



Supporting Information

for

Deciphering the mechanism of γ -cyclodextrin's hydrophobic cavity hydration: an integrated experimental and theoretical study

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Figure S1. Schematic representation of γ -CD-H₂O complexes with water molecule located at different positions, and M062X/6-311++G(d,p)//M062X/6-31G(d,p) calculated relative enthalpies (ΔH^{78}) of the respective complexes, in kcal mol⁻¹. γ -CD-H₂O (*f*) is a complex in which a single water molecule is located outside the CD cavity, near the oxygen atom of one of the glucopyranose units.

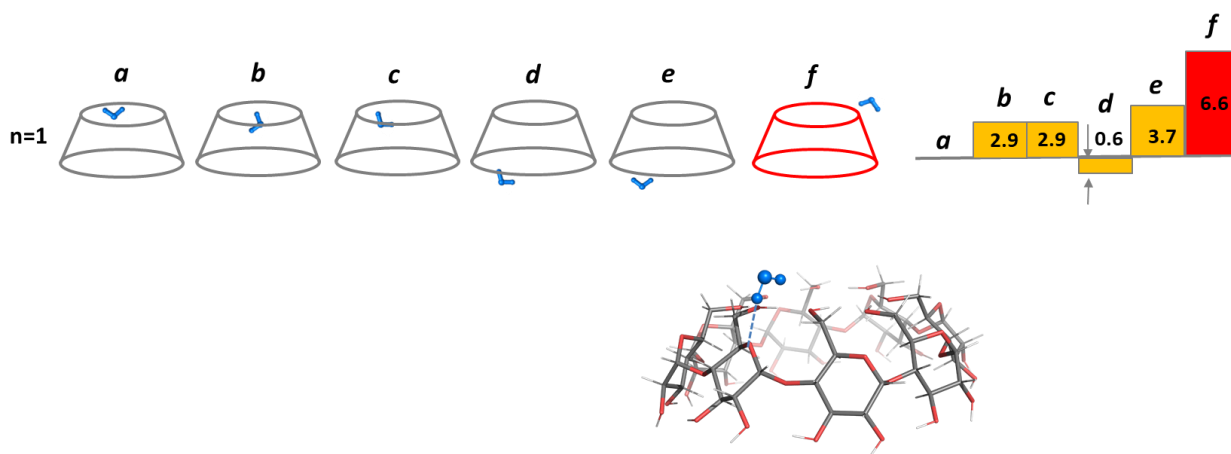


Figure S2. H-bonds in γ -CD-H₂O (*a*) and γ -CD-H₂O (*d*) complexes.

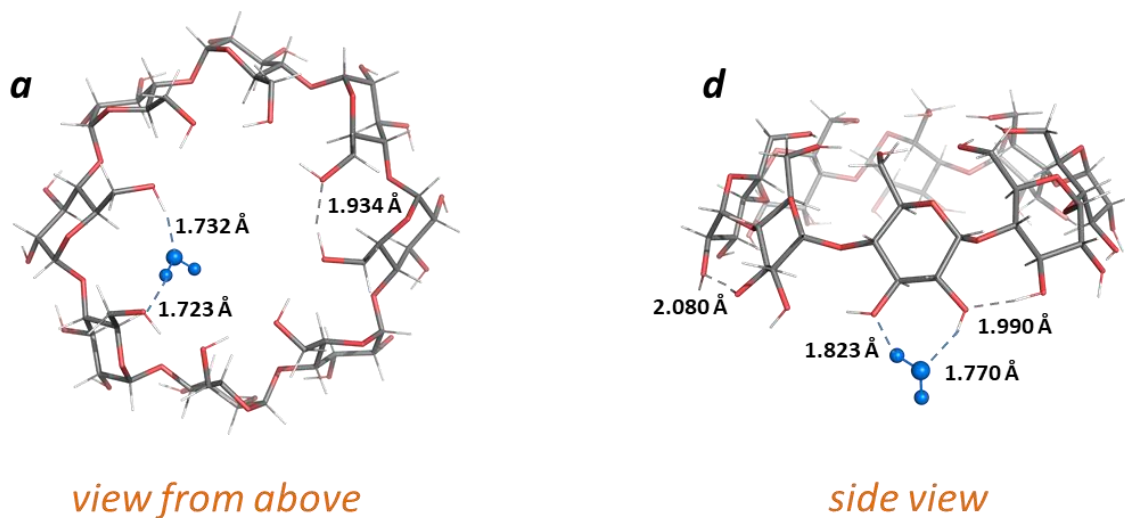


Table S1. M062X/6-31G(d,p) optimized geometries of γ -CD, selected γ -CD- n H₂O ($n = 1-7$) complexes, and a cluster of 7 water molecules.

