Supporting Information II for:

How are N-methylcarbamates encapsulated by β-cyclodextrin: Insight into binding mechanism

Xiaofang Bao[a], Xiao Liu[a], Ran Dou[a], Sen Xu[a], Dabin Liu[a], Jun Luo[a], Xuedong Gong[a], Chung F. Wong[b], Baojing Zhou[a],*

[a] Computational Institute for Molecules and Materials, School of Chemistry and Chemical Engineering, Nanjing University of Science and Technology, Nanjing 210094, China

[b] Department of Chemistry and Biochemistry and Center for Nanoscience, University of Missouri-Saint Louis, One University Boulevard, Saint Louis, MO 63121, United States

Contents:

1. Cartesian coordinates of the β-CD/PC complexe

Table S1. ONIOM2(B971/6-31G(d):PM6) Optimized Model Cartesian coordinates for the Complex of PC with β-CD.

180

C	-12.907000	3.869000	21.681000
H	-13.990000	3.648000	21.739000
O	-12.656000	5.225000	22.035999
C	-12.144000	2.886000	22.579000
H	-12.396000	1.868000	22.273001
O	-12.502000	3.067000	23.962999
H	-12.207000	3.961000	24.238001
C	-10.645000	3.091000	22.457001
H	-10.377000	4.045000	22.921000
O	-10.018000	1.997000	23.145000
H	-9.052000	2.161000	23.174999
C	-10.175000	3.092000	21.002001
H	-10.175000	2.075000	20.601999
C	-11.073000	3.976000	20.120001
H	-10.905000	5.018000	20.398001
O	-12.456000	3.643000	20.344999
C	-10.773000	3.861000	18.624001
H	-11.157000	2.924000	18.212999
H	-9.695000	3.903000	18.451000
O	-11.395000	4.982000	17.974001
H	-10.903000	5.188000	17.152000
C	-14.201000	8.456000	24.014000
H	-14.766000	9.091000	24.724001
O	-13.399000	9.262000	23.148001
C	-13.329000	7.508000	24.834000
H	-13.960000	6.927000	25.510000
O	-12.395000	8.263000	25.608000
H	-11.985000	8.935000	25.044001
C	-12.552000	6.571000	23.934000
H	-11.838000	7.147000	23.336000
O	-11.869000	5.623000	24.777000
H	-11.543000	6.086000	25.573000
C	-13.503000	5.814000	23.013000
H	-14.055000	5.063000	23.586000
C	-14.497000	6.758000	22.309999
H	-13.963000	7.350000	21.563999
O	-15.106000	7.642000	23.271000
C	-15.609000	5.990000	21.598000
H	-16.261000	5.486000	22.315001
H	-15.184000	5.242000	20.926001
O	-16.370001	6.916000	20.815001
H	-16.916000	6.378000	20.197001
C	-12.824000	13.221000	22.132999
H	-13.006000	14.309000	22.025000
O	-11.565000	12.871000	21.569000
C	-12.851000	12.912000	23.629000
H	-13.763000	13.334000	24.059000
O	-11.705000	13.512000	24.254999
H	-11.318000	14.161000	23.638000
C	-12.799000	11.421000	23.903000
H	-11.787000	11.068000	23.677000

