Supporting Information

Encapsulation of Greenhouse Gases in Clathrate Hydrates: Structural Insights, Energetics, Chemical Interactions, and Environmental Implications

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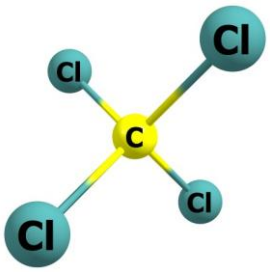
Table S1. Cartesian coordinates for optimized geometries of the guest molecule monomers computes at B3LYP/6-31G(d) level of theory and basis set.

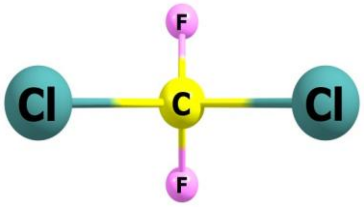
CCl_4

C	0.000000000	0.000000000	0.000000000
Cl	1.034552000	1.034552000	1.034552000
Cl	-1.034552000	-1.034552000	1.034552000
Cl	1.034552000	-1.034552000	-1.034552000
Cl	-1.034552000	1.034552000	-1.034552000



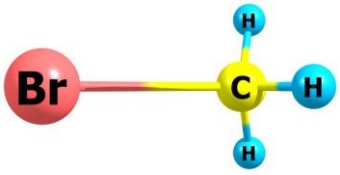
CF_2Cl_2

C	0.000000000	0.000000000	0.344814000
Cl	0.000000000	1.479072000	-0.655712000
Cl	0.000000000	-1.479072000	-0.655712000
F	-1.082744000	0.000063000	1.123629000
F	1.082744000	-0.000063000	1.123629000



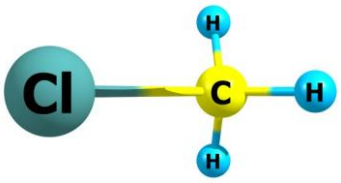
CH_3Br

C	0.000000000	0.000000000	-1.540232000
H	0.000000000	1.036877000	-1.871692000
H	0.897962000	-0.518439000	-1.871692000
H	-0.897962000	-0.518439000	-1.871692000
Br	0.000000000	0.000000000	0.424471000



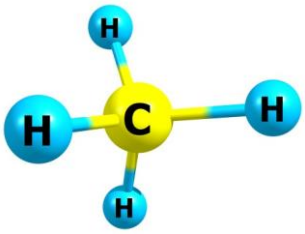
CH_3Cl

C	0.000000000	0.000000000	-1.139207000
H	0.000000000	1.033884000	-1.485431000
H	0.895369000	-0.516942000	-1.485431000
H	-0.895369000	-0.516942000	-1.485431000
Cl	0.000000000	0.000000000	0.664208000



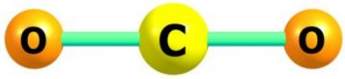
CH_4

C	0.000000000	0.000000000	0.000000000
H	0.631339000	0.631339000	0.631339000
H	-0.631339000	-0.631339000	0.631339000
H	-0.631339000	0.631339000	-0.631339000
H	0.631339000	-0.631339000	-0.631339000



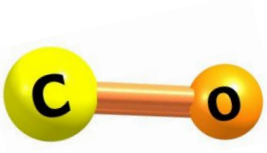
CO_2

C	0.000000000	0.000000000	-0.000083000
O	0.000000000	0.000000000	1.169178000
O	0.000000000	0.000000000	-1.169116000



CO

C	0.000000000	0.000000000	-0.650252000
O	0.000000000	0.000000000	0.487689000



H_2S

S	0.000000000	0.000000000	0.103381000
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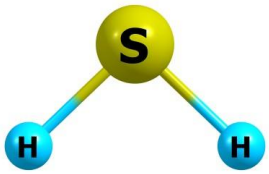
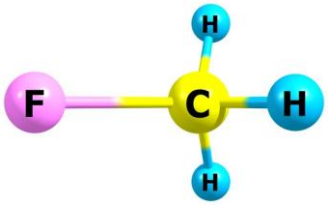
H	0.000000000	-0.977095000	-0.827050000



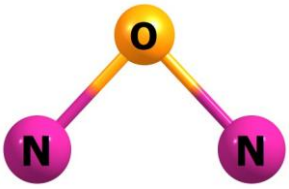
CH_3F

C	0.000000000	0.000000000	-0.630032000
H	0.000000000	1.032925000	-0.998065000
H	0.894540000	-0.516463000	-0.998065000
H	-0.894540000	-0.516463000	-0.998065000
F	0.000000000	0.000000000	0.752710000



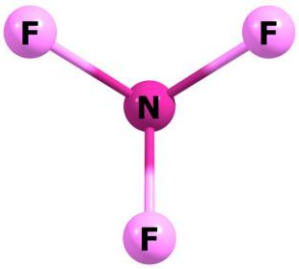
N_2O

O	0.000000000	0.000000000	0.599046000
N	0.000000000	-0.884567000	-0.342312000
N	0.000000000	0.884567000	-0.342312000



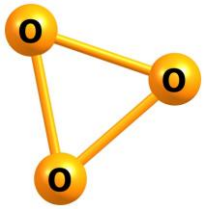
NF_3

N	0.000000000	0.000000000	0.487404000
F	0.000000000	1.240504000	-0.126364000
F	1.074308000	-0.620252000	-0.126364000
F	-1.074308000	-0.620252000	-0.126364000



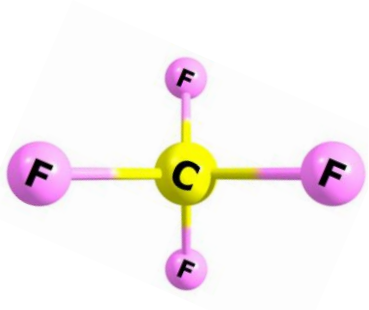
O_3

O	-0.719128000	-0.415187000	0.000000000
O	0.000000000	0.830376000	0.000000000
O	0.719128000	-0.415189000	0.000000000



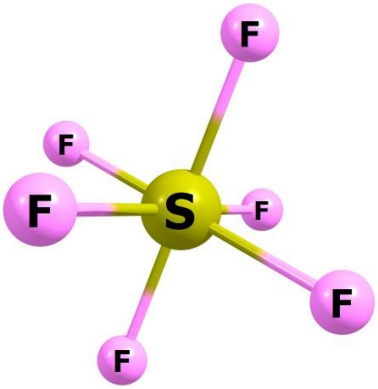
CF_4

C	0.000000000	0.000000000	0.000000000
F	-0.767523000	-0.767523000	0.767523000
F	0.767523000	0.767523000	0.767523000
F	-0.767523000	0.767523000	-0.767523000
F	0.767523000	-0.767523000	-0.767523000



SF_6

S	0.000000000	0.000000000	0.000000000
F	0.000000000	0.000000000	1.600359000
F	0.000000000	1.600359000	0.000000000
F	1.600359000	0.000000000	0.000000000
F	0.000000000	0.000000000	-1.600359000
F	-1.600359000	0.000000000	0.000000000
F	0.000000000	-1.600359000	0.000000000



SO_2

S	0.000000000	0.000000000	0.370851000
O	0.000000000	-1.261655000	-0.370851000
O	0.000000000	1.261655000	-0.370851000

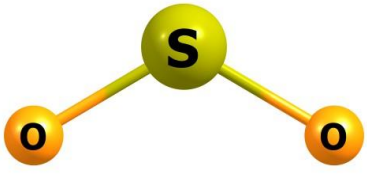
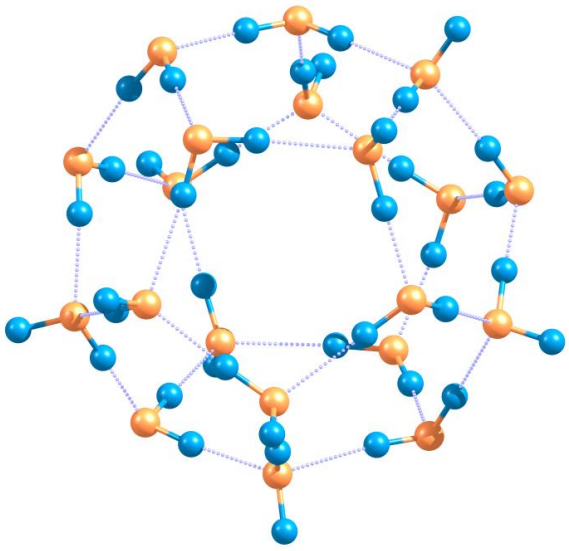


Table S2. Cartesian coordinates for optimized geometries of the empty 5^{12}, $5^{12}6^2$ and $5^{12}6^4$ clathrate hydrate monomers computes at B3LYP/6-31G(d) level of theory and basis set.

5^{12} Clathrate Hydate

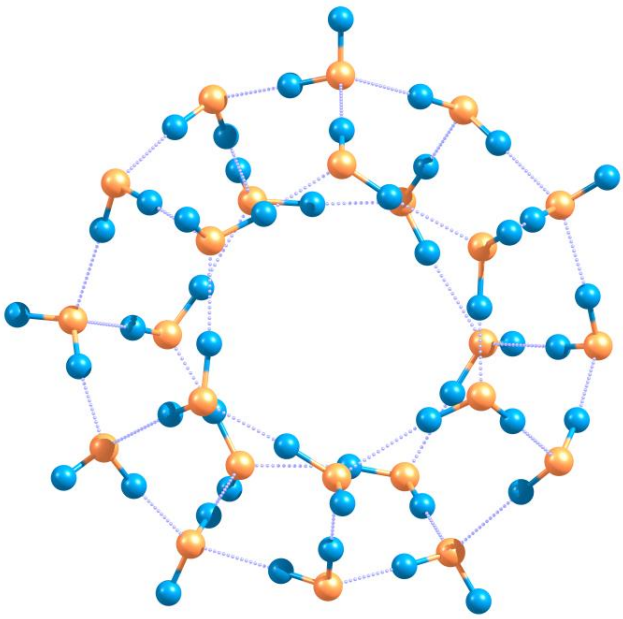


O	-0.807577000	3.763614000	-0.197525000
H	0.033759000	3.646888000	-0.739898000
H	-1.489303000	3.214763000	-0.641502000
O	-1.551322000	-3.222440000	1.739266000
H	-0.689809000	-3.295212000	1.284180000
H	-2.140813000	-2.797739000	1.075239000
O	1.413633000	3.377377000	-1.602252000
H	2.117106000	3.005161000	-1.018090000
H	1.275897000	2.699508000	-2.305179000
O	0.964264000	-3.657368000	0.371278000
H	0.821396000	-3.505735000	-0.596659000
H	1.034491000	-4.616986000	0.486410000
O	-2.569887000	0.928763000	2.787521000
H	-1.861318000	1.555542000	2.534554000
H	-2.085940000	0.129170000	3.126911000
O	3.749216000	-0.528969000	-0.549899000
H	3.468273000	-1.141628000	0.220329000
H	4.717658000	-0.566792000	-0.567274000
O	-3.871058000	0.315406000	0.542311000
H	-3.430683000	0.540243000	1.418013000
H	-3.530765000	0.983251000	-0.090431000
O	2.368082000	-1.079008000	-2.741412000
H	2.943499000	-0.882220000	-1.941778000

