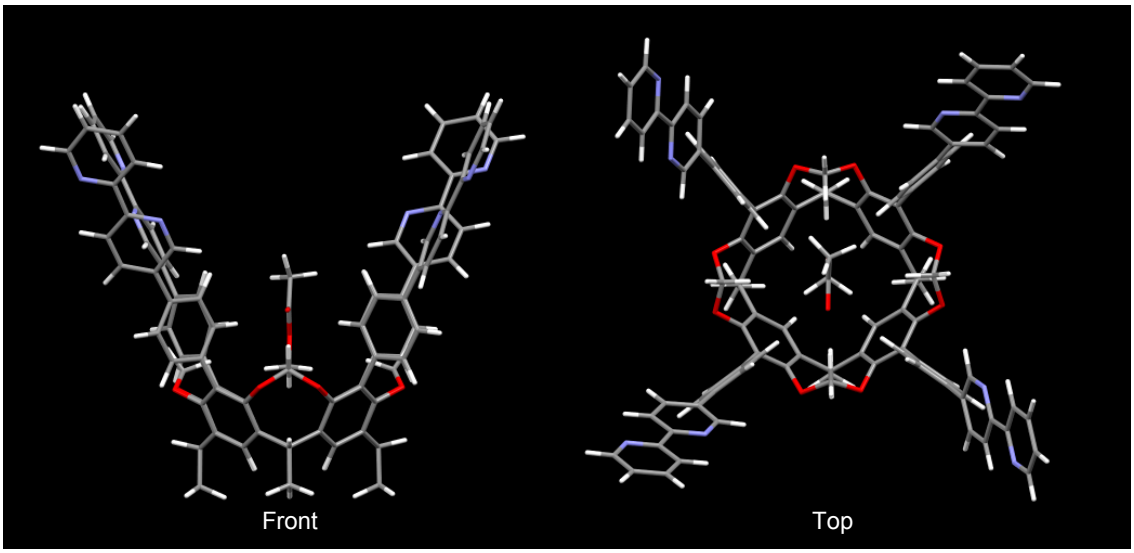

Figure S9. Front and top views of the energy minimized structure of **8⊂16** (Table S4-2). Color scheme: gray (carbon), white (hydrogen), light-blue (nitrogen), red (oxygen).

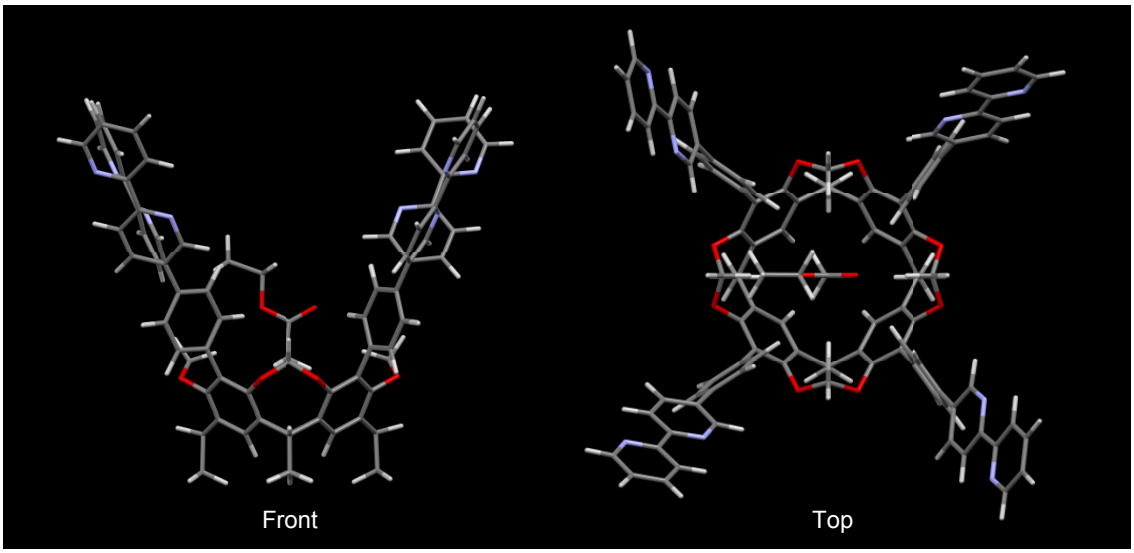

Figure S10. Front and top views of the energy minimized structure of **9⊂16** (Table S5-1). Color scheme: gray (carbon), white (hydrogen), light-blue (nitrogen), red (oxygen).