O	-13.114000	11.238000	25.296000
H	-12.261000	11.198000	25.785999
C	-13.806000	10.630000	23.070999
H	-14.818000	10.777000	23.455999
C	-13.787000	11.065000	21.598000
H	-12.856000	10.724000	21.139000
O	-13.876000	12.498000	21.503000
C	-14.961000	10.482000	20.813999
H	-15.905000	10.914000	21.153999
H	-15.007000	9.399000	20.941000
O	-14.754000	10.786000	19.427999
H	-14.745000	11.755000	19.320999
C	-8.667000	14.659000	19.261000
H	-8.164000	15.353000	18.559000
O	-7.779000	13.640000	19.697001
C	-9.117000	15.455000	20.489000
H	-9.714000	16.316999	20.180000
O	-7.936000	15.901000	21.181000
H	-7.257000	15.210000	21.104000
C	-9.924000	14.572000	21.431999
H	-9.263000	13.828000	21.877001
O	-10.498000	15.395000	22.465000
H	-9.777000	15.740000	23.042000
C	-11.053000	13.866000	20.688000
H	-11.812000	14.600000	20.403000
C	-10.569000	13.163000	19.413000
H	-9.935000	12.320000	19.684000
O	-9.810000	14.089000	18.622000
C	-11.744000	12.635000	18.584000
H	-12.366000	13.461000	18.232000
H	-12.360000	11.971000	19.191999
O	-11.240000	11.896000	17.461000
H	-11.073000	12.544000	16.747000
C	-4.599000	11.425000	18.601000
H	-3.650000	11.049000	18.173000
O	-5.302000	10.363000	19.245001
C	-4.277000	12.573000	19.566999
H	-3.702000	13.334000	19.033001
O	-3.509000	12.096000	20.684000
H	-4.057000	11.454000	21.186001
C	-5.546000	13.182000	20.127001
H	-6.012000	12.452000	20.795000
O	-5.194000	14.389000	20.837999
H	-4.599000	14.174000	21.594999
C	-6.528000	13.569000	19.028999
H	-6.224000	14.540000	18.632000
C	-6.651000	12.544000	17.882999
H	-7.313000	11.742000	18.219999
O	-5.383000	11.960000	17.538000
C	-7.245000	13.135000	16.598000
H	-8.282000	13.435000	16.754000
H	-7.227000	12.395000	15.794000
O	-6.470000	14.284000	16.209000
H	-5.615000	13.956000	15.862000
C	-4.280000	6.651000	20.836000
H	-3.618000	5.878000	21.271999
O	-5.606000	6.169000	20.712999
C	-4.251000	7.852000	21.780001

H	-3.211000	8.139000	21.959999
O	-4.872000	7.510000	23.034000
H	-5.022000	6.549000	23.058001
C	-5.013000	9.023000	21.190001
H	-6.075000	8.770000	21.118000
O	-4.796000	10.131000	22.084000
H	-4.877000	9.786000	22.990000
C	-4.456000	9.360000	19.811001
H	-3.427000	9.712000	19.926001
C	-4.442000	8.123000	18.898001
H	-5.475000	7.827000	18.698000
O	-3.776000	7.037000	19.559000
C	-3.744000	8.328000	17.549000
H	-4.319000	9.015000	16.927000
H	-3.653000	7.378000	17.017000
O	-2.439000	8.885000	17.775999
H	-2.001000	9.050000	16.927999
C	-7.780000	2.766000	20.850000
H	-8.136000	1.718000	20.846001
O	-8.874000	3.673000	21.007000
C	-6.774000	2.923000	21.997999
H	-5.942000	2.232000	21.840000
O	-7.415000	2.626000	23.249001
H	-6.738000	2.481000	23.947001
C	-6.271000	4.354000	22.041000
H	-7.114000	5.013000	22.261999
O	-5.265000	4.481000	23.070000
H	-4.665000	3.704000	23.073000
C	-5.680000	4.752000	20.690001
H	-4.700000	4.285000	20.556999
C	-6.585000	4.374000	19.506001
H	-7.443000	5.052000	19.520000
O	-7.079000	3.031000	19.634001
C	-5.943000	4.540000	18.125000
H	-5.635000	5.577000	17.981001
H	-6.671000	4.293000	17.349001
O	-4.791000	3.686000	17.980000
H	-4.630000	3.180000	18.801001
O	-8.131000	6.723000	23.917999
O	-9.524000	7.637000	25.438999
N	-8.133000	5.956000	26.277000
H	-7.306000	6.446000	26.671000
H	-8.853000	5.975000	27.021999
C	-9.974000	7.884000	19.497999
H	-9.724000	6.842000	19.285999
C	-9.282000	8.282000	20.799999
C	-9.013000	9.623000	21.091999
H	-9.287000	10.399000	20.386999
C	-9.503000	8.711000	18.284000
H	-9.893000	8.282000	17.358999
H	-8.413000	8.714000	18.226000
H	-9.849000	9.744000	18.339001
C	-11.505000	7.989000	19.642000
H	-11.999000	7.645000	18.732000
H	-11.809000	9.021000	19.827999
H	-11.853000	7.372000	20.472000
C	-8.957000	7.304000	21.743999
H	-9.185000	6.259000	21.556000

C	-8.401000	9.983000	22.290001
C	-8.371000	7.668000	22.952000
C	-8.070000	9.000000	23.211000
H	-7.604000	9.279000	24.152000
C	-8.124000	11.433000	22.615999
H	-8.047000	12.019000	21.702999
H	-8.926000	11.841000	23.236000
H	-7.185000	11.535000	23.165001
C	-8.630000	6.865000	25.164000
C	-7.751000	4.567000	25.816999
H	-7.338000	4.024000	26.667999
H	-7.003000	4.655000	25.023001
H	-8.648000	4.060000	25.448000

2. Cartesian coordinates of the β-CD/BC complexe (RC_{QM})

Table S2. ONIOM2(B971/6-31G(d):PM6) Optimized Model Cartesian coordinates for the Complex of BC with β-CD.