H	2.954137000	-1.057891000	-3.512858000
O	1.897263000	2.036300000	2.632716000
H	0.964568000	2.395613000	2.479076000
H	2.332087000	2.666011000	3.227134000
O	-1.780330000	0.621440000	-3.320016000
H	-1.856307000	-0.359643000	-3.057845000
H	-2.172595000	0.678524000	-4.204408000
O	1.709566000	-0.587100000	3.250137000
H	1.798972000	0.390552000	3.087626000
H	1.924094000	-0.724729000	4.185057000
O	-1.993027000	-1.894973000	-2.676399000
H	-2.464723000	-1.963222000	-1.804008000
H	-1.106040000	-2.276955000	-2.511180000
O	-0.547199000	2.868839000	2.169973000
H	-0.637031000	3.213235000	1.192339000
H	-0.875516000	3.597510000	2.718898000
O	-3.158561000	-2.025927000	-0.222592000
H	-3.997474000	-2.512237000	-0.220276000
H	-3.413782000	-1.077207000	0.095327000
O	0.962206000	1.340106000	-3.471994000
H	0.004323000	1.134069000	-3.425207000
H	1.396848000	0.541300000	-3.116549000
O	3.056606000	-2.107375000	1.381532000
H	2.344278000	-2.702614000	1.054572000
H	2.627175000	-1.575971000	2.094726000
O	0.601616000	-3.040756000	-2.275954000
H	0.688697000	-3.729709000	-2.952102000
H	1.280199000	-2.344464000	-2.502440000
O	3.265415000	2.218064000	0.129949000
H	3.383657000	1.280769000	-0.124790000

H	2.791634000	2.177104000	0.986113000
O	-1.097840000	-1.230126000	3.591618000
H	-1.315511000	-1.990870000	2.995632000
H	-0.174413000	-1.006531000	3.365918000
O	-2.819942000	2.147594000	-1.347338000
H	-2.474166000	1.614955000	-2.113274000
H	-3.515538000	2.716503000	-1.709670000

$5^{12}6^2$ Clathrate Hydate

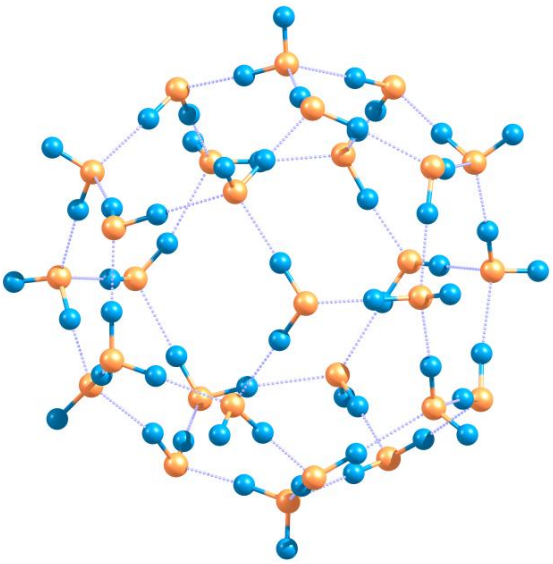


O	-0.345203000	2.481350000	-2.919374000
H	-1.096856000	1.809772000	-2.991477000
H	-0.321095000	2.922608000	-3.782394000
O	0.644304000	-2.757779000	-2.868436000
H	1.349687000	-2.073914000	-2.784163000
H	0.739074000	-3.325178000	-2.063525000
O	-0.817528000	4.308105000	-0.904330000
H	-0.656777000	3.683530000	-1.653866000
H	-1.566434000	3.917903000	-0.408712000
O	0.873225000	-4.244915000	-0.565567000
H	-0.008782000	-4.219572000	-0.048767000
H	1.038526000	-5.187042000	-0.722477000
O	-2.372808000	0.816525000	-3.124882000
H	-2.100343000	-0.134388000	-3.080825000
H	-2.961099000	0.945484000	-2.353360000
O	-1.783804000	-1.857683000	-2.943337000
H	-0.807581000	-2.154185000	-2.882220000
H	-2.109478000	-2.285936000	-3.750176000
O	-4.180995000	1.329050000	-0.954304000

H	-3.794204000	2.061844000	-0.399704000
H	-4.943414000	1.710572000	-1.415283000
O	-3.221704000	-3.086250000	-0.868769000
H	-2.702308000	-2.666710000	-1.591913000
H	-3.586242000	-2.334678000	-0.359936000
O	-3.012874000	3.214457000	0.574194000
H	-3.531310000	3.976918000	0.873336000
H	-2.631424000	2.793243000	1.407690000
O	-1.348417000	-4.205013000	0.767234000
H	-1.239652000	-3.541182000	1.486535000
H	-2.069582000	-3.848174000	0.183202000
O	2.314988000	1.535830000	-2.903515000
H	1.366880000	1.781941000	-2.843826000
H	2.768470000	2.051302000	-2.166945000
O	2.765969000	-0.966733000	-2.687684000
H	2.542147000	0.043656000	-2.732507000
H	3.260744000	-1.133769000	-3.504874000
O	3.429465000	2.874035000	-0.893150000
H	2.701398000	3.282784000	-0.380674000
H	3.848832000	2.236674000	-0.255026000
O	4.189227000	-1.426488000	-0.441844000
H	3.686385000	-1.267276000	-1.288637000
H	5.059819000	-1.757372000	-0.708255000
O	1.337992000	4.108803000	0.616923000
H	1.667923000	5.012160000	0.736538000
H	0.521521000	4.199255000	0.032977000
O	2.835198000	-3.294140000	1.204394000
H	2.149713000	-3.649729000	0.595013000
H	3.327205000	-2.642960000	0.659648000
O	-2.812927000	-0.359035000	2.903060000

H	-2.102181000	-1.054984000	2.913789000
H	-3.371893000	-0.581814000	2.126215000
O	2.489744000	0.703983000	2.924177000
H	1.822783000	1.459141000	2.927184000
H	2.980897000	0.803376000	3.753953000
O	-4.348306000	-0.899473000	0.616196000
H	-4.378049000	-0.106226000	0.025008000
H	-5.269562000	-1.147187000	0.785888000
O	4.419159000	1.060241000	0.889148000
H	4.389264000	0.194418000	0.429459000
H	3.743017000	0.970798000	1.596217000
O	-1.965176000	2.052194000	2.703428000
H	-2.251815000	1.063069000	2.758027000
H	-2.218160000	2.426989000	3.561596000
O	0.778503000	2.724046000	2.944513000
H	-0.130958000	2.391502000	2.791268000
H	0.990777000	3.260224000	2.142903000
O	-0.991221000	-2.369930000	2.858962000
H	0.011214000	-2.136992000	2.916461000
H	-1.145514000	-2.920341000	3.642525000
O	1.521136000	-1.916745000	3.120010000
H	1.807722000	-0.982781000	3.003007000
H	2.037147000	-2.442277000	2.444733000

$5^{12}6^4$ Clathrate Hydate



O	-1.008193000	-1.028248000	4.366167000
H	-0.064179000	-1.220972000	4.165992000
H	-1.521982000	-1.594714000	3.745554000
O	3.670766000	0.143197000	2.837518000
H	3.303834000	1.044057000	2.682586000
H	2.909471000	-0.396626000	3.134116000
O	2.724541000	2.731944000	2.389823000
H	3.240164000	3.299291000	2.983355000
H	1.751948000	2.936802000	2.625921000
O	0.298707000	3.391332000	3.021988000
H	-0.136079000	3.821393000	2.235958000
H	-0.293597000	2.647055000	3.266878000
O	3.228322000	3.469947000	-0.212173000
H	3.562578000	2.642155000	-0.636219000
H	3.060914000	3.222841000	0.731276000
O	4.121087000	1.135168000	-1.391287000
H	3.556967000	0.949849000	-2.218322000
H	5.013444000	1.292929000	-1.736141000
O	1.016926000	4.213470000	-1.301284000
H	1.170894000	5.155475000	-1.473753000
H	1.888055000	3.890255000	-0.860440000
O	-3.747874000	1.660469000	-1.947822000
H	-4.496074000	2.057309000	-2.418837000
H	-3.583106000	2.243697000	-1.154652000
O	-3.306617000	3.125338000	0.267466000
H	-3.897478000	3.883191000	0.398575000
H	-3.500682000	2.508167000	1.059876000
O	-0.853493000	4.447945000	0.801214000

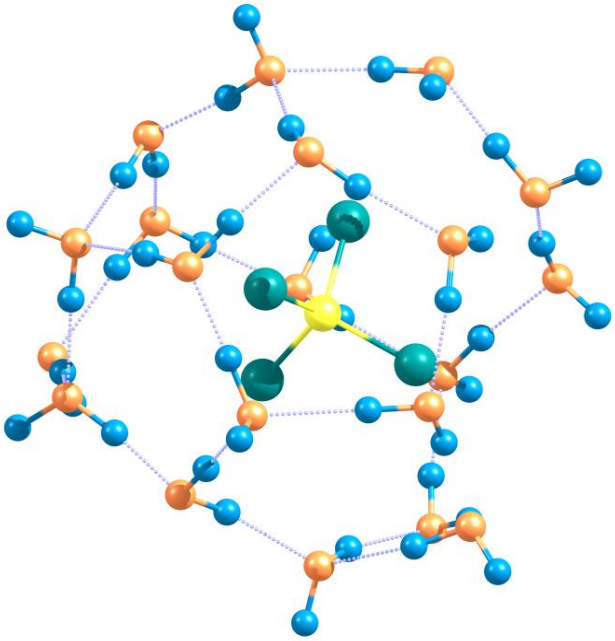
H	-0.233451000	4.296329000	0.054872000
H	-1.654692000	3.926704000	0.580879000
O	0.676480000	2.704828000	-3.504908000
H	0.771208000	3.287523000	-2.699294000
H	0.792590000	3.290877000	-4.267997000
O	-3.849721000	1.591069000	2.283364000
H	-4.003611000	0.666694000	1.977727000
H	-3.049597000	1.544279000	2.862899000
O	-4.279903000	-1.019844000	1.400415000
H	-4.267805000	-1.006395000	0.369648000
H	-5.196135000	-1.243763000	1.626011000
O	-1.588295000	1.478455000	3.856224000
H	-1.809642000	1.833214000	4.731089000
H	-1.326830000	0.514755000	4.028969000
O	1.737174000	-3.491705000	-2.304870000
H	2.171990000	-3.206501000	-1.474015000
H	0.850199000	-3.866981000	-2.026409000
O	3.222882000	-3.040166000	0.054609000
H	3.712871000	-2.141263000	0.213763000
H	3.920600000	-3.659257000	-0.210613000
O	4.515825000	-0.883281000	0.486222000
H	4.321156000	-0.190609000	-0.186920000
H	4.248698000	-0.488158000	1.363534000
O	2.742544000	0.806830000	-3.574225000
H	2.290467000	-0.067888000	-3.673891000
H	2.010987000	1.463732000	-3.560106000
O	1.830938000	-3.755448000	2.175368000
H	2.384379000	-3.507675000	1.368878000
H	2.206383000	-4.583893000	2.510000000
O	1.676858000	-1.624297000	3.837119000

H	1.747129000	-2.432867000	3.260810000
H	2.108223000	-1.862525000	4.672079000
O	-0.773570000	-4.465296000	1.221436000
H	0.122116000	-4.213649000	1.526033000
H	-1.349640000	-3.745812000	1.551792000
O	-2.449055000	-2.613185000	2.574819000
H	-3.131230000	-2.060991000	2.100310000
H	-2.949583000	-3.288976000	3.056851000
O	-0.672139000	-4.380658000	-1.546346000
H	-1.320907000	-3.685841000	-1.790181000
H	-0.734744000	-4.458770000	-0.562884000
O	-2.601760000	-2.521919000	-2.468960000
H	-3.111038000	-3.158089000	-2.995400000
H	-2.111406000	-1.960901000	-3.171706000
O	-4.393161000	-0.936851000	-1.159723000
H	-3.737536000	-1.527054000	-1.616774000
H	-4.172744000	-0.025176000	-1.459017000
O	-1.381083000	-1.179151000	-4.315951000
H	-1.554362000	-0.202004000	-4.262856000
H	-0.409855000	-1.282782000	-4.186173000
O	-1.832698000	1.502221000	-4.033734000
H	-2.411713000	1.577620000	-3.247099000
H	-0.979512000	1.908162000	-3.771103000
O	1.364328000	-1.539027000	-3.957665000
H	1.506339000	-2.284453000	-3.269764000
H	1.667072000	-1.924851000	-4.794110000

Table S3. Cartesian coordinates for optimized geometries of the Greenhouse gases encapsulated within 5^{12} clathrate hydrate computes at B3LYP/6-31G(d) level of theory and basis set.