γ-CD			
6	1.065743000	-6.749738000	0.139061000
6	0.197080000	-7.342359000	-0.969302000
6	-0.966496000	-6.424075000	-1.291448000
6	-1.684189000	-6.050316000	-0.003626000
6	-0.690933000	-5.392729000	0.954952000
6	-1.269603000	-4.871614000	2.275235000
8	1.736368000	-5.637251000	-0.375387000
8	1.009378000	-7.571892000	-2.101331000
8	-1.805098000	-7.112188000	-2.184971000
8	0.282994000	-6.403875000	1.253388000
8	-1.177108000	-3.461214000	2.362789000
1	-2.068260000	-6.964735000	0.473576000
1	1.782808000	-7.498511000	0.494820000
1	-0.219607000	-8.288697000	-0.593231000
1	-0.570470000	-5.499009000	-1.741899000
1	-0.198377000	-4.548157000	0.455466000
1	-2.329243000	-5.122882000	2.367863000
1	-0.720384000	-5.353350000	3.094392000
1	0.408773000	-7.792827000	-2.826360000
1	-2.634761000	-6.610580000	-2.275964000
1	-0.224891000	-3.247583000	2.407736000
6	-4.021894000	-5.528366000	0.130327000
6	-5.051683000	-5.328471000	-0.980630000
6	-5.226142000	-3.854905000	-1.296093000
6	-5.472129000	-3.089673000	-0.004877000
6	-4.306957000	-3.330994000	0.955638000
6	-4.351480000	-2.559184000	2.279392000
8	-2.758907000	-5.212115000	-0.377076000
8	-4.635404000	-6.060613000	-2.114132000
8	-6.305697000	-3.746116000	-2.189556000
8	-4.334341000	-4.735982000	1.247709000
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1	-6.390899000	-3.467765000	0.468883000
1	-4.044759000	-6.566706000	0.480685000
1	-6.016516000	-5.705185000	-0.609277000
1	-4.292406000	-3.476065000	-1.743648000
1	-3.359835000	-3.080803000	0.459970000
1	-5.280652000	-1.991548000	2.373470000
1	-4.301959000	-3.291681000	3.095463000
1	-5.215743000	-5.792291000	-2.839564000
1	-6.543486000	-2.805424000	-2.272164000
1	-2.464898000	-2.141474000	2.412714000
6	-6.752577000	-1.065444000	0.141203000
6	-7.346179000	-0.197107000	-0.966808000
6	-6.427960000	0.966232000	-1.290189000
6	-6.052578000	1.684090000	-0.002900000
6	-5.394523000	0.690827000	0.955521000
6	-4.872119000	1.269303000	2.275308000

8	-5.640475000	-1.736065000	-0.373992000
8	-7.576915000	-1.009697000	-2.098386000
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1	-7.500993000	-1.782465000	0.497805000
1	-8.292079000	0.219826000	-0.589897000
1	-5.503507000	0.569833000	-1.741564000
1	-4.550655000	0.197699000	0.455388000
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1	-7.798092000	-0.409213000	-2.823447000
1	-6.614958000	2.634008000	-2.275534000
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6	-5.329258000	5.050917000	-0.981148000
6	-3.855579000	5.223768000	-1.297057000
6	-3.090197000	5.470019000	-0.005979000
6	-3.332078000	4.305455000	0.955199000
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8	-3.745888000	6.302569000	-2.191313000
8	-4.737051000	4.334078000	1.247480000
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1	-3.291869000	4.300062000	3.095067000
1	-5.793366000	5.214452000	-2.840101000
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6	0.966732000	6.425370000	-1.290637000
6	1.684187000	6.050550000	-0.002995000
6	0.690625000	5.392262000	0.954774000
6	1.268603000	4.869645000	2.274719000
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8	-1.009127000	7.573618000	-2.099968000
8	1.805520000	7.114162000	-2.183463000
8	-0.283012000	6.403358000	1.254065000
8	1.177259000	3.459085000	2.359770000
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1	0.219679000	8.289541000	-0.591311000
1	0.570769000	5.500639000	-1.741842000
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1	2.327917000	5.121794000	2.368792000

1	0.718166000	5.349489000	3.094158000
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6	5.471902000	3.089638000	-0.004615000
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1	6.544041000	2.805950000	-2.272093000
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1	5.504163000	-0.569835000	-1.741183000
1	4.550816000	-0.197627000	0.455834000
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1	5.352770000	-0.721337000	3.095305000
1	7.799515000	0.408378000	-2.822437000
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6	5.328934000	-5.050154000	-0.982222000
6	3.855137000	-5.222537000	-1.297687000
6	3.090183000	-5.469640000	-0.006537000
6	3.332545000	-4.305925000	0.955532000
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8	6.061319000	-4.633507000	-2.115432000
8	3.745042000	-6.300570000	-2.192824000
8	4.737676000	-4.334621000	1.247130000
8	1.625749000	-3.292819000	2.374041000
1	3.468144000	-6.389149000	0.465905000
1	6.568364000	-4.045520000	0.479587000
1	5.704659000	-6.015781000	-0.611943000
1	3.477212000	-4.287717000	-1.743744000
1	3.082979000	-3.357779000	0.461500000
1	1.993374000	-5.281063000	2.372787000
1	3.293788000	-4.303192000	3.095366000
1	5.792333000	-5.212859000	-2.841406000
1	2.804174000	-6.537791000	-2.275092000
1	2.143660000	-2.465409000	2.414698000
γ-CD-H₂O(a)			
6	6.615442000	1.871140000	0.207943000
6	7.383801000	0.998953000	-0.781648000
6	6.650742000	-0.307177000	-0.996670000
6	6.383035000	-0.982693000	0.336513000
6	5.655612000	-0.026547000	1.284688000
6	5.508717000	-0.589011000	2.686507000
8	5.402165000	2.244773000	-0.383473000
8	7.520545000	1.706419000	-1.997344000
8	7.445419000	-1.100106000	-1.841240000
8	6.411739000	1.182904000	1.411800000
8	4.520227000	0.081432000	3.447250000
1	7.340559000	-1.297263000	0.780796000
1	7.204581000	2.758928000	0.464957000
1	8.370768000	0.780670000	-0.347953000
1	5.673739000	-0.083863000	-1.455652000
1	4.661629000	0.192540000	0.873119000
1	5.205276000	-1.638450000	2.625953000
1	6.487726000	-0.532311000	3.182795000
1	7.841871000	1.062614000	-2.644846000
1	7.081384000	-2.003924000	-1.847115000
1	4.546178000	1.038413000	3.255105000
6	5.882832000	-3.343459000	0.608965000
6	5.908374000	-4.394446000	-0.502014000
6	4.513534000	-4.603788000	-1.061544000
6	3.557064000	-4.886188000	0.085357000
6	3.589010000	-3.722106000	1.072957000
6	2.633415000	-3.851410000	2.259399000
8	5.587026000	-2.110090000	0.023087000
8	6.808595000	-3.973515000	-1.506970000
8	4.588824000	-5.675222000	-1.969510000
8	4.930213000	-3.682082000	1.585220000
8	1.426952000	-3.157170000	2.014949000
1	3.899984000	-5.780987000	0.626761000
1	6.848959000	-3.304891000	1.126161000
1	6.242528000	-5.344814000	-0.060433000
1	4.191232000	-3.675523000	-1.560443000
1	3.365825000	-2.774658000	0.566081000