177

C	-20.882999	-19.437000	23.862000
H	-21.273001	-18.955999	22.947001
O	-19.653000	-18.849001	24.278999
C	-21.940001	-19.266001	24.948000
H	-22.882999	-19.688000	24.594999
O	-22.120001	-17.867001	25.240000
H	-22.872999	-17.775000	25.857000
C	-21.507000	-19.975000	26.214001
H	-20.625000	-19.469000	26.615000
O	-22.607000	-19.902000	27.143999
H	-22.527000	-20.627001	27.794001
C	-21.173000	-21.441999	25.931000
H	-22.096001	-22.003000	25.763000
C	-20.235001	-21.604000	24.716999
H	-19.243999	-21.242001	25.002001
O	-20.716000	-20.827000	23.614000
C	-20.101000	-23.048000	24.223000
H	-20.954000	-23.320000	23.596001
H	-20.056000	-23.740999	25.065001
O	-18.879999	-23.159000	23.468000
H	-18.139000	-23.100000	24.101999
C	-16.812000	-16.205000	22.940001
H	-16.285000	-15.495000	22.273001
O	-16.134001	-16.311001	24.193001
C	-18.239000	-15.666000	23.112000
H	-18.712999	-15.607000	22.129000
O	-18.230000	-14.350000	23.698999
H	-18.014999	-13.703000	22.997000
C	-19.054001	-16.601999	23.976999
H	-18.608000	-16.665001	24.973000
O	-20.412001	-16.118000	24.033001
H	-20.958000	-16.794001	24.497000
C	-19.082001	-17.972000	23.319000
H	-19.674000	-17.910999	22.402000
C	-17.679001	-18.490999	22.969999
H	-17.180000	-18.753000	23.905001

O	-16.892000	-17.483999	22.309000
C	-17.690001	-19.745001	22.086000
H	-18.107000	-20.587999	22.639999
H	-16.672001	-20.004000	21.787001
O	-18.490999	-19.511999	20.912001
H	-18.207001	-18.688999	20.473000
C	-12.427000	-15.406000	25.784000
H	-11.342000	-15.219000	25.906000
O	-13.075000	-15.425000	27.056999
C	-13.034000	-14.354000	24.847000
H	-12.545000	-14.431000	23.872000
O	-12.827000	-13.024000	25.358999
H	-13.324000	-12.921000	26.195999
C	-14.525000	-14.618000	24.688999
H	-15.012000	-14.558000	25.666000
O	-15.067000	-13.620000	23.799999
H	-14.758000	-13.769000	22.882999
C	-14.736000	-16.021999	24.111000
H	-14.372000	-16.066999	23.082001
C	-13.971000	-17.076000	24.938000
H	-14.455000	-17.165001	25.910999
O	-12.604000	-16.666000	25.135000
C	-13.960000	-18.462999	24.291000
H	-13.222000	-18.516001	23.487000
H	-14.941000	-18.697001	23.875000
O	-13.650000	-19.424999	25.313000
H	-14.015000	-20.296000	25.055000
C	-12.910000	-14.198000	30.934999
H	-12.676000	-13.680000	31.882000
O	-13.846000	-15.256000	31.148001
C	-13.491000	-13.173000	29.958000
H	-12.773000	-12.363000	29.802999
O	-14.714000	-12.636000	30.487000
H	-14.529000	-12.197000	31.330999
C	-13.809000	-13.842000	28.634001
H	-14.603000	-14.574000	28.799999
O	-14.238000	-12.827000	27.708000
H	-15.045000	-12.411000	28.079000
C	-12.581000	-14.534000	28.055000
H	-11.915000	-13.775000	27.635000
C	-11.826000	-15.373000	29.105000
H	-12.387000	-16.295000	29.273001
O	-11.701000	-14.683000	30.360001
C	-10.415000	-15.754000	28.666000
H	-10.449000	-16.348000	27.750999
H	-9.919000	-16.339001	29.443001
O	-9.683000	-14.541000	28.431000
H	-9.801000	-13.962000	29.204000
C	-15.325000	-17.990000	33.797001
H	-15.545000	-18.552999	34.724998
O	-15.998000	-18.587000	32.688999
C	-15.768000	-16.544001	34.026001
H	-15.252000	-16.166000	34.910999
O	-17.184999	-16.489000	34.256001
H	-17.356001	-16.884001	35.127998
C	-15.434000	-15.647000	32.849998
H	-16.046000	-15.943000	31.992001
O	-15.720000	-14.285000	33.259998