CCl_4 within 5^{12} clathrate hydrate

O	3.103269000	0.310240000	-2.405422000
H	2.480067000	1.044335000	-2.648012000
H	3.400336000	0.495119000	-1.491438000
O	-0.967257000	-2.351909000	3.212136000
H	-1.694701000	-1.705288000	3.130024000
H	-0.158906000	-1.808785000	3.342075000
O	1.530894000	2.498914000	-2.968483000
H	0.555389000	2.549604000	-3.028430000
H	1.778075000	3.161595000	-2.285891000
O	-3.176329000	-0.294228000	3.148679000
H	-2.628980000	0.511710000	3.306115000
H	-3.661314000	-0.443828000	3.974849000
O	2.317149000	-3.416945000	0.206486000
H	2.386051000	-2.925906000	-0.641269000
H	1.353483000	-3.425064000	0.436105000
O	-3.514751000	1.505088000	-1.646502000
H	-3.596064000	0.528458000	-1.834496000
H	-4.288361000	1.904628000	-2.073958000
O	3.301513000	-1.579292000	1.959671000
H	3.018749000	-2.317387000	1.349035000
H	3.691880000	-0.884223000	1.388245000
O	-3.837730000	1.993065000	1.191011000
H	-3.657533000	1.843286000	0.234062000

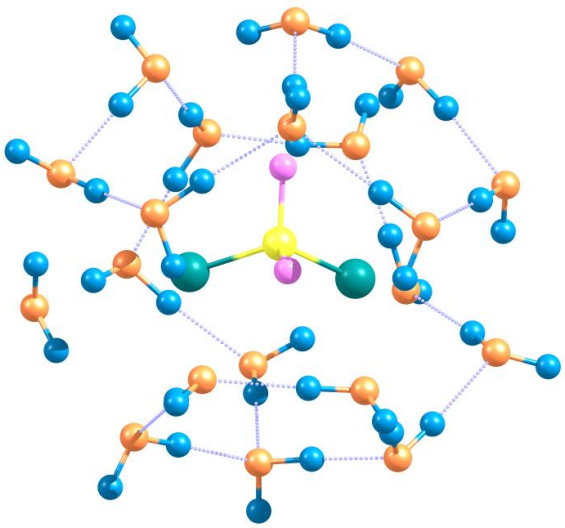


H	-3.997447000	1.105139000	1.558949000
O	0.309163000	-3.941098000	-2.321474000
H	0.974513000	-3.236087000	-2.510099000
H	0.644696000	-4.340582000	-1.500551000
O	2.768149000	2.726730000	1.450844000
H	2.030316000	2.391771000	2.062507000
H	3.313775000	3.293181000	2.017972000
O	-2.132141000	-3.206479000	-1.546127000
H	-1.226889000	-3.373315000	-1.946586000
H	-2.581179000	-4.061619000	-1.635060000
O	0.992762000	1.903809000	3.197552000
H	1.130773000	0.942427000	3.383701000
H	0.040540000	1.993292000	2.983771000
O	2.446568000	-2.227128000	-2.378383000
H	2.595590000	-1.225768000	-2.418896000
H	3.195325000	-2.608322000	-2.860899000
O	1.400029000	-0.804704000	3.622458000
H	1.746437000	-1.041842000	4.496357000
H	2.114063000	-1.105303000	2.972242000
O	2.192603000	4.244589000	-0.843720000
H	2.319838000	3.688869000	-0.041548000
H	1.417292000	4.790339000	-0.647744000
O	-3.929197000	-1.156457000	-2.124435000
H	-4.565094000	-1.442237000	-1.451384000
H	-3.185787000	-1.802495000	-2.021421000
O	-1.865181000	2.144940000	3.001434000
H	-2.113409000	2.858146000	3.609579000
H	-2.463009000	2.258049000	2.207387000
O	-1.410368000	2.773949000	-3.312121000
H	-2.017603000	2.323798000	-2.687979000

H	-1.517191000	2.284530000	-4.141465000
O	-0.381057000	-3.654875000	0.815400000
H	-0.625009000	-3.242905000	1.681684000
H	-1.066935000	-3.364222000	0.186627000
O	4.104628000	0.618918000	0.305826000
H	3.653921000	1.392617000	0.734790000
H	5.039460000	0.864624000	0.234240000
C	-0.400148000	0.235345000	-0.385797000
Cl	-1.797924000	-0.471637000	0.477382000
Cl	-0.459297000	-0.228966000	-2.115112000
Cl	-0.446156000	2.024947000	-0.223438000
Cl	1.088319000	-0.381956000	0.353693000

CF_2Cl_2 within 5^{12} clathrate hydrate

O	-1.98606200	-1.02345900	-3.29441500
H	-1.01790500	-1.30276900	-3.27917300
H	-2.30698200	-1.30278600	-4.16558100
O	2.40145300	2.19044500	-2.72047900
H	1.45100200	2.42566200	-2.62004000
H	2.82729100	2.44381100	-1.86643900
O	-3.39401200	-2.41353300	-1.31565900
H	-2.90459000	-1.90866100	-2.00856500
H	-2.71200200	-2.92943300	-0.83931500
O	3.55255300	2.79523200	-0.25052700
H	3.91777600	1.97310600	0.22550800
H	4.29645100	3.41542400	-0.28942900
O	0.48875000	-1.95434500	-3.32014500

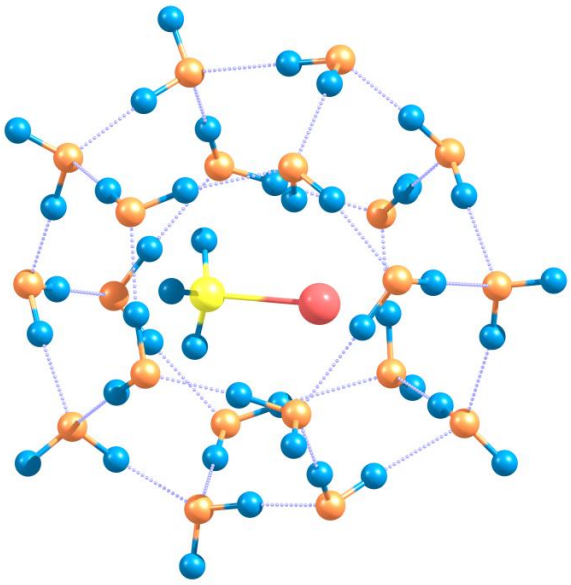


H	1.26111000	-1.34202300	-3.25174800
H	0.58581500	-2.58488300	-2.57867500
O	2.77054500	-0.38030600	-3.11845600
H	2.59949300	0.60757400	-2.96417900
H	3.27675300	-0.41844100	-3.94444800
O	0.68305900	-4.07957700	-1.39854900
H	-0.15244000	-4.15488100	-0.86273000
H	0.70190500	-4.84897700	-1.98720400
O	4.34232900	-1.31811100	-0.93557000
H	3.83510800	-0.97919800	-1.70613400
H	3.75779900	-1.99337300	-0.53530500
O	-1.57114600	-4.12871700	0.10099200
H	-2.08061900	-4.94072900	0.24295400
H	-1.39163700	-3.74661100	1.01315400
O	4.45078700	0.66277300	0.96420800
H	3.81434400	0.37194600	1.65652800
H	4.47730800	-0.07404300	0.29874300
O	-2.42449100	1.77229600	-3.09103600
H	-2.24415500	0.81012600	-3.17757800
H	-3.05791900	1.83504100	-2.32539200
O	-0.26949100	3.11863800	-2.55560700
H	-1.09343000	2.53656900	-2.73863100
H	-0.27199500	3.76305400	-3.28054700
O	-4.02587300	1.84246200	-0.88227200
H	-4.27954700	0.99422900	-0.46235700
H	-3.71874400	2.41705200	-0.12983100
O	-0.61583200	4.27028600	-0.11601400
H	-0.50028900	3.86318800	-1.01759900
H	-0.68442500	5.22528000	-0.26379400
O	-4.47036700	-0.69390200	0.40923900

H	-5.40228400	-0.94725400	0.49062400
H	-4.07722000	-1.33804100	-0.25567600
O	1.61674800	3.77954100	1.56803800
H	2.30470300	3.44395000	0.95240700
H	0.83300200	3.93361200	0.99884300
O	1.49308300	-2.66109700	2.70430200
H	1.82208700	-1.74182800	2.87387100
H	1.94263500	-2.92430900	1.87138900
O	-1.85989200	1.57917500	3.13112200
H	-2.25396900	0.66511200	3.00606900
H	-2.19754200	1.88190300	3.98782600
O	2.73100600	-3.38111600	0.27282400
H	2.03428300	-3.68747500	-0.35952000
H	3.34605500	-4.12330600	0.37340400
O	-2.97017700	3.31453700	1.15714200
H	-2.16201100	3.67775800	0.73641500
H	-2.62177100	2.70152400	1.84174300
O	-1.08062400	-3.03142200	2.48165000
H	-0.08602200	-2.81162100	2.55793500
H	-1.27714700	-3.55922500	3.27096300
O	-2.97784500	-0.83971700	2.79714900
H	-2.29069600	-1.51730600	2.63365900
H	-3.51771700	-0.80038500	1.97321600
O	2.61526700	-0.14644900	3.01153700
H	1.93866800	0.61133600	3.11743700
H	3.13539700	-0.11355200	3.82947500
O	0.98616900	1.85215500	3.37744400
H	0.02664800	1.68853500	3.25154600
H	1.21680400	2.58581400	2.74340000
C	-0.11628600	-0.37805300	0.38443100

Cl	-1.49472000	0.54596200	-0.20904300
Cl	1.43078900	0.28105000	-0.15815900
F	-0.21648200	-1.65668200	-0.04747000
F	-0.13933100	-0.40750500	1.72339200

CH_3Br within 5^{12} clathrate hydrate



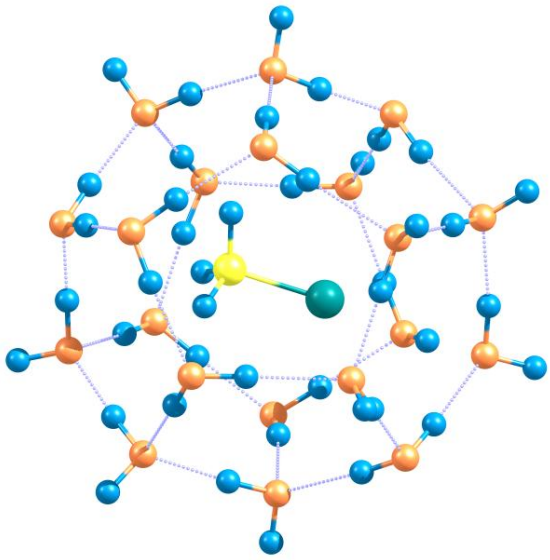
O	-4.110479000	-0.525289000	-0.063101000
H	-3.869064000	-0.368628000	-1.024868000
H	-3.665287000	-1.362099000	0.182354000
O	2.906064000	0.092000000	2.892245000
H	3.282394000	0.296777000	2.012870000
H	2.449260000	-0.770063000	2.757542000
O	-3.303471000	-0.062310000	-2.585361000
H	-2.865868000	0.821437000	-2.567858000
H	-2.593103000	-0.684827000	-2.860375000
O	3.888987000	0.723714000	0.189373000
H	3.816951000	-0.025525000	-0.450953000
H	4.825708000	0.971662000	0.210475000
O	-1.675172000	0.371724000	3.494764000
H	-2.304068000	0.771352000	2.856975000
H	-0.848555000	0.901057000	3.420545000
O	0.883778000	2.090918000	-2.754158000
H	1.434984000	2.408436000	-1.947374000
H	1.064356000	2.746993000	-3.445548000
O	-0.996997000	-2.177809000	2.921600000
H	-1.292194000	-1.264713000	3.190054000
H	-1.608818000	-2.454835000	2.207560000