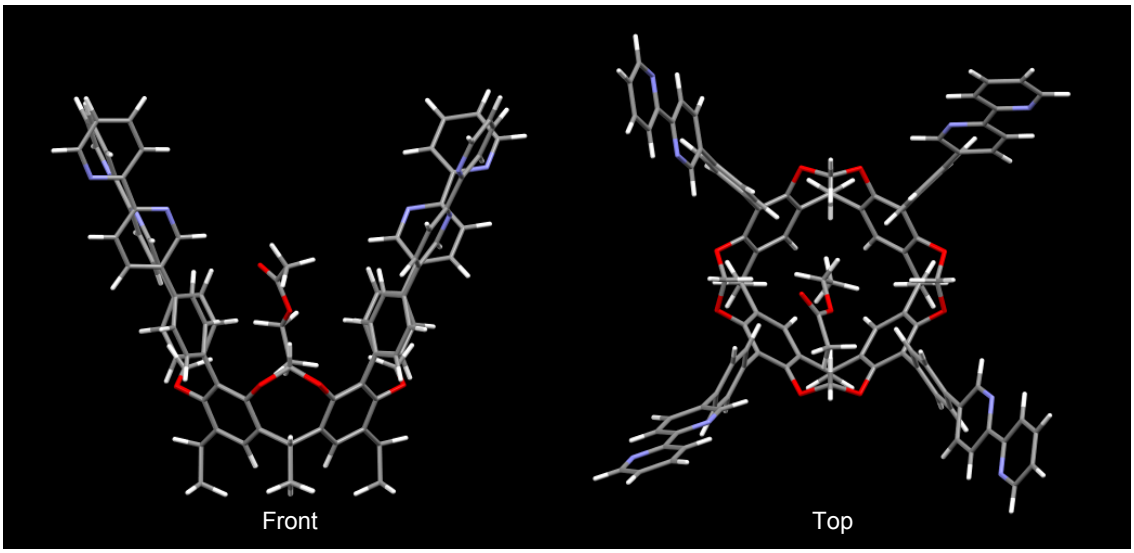

Figure S11. Front and top views of the energy minimized structure of **9⊂16** (Table S5-2). Color scheme: gray (carbon), white (hydrogen), light-blue (nitrogen), red (oxygen).