1	2.370679000	-4.898944000	2.439744000
1	3.146683000	-3.459781000	3.148249000
1	6.663361000	-4.565948000	-2.258168000
1	3.691161000	-5.871280000	-2.292513000
1	1.645995000	-2.200746000	1.973076000
6	1.732919000	-6.385105000	-0.232443000
6	1.006101000	-6.858269000	-1.491184000
6	-0.264141000	-6.062543000	-1.721658000
6	-1.086714000	-6.063678000	-0.443653000
6	-0.249752000	-5.473624000	0.690021000
6	-0.959814000	-5.329909000	2.041809000
8	2.281780000	-5.122098000	-0.476279000
8	1.892752000	-6.761393000	-2.586021000
8	-0.947860000	-6.663783000	-2.793068000
8	0.866407000	-6.359379000	0.870877000
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1	-1.351106000	-7.100479000	-0.185191000
1	2.523320000	-7.100538000	0.022826000
1	0.713368000	-7.906069000	-1.324217000
1	0.007421000	-5.019302000	-1.952408000
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1	-1.956435000	-5.776828000	2.018405000
1	-0.355405000	-5.860710000	2.789382000
1	1.363424000	-6.905233000	-3.382105000
1	-1.848747000	-6.295852000	-2.823625000
1	-0.235403000	-3.579851000	2.420799000
6	-3.479806000	-5.867193000	-0.330914000
6	-4.498702000	-5.637617000	-1.447659000
6	-4.877165000	-4.171086000	-1.548678000
6	-5.251277000	-3.647487000	-0.171021000
6	-4.083933000	-3.874494000	0.789369000
6	-4.251613000	-3.319070000	2.208977000
8	-2.257113000	-5.322238000	-0.729841000
8	-3.950606000	-6.120510000	-2.656401000
8	-5.946738000	-4.073552000	-2.456202000
8	-3.926790000	-5.297781000	0.872930000
8	-3.319563000	-2.286757000	2.477801000
1	-6.123730000	-4.206539000	0.201192000
1	-3.374086000	-6.940831000	-0.135635000
1	-5.408888000	-6.196499000	-1.183490000
1	-3.998869000	-3.604622000	-1.900197000
1	-3.171003000	-3.431267000	0.371213000
1	-5.245096000	-2.892954000	2.359287000
1	-4.115477000	-4.153918000	2.908076000
1	-4.553905000	-5.844462000	-3.359600000
1	-6.354327000	-3.195429000	-2.351870000
1	-2.454002000	-2.737900000	2.512800000
6	-6.710622000	-1.804209000	0.328828000
6	-7.518484000	-0.929921000	-0.629300000
6	-6.784498000	0.363668000	-0.927968000
6	-6.338117000	1.013957000	0.372272000
6	-5.473881000	0.030022000	1.159894000
6	-4.860181000	0.555845000	2.462314000

8	-5.593612000	-2.288297000	-0.356342000
8	-7.765747000	-1.671607000	-1.805351000
8	-7.662973000	1.185646000	-1.655033000
8	-6.334430000	-1.074510000	1.468518000
8	-3.442832000	0.547806000	2.408157000
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1	-7.327012000	-2.635566000	0.690712000
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1	-4.646783000	-0.316478000	0.526954000
1	-5.160839000	1.588495000	2.653590000
1	-5.221079000	-0.078133000	3.281548000
1	-8.159686000	-1.055033000	-2.437612000
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6	-6.042086000	4.500227000	-0.351731000
6	-4.660082000	4.791171000	-0.903572000
6	-3.687252000	4.992013000	0.248684000
6	-3.687022000	3.757497000	1.149622000
6	-2.709604000	3.798011000	2.330543000
8	-5.656373000	2.193809000	-0.002718000
8	-6.942541000	4.123640000	-1.371832000
8	-4.765402000	5.937383000	-1.710749000
8	-5.021017000	3.662470000	1.668598000
8	-1.685940000	2.824530000	2.202754000
1	-4.016078000	5.850515000	0.853490000
1	-6.932564000	3.271673000	1.195990000
1	-6.396700000	5.404286000	0.165614000
1	-4.324583000	3.917695000	-1.486149000
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1	-2.212109000	4.770400000	2.389396000
1	-3.287770000	3.642239000	3.250276000
1	-6.836728000	4.774446000	-2.079435000
1	-3.873068000	6.188942000	-2.008032000
1	-2.121231000	1.954360000	2.280942000
6	-1.803928000	6.452793000	0.048336000
6	-1.121627000	7.047497000	-1.182985000
6	0.051057000	6.183759000	-1.600933000
6	0.941909000	5.949889000	-0.391026000
6	0.135083000	5.275105000	0.718541000
6	0.924729000	4.910420000	1.979638000
8	-2.428412000	5.264207000	-0.333339000
8	-2.080935000	7.168747000	-2.211344000
8	0.729037000	6.862302000	-2.629570000
8	-0.876772000	6.225712000	1.081833000
8	1.104021000	3.508390000	2.103038000
1	1.283237000	6.920112000	-0.000380000
1	-2.535915000	7.162184000	0.450300000
1	-0.728015000	8.035884000	-0.901792000
1	-0.331177000	5.209274000	-1.944789000
1	-0.341181000	4.358911000	0.344131000
1	1.923706000	5.357006000	1.951442000