O	1.473261000	-0.447058000	-3.339087000
H	1.261735000	0.510736000	-3.120221000
H	1.626691000	-0.466690000	-4.296611000
O	-2.044169000	3.400239000	0.301790000
H	-2.588879000	2.718613000	0.783326000
H	-2.540047000	4.229893000	0.372683000
O	-0.672551000	-3.632268000	-1.045127000
H	0.267206000	-3.469982000	-0.689523000
H	-0.663980000	-4.553655000	-1.346327000
O	0.675753000	3.901607000	1.119137000
H	-0.253166000	3.739443000	0.849701000
H	0.792826000	3.335757000	1.913117000
O	1.773588000	-3.344759000	-0.150207000
H	1.729237000	-3.008802000	0.781229000
H	2.271368000	-2.652068000	-0.632106000
O	-3.456822000	1.430554000	1.529690000
H	-3.702446000	0.672270000	0.888714000
H	-4.290547000	1.671642000	1.961702000
O	1.555411000	-2.341122000	2.404491000
H	1.806668000	-2.981840000	3.088177000
H	0.557414000	-2.211852000	2.548274000
O	-1.104897000	-1.785058000	-3.166480000
H	-0.977193000	-2.494159000	-2.501591000
H	-0.248696000	-1.311197000	-3.180737000
O	2.342071000	2.976301000	-0.815487000
H	2.842690000	2.237465000	-0.412929000
H	1.755068000	3.336302000	-0.091415000
O	3.357270000	-1.358267000	-1.592591000
H	4.041313000	-1.827303000	-2.094688000
H	2.704447000	-1.020718000	-2.265326000

O	-1.919748000	2.363117000	-2.334705000
H	-0.951944000	2.263595000	-2.460745000
H	-2.012229000	2.808485000	-1.466316000
O	0.722838000	1.682643000	2.817674000
H	1.563921000	1.215703000	3.085667000
H	0.613999000	1.311058000	1.922533000
O	-2.636244000	-2.907047000	0.717117000
H	-1.952782000	-3.220850000	0.067219000
H	-3.205709000	-3.670911000	0.893867000
C	-1.075465000	-0.168904000	-0.171174000
Br	0.886972000	-0.033836000	-0.052720000
H	-1.426027000	0.782695000	-0.555487000
H	-1.288275000	-0.961731000	-0.878027000
H	-1.418360000	-0.385860000	0.834053000

CH_3Cl within 5^{12} clathrate hydrate

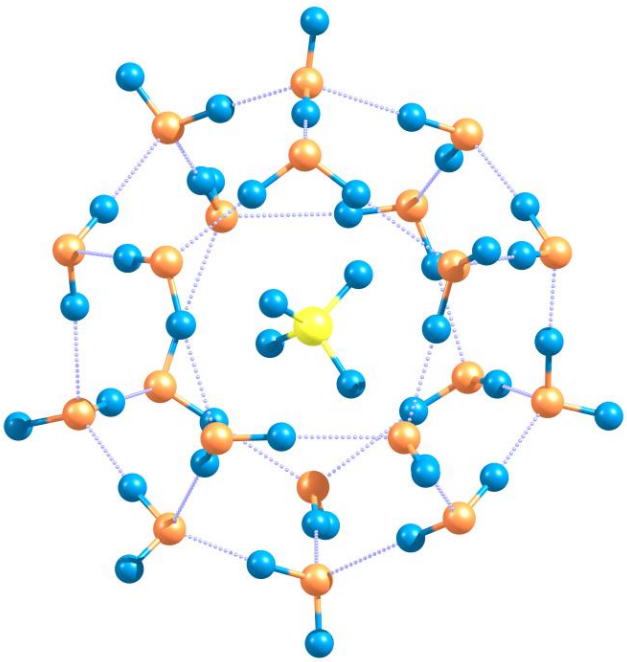
O	-3.954632000	0.203912000	-0.636027000
H	-3.532072000	0.548838000	-1.479662000
H	-3.672031000	-0.731674000	-0.562713000
O	2.419150000	-1.169587000	2.975045000
H	2.866508000	-0.760982000	2.209300000
H	1.852671000	-1.868749000	2.578236000
O	-2.697172000	1.126391000	-2.815714000
H	-2.138334000	1.891978000	-2.546600000
H	-2.056441000	0.461693000	-3.161292000
O	3.952254000	0.010963000	0.699063000
H	3.805257000	-0.571812000	-0.085669000
H	4.872545000	-0.126106000	0.969106000



O	-1.984683000	-0.293661000	3.212141000
H	-2.445886000	0.370937000	2.663167000
H	-1.082429000	0.084374000	3.403184000
O	1.777211000	2.574154000	-2.087520000
H	2.255494000	2.582690000	-1.186624000
H	2.145946000	3.326342000	-2.575755000
O	-1.735495000	-2.755271000	2.168540000
H	-1.872156000	-1.865526000	2.602154000
H	-2.227791000	-2.701611000	1.323043000
O	1.961051000	0.140894000	-3.202646000
H	1.895157000	1.052386000	-2.791942000
H	2.247408000	0.285265000	-4.117478000
O	-1.549292000	3.511932000	0.931561000
H	-2.237918000	2.814622000	1.151214000
H	-1.990730000	4.366391000	1.049517000
O	-0.976747000	-3.112512000	-2.041558000
H	-0.089605000	-3.232165000	-1.551301000
H	-1.060069000	-3.898955000	-2.602051000
O	0.942411000	3.071811000	2.020187000
H	0.043138000	3.260107000	1.652006000
H	1.050901000	3.667628000	2.776322000
O	1.299987000	-3.483279000	-0.827292000
H	1.147179000	-3.421077000	0.151844000
H	1.947416000	-2.774249000	-1.024814000
O	-3.317116000	1.582927000	1.457260000
H	-3.559841000	1.039623000	0.619918000
H	-4.166201000	1.822192000	1.858794000
O	0.806780000	-3.209871000	1.843614000
H	0.936850000	-4.009659000	2.375785000
H	-0.182756000	-2.988330000	1.956080000

O	-0.765178000	-0.757975000	-3.618347000
H	-0.850587000	-1.602755000	-3.128094000
H	0.137910000	-0.443260000	-3.413556000
O	3.036477000	2.662530000	0.199973000
H	3.380682000	1.764197000	0.403383000
H	2.331884000	2.819422000	0.870491000
O	3.319421000	-1.527937000	-1.528793000
H	3.983002000	-1.991467000	-2.062014000
H	2.844180000	-0.918154000	-2.155470000
O	-1.017634000	3.164354000	-1.858355000
H	-0.065882000	2.933812000	-1.905378000
H	-1.192459000	3.334615000	-0.910463000
O	0.501786000	0.722292000	3.658340000
H	1.191726000	0.032751000	3.484565000
H	0.685153000	1.417925000	2.998003000
O	-3.038242000	-2.515304000	-0.358569000
H	-2.324146000	-2.783722000	-0.995794000
H	-3.757334000	-3.153470000	-0.479005000
C	-0.859126000	0.030936000	-0.174088000
H	-1.127987000	1.037281000	-0.481450000
H	-1.078437000	-0.661641000	-0.980823000
H	-1.332420000	-0.259780000	0.759989000
Cl	0.925563000	0.005315000	0.109361000

CH_4 within 5^{12} clathrate hydrate

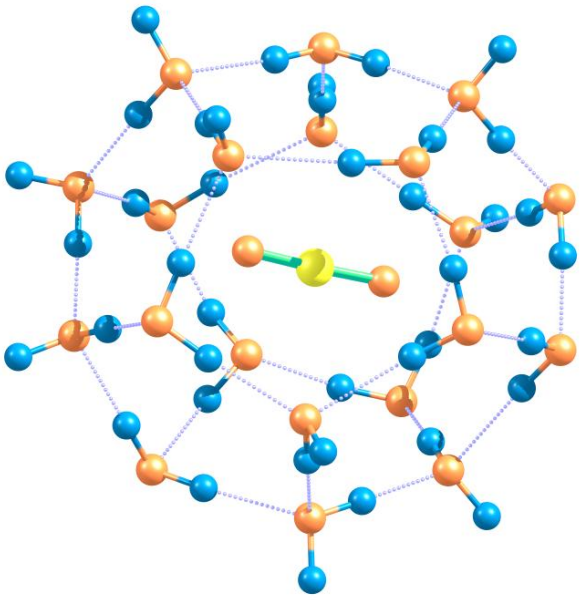


O	-1.721426000	2.697216000	-2.144278000
H	-0.912505000	2.378137000	-2.647768000
H	-2.285592000	1.902117000	-2.030152000
O	-0.627081000	-1.628749000	3.516898000
H	0.186981000	-1.862906000	3.030284000
H	-1.353159000	-1.803479000	2.876198000
O	0.447373000	1.793087000	-3.390179000
H	1.277088000	1.975498000	-2.886485000
H	0.444743000	0.821151000	-3.559645000
O	1.814914000	-2.504504000	2.235067000
H	1.575745000	-3.001603000	1.413179000
H	2.104059000	-3.167670000	2.879609000
O	-2.468178000	2.042408000	2.108075000
H	-1.980317000	2.567958000	1.441226000
H	-1.776371000	1.728942000	2.750430000
O	3.751264000	-0.236567000	-0.898014000
H	3.649569000	-0.270352000	0.116693000
H	4.703058000	-0.154209000	-1.061956000
O	-3.797152000	0.013626000	0.984378000
H	-3.338620000	0.783705000	1.434532000
H	-3.680300000	0.179310000	0.024739000
O	2.375934000	-2.225051000	-1.998234000
H	2.939613000	-1.491772000	-1.609001000
H	2.878993000	-2.592808000	-2.740254000
O	1.539314000	3.493024000	0.522169000
H	0.543119000	3.566216000	0.374968000
H	1.878670000	4.400444000	0.503072000
O	-2.121152000	-1.814387000	-2.667429000

H	-1.937400000	-2.411650000	-1.867421000
H	-2.577335000	-2.378409000	-3.310064000
O	2.071938000	1.830008000	2.588082000
H	1.888359000	2.490517000	1.867305000
H	2.418057000	2.337045000	3.337643000
O	-1.659123000	-3.366415000	-0.615095000
H	-2.045415000	-2.971383000	0.211612000
H	-0.702770000	-3.470070000	-0.429570000
O	-1.067363000	3.592336000	0.153287000
H	-1.319437000	3.207348000	-0.776826000
H	-1.489442000	4.464532000	0.184191000
O	-2.630985000	-2.183526000	1.628504000
H	-3.329958000	-2.680710000	2.080480000
H	-3.074936000	-1.290169000	1.368923000
O	0.392220000	-0.979041000	-3.692958000
H	-0.493671000	-1.244824000	-3.366221000
H	1.012261000	-1.332846000	-3.026668000
O	3.496336000	-0.351939000	1.679976000
H	2.929984000	-1.117033000	1.929638000
H	3.029939000	0.443332000	2.033536000
O	1.142164000	-3.713675000	-0.135755000
H	1.350440000	-4.648755000	-0.283016000
H	1.623562000	-3.208967000	-0.849584000
O	2.670421000	2.265099000	-1.798616000
H	3.000578000	1.395164000	-1.495437000
H	2.270293000	2.668771000	-1.000881000
O	-0.494755000	1.115247000	3.738855000
H	-0.571531000	0.127262000	3.736302000
H	0.354886000	1.294489000	3.292084000
O	-3.366108000	0.426624000	-1.783361000