H	-16.646999	-14.061000	33.030998
C	-13.952000	-15.763000	32.478001
H	-13.359000	-15.188000	33.191002
C	-13.446000	-17.219000	32.456001
H	-13.809000	-17.691000	31.542000
O	-13.919000	-17.962999	33.590000
C	-11.921000	-17.309000	32.488998
H	-11.535000	-16.898001	33.424000
H	-11.477000	-16.763000	31.658001
O	-11.556000	-18.693001	32.383999
H	-12.052000	-19.177000	33.070000
C	-17.683001	-22.312000	31.806000
H	-17.829000	-23.403999	31.916000
O	-18.485001	-21.785999	30.750999
C	-18.070999	-21.658001	33.127998
H	-17.565001	-22.167999	33.952000
O	-19.490000	-21.774000	33.292999
H	-19.903000	-21.663000	32.422001
C	-17.719000	-20.184000	33.158001
H	-18.306000	-19.643999	32.410000
O	-18.055000	-19.742001	34.488998
H	-18.966000	-20.059999	34.667999
C	-16.230000	-19.990999	32.862999
H	-15.629000	-20.410999	33.674999
C	-15.856000	-20.712000	31.551001
H	-16.351000	-20.193001	30.726999
O	-16.302999	-22.076000	31.561001
C	-14.358000	-20.763000	31.243000
H	-13.942000	-19.757000	31.181000
H	-14.190000	-21.261000	30.285000
O	-13.690000	-21.497000	32.282001
H	-14.063000	-22.396999	32.300999
C	-20.879000	-23.094000	27.700001
H	-21.542000	-23.677000	27.030001
O	-20.458000	-21.884001	27.077999
C	-21.594999	-22.792999	29.018000
H	-21.843000	-23.733000	29.511999
O	-22.802000	-22.055000	28.773001
H	-23.388000	-22.568001	28.164000
C	-20.680000	-21.964001	29.908001
H	-20.455999	-21.020000	29.403999
O	-21.350000	-21.719999	31.170000
H	-21.634001	-22.584000	31.552999
C	-19.374001	-22.725000	30.152000
H	-19.577999	-23.569000	30.813000
C	-18.742001	-23.247999	28.844999
H	-18.323999	-22.400999	28.295000
O	-19.746000	-23.893000	28.034000
C	-17.615999	-24.260000	29.083000
H	-18.006001	-25.172001	29.541000
H	-16.850000	-23.841999	29.738001
O	-17.016001	-24.568001	27.816000
H	-16.283001	-25.211000	27.969000
O	-18.135000	-16.878000	27.413000
O	-18.007999	-18.516001	29.061001
O	-20.677000	-15.370000	26.825001
O	-19.125999	-13.875000	27.534000
N	-20.201000	-13.328000	25.507000

H	-19.570999	-13.706000	24.777000
H	-19.836000	-12.378000	25.694000
C	-17.257000	-17.872000	28.002001
C	-19.341000	-17.007000	28.049000
C	-19.259001	-17.973000	29.021000
C	-16.032000	-17.181999	28.596001
H	-15.330000	-17.920000	28.987000
H	-15.529000	-16.587000	27.834000
H	-16.332001	-16.525000	29.412001
C	-16.903999	-18.909000	26.937000
H	-16.407000	-18.427999	26.096001
H	-16.236000	-19.669001	27.348000
H	-17.806999	-19.400000	26.570999
C	-20.535999	-16.327999	27.808001
C	-20.348000	-18.309999	29.813000
H	-20.245001	-19.048000	30.605000
C	-21.652000	-16.681999	28.568001
H	-22.597000	-16.170000	28.388000
C	-21.561001	-17.656000	29.573999
H	-22.438999	-17.891001	30.176001
C	-19.959999	-14.233000	26.724001
C	-21.620001	-13.344000	24.971001
H	-21.917999	-14.381000	24.806000
H	-21.645000	-12.783000	24.033001
H	-22.278000	-12.877000	25.708000