1	0.385311000	5.317887000	2.844470000
1	-1.590840000	7.372352000	-3.019683000
1	1.514601000	6.343245000	-2.877510000
1	0.216389000	3.118495000	2.221941000
6	3.297184000	5.806344000	-0.692863000
6	4.173040000	5.398000000	-1.872804000
6	4.543508000	3.925912000	-1.802723000
6	5.090211000	3.622879000	-0.416803000
6	4.059366000	4.025586000	0.634311000
6	4.427482000	3.683147000	2.077542000
8	2.048874000	5.193955000	-0.834939000
8	3.482446000	5.712061000	-3.063448000
8	5.487192000	3.690409000	-2.816211000
8	3.897932000	5.444088000	0.526166000
8	3.745134000	2.523432000	2.511446000
1	6.001586000	4.219968000	-0.258267000
1	3.190380000	6.896672000	-0.668570000
1	5.107684000	5.974446000	-1.803055000
1	3.632409000	3.323151000	-1.952561000
1	3.101669000	3.533681000	0.418350000
1	5.495756000	3.473495000	2.184680000
1	4.184671000	4.550397000	2.705466000
1	3.991010000	5.326514000	-3.789466000
1	5.980487000	2.879002000	-2.600143000
1	2.795197000	2.744849000	2.549790000
8	2.446392000	-0.666134000	1.915095000
1	2.150512000	0.140187000	1.481152000
1	3.090145000	-0.380509000	2.603520000
γ-CD-2H₂O(a)			
6	6.961810000	-0.651159000	-0.246784000
6	7.535407000	0.412567000	0.686503000
6	6.545503000	1.545437000	0.854323000
6	6.116382000	2.072981000	-0.503631000
6	5.597295000	0.933649000	-1.381972000
6	5.290388000	1.380042000	-2.799728000
8	5.862234000	-1.241473000	0.386949000
8	7.825820000	-0.191885000	1.930901000
8	7.169262000	2.534249000	1.634213000
8	6.601376000	-0.082359000	-1.475867000
8	4.453764000	0.472581000	-3.490476000
1	6.977331000	2.559179000	-0.989096000
1	7.724728000	-1.405249000	-0.473273000
1	8.450862000	0.813255000	0.226992000
1	5.647397000	1.146225000	1.353574000
1	4.686292000	0.522150000	-0.927753000
1	4.759128000	2.336078000	-2.769009000
1	6.242965000	1.519902000	-3.330564000
1	8.032131000	0.532548000	2.538408000
1	6.649487000	3.355236000	1.564919000
1	4.729905000	-0.444195000	-3.289284000
6	5.091268000	4.232185000	-0.924847000
6	5.004100000	5.363325000	0.101485000

6	3.652742000	5.341277000	0.789088000
6	2.559643000	5.324534000	-0.266374000
6	2.733967000	4.111486000	-1.176511000
6	1.671606000	3.972252000	-2.271215000
8	5.102901000	3.021972000	-0.226449000
8	6.057399000	5.213813000	1.031949000
8	3.581863000	6.483954000	1.606506000
8	4.006958000	4.290402000	-1.816931000
8	0.671199000	3.038660000	-1.908498000
1	2.658582000	6.219463000	-0.899257000
1	5.995143000	4.335027000	-1.537038000
1	5.097792000	6.318864000	-0.435314000
1	3.575449000	4.416215000	1.382753000
1	2.746803000	3.180614000	-0.595691000
1	1.169213000	4.929016000	-2.448225000
1	2.182638000	3.667139000	-3.193901000
1	5.870286000	5.838738000	1.746752000
1	2.705845000	6.506558000	2.030932000
1	1.102631000	2.157247000	-1.903315000
6	0.527183000	6.477176000	0.176126000
6	-0.180940000	6.858179000	1.475755000
6	-1.236776000	5.830974000	1.832428000
6	-2.134210000	5.612345000	0.624882000
6	-1.285869000	5.147667000	-0.556533000
6	-2.060812000	4.807203000	-1.832377000
8	1.320635000	5.351308000	0.413226000
8	0.790507000	6.992716000	2.491369000
8	-1.951284000	6.323644000	2.939427000
8	-0.395781000	6.233749000	-0.854510000
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1	-2.610542000	6.564647000	0.346687000
1	1.144703000	7.316477000	-0.163531000
1	-0.693007000	7.816827000	1.302311000
1	-0.737623000	4.877034000	2.067755000
1	-0.698944000	4.264486000	-0.275389000
1	-3.106594000	5.119467000	-1.750498000
1	-1.596676000	5.354628000	-2.662963000
1	0.308365000	7.060951000	3.326492000
1	-2.677593000	5.705396000	3.134163000
1	-1.129211000	3.141285000	-2.171919000
6	-4.447688000	5.091468000	0.917944000
6	-5.226766000	4.469431000	2.071797000
6	-5.339796000	2.964188000	1.902927000
6	-5.844745000	2.650644000	0.503317000
6	-4.941054000	3.308064000	-0.535125000
6	-5.309797000	3.023555000	-1.993160000
8	-3.117747000	4.673470000	1.011553000
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8	-6.212500000	2.499524000	2.902043000
8	-5.012332000	4.721758000	-0.316205000
8	-4.443931000	2.063716000	-2.560127000
1	-6.863568000	3.054201000	0.395410000
1	-4.512619000	6.184435000	0.967751000