H	-2.942501000	-0.394856000	-2.149688000
H	-4.188104000	0.548389000	-2.281509000
C	-0.004472000	0.010745000	0.022634000
H	0.980282000	-0.094505000	0.486907000
H	0.087081000	0.573873000	-0.910145000
H	-0.415301000	-0.980410000	-0.188852000
H	-0.674316000	0.532143000	0.710804000

CO_2 within 5^{12} clathrate hydrate



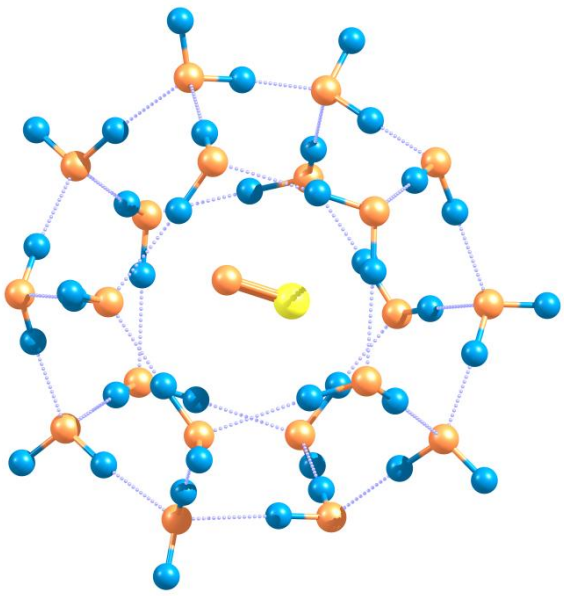
O	-2.360130000	0.572211000	-3.037786000
H	-1.374549000	0.423275000	-3.071131000
H	-2.693648000	-0.232275000	-2.582517000
O	-0.422532000	-0.157880000	3.822404000
H	0.495277000	-0.206095000	3.489464000
H	-0.914347000	-0.848566000	3.323084000
O	0.267839000	0.185282000	-2.714625000
H	0.891419000	0.934806000	-2.883841000
H	0.720497000	-0.641317000	-3.012329000
O	2.348458000	-0.364991000	3.008987000
H	2.456406000	-1.175186000	2.451996000
H	2.794411000	-0.552203000	3.848654000
O	-3.598617000	1.503073000	1.126764000
H	-3.221053000	1.807166000	0.276945000
H	-2.896606000	1.732584000	1.790182000
O	3.714663000	1.069702000	-0.870939000
H	3.475716000	1.369559000	0.074687000
H	4.592228000	1.445674000	-1.040042000
O	-3.747512000	-1.175510000	1.010805000

H	-3.734429000	-0.172658000	1.070435000
H	-3.563802000	-1.371732000	0.068038000
O	3.473543000	-1.604691000	-1.028742000
H	3.537588000	-0.604785000	-0.997046000
H	4.305739000	-1.908099000	-1.422118000
O	-0.126653000	3.686383000	-1.182094000
H	-1.031408000	3.251059000	-1.286363000
H	-0.227133000	4.586876000	-1.525352000
O	-0.793017000	-3.311878000	-1.670877000
H	-0.502060000	-3.372523000	-0.699355000
H	-0.926488000	-4.232435000	-1.944856000
O	0.726622000	3.241047000	1.340715000
H	0.415899000	3.488757000	0.429386000
H	0.647594000	4.042256000	1.880397000
O	-0.052439000	-3.507995000	0.818931000
H	-0.694580000	-3.036621000	1.412675000
H	0.829836000	-3.127981000	1.013092000
O	-2.507138000	2.533411000	-1.369536000
H	-2.463888000	1.735013000	-2.019043000
H	-3.221212000	3.093600000	-1.710744000
O	-1.788082000	-2.121197000	2.375169000
H	-2.236962000	-2.672450000	3.034537000
H	-2.555769000	-1.709177000	1.818375000
O	1.475406000	-2.255411000	-3.027166000
H	0.711578000	-2.680373000	-2.579237000
H	2.115438000	-2.072817000	-2.310045000
O	3.150368000	1.886407000	1.537084000
H	2.899573000	1.108792000	2.085361000
H	2.318300000	2.410544000	1.468854000
O	2.582076000	-2.544365000	1.342968000

H	3.117237000	-3.319800000	1.570260000
H	2.939158000	-2.207643000	0.474769000
O	1.925970000	2.354574000	-2.694641000
H	2.533120000	1.957121000	-2.034372000
H	1.267055000	2.851078000	-2.166256000
O	-1.515900000	2.148769000	2.801773000
H	-1.170158000	1.344963000	3.265641000
H	-0.779123000	2.411719000	2.218466000
O	-3.098478000	-1.815101000	-1.702147000
H	-2.264318000	-2.353651000	-1.713825000
H	-3.759947000	-2.344499000	-2.172004000
C	-0.001388000	-0.075767000	0.017016000
O	1.152506000	-0.153913000	0.202897000
O	-1.159985000	-0.005096000	-0.089560000

CO within 5^{12} clathrate hydrate

O	-1.856366000	2.748389000	-1.847231000
H	-1.165747000	2.374381000	-2.476751000
H	-2.479297000	2.012428000	-1.662666000
O	-0.174283000	-1.592024000	3.640379000
H	0.544057000	-1.876688000	3.042261000
H	-0.993255000	-1.705169000	3.106273000
O	0.011058000	1.723538000	-3.420397000
H	0.919727000	1.853147000	-3.055600000
H	-0.086817000	0.752055000	-3.557537000
O	1.965999000	-2.597612000	1.979714000



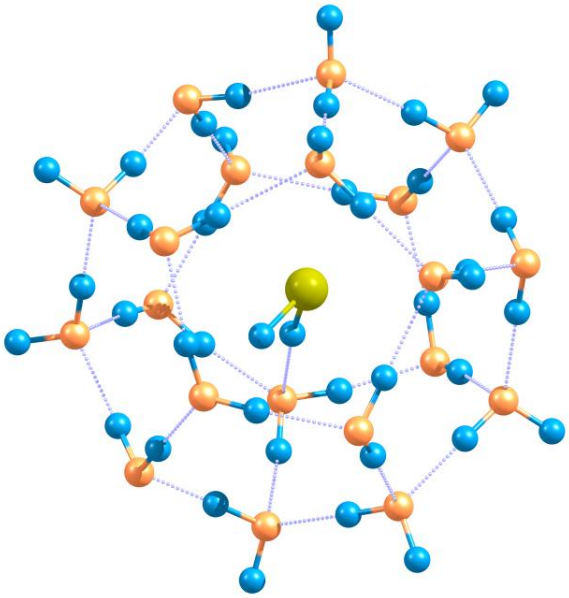
H	1.564945000	-3.084074000	1.216548000
H	2.330500000	-3.274415000	2.569675000
O	-1.980360000	2.206334000	2.462857000
H	-1.553331000	2.672999000	1.715799000
H	-1.227304000	1.829544000	2.991786000
O	3.511389000	-0.509155000	-1.431174000
H	3.584448000	-0.531286000	-0.409945000
H	4.425465000	-0.494138000	-1.753647000
O	-3.562455000	0.272514000	1.542739000
H	-2.999093000	1.018550000	1.911290000
H	-3.614122000	0.434989000	0.576834000
O	1.868159000	-2.399506000	-2.285578000
H	2.528016000	-1.699135000	-1.992991000
H	2.235249000	-2.803574000	-3.086170000
O	1.839624000	3.394059000	0.222915000
H	0.839332000	3.525861000	0.236182000
H	2.226419000	4.279865000	0.155862000
O	-2.688091000	-1.694061000	-2.267623000
H	-2.406673000	-2.285625000	-1.491067000
H	-3.271456000	-2.245782000	-2.810418000
O	2.539973000	1.667173000	2.185550000
H	2.309469000	2.346379000	1.497173000
H	2.991550000	2.146191000	2.896558000
O	-1.975615000	-3.256966000	-0.300210000
H	-2.191666000	-2.823465000	0.567719000
H	-1.006550000	-3.395699000	-0.275803000
O	-0.783244000	3.618658000	0.287288000
H	-1.216653000	3.250643000	-0.582078000
H	-1.155729000	4.506842000	0.397934000
O	-2.446826000	-1.974996000	2.044540000

H	-3.099644000	-2.417896000	2.608430000
H	-2.871589000	-1.057718000	1.831453000
O	-0.295977000	-1.034087000	-3.617135000
H	-1.144242000	-1.253574000	-3.174753000
H	0.393592000	-1.464855000	-3.076961000
O	3.727895000	-0.596340000	1.144539000
H	3.136892000	-1.308902000	1.477761000
H	3.357868000	0.234210000	1.529630000
O	0.843198000	-3.768167000	-0.229411000
H	0.927525000	-4.722558000	-0.375576000
H	1.255562000	-3.327179000	-1.024218000
O	2.487611000	2.049655000	-2.212971000
H	2.798143000	1.164487000	-1.933967000
H	2.263111000	2.506935000	-1.376604000
O	0.171058000	1.138472000	3.758593000
H	0.030226000	0.159232000	3.811074000
H	0.923578000	1.242236000	3.144669000
O	-3.642433000	0.644709000	-1.261162000
H	-3.318741000	-0.206048000	-1.659983000
H	-4.526900000	0.794414000	-1.626995000
C	-0.451616000	0.100220000	-0.420250000
O	0.621290000	0.243297000	-0.066182000

H_2S within 5^{12} clathrate hydrate

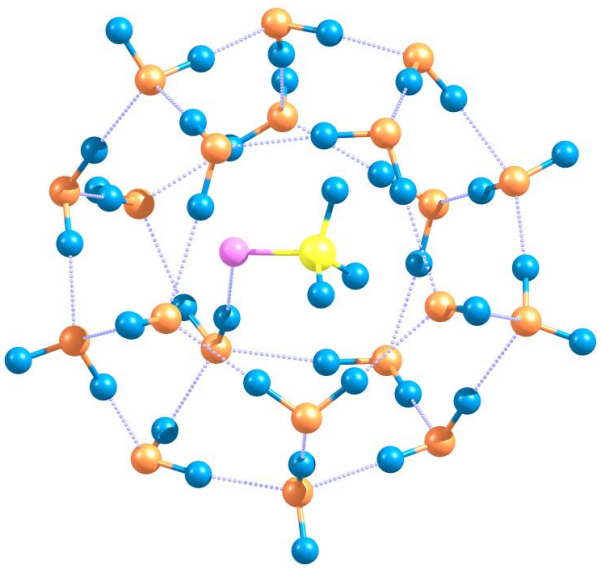
O	1.658986000	2.950816000	2.063290000
H	1.029459000	2.368540000	2.568120000
H	2.331286000	2.322753000	1.716143000