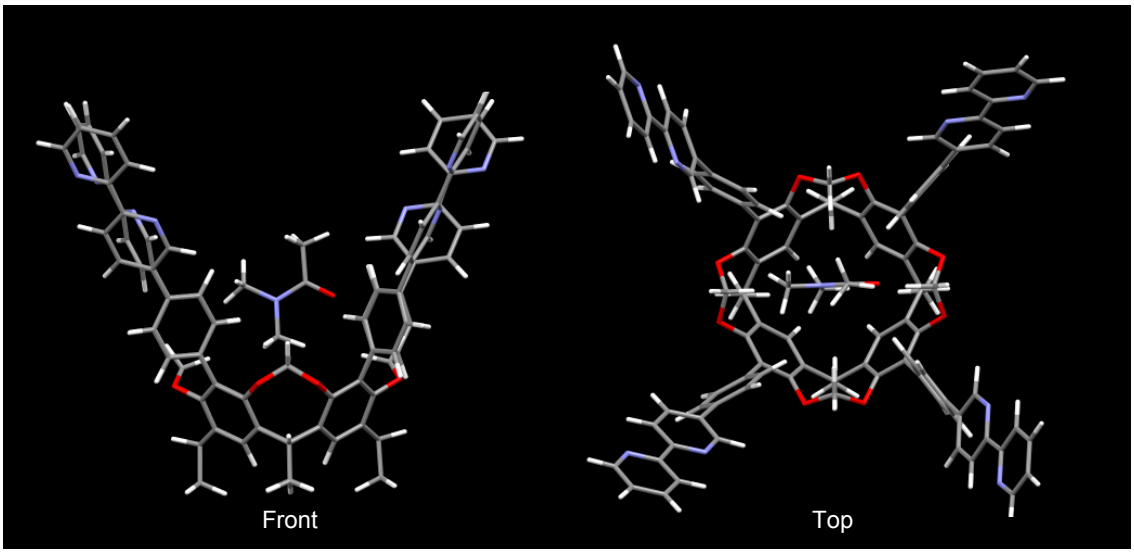

Figure S12. Front and top views of the energy minimized structure of **11⊂16** (Table S6-1). Color scheme: gray (carbon), white (hydrogen), light-blue (nitrogen), red (oxygen).

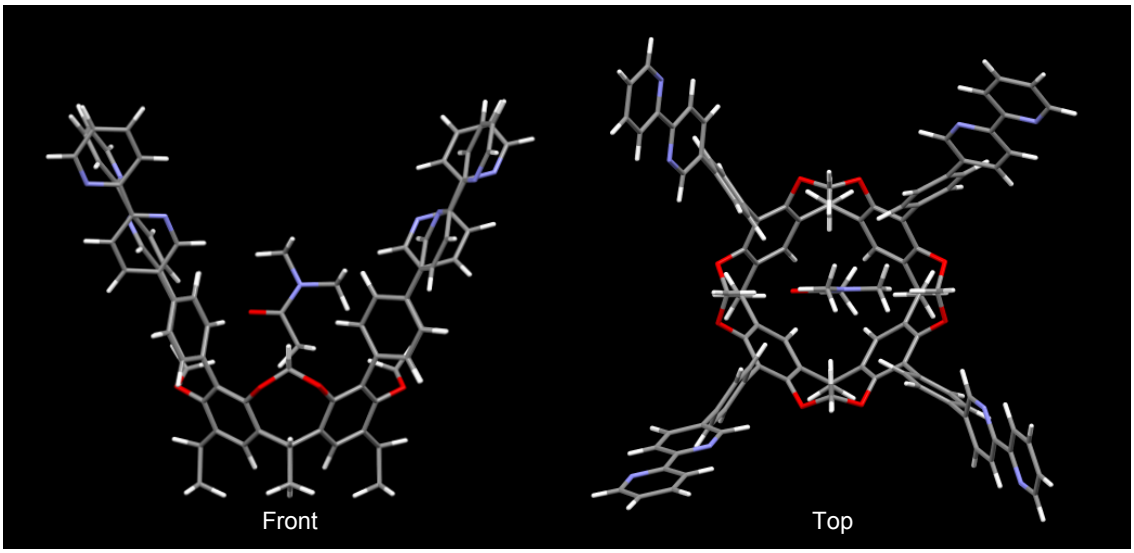

Figure S13. Front and top views of the energy minimized structure of **11⊂16** (Table S6-2). Color scheme: gray (carbon), white (hydrogen), light-blue (nitrogen), red (oxygen).