3. Cartesian coordinates of the β-CD/CY complexe (RC_{QM})

Table S3. ONIOM2(B971/6-31G(d):PM6) Optimized Model Cartesian coordinates for the Complex of CY with β-CD.

174

C	0.364000	5.595000	-0.886000
H	0.892000	6.502000	-1.255000
O	1.246000	4.487000	-0.647000
C	-0.337000	5.779000	0.489000
H	-0.804000	6.790000	0.590000
O	0.646000	5.747000	1.531000
H	1.553000	5.418000	1.185000
C	-1.381000	4.667000	0.716000
H	-0.909000	3.682000	0.951000
O	-2.168000	5.043000	1.859000
H	-3.101000	4.632000	1.770000
C	-2.278000	4.567000	-0.540000
H	-2.791000	5.533000	-0.756000
C	-1.403000	4.129000	-1.732000
H	-0.795000	3.220000	-1.510000
O	-0.497000	5.257000	-1.951000
C	-2.141000	3.977000	-3.068000
H	-1.883000	4.803000	-3.761000
H	-3.244000	3.913000	-2.937000
O	-1.819000	2.725000	-3.664000
H	-0.847000	2.672000	-3.905000
C	5.056000	3.235000	-1.741000
H	6.002000	3.167000	-2.314000
O	4.762000	2.074000	-0.955000

C	4.989000	4.385000	-0.703000
H	5.284000	5.364000	-1.152000
O	5.918000	4.195000	0.345000
H	6.082000	3.214000	0.518000
C	3.556000	4.434000	-0.122000
H	3.349000	3.546000	0.518000
O	3.354000	5.611000	0.677000
H	4.144000	5.759000	1.258000
C	2.546000	4.570000	-1.279000
H	2.667000	5.548000	-1.798000
C	2.675000	3.380000	-2.253000
H	2.463000	2.402000	-1.751000
O	4.051000	3.353000	-2.736000
C	1.841000	3.537000	-3.532000
H	2.494000	3.642000	-4.422000
H	1.128000	4.387000	-3.473000
O	0.984000	2.408000	-3.694000
H	1.513000	1.561000	-3.777000
C	5.831000	-1.950000	-0.683000
H	6.362000	-2.871000	-1.015000
O	4.729000	-2.205000	0.206000
C	6.717000	-0.940000	0.094000
H	7.756000	-0.916000	-0.318000
O	6.894000	-1.413000	1.421000
H	6.007000	-1.632000	1.839000
C	6.106000	0.478000	0.137000
H	5.344000	0.564000	0.947000
O	7.125000	1.459000	0.378000
H	7.672000	1.196000	1.159000
C	5.517000	0.878000	-1.232000
H	6.320000	1.068000	-1.976000
C	4.510000	-0.191000	-1.704000
H	3.711000	-0.355000	-0.942000
O	5.259000	-1.428000	-1.871000
C	3.896000	0.087000	-3.081000
H	4.138000	-0.718000	-3.801000
H	4.202000	1.074000	-3.491000
O	2.480000	0.225000	-2.944000
H	2.039000	-0.647000	-2.724000
C	2.126000	-5.257000	1.013000
H	1.686000	-6.267000	1.201000
O	1.167000	-4.329000	0.496000
C	2.787000	-4.595000	2.242000
H	3.392000	-5.363000	2.785000
O	1.709000	-4.182000	3.087000
H	2.079000	-3.735000	3.890000
C	3.654000	-3.370000	1.879000
H	3.018000	-2.450000	1.775000
O	4.496000	-3.032000	2.981000
H	5.150000	-3.740000	3.177000
C	4.506000	-3.577000	0.608000
H	5.483000	-4.065000	0.829000
C	3.752000	-4.304000	-0.520000
H	2.955000	-3.632000	-0.944000
O	3.107000	-5.489000	0.004000
C	4.660000	-4.844000	-1.637000
H	4.813000	-4.080000	-2.428000
H	4.232000	-5.765000	-2.078000