O	0.257562000	-1.063971000	-3.634706000
H	-0.369919000	-1.579111000	-3.089431000
H	1.119236000	-1.134733000	-3.166503000
O	-0.094243000	1.214560000	3.101167000
H	-1.078056000	1.301396000	3.020273000
H	0.105900000	0.301763000	3.429409000
O	-1.625644000	-2.670145000	-2.165994000
H	-1.129855000	-3.119093000	-1.436131000
H	-1.893644000	-3.370052000	-2.779931000
O	1.287519000	2.238784000	-1.847094000
H	0.964052000	2.981424000	-1.295873000
H	0.618783000	2.088892000	-2.578278000
O	-3.388507000	-1.123514000	1.438422000
H	-3.447829000	-1.057563000	0.417495000
H	-4.293775000	-1.311885000	1.730074000
O	3.658788000	0.972197000	-1.621218000
H	2.875865000	1.550903000	-1.808140000
H	3.716551000	0.990504000	-0.640947000
O	-1.474525000	-2.838788000	2.142889000
H	-2.209331000	-2.201904000	1.892211000
H	-1.844159000	-3.417050000	2.827048000
O	-2.285636000	3.157966000	0.206941000
H	-1.329099000	3.458670000	0.200533000
H	-2.808317000	3.956398000	0.375326000
O	2.883989000	-1.451157000	2.002703000
H	2.683295000	-2.005488000	1.170515000
H	3.581243000	-1.944238000	2.461974000
O	-2.915559000	1.576146000	-1.948068000
H	-2.672447000	2.149338000	-1.176352000
H	-3.608026000	2.057552000	-2.425286000



O	2.449703000	-2.957374000	-0.085656000
H	2.582268000	-2.400431000	-0.894812000
H	1.492913000	-3.171061000	-0.094267000
O	0.274104000	3.937515000	0.130914000
H	0.829542000	3.533042000	0.900111000
H	0.466341000	4.887086000	0.154298000
O	2.740026000	-1.373047000	-2.311732000
H	3.377847000	-1.692469000	-2.968085000
H	3.095345000	-0.460714000	-2.028081000
O	0.550467000	-1.397081000	3.614788000
H	1.366134000	-1.424723000	3.066949000
H	-0.118039000	-1.866547000	3.076729000
O	-3.630105000	-0.999295000	-1.139684000
H	-2.936165000	-1.580510000	-1.526667000
H	-3.372221000	-0.089642000	-1.420519000
O	-0.282345000	-3.837573000	-0.072450000
H	-0.242106000	-4.800768000	0.026314000
H	-0.715131000	-3.494613000	0.756072000
O	-2.744808000	1.457534000	2.472798000
H	-2.951796000	0.573558000	2.101338000
H	-2.589916000	2.019521000	1.684930000
O	-0.568944000	1.553983000	-3.636414000
H	-0.283762000	0.607031000	-3.727094000
H	-1.376102000	1.509411000	-3.084721000
O	3.574018000	1.048238000	1.203319000
H	3.308888000	0.140452000	1.518863000
H	4.408552000	1.247174000	1.653848000
S	-0.112730000	-0.149640000	-0.022286000
H	-0.005423000	0.484021000	1.177921000
H	0.526526000	0.821061000	-0.742506000

CH_3F within 5^{12} clathrate hydrate



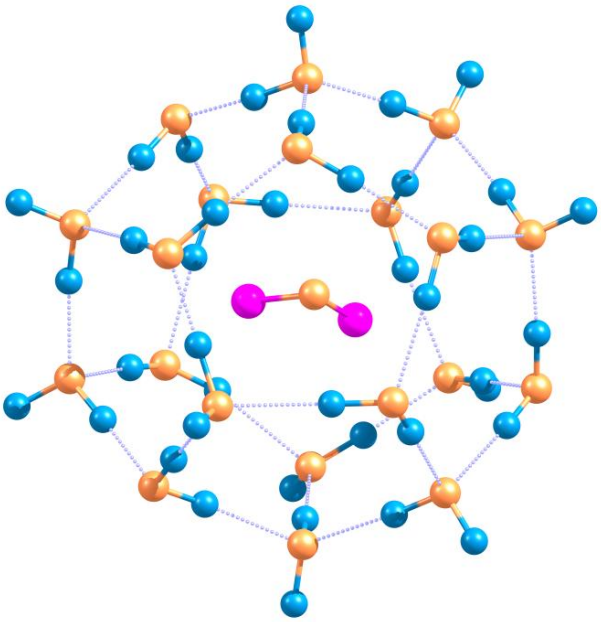
O	-0.949519000	2.464052000	2.666180000
H	-0.895165000	1.591117000	3.158880000
H	-0.045476000	2.618128000	2.316988000
O	0.513924000	0.135019000	-3.677919000
H	0.554052000	-0.756022000	-3.276515000
H	1.220391000	0.643028000	-3.218886000
O	-0.728605000	0.075608000	3.815906000
H	-1.420543000	-0.528954000	3.445601000
H	0.124084000	-0.312699000	3.528628000
O	0.675704000	-2.501169000	-2.592211000
H	1.432335000	-2.533037000	-1.943051000
H	0.951047000	-3.042019000	-3.347527000
O	-1.357777000	3.288883000	-1.506948000
H	-1.875553000	3.059452000	-0.709088000
H	-1.608218000	2.603440000	-2.183529000
O	-1.121981000	-3.482394000	1.108081000
H	-1.380153000	-3.361217000	0.138904000
H	-1.504445000	-4.334323000	1.369126000
O	1.300502000	3.444154000	-1.081589000
H	0.318262000	3.432058000	-1.260718000
H	1.392920000	3.304512000	-0.115715000
O	1.644248000	-3.443950000	1.441151000
H	0.666519000	-3.527672000	1.329928000
H	1.747309000	-2.673121000	2.046181000
O	-3.916921000	0.138818000	0.623452000
H	-3.540371000	1.065648000	0.734121000

H	-4.813130000	0.167307000	0.991261000
O	3.506940000	0.941461000	1.867967000
H	3.662793000	0.563786000	0.926515000
H	4.388683000	1.130860000	2.222332000
O	-3.363060000	-0.882632000	-1.834039000
H	-3.665509000	-0.501975000	-0.968809000
H	-4.158448000	-0.989150000	-2.377242000
O	3.887495000	-0.038037000	-0.496792000
H	3.415927000	0.532060000	-1.157215000
H	3.450154000	-0.915710000	-0.572618000
O	-2.775711000	2.518648000	0.870713000
H	-2.034210000	2.487860000	1.587870000
H	-3.332078000	3.273849000	1.115994000
O	2.518735000	1.513805000	-2.296162000
H	3.086235000	1.973418000	-2.933818000
H	2.018414000	2.261593000	-1.809325000
O	1.610471000	-0.911185000	2.521589000
H	2.411629000	-0.340987000	2.584923000
H	1.289689000	-0.688890000	1.625533000
O	-1.754795000	-3.145255000	-1.422016000
H	-0.921256000	-2.942178000	-1.906407000
H	-2.359321000	-2.390217000	-1.601008000
O	2.688403000	-2.593754000	-0.787067000
H	3.399995000	-3.225614000	-0.973683000
H	2.268483000	-2.923354000	0.083054000
O	-2.560208000	-1.520630000	2.545376000
H	-2.058901000	-2.207878000	2.054226000
H	-3.002779000	-0.981087000	1.860051000
O	-1.937220000	1.262404000	-3.221732000
H	-1.056214000	0.874396000	-3.463671000

H	-2.402347000	0.538821000	-2.760426000
O	1.659127000	2.929254000	1.674370000
H	2.353074000	2.222694000	1.769988000
H	2.016120000	3.711078000	2.121759000
C	-0.436664000	0.112305000	-0.162556000
H	-0.927832000	-0.740943000	-0.631297000
H	-0.556690000	1.014107000	-0.762307000
H	-0.810385000	0.263418000	0.852677000
F	0.944766000	-0.181578000	-0.073647000

N_2O within 5^{12} clathrate hydrate

O	-2.035317000	2.549271000	-1.930079000
H	-1.535128000	2.018568000	-2.628162000
H	-2.644782000	1.918237000	-1.491321000
O	0.599131000	-0.927662000	3.694303000
H	1.154254000	-1.429817000	3.065657000
H	-0.326043000	-1.104808000	3.412637000
O	-0.677616000	1.145688000	-3.714093000
H	0.287606000	1.216083000	-3.516195000
H	-0.890064000	0.187133000	-3.618968000
O	2.235941000	-2.469229000	1.894702000
H	1.624345000	-2.980079000	1.306177000
H	2.667806000	-3.122205000	2.465944000
O	-1.231082000	2.781310000	2.339112000
H	-0.964237000	3.099787000	1.452058000
H	-0.391832000	2.447611000	2.753498000
O	3.184010000	-1.065446000	-2.064726000
H	3.469353000	-0.939397000	-1.093677000

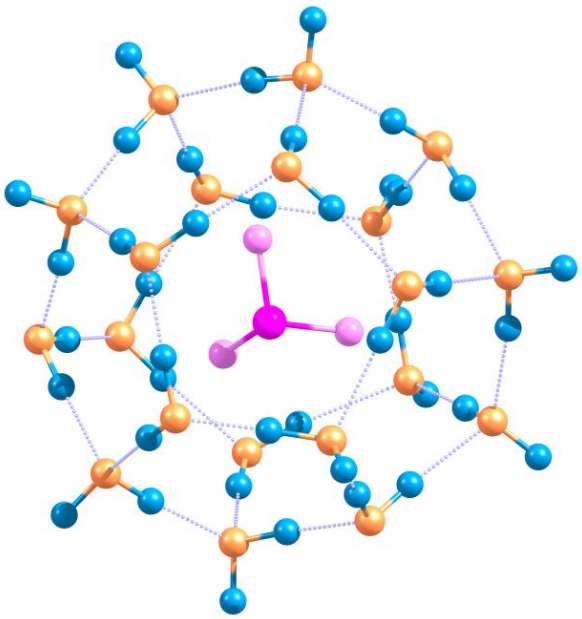


H	4.003114000	-1.206309000	-2.562980000
O	-3.021044000	0.824337000	2.104270000
H	-2.379849000	1.588810000	2.217633000
H	-3.345661000	0.867526000	1.180043000
O	1.164801000	-2.782692000	-2.198014000
H	1.956685000	-2.168313000	-2.191841000
H	1.178876000	-3.255492000	-3.043434000
O	2.067663000	3.139272000	-0.769218000
H	1.103290000	3.371000000	-0.584907000
H	2.471871000	3.941617000	-1.132080000
O	-3.302295000	-1.752280000	-1.350041000
H	-2.876000000	-2.249215000	-0.574083000
H	-4.009322000	-2.333631000	-1.668385000
O	3.163221000	1.752664000	1.282225000
H	2.798280000	2.304366000	0.539696000
H	3.849851000	2.291658000	1.703287000
O	-2.221208000	-3.084707000	0.628376000
H	-2.202107000	-2.520800000	1.444042000
H	-1.278821000	-3.287796000	0.451755000
O	-0.468458000	3.642914000	-0.260707000
H	-1.097770000	3.163602000	-0.939267000
H	-0.737090000	4.573918000	-0.293793000
O	-2.016903000	-1.435277000	2.793083000
H	-2.542190000	-1.700160000	3.563832000
H	-2.410019000	-0.529338000	2.509005000
O	-1.197907000	-1.557408000	-3.245681000
H	-1.955278000	-1.596194000	-2.623263000
H	-0.422773000	-1.804577000	-2.706304000
O	3.920046000	-0.780884000	0.413637000
H	3.359132000	-1.375296000	0.961163000

H	3.694423000	0.128773000	0.721015000
O	0.523380000	-3.772416000	0.189972000
H	0.541990000	-4.741159000	0.161857000
H	0.772240000	-3.466734000	-0.727923000
O	2.007288000	1.369230000	-3.011257000
H	2.369876000	0.520400000	-2.686307000
H	2.007274000	1.950396000	-2.223652000
O	1.099552000	1.754373000	3.326588000
H	0.930981000	0.804026000	3.546695000
H	1.789981000	1.727976000	2.636381000
O	-3.829741000	0.799757000	-0.600685000
H	-3.700412000	-0.139347000	-0.900168000
H	-4.750122000	1.025380000	-0.801792000
O	-0.118598000	0.319007000	0.806972000
N	0.853069000	-0.088880000	0.046332000
N	-0.900304000	-0.024661000	-0.148300000