1	-6.245166000	4.885043000	2.043518000
1	-4.335509000	2.522244000	2.009111000
1	-3.907882000	2.968060000	-0.387762000
1	-6.323389000	2.622271000	-2.084149000
1	-5.269420000	3.973857000	-2.542114000
1	-4.997370000	4.292125000	3.976052000
1	-6.548927000	1.624720000	2.637849000
1	-3.549417000	2.456864000	-2.574377000
6	-6.962012000	0.651317000	-0.247034000
6	-7.535852000	-0.412533000	0.685957000
6	-6.545974000	-1.545406000	0.853926000
6	-6.116321000	-2.072693000	-0.503965000
6	-5.596935000	-0.933236000	-1.381918000
6	-5.289419000	-1.379167000	-2.799700000
8	-5.862735000	1.241620000	0.387185000
8	-7.826612000	0.191831000	1.930318000
8	-7.170004000	-2.534381000	1.633385000
8	-6.601045000	0.082771000	-1.476048000
8	-4.452202000	-0.471448000	-3.489530000
1	-6.977056000	-2.558875000	-0.989813000
1	-7.724935000	1.405370000	-0.473672000
1	-8.451168000	-0.813219000	0.226167000
1	-5.648068000	-1.146251000	1.353574000
1	-4.686144000	-0.521728000	-0.927274000
1	-4.758258000	-2.335261000	-2.769200000
1	-6.241703000	-1.518531000	-3.331137000
1	-8.033175000	-0.532638000	2.537699000
1	-6.649927000	-3.355220000	1.564540000
1	-4.729286000	0.445234000	-3.289196000
6	-5.091384000	-4.232066000	-0.924626000
6	-5.004104000	-5.362922000	0.102000000
6	-3.652634000	-5.340790000	0.789408000
6	-2.559734000	-5.324501000	-0.266269000
6	-2.734107000	-4.111689000	-1.176694000
6	-1.672004000	-3.972834000	-2.271627000
8	-5.102872000	-3.021670000	-0.226551000
8	-6.057228000	-5.213150000	1.032617000
8	-3.581823000	-6.483207000	1.607170000
8	-4.007236000	-4.290618000	-1.816875000
8	-0.670938000	-3.040009000	-1.908852000
1	-2.658931000	-6.219603000	-0.898862000
1	-5.995365000	-4.335050000	-1.536635000
1	-5.097915000	-6.318595000	-0.434538000
1	-3.575123000	-4.415545000	1.382760000
1	-2.746771000	-3.180648000	-0.596135000
1	-1.170250000	-4.929846000	-2.449137000
1	-2.183114000	-3.667027000	-3.194035000
1	-5.869888000	-5.837782000	1.747617000
1	-2.705690000	-6.505940000	2.031355000
1	-1.101761000	-2.158249000	-1.903887000
6	-0.527159000	-6.477148000	0.175876000
6	0.180884000	-6.858353000	1.475503000
6	1.236874000	-5.831353000	1.832214000

6	2.134486000	-5.612910000	0.624749000
6	1.286329000	-5.147991000	-0.556705000
6	2.061400000	-4.807825000	-1.832581000
8	-1.320533000	-5.351214000	0.413005000
8	-0.790548000	-6.992768000	2.491153000
8	1.951196000	-6.324044000	2.939321000
8	0.395857000	-6.233770000	-0.854710000
8	2.065800000	-3.411583000	-2.082355000
1	2.610798000	-6.565258000	0.346675000
1	-1.144761000	-7.316346000	-0.163877000
1	0.692769000	-7.817084000	1.301996000
1	0.737879000	-4.877297000	2.067413000
1	0.699727000	-4.264615000	-0.275488000
1	3.107297000	-5.119555000	-1.750228000
1	1.597744000	-5.355983000	-2.662954000
1	-0.308391000	-7.061166000	3.326254000
1	2.677615000	-5.705919000	3.134039000
1	1.129092000	-3.142390000	-2.172708000
6	4.448010000	-5.091788000	0.917549000
6	5.227180000	-4.469782000	2.071355000
6	5.339961000	-2.964444000	1.902801000
6	5.844326000	-2.650517000	0.503053000
6	4.940298000	-3.307884000	-0.535080000
6	5.307856000	-3.022427000	-1.993177000
8	3.118028000	-4.674136000	1.011679000
8	4.581032000	-4.816387000	3.278203000
8	6.213052000	-2.500063000	2.901713000
8	5.012320000	-4.721605000	-0.316650000
8	4.442305000	-2.060939000	-2.557909000
1	6.863095000	-3.054049000	0.394632000
1	4.513217000	-6.184754000	0.967056000
1	6.245660000	-4.885170000	2.042806000
1	4.335695000	-2.522598000	2.009521000
1	3.907043000	-2.968450000	-0.387067000
1	6.321849000	-2.622322000	-2.084971000
1	5.265608000	-3.972073000	-2.543109000
1	4.998122000	-4.292947000	3.975677000
1	6.549146000	-1.625046000	2.637802000
1	3.548050000	-2.454607000	-2.574037000
8	2.281309000	0.849350000	-1.926472000
1	2.195302000	0.013541000	-1.456572000
1	2.954378000	0.685572000	-2.625999000
8	-2.280616000	-0.851225000	-1.926486000
1	-2.191327000	-0.015840000	-1.456541000
1	-2.953875000	-0.685607000	-2.625501000
γ-CD-3H₂O(b)			
6	-5.686416000	-3.679007000	-0.423323000
6	-5.504876000	-4.915445000	0.454855000
6	-4.040539000	-5.158020000	0.761762000
6	-3.237285000	-5.152809000	-0.529767000
6	-3.467713000	-3.828989000	-1.257110000
6	-2.726290000	-3.691632000	-2.571568000