O	5.985000	-5.089000	-1.158000
H	6.032000	-5.970000	-0.721000
C	-2.443000	-4.754000	-1.565000
H	-3.096000	-4.988000	-2.439000
O	-3.029000	-3.809000	-0.650000
C	-2.043000	-5.976000	-0.704000
H	-1.802000	-6.855000	-1.354000
O	-3.153000	-6.423000	0.054000
H	-3.619000	-5.654000	0.506000
C	-0.860000	-5.671000	0.245000
H	-1.194000	-5.140000	1.165000
O	-0.246000	-6.912000	0.629000
H	-0.929000	-7.520000	1.005000
C	0.259000	-4.902000	-0.483000
H	0.827000	-5.583000	-1.158000
C	-0.301000	-3.663000	-1.213000
H	-0.757000	-2.941000	-0.494000
O	-1.324000	-4.100000	-2.144000
C	0.739000	-2.986000	-2.112000
H	0.632000	-3.304000	-3.167000
H	1.779000	-3.171000	-1.745000
O	0.620000	-1.558000	-2.019000
H	-0.233000	-1.257000	-2.414000
C	-6.291000	-1.256000	-0.678000
H	-7.292000	-0.853000	-0.927000
O	-5.392000	-0.257000	-0.153000
C	-6.282000	-2.339000	0.428000
H	-7.131000	-3.056000	0.291000
O	-6.561000	-1.727000	1.678000
H	-6.002000	-0.908000	1.807000
C	-4.940000	-3.104000	0.493000
H	-4.182000	-2.555000	1.096000
O	-5.169000	-4.390000	1.089000
H	-5.533000	-4.284000	1.999000
C	-4.403000	-3.446000	-0.912000
H	-4.953000	-4.314000	-1.351000
C	-4.412000	-2.226000	-1.852000
H	-3.752000	-1.408000	-1.478000
O	-5.777000	-1.706000	-1.910000
C	-4.076000	-2.566000	-3.309000
H	-2.978000	-2.692000	-3.437000
H	-4.439000	-1.775000	-3.995000
O	-4.598000	-3.844000	-3.684000
H	-5.570000	-3.789000	-3.818000
C	-4.597000	3.819000	-0.546000
H	-4.772000	4.866000	-0.870000
O	-3.234000	3.560000	-0.169000
C	-5.462000	3.374000	0.657000
H	-6.514000	3.719000	0.519000
O	-4.926000	4.072000	1.791000
H	-5.305000	3.680000	2.620000
C	-5.389000	1.846000	0.873000
H	-4.394000	1.543000	1.291000
O	-6.282000	1.471000	1.911000
H	-7.221000	1.471000	1.619000
C	-5.670000	1.116000	-0.463000
H	-6.719000	1.245000	-0.802000
C	-4.661000	1.599000	-1.532000

H	-3.609000	1.428000	-1.199000
O	-4.873000	3.038000	-1.691000
C	-4.874000	1.044000	-2.946000
H	-5.237000	1.831000	-3.636000
H	-5.569000	0.175000	-2.958000
O	-3.649000	0.489000	-3.418000
H	-3.006000	1.219000	-3.657000
O	-0.573000	2.386000	2.824000
O	1.211000	2.790000	4.219000
N	-0.354000	4.471000	3.705000
H	-1.342000	4.465000	3.364000
H	0.156000	5.052000	2.985000
C	-0.602000	0.022000	3.476000
C	-0.278000	-1.332000	3.118000
C	-0.235000	1.018000	2.534000
C	0.350000	-1.603000	1.869000
H	0.587000	-2.644000	1.627000
C	-1.256000	0.277000	4.713000
H	-1.527000	1.296000	4.984000
C	-0.609000	-2.376000	4.027000
H	-0.355000	-3.399000	3.748000
C	0.356000	0.759000	1.324000
H	0.590000	1.571000	0.640000
C	0.652000	-0.588000	0.987000
H	1.105000	-0.807000	0.020000
C	-1.564000	-0.763000	5.566000
H	-2.066000	-0.558000	6.508000
C	-1.235000	-2.100000	5.224000
H	-1.483000	-2.904000	5.910000
C	0.217000	3.072000	3.625000
C	-0.211000	5.097000	5.066000
H	-0.544000	6.133000	4.983000
H	0.839000	5.039000	5.346000
H	-0.833000	4.542000	5.766000

4. Cartesian coordinates of the β-CD/CF complexe (RC_{QM})

Table S4. ONIOM2(B971/6-31G(d):PM6) Optimized Model Cartesian coordinates for the Complex of CF with β-CD.