NF_3 within 5^{12} clathrate hydrate

O	-3.255362000	-2.160379000	-0.345498000
H	-2.862167000	-2.128945000	-1.271768000
H	-2.576564000	-2.601480000	0.208325000
O	1.833461000	1.868965000	2.756606000
H	2.258869000	1.972784000	1.883757000
H	1.822978000	0.899288000	2.921596000
O	-2.143804000	-1.970596000	-2.752925000
H	-2.096293000	-1.007636000	-2.965088000
H	-1.210005000	-2.285641000	-2.773889000
O	3.195363000	2.314241000	0.257203000



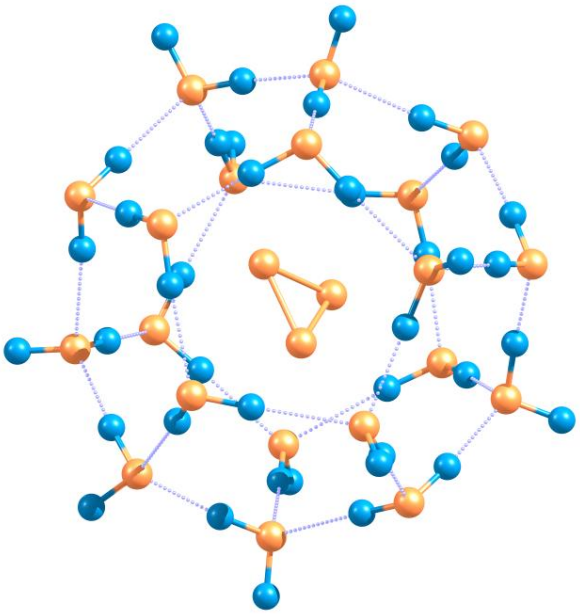
H	3.556411000	1.457472000	-0.080275000
H	3.959414000	2.858275000	0.499234000
O	-2.199395000	0.453618000	3.045084000
H	-2.662579000	0.364481000	2.187575000
H	-1.698679000	1.310401000	2.982017000
O	0.803871000	1.545473000	-3.115758000
H	0.951104000	2.269199000	-2.408876000
H	0.784677000	2.018005000	-3.962084000
O	-0.609381000	-1.645929000	3.451690000
H	-1.216690000	-0.852203000	3.349199000
H	-0.875317000	-2.260744000	2.735456000
O	2.414124000	-0.543605000	-2.850369000
H	1.829718000	0.260561000	-2.988652000
H	2.749797000	-0.787105000	-3.726423000
O	-3.135351000	2.189812000	-1.009616000
H	-3.378337000	1.435327000	-0.386101000
H	-3.974229000	2.539917000	-1.345153000
O	1.052650000	-3.711765000	-0.031520000
H	1.761985000	-3.098604000	0.359809000
H	1.456193000	-4.592930000	-0.028364000
O	-1.169411000	3.766753000	0.031524000
H	-1.934156000	3.257875000	-0.345617000
H	-1.483454000	4.673961000	0.160621000
O	2.915237000	-2.210321000	1.019981000
H	2.559914000	-1.760341000	1.830809000
H	3.236032000	-1.485539000	0.445036000
O	-3.662062000	0.173139000	0.605848000
H	-3.464722000	-0.758111000	0.192744000
H	-4.562490000	0.099181000	0.957368000
O	1.826038000	-0.903670000	3.138810000

H	2.231117000	-1.093583000	3.998911000
H	0.840850000	-1.190440000	3.245434000
O	0.553399000	-2.762608000	-2.661239000
H	0.687520000	-3.159111000	-1.774780000
H	1.113669000	-1.963099000	-2.644226000
O	1.206065000	3.420534000	-1.380373000
H	1.885604000	3.094219000	-0.749459000
H	0.384634000	3.565168000	-0.854133000
O	3.975813000	-0.151837000	-0.700795000
H	4.897153000	-0.386576000	-0.888362000
H	3.469835000	-0.307998000	-1.546211000
O	-1.924466000	0.771864000	-3.182107000
H	-0.973882000	0.970330000	-3.060252000
H	-2.363693000	1.239142000	-2.442266000
O	-0.771650000	2.758736000	2.740553000
H	0.178053000	2.484408000	2.794325000
H	-0.886721000	3.065613000	1.821237000
O	-1.284878000	-3.368505000	1.304869000
H	-0.440117000	-3.544907000	0.811113000
H	-1.594506000	-4.230668000	1.620506000
N	0.028176000	-0.090435000	0.440267000
F	-0.446813000	-1.056777000	-0.424252000
F	1.244769000	0.237706000	-0.159412000
F	-0.744653000	0.999265000	0.092475000

O_3 within 5^{12} clathrate hydrate

O	0.502192000	3.203562000	-2.088923000
H	0.882755000	2.435626000	-2.616387000

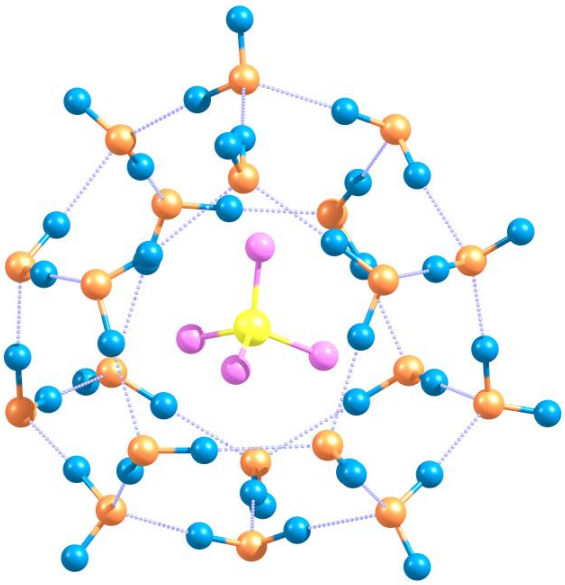
H	-0.438895000	2.967971000	-1.938923000
O	-1.409510000	-0.902108000	3.553055000
H	-0.998637000	-1.626413000	3.041675000
H	-2.087011000	-0.524142000	2.947424000
O	1.465895000	1.110375000	-3.405786000
H	2.218439000	0.677912000	-2.935894000
H	0.782921000	0.408550000	-3.516628000
O	-0.275064000	-3.152765000	2.160276000
H	-0.821496000	-3.319497000	1.351574000
H	-0.470117000	-3.877885000	2.772632000
O	-0.354679000	3.186470000	2.238931000
H	0.301201000	3.201252000	1.511815000
H	-0.055381000	2.439224000	2.820854000
O	2.505120000	-2.650942000	-1.035646000
H	2.461910000	-2.654922000	-0.013112000
H	3.259354000	-3.217027000	-1.260520000
O	-2.708342000	2.541414000	1.165187000
H	-1.843559000	2.812100000	1.602126000
H	-2.531860000	2.594627000	0.201607000
O	0.140376000	-3.224743000	-2.087700000
H	1.052808000	-3.034811000	-1.711023000
H	0.270961000	-3.857624000	-2.809681000
O	3.541812000	1.553463000	0.441516000
H	2.842769000	2.277205000	0.335520000
H	4.400278000	2.002183000	0.418883000
O	-2.943719000	0.150217000	-2.560362000
H	-3.183663000	-0.430959000	-1.762432000
H	-3.693384000	0.079228000	-3.170235000
O	2.858879000	-0.122874000	2.444420000
H	3.165441000	0.516377000	1.746374000



H	3.461154000	-0.010708000	3.195094000
O	-3.550311000	-1.348553000	-0.513364000
H	-3.508558000	-0.809655000	0.320864000
H	-2.904149000	-2.073018000	-0.382302000
O	1.636318000	3.337525000	0.183543000
H	1.172183000	3.258391000	-0.745132000
H	1.886068000	4.271298000	0.259402000
O	-3.289429000	0.121712000	1.753399000
H	-4.121564000	0.215781000	2.242373000
H	-3.020538000	1.093075000	1.516223000
O	-0.506432000	-0.849792000	-3.581510000
H	-1.368288000	-0.500685000	-3.270471000
H	-0.320057000	-1.624564000	-3.017603000
O	2.411337000	-2.701570000	1.549472000
H	1.479192000	-2.872604000	1.814563000
H	2.609968000	-1.796411000	1.889061000
O	-1.697500000	-3.498051000	-0.157180000
H	-2.189216000	-4.321553000	-0.297087000
H	-1.031480000	-3.445418000	-0.898875000
O	3.454070000	-0.092934000	-1.890914000
H	3.075736000	-0.940774000	-1.580638000
H	3.488704000	0.471310000	-1.091465000
O	0.523178000	1.043187000	3.686434000
H	-0.186207000	0.352825000	3.723786000
H	1.262958000	0.614705000	3.215321000
O	-2.216290000	2.591322000	-1.620119000
H	-2.498010000	1.717650000	-2.000968000
H	-2.754193000	3.261925000	-2.066935000
O	-0.174695000	0.104861000	0.748514000
O	0.685566000	0.307239000	-0.394014000

O	-0.604839000	-0.298335000	-0.569338000

CF_4 within 5^{12} clathrate hydrate

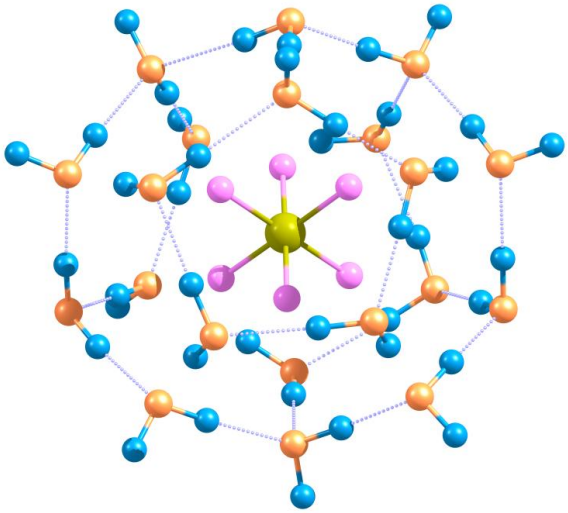


O	2.058661000	2.320708000	2.256780000
H	1.096492000	2.279448000	2.533009000
H	2.406635000	1.412472000	2.383083000
O	0.846166000	-2.438451000	-3.244719000
H	-0.104717000	-2.412711000	-3.026077000
H	1.285156000	-2.646236000	-2.389818000
O	-0.534905000	2.219427000	2.845382000
H	-1.131551000	2.632849000	2.177998000
H	-0.989704000	1.414897000	3.185288000
O	-2.000580000	-2.272104000	-2.493785000
H	-2.130453000	-2.579938000	-1.563428000
H	-2.580809000	-2.823486000	-3.039901000
O	3.431717000	0.788775000	-1.527601000
H	2.979165000	1.525774000	-1.069536000
H	2.833824000	0.558588000	-2.286897000
O	-3.639723000	1.032986000	-0.068007000
H	-3.310111000	0.767604000	-0.995664000
H	-4.491138000	1.471786000	-0.218186000
O	3.791021000	-1.340536000	0.052722000
H	3.709321000	-0.533871000	-0.538714000
H	3.586520000	-1.014930000	0.953767000
O	-3.555320000	-1.055834000	1.601811000
H	-3.625001000	-0.251713000	1.008109000
H	-4.425836000	-1.161919000	2.014009000