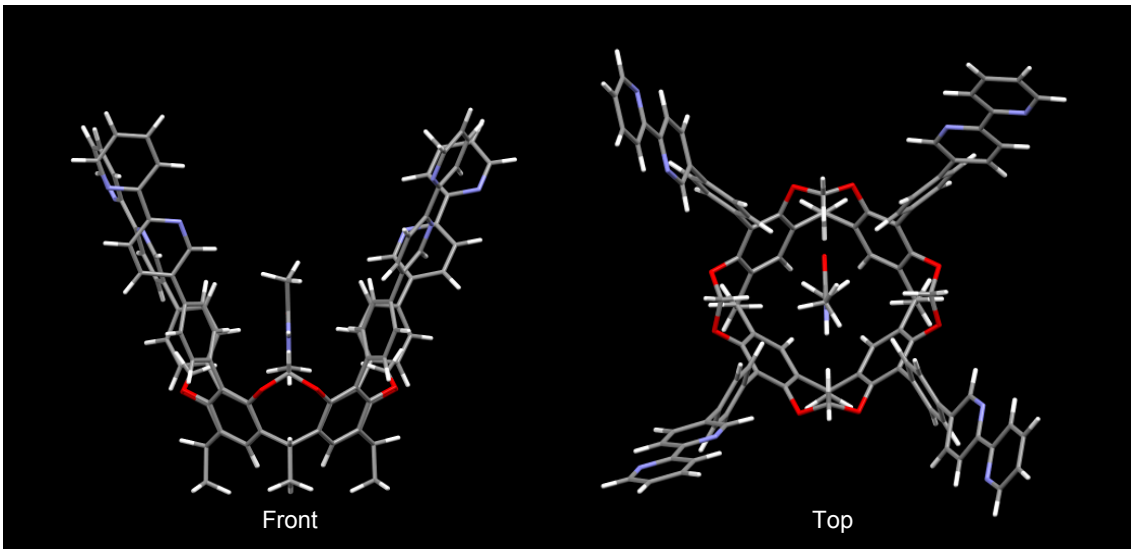

Figure S14. Front and top views of the energy minimized structure of **12⊂16** (Table S7-1). Color scheme: gray (carbon), white (hydrogen), light-blue (nitrogen), red (oxygen).

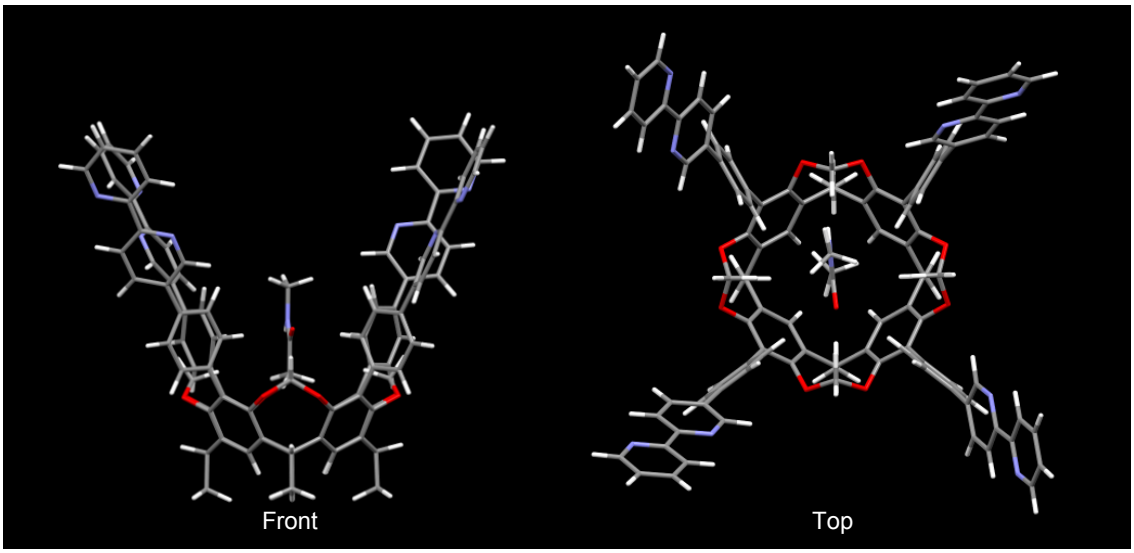

Figure S15. Front and top views of the energy minimized structure of **12⊂16** (Table S7-2). Color scheme: gray (carbon), white (hydrogen), light-blue (nitrogen), red (oxygen).

Reference

[1] F. Mohamadi, N. G. J. Richards, W. C. Guida,. R. Liskamp, M. Lipton, C. Caufield, G. Chang, T. Hendrickson, and W. C. Still, *J. Comput. Chem*., **1990**, *11*, 440-467.