8	-5.399968000	-2.546398000	0.343328000
8	-6.251681000	-4.730473000	1.639991000
8	-3.965187000	-6.385920000	1.439382000
8	-4.866252000	-3.740182000	-1.556952000
8	-2.676560000	-2.352944000	-3.010243000
1	-3.572607000	-5.982182000	-1.171125000
1	-6.717436000	-3.640070000	-0.793568000
1	-5.877314000	-5.785150000	-0.107261000
1	-3.671545000	-4.327957000	1.387288000
1	-3.170998000	-2.996200000	-0.603994000
1	-1.695620000	-4.034109000	-2.439243000
1	-3.209839000	-4.341548000	-3.316032000
1	-6.011314000	-5.464617000	2.222488000
1	-3.031520000	-6.659357000	1.489013000
1	-3.570563000	-1.954744000	-2.952463000
6	-1.147127000	-6.323659000	-0.819857000
6	-0.410474000	-7.155565000	0.229340000
6	0.670166000	-6.325169000	0.892403000
6	1.554114000	-5.719763000	-0.185885000
6	0.707178000	-4.863032000	-1.125736000
6	1.480028000	-4.189771000	-2.262423000
8	-1.883743000	-5.338172000	-0.155997000
8	-1.342624000	-7.636427000	1.174988000
8	1.385806000	-7.185356000	1.745486000
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8	1.863415000	-2.877873000	-1.919876000
1	1.985218000	-6.530366000	-0.792799000
1	-1.808973000	-6.962112000	-1.415825000
1	0.077359000	-7.994650000	-0.288665000
1	0.193939000	-5.505516000	1.453944000
1	0.172834000	-4.082823000	-0.565411000
1	2.393497000	-4.750944000	-2.491327000
1	0.836135000	-4.200764000	-3.152371000
1	-0.819065000	-7.986592000	1.909558000
1	2.104916000	-6.679716000	2.163933000
1	1.052523000	-2.297892000	-1.911321000
6	3.878019000	-5.504817000	0.275515000
6	4.657172000	-5.350254000	1.580791000
6	4.901418000	-3.884236000	1.869043000
6	5.543194000	-3.229276000	0.655345000
6	4.640856000	-3.424732000	-0.562487000
6	5.145555000	-2.804123000	-1.870490000
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8	5.723552000	-3.799947000	3.007959000
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1	3.928702000	-3.395845000	2.039543000
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6	6.177272000	1.427150000	0.443983000
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8	5.692430000	-1.865038000	1.001293000
8	6.921770000	-0.955003000	3.224246000
8	6.390561000	1.821375000	2.833552000
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8	4.697523000	0.795324000	-2.575908000
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1	5.076823000	0.444018000	1.993866000
1	5.051843000	-0.201837000	-0.411756000
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1	6.883154000	-0.282078000	3.917269000
1	6.030265000	2.680712000	2.553233000
1	4.455450000	-0.153866000	-2.696250000
6	5.523382000	3.595669000	-0.375345000
6	5.355665000	4.807299000	0.539038000
6	3.893518000	5.108151000	0.787632000
6	3.152539000	5.215027000	-0.535347000
6	3.362120000	3.931528000	-1.334360000
6	2.722090000	3.914157000	-2.707673000
8	5.169887000	2.426005000	0.325795000
8	6.037215000	4.550608000	1.749100000
8	3.836129000	6.297617000	1.529385000
8	4.766455000	3.735595000	-1.541860000
8	2.670885000	2.606312000	-3.241308000
1	3.527676000	6.083374000	-1.098398000
1	6.566961000	3.528466000	-0.700133000
1	5.796003000	5.673978000	0.023718000
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1	3.280529000	4.592261000	-3.368962000
1	5.809871000	5.278375000	2.345228000
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1	3.546568000	2.183308000	-3.165228000
6	1.042628000	6.363153000	-0.859213000
6	0.315632000	7.197393000	0.195959000
6	-0.736897000	6.354355000	0.888823000
6	-1.627925000	5.711023000	-0.161374000
6	-0.778291000	4.858902000	-1.101487000
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8	1.266796000	7.692595000	1.116499000
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8	0.129156000	5.767187000	-1.743915000
8	-1.859653000	2.803724000	-1.824485000
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1	1.691165000	6.997941000	-1.473741000
1	-0.192346000	8.027361000	-0.316633000
1	-0.232319000	5.552360000	1.451151000
1	-0.207150000	4.109999000	-0.535385000
1	-2.507334000	4.635263000	-2.396247000
1	-0.950112000	4.160469000	-3.115373000
1	0.756524000	8.055788000	1.854317000
1	-2.133996000	6.678280000	2.207433000
1	-1.027078000	2.282201000	-1.797880000
6	-3.924672000	5.472291000	0.389392000
6	-4.663862000	5.243410000	1.705012000
6	-4.901570000	3.763137000	1.931209000
6	-5.558953000	3.167709000	0.694762000
6	-4.674997000	3.429489000	-0.521916000
6	-5.169994000	2.839717000	-1.845857000
8	-2.620966000	4.975813000	0.519878000
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8	-5.708092000	3.632337000	3.075258000
8	-4.590026000	4.854480000	-0.678883000
8	-4.355799000	1.764007000	-2.271407000
1	-6.539031000	3.643180000	0.537006000
1	-3.904098000	6.543751000	0.159729000
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1	-6.184642000	2.442481000	-1.748979000
1	-5.179356000	3.649450000	-2.588077000
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1	-3.422272000	2.057011000	-2.241163000
6	-6.988049000	1.232408000	0.775853000
6	-7.231991000	0.238587000	1.907156000
6	-6.287838000	-0.941592000	1.779823000
6	-6.366430000	-1.514227000	0.374481000
6	-6.107586000	-0.428277000	-0.668486000
6	-6.210349000	-0.885920000	-2.131922000
8	-5.720133000	1.789282000	0.960959000
8	-7.060919000	0.911062000	3.138302000
8	-6.660775000	-1.890159000	2.749952000
8	-7.095197000	0.594484000	-0.469911000
8	-4.973010000	-0.840188000	-2.803433000
1	-7.373603000	-1.933429000	0.221876000
1	-7.757223000	2.014057000	0.784309000
1	-8.261613000	-0.135727000	1.808786000
1	-5.258401000	-0.583905000	1.943542000
1	-5.105901000	-0.008495000	-0.514606000
1	-6.568389000	-1.915624000	-2.208506000
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1	-1.144196000	-1.601485000	-2.342620000
8	0.527784000	1.455401000	-1.868994000
1	1.096221000	1.257246000	-1.099709000
1	1.175429000	1.753319000	-2.538556000
8	2.782367000	0.800991000	-0.390011000
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γ-CD-4H₂O(a)			
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1	-6.561478000	-3.211485000	-0.975997000
1	-7.686284000	0.623766000	-0.685763000
1	-8.266605000	-1.606346000	0.066868000
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1	-4.093385000	-2.818445000	-2.500622000
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6	-3.065848000	-5.690148000	1.088933000
6	-2.063364000	-5.718151000	-0.053395000
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8	-4.752612000	-3.564875000	-0.024366000
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6	0.940618000	-6.960450000	1.445940000
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8	6.503286000	-2.072356000	2.851583000
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1	3.679021000	-1.906176000	-2.458864000
6	6.957048000	0.026999000	-0.169125000
6	7.397284000	1.107133000	0.815625000
6	6.280245000	2.108392000	1.023459000
6	5.822280000	2.651800000	-0.318054000
6	5.439030000	1.509656000	-1.261773000
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1	4.662492000	0.172957000	-3.199572000
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6	4.416365000	5.792561000	0.435716000
6	3.040238000	5.621920000	1.049120000
6	2.009687000	5.613778000	-0.065589000
6	2.309041000	4.492850000	-1.058776000
6	1.319499000	4.415682000	-2.227877000
8	4.713279000	3.489746000	-0.037837000
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8	2.850143000	6.695333000	1.937987000
8	3.604923000	4.786904000	-1.601227000
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1	4.456838000	6.784880000	-0.037166000
1	3.001987000	4.652659000	1.571217000
1	2.331410000	3.515452000	-0.559158000
1	0.734927000	5.338713000	-2.299627000
1	1.905399000	4.298946000	-3.148570000
1	5.155444000	6.226447000	2.152231000
1	1.949124000	6.643156000	2.303136000
1	0.940676000	2.504462000	-2.219131000
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6	-1.829257000	5.153682000	-0.540714000
6	-2.559194000	4.843391000	-1.851518000
8	0.732936000	5.505437000	0.533523000
8	0.005683000	7.030018000	2.651014000
8	-2.672438000	6.123352000	2.981488000
8	-1.004661000	6.305063000	-0.760192000
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1	0.426041000	7.471588000	0.020259000
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8	-5.211271000	4.489499000	3.158341000
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γ-CD-5H₂O(a)			
6	6.894554000	0.277195000	-0.554090000
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6	5.138023000	1.633778000	-1.398210000
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8	6.006136000	-0.482090000	0.213693000
8	7.974232000	0.844530000	1.493768000
8	6.937542000	3.463388000	1.337572000
8	6.254984000	0.785362000	-1.694324000
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6	4.202304000	5.940289000	0.353299000
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8	6.606993000	-1.966060000	-0.613768000
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1	7.726046000	0.378647000	0.181784000
1	6.887532000	-3.547457000	0.570780000
1	8.006604000	-1.703024000	1.643826000
1	5.274276000	-0.378981000	1.820890000
1	4.967240000	-0.670965000	-0.627836000
1	6.720741000	0.778914000	-2.281122000
1	7.084913000	-0.923594000	-2.615503000
1	6.787128000	-1.730289000	3.683796000
1	6.852864000	1.349568000	2.494863000
1	4.736878000	-1.129950000	-2.883819000
6	6.456935000	2.539208000	-0.438803000
6	6.561972000	3.825410000	0.380099000
6	5.188932000	4.363644000	0.737563000
6	4.315849000	4.439087000	-0.506139000
6	4.245856000	3.049641000	-1.133876000
6	3.384038000	2.918202000	-2.371953000
8	6.011574000	1.520531000	0.399867000
8	7.322706000	3.549596000	1.535892000
8	5.383837000	5.622119000	1.330119000
8	5.581916000	2.704324000	-1.524395000
8	3.128435000	1.555967000	-2.654565000
1	4.764106000	5.138248000	-1.227756000
1	7.436326000	2.288916000	-0.864965000
1	7.059687000	4.579689000	-0.248498000
1	4.709565000	3.659243000	1.437935000
1	3.873586000	2.329773000	-0.391144000
1	2.421989000	3.404002000	-2.191805000
1	3.876781000	3.418532000	-3.216625000
1	7.270063000	4.344645000	2.084159000
1	4.515432000	6.046963000	1.449309000
1	3.971419000	1.056643000	-2.751242000
6	2.514808000	6.016111000	-0.750634000
6	1.941739000	6.983149000	0.287230000
6	0.705945000	6.395690000	0.941107000
6	-0.258449000	5.958355000	-0.148866000
6	0.425448000	4.930162000	-1.046311000
6	-0.443644000	4.368334000	-2.171698000
8	3.056102000	4.919454000	-0.074853000
8	2.944716000	7.279175000	1.235919000
8	0.156144000	7.395503000	1.764953000
8	1.523922000	5.618580000	-1.663585000
8	-1.059358000	3.150239000	-1.801192000
1	-0.506260000	6.825551000	-0.779102000
1	3.285622000	6.519319000	-1.345572000
1	1.635513000	7.896313000	-0.245023000
1	0.999155000	5.508839000	1.525371000