179

C	-2.529000	-5.220000	0.517000
H	-2.395000	-6.264000	0.873000
O	-1.286000	-4.491000	0.462000
C	-3.164000	-5.120000	-0.899000
H	-3.788000	-6.028000	-1.102000
O	-2.108000	-5.051000	-1.861000
H	-1.531000	-5.867000	-1.792000
C	-3.999000	-3.855000	-1.166000
H	-3.400000	-3.090000	-1.717000
O	-5.079000	-4.307000	-1.989000
H	-5.560000	-3.519000	-2.368000
C	-4.629000	-3.252000	0.111000
H	-5.575000	-3.787000	0.358000
C	-3.659000	-3.230000	1.305000
H	-2.744000	-2.636000	1.086000
O	-3.276000	-4.610000	1.556000

C	-4.332000	-2.770000	2.602000
H	-4.826000	-3.606000	3.129000
H	-5.063000	-1.951000	2.406000
O	-3.352000	-2.151000	3.455000
H	-2.953000	-2.822000	4.050000
C	2.799000	-5.057000	0.845000
H	3.772000	-5.383000	1.268000
O	2.900000	-3.826000	0.108000
C	2.081000	-6.109000	-0.040000
H	2.106000	-7.113000	0.458000
O	2.807000	-6.328000	-1.236000
H	2.826000	-5.502000	-1.810000
C	0.632000	-5.685000	-0.361000
H	0.600000	-4.910000	-1.164000
O	-0.125000	-6.820000	-0.819000
H	0.428000	-7.374000	-1.428000
C	-0.114000	-5.203000	0.903000
H	-0.387000	-6.064000	1.553000
C	0.717000	-4.134000	1.645000
H	0.878000	-3.231000	1.005000
O	2.012000	-4.712000	1.975000
C	0.120000	-3.760000	3.003000
H	0.321000	-4.530000	3.773000
H	-0.971000	-3.567000	2.920000
O	0.663000	-2.505000	3.447000
H	1.627000	-2.616000	3.655000
C	5.467000	-1.064000	-1.338000
H	6.354000	-0.525000	-1.741000
O	4.583000	-0.193000	-0.608000
C	4.542000	-1.701000	-2.399000
H	5.147000	-2.144000	-3.232000
O	3.792000	-0.675000	-3.036000
H	3.319000	-0.109000	-2.353000
C	3.575000	-2.754000	-1.815000
H	2.596000	-2.281000	-1.543000
O	3.338000	-3.772000	-2.805000
H	2.895000	-3.385000	-3.596000
C	4.123000	-3.565000	-0.622000
H	4.587000	-4.515000	-0.977000
C	5.032000	-2.763000	0.325000
H	4.415000	-2.039000	0.927000
O	6.009000	-2.009000	-0.435000
C	5.889000	-3.638000	1.251000
H	6.849000	-3.919000	0.778000
H	5.343000	-4.549000	1.576000
O	6.109000	-2.925000	2.471000
H	6.895000	-2.343000	2.384000
C	4.700000	3.454000	1.238000
H	4.872000	4.259000	1.981000
O	3.530000	3.633000	0.446000
C	5.881000	3.228000	0.266000
H	6.842000	3.224000	0.834000
O	5.860000	4.378000	-0.585000
H	6.551000	4.287000	-1.289000
C	5.717000	1.938000	-0.563000
H	5.029000	2.108000	-1.434000
O	6.948000	1.614000	-1.204000
H	7.677000	1.471000	-0.560000