1	0.807245000	4.087799000	-0.453710000
1	-1.246517000	5.068898000	-2.428243000
1	0.197737000	4.239219000	-3.054079000
1	2.503858000	7.750075000	1.956815000
1	-0.660846000	7.050856000	2.166936000
1	-0.355261000	2.511069000	-1.526674000
6	-2.590427000	6.211556000	0.237817000
6	-3.438649000	6.230578000	1.509293000
6	-4.006163000	4.854414000	1.795116000
6	-4.704604000	4.335269000	0.547950000
6	-3.710920000	4.314538000	-0.609681000
6	-4.256250000	3.743211000	-1.920678000
8	-1.427432000	5.475999000	0.484748000
8	-2.637396000	6.702622000	2.571225000
8	-4.886518000	4.970258000	2.885299000
8	-3.309832000	5.670742000	-0.841870000
8	-3.611963000	2.525879000	-2.275879000
1	-5.544757000	4.997273000	0.288590000
1	-2.340608000	7.238866000	-0.050161000
1	-4.283531000	6.912743000	1.329410000
1	-3.172034000	4.171460000	2.024070000
1	-2.831903000	3.724383000	-0.323207000
1	-5.323761000	3.516619000	-1.833993000
1	-4.120817000	4.498427000	-2.704336000
1	-3.134422000	6.540744000	3.384532000
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6	-6.931671000	1.850188000	1.876928000
6	-6.245914000	0.504474000	1.704514000
6	-6.504994000	-0.025154000	0.302699000
6	-6.094570000	1.021615000	-0.730782000
6	-6.265978000	0.591280000	-2.191622000
8	-5.174064000	3.039582000	0.857370000
8	-6.574933000	2.459155000	3.101158000
8	-6.752318000	-0.344326000	2.703948000
8	-6.861079000	2.207522000	-0.500362000
8	-5.030945000	0.205522000	-2.772407000
1	-7.577850000	-0.251525000	0.199711000
1	-7.115868000	3.724901000	0.799032000
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1	-6.934717000	-0.269012000	-2.285947000
1	-6.713836000	1.427955000	-2.742476000
1	-6.648039000	1.773451000	3.779325000
1	-6.625716000	-1.266508000	2.418524000
1	-4.492402000	1.015210000	-2.867802000
8	-0.754804000	-1.745449000	-2.013901000
1	-1.029784000	-1.762397000	-1.060210000
1	-1.569564000	-1.576576000	-2.522556000
8	0.960391000	1.713930000	-0.808955000
1	0.741898000	1.082006000	-0.096878000