C	5.229000	0.742000	0.286000
H	6.076000	0.238000	0.801000
C	4.087000	1.114000	1.257000
H	3.154000	1.363000	0.691000
O	4.487000	2.281000	2.025000
C	3.837000	0.036000	2.317000
H	4.580000	0.075000	3.136000
H	3.827000	-0.985000	1.858000
O	2.519000	0.177000	2.868000
H	2.481000	0.986000	3.447000
C	-0.013000	5.817000	0.632000
H	-0.635000	6.647000	1.026000
O	-0.785000	4.791000	-0.028000
C	1.027000	6.263000	-0.430000
H	1.357000	7.324000	-0.259000
O	0.358000	6.334000	-1.677000
H	-0.123000	5.478000	-1.887000
C	2.279000	5.361000	-0.507000
H	2.187000	4.586000	-1.309000
O	3.339000	6.262000	-0.828000
H	4.184000	5.751000	-0.970000
C	2.635000	4.696000	0.848000
H	3.151000	5.426000	1.511000
C	1.401000	4.082000	1.531000
H	0.871000	3.356000	0.871000
O	0.519000	5.213000	1.796000
C	1.670000	3.484000	2.913000
H	1.539000	4.236000	3.716000
H	2.682000	3.025000	2.974000
O	0.787000	2.378000	3.153000
H	-0.153000	2.716000	3.294000
C	-4.860000	3.775000	-0.145000
H	-5.933000	3.964000	0.065000
O	-4.564000	2.418000	-0.460000
C	-4.282000	4.628000	-1.304000
H	-4.629000	5.684000	-1.217000
O	-4.856000	4.080000	-2.492000
H	-4.342000	4.388000	-3.283000
C	-2.739000	4.531000	-1.328000
H	-2.407000	3.504000	-1.631000
O	-2.199000	5.342000	-2.360000
H	-2.232000	6.305000	-2.144000
C	-2.213000	4.913000	0.075000
H	-2.494000	5.955000	0.349000
C	-2.764000	3.902000	1.107000
H	-2.517000	2.848000	0.826000
O	-4.214000	4.069000	1.093000
C	-2.377000	4.199000	2.559000
H	-3.202000	4.699000	3.104000
H	-1.445000	4.802000	2.633000
O	-2.022000	2.987000	3.234000
H	-2.825000	2.411000	3.387000
C	-6.188000	-1.377000	-0.002000
H	-6.913000	-2.152000	0.320000
O	-4.881000	-1.883000	-0.271000
C	-6.628000	-0.583000	-1.255000
H	-7.700000	-0.279000	-1.176000
O	-6.495000	-1.512000	-2.335000

H	-6.742000	-1.059000	-3.182000
C	-5.732000	0.652000	-1.480000
H	-4.733000	0.372000	-1.885000
O	-6.436000	1.435000	-2.444000
H	-5.926000	2.277000	-2.628000
C	-5.602000	1.457000	-0.165000
H	-6.560000	1.963000	0.084000
C	-5.102000	0.563000	0.987000
H	-4.100000	0.129000	0.754000
O	-6.060000	-0.526000	1.138000
C	-5.108000	1.252000	2.355000
H	-6.025000	1.019000	2.928000
H	-4.980000	2.354000	2.261000
O	-3.951000	0.852000	3.102000
H	-4.043000	-0.081000	3.426000
O	1.212000	0.800000	-1.624000
O	0.165000	-1.180000	0.166000
O	-1.179000	0.677000	0.337000
N	0.012000	-0.147000	2.184000
H	0.562000	-1.009000	2.392000
H	0.667000	0.660000	2.303000
C	1.298000	1.735000	-2.779000
C	1.132000	0.814000	-4.030000
H	2.110000	0.536000	-4.453000
H	0.554000	1.309000	-4.818000
C	0.441000	-0.403000	-3.451000
C	0.559000	-0.306000	-2.062000
C	0.133000	2.720000	-2.638000
H	-0.823000	2.187000	-2.711000
H	0.171000	3.224000	-1.663000
H	0.170000	3.474000	-3.434000
C	2.662000	2.413000	-2.691000
H	2.739000	3.022000	-1.774000
H	3.466000	1.664000	-2.695000
H	2.804000	3.075000	-3.555000
C	-0.192000	-1.507000	-4.021000
H	-0.291000	-1.590000	-5.099000
C	0.028000	-1.298000	-1.246000
C	-0.705000	-2.513000	-3.186000
H	-1.215000	-3.378000	-3.606000
C	-0.596000	-2.414000	-1.793000
H	-1.013000	-3.195000	-1.145000
C	-0.425000	-0.151000	0.749000
C	-1.151000	-0.003000	3.134000
H	-1.766000	-0.904000	3.053000
H	-1.714000	0.886000	2.840000
H	-0.736000	0.094000	4.137000