1	1.704117000	1.332935000	-1.303145000
8	1.745087000	-0.819745000	-2.310065000
1	0.768168000	-0.917912000	-2.266846000
1	1.960216000	-0.017650000	-2.807657000
8	-2.974433000	0.101077000	-0.731237000
1	-2.935875000	1.046766000	-0.928610000
1	-3.672373000	-0.229444000	-1.317875000
1	2.580512000	-0.939718000	-0.756638000
8	2.851222000	-0.888473000	0.186959000
1	3.481242000	-1.609952000	0.335197000
8	0.609111000	-0.175416000	1.264704000
1	0.754839000	0.251952000	2.114759000
1	1.483793000	-0.569125000	0.996070000
8	-1.525332000	-1.813510000	0.555960000
1	-0.769410000	-1.378727000	0.992058000
1	-2.148188000	-1.082060000	0.390346000
7H₂O (cluster)			
8	-0.451772000	-1.835357000	-2.064106000
1	-0.494223000	-2.030703000	-1.099714000
1	-1.270847000	-1.321550000	-2.176872000
8	-0.236652000	1.442135000	-0.746576000
1	0.105151000	1.196067000	0.132653000
1	0.443517000	1.120665000	-1.364713000
8	1.502543000	-0.192547000	-2.185795000
1	0.735130000	-0.853008000	-2.240660000
1	1.920778000	-0.156597000	-3.051105000
8	-2.341762000	-0.079228000	-1.155697000
1	-1.599378000	0.571307000	-1.012559000
1	-3.141251000	0.434446000	-1.298789000
1	2.314980000	-0.880454000	-0.809330000
8	2.490920000	-1.258373000	0.081828000
1	2.139762000	-2.155258000	0.052786000
8	0.783558000	0.153099000	1.491118000
1	1.089872000	0.433610000	2.358052000
1	1.525819000	-0.346674000	1.056730000
8	-1.011229000	-1.799249000	0.590698000
1	-0.475290000	-1.156541000	1.086949000
1	-1.768793000	-1.283279000	0.266583000