O	-0.114111000	3.826390000	-1.252421000
H	0.766143000	3.570067000	-0.836475000
H	-0.061540000	4.777898000	-1.426885000
O	0.734720000	-1.740099000	3.265914000
H	0.545285000	-2.348947000	2.477486000
H	0.803714000	-2.337059000	4.026820000
O	-0.667520000	1.960011000	-3.163764000
H	-0.450550000	2.687720000	-2.522896000
H	-0.635783000	2.357502000	-4.046644000
O	0.230067000	-3.371815000	1.278783000
H	0.900806000	-3.299732000	0.549489000
H	-0.633354000	-3.178563000	0.858630000
O	2.189869000	3.020445000	-0.205683000
H	2.113217000	2.719811000	0.780131000
H	2.926068000	3.651357000	-0.211494000
O	2.029107000	-3.052856000	-0.738851000
H	2.569909000	-3.842830000	-0.893586000
H	2.706240000	-2.342499000	-0.430321000
O	-1.649468000	-0.210192000	3.710018000
H	-0.834703000	-0.733499000	3.553933000
H	-2.266894000	-0.503098000	3.013596000
O	-2.836195000	0.394734000	-2.451475000
H	-2.509116000	-0.530933000	-2.520454000
H	-2.084949000	0.967774000	-2.735200000
O	-2.370021000	-3.000225000	0.144929000
H	-2.771426000	-3.853175000	0.370027000
H	-2.850924000	-2.316111000	0.688989000
O	-2.095340000	3.292664000	0.805015000
H	-2.562551000	2.495837000	0.481805000
H	-1.434901000	3.493901000	0.111378000

O	1.631667000	0.213886000	-3.500255000
H	1.361201000	-0.737866000	-3.482401000
H	0.820360000	0.719319000	-3.302730000
O	3.000527000	-0.350016000	2.632001000
H	2.196562000	-0.858355000	2.918845000
H	3.627429000	-0.399237000	3.368832000
C	-0.021657000	-0.013464000	0.013051000
F	1.150964000	-0.101706000	0.617085000
F	-0.050651000	-0.836880000	-1.029911000
F	-0.990363000	-0.360038000	0.861355000
F	-0.227820000	1.229704000	-0.400815000

SF_6 within 5^{12} clathrate hydrate



O	2.744978000	2.753857000	-1.260277000
H	1.914364000	3.276929000	-1.077409000
H	2.999292000	2.349227000	-0.403881000
O	-0.026437000	-4.130897000	0.558705000
H	-0.895872000	-3.706636000	0.677163000
H	0.583332000	-3.610691000	1.126950000
O	0.391066000	4.079959000	-0.749473000
H	-0.348818000	3.702889000	-1.276945000
H	0.097182000	3.971369000	0.183593000
O	-2.808430000	-2.716129000	0.989237000
H	-2.678831000	-2.053434000	1.709126000
H	-3.449499000	-3.356026000	1.333689000
O	3.137645000	-1.876085000	-1.770910000
H	2.854875000	-1.013112000	-2.131671000
H	2.356014000	-2.471938000	-1.889726000

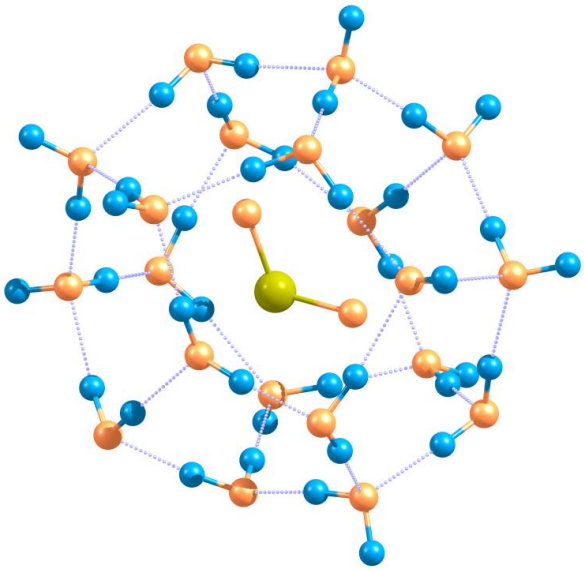
O	-3.833334000	1.288973000	-0.692404000
H	-3.804390000	0.307669000	-0.933226000
H	-4.690496000	1.608385000	-1.012127000
O	3.740926000	-1.539718000	0.860430000
H	3.563962000	-1.691434000	-0.111646000
H	3.760518000	-0.566848000	0.961332000
O	-3.110889000	1.728817000	1.899241000
H	-3.387509000	1.592952000	0.950690000
H	-3.819920000	2.253211000	2.300867000
O	-0.265826000	0.649242000	-3.656587000
H	0.703883000	0.696336000	-3.403567000
H	-0.314313000	0.998297000	-4.559414000
O	1.523025000	1.772175000	3.040340000
H	1.125583000	0.872476000	3.264034000
H	1.770520000	2.153484000	3.896569000
O	-1.507257000	-1.762884000	-3.043012000
H	-1.056624000	-0.920472000	-3.303429000
H	-1.703709000	-2.219731000	-3.874890000
O	0.475147000	-0.596606000	3.679967000
H	0.942402000	-1.327197000	3.202202000
H	-0.458595000	-0.659399000	3.395380000
O	2.317471000	0.768258000	-2.904481000
H	2.464388000	1.544173000	-2.254187000
H	2.979275000	0.903560000	-3.599842000
O	1.762364000	-2.602332000	2.233986000
H	2.212176000	-3.256008000	2.791322000
H	2.510778000	-2.182533000	1.686110000
O	-0.508132000	3.552370000	1.919598000
H	0.167605000	2.946309000	2.288724000
H	-1.314948000	3.009274000	1.866952000

O	-3.743059000	-1.303183000	-1.316271000
H	-3.453680000	-1.814862000	-0.527408000
H	-3.020265000	-1.452642000	-1.967799000
O	-2.405209000	-0.724481000	2.946468000
H	-2.860656000	-0.813313000	3.797485000
H	-2.672087000	0.167025000	2.595218000
O	-1.697641000	2.753791000	-2.213964000
H	-2.376672000	2.297165000	-1.680497000
H	-1.219669000	2.031131000	-2.667554000
O	0.826941000	-3.468685000	-2.041004000
H	0.553595000	-3.779258000	-1.143681000
H	0.071074000	-2.930550000	-2.341024000
O	3.563780000	1.420922000	1.186732000
H	2.872021000	1.571257000	1.880190000
H	4.363345000	1.859524000	1.514573000
S	-0.020791000	-0.008991000	0.015336000
F	-0.474310000	-1.373759000	0.715266000
F	-0.641491000	0.807887000	1.249327000
F	-1.436893000	0.068901000	-0.729297000
F	0.416490000	1.359598000	-0.666554000
F	1.380009000	-0.090512000	0.770472000
F	0.575751000	-0.830073000	-1.210123000

SO_2 within 5^{12} clathrate hydrate

O	-2.002336000	2.897931000	1.490533000
H	-2.276927000	2.133932000	2.084783000
H	-1.027703000	2.962475000	1.562701000
O	2.300907000	-0.673339000	-3.091097000

H	2.218935000	-1.479931000	-2.539522000
H	2.787140000	-0.029171000	-2.524811000
O	-2.581422000	0.795572000	3.027315000
H	-3.030372000	0.092840000	2.492081000
H	-1.650768000	0.492593000	3.087434000
O	1.836663000	-3.018308000	-1.522709000
H	2.221061000	-2.811403000	-0.634832000
H	2.308913000	-3.803813000	-1.837708000
O	-0.521023000	3.058493000	-2.568468000
H	-1.301572000	2.993798000	-1.977563000
H	-0.387066000	2.120461000	-2.833055000
O	-1.611811000	-3.280422000	1.209332000
H	-1.368093000	-3.303849000	0.222304000
H	-2.026206000	-4.139919000	1.381322000
O	1.761751000	3.209456000	-1.102113000
H	0.935605000	3.217207000	-1.661465000
H	1.442932000	3.299404000	-0.179315000
O	0.620537000	-2.674878000	2.505036000
H	-0.218278000	-2.944293000	2.016939000
H	0.549120000	-3.062875000	3.389854000
O	-3.892993000	0.072035000	-1.169238000
H	-3.478966000	0.977589000	-1.064417000
H	-4.823501000	0.231560000	-1.386581000
O	2.487634000	1.487893000	2.696098000
H	3.063705000	0.972828000	2.026902000
H	3.070083000	1.691771000	3.442429000
O	-2.245249000	-1.442646000	-2.733759000
H	-2.865246000	-0.925992000	-2.151782000
H	-2.740702000	-1.643490000	-3.541574000
O	3.972521000	0.132423000	1.040949000

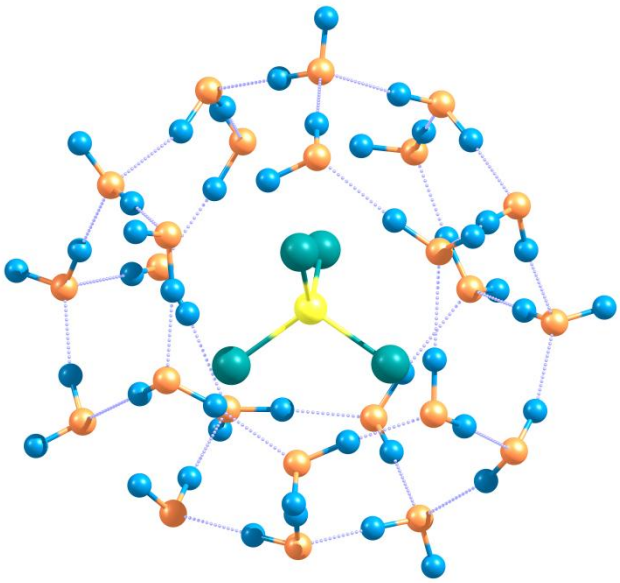


H	3.828206000	0.530010000	0.144938000
H	3.564469000	-0.756847000	0.977945000
O	-2.807445000	2.531711000	-0.916366000
H	-2.466944000	2.654290000	0.048319000
H	-3.442082000	3.254504000	-1.040090000
O	3.479095000	1.262364000	-1.433683000
H	4.222305000	1.734565000	-1.838994000
H	2.765110000	1.974720000	-1.308757000
O	0.099403000	0.097854000	2.703279000
H	0.952351000	0.553856000	2.873430000
H	0.310620000	-0.858124000	2.651773000
O	-0.949265000	-3.509674000	-1.316116000
H	0.005670000	-3.289077000	-1.399026000
H	-1.418989000	-2.803726000	-1.814634000
O	2.907130000	-2.578487000	1.004379000
H	3.504541000	-3.236067000	1.391548000
H	2.088974000	-2.596895000	1.564825000
O	-3.692604000	-1.214434000	1.443236000
H	-2.949967000	-1.847108000	1.366346000
H	-3.711012000	-0.778027000	0.567518000
O	-0.109618000	0.354764000	-2.651518000
H	0.770641000	-0.048727000	-2.923270000
H	-0.814800000	-0.305280000	-2.835736000
O	0.842671000	3.333633000	1.562841000
H	1.469821000	2.718012000	2.024631000
H	0.982321000	4.206465000	1.959545000
S	-0.021079000	0.238154000	-0.127200000
O	-1.236453000	-0.585012000	-0.065862000
O	1.251151000	-0.501767000	-0.080724000

Table S4. Cartesian coordinates for optimized geometries of the Greenhouse gases encapsulated within $5^{12}6^2$ clathrate hydrate computes at B3LYP/6-31G(d) level of theory and basis set.

CCl_4 within $5^{12}6^2$ clathrate hydrate

O	1.418021000	-2.280373000	-3.498446000
H	1.758496000	-1.338747000	-3.478324000
H	1.843261000	-2.683824000	-4.270496000
O	-1.825271000	2.158483000	-2.800106000
H	-2.178932000	1.243893000	-2.777066000
H	-2.185707000	2.608270000	-2.000260000
O	2.426094000	-3.374842000	-1.066894000
H	2.023664000	-3.018875000	-1.893839000
H	2.824252000	-2.607154000	-0.610329000
O	-2.777043000	3.523051000	-0.505328000
H	-1.927224000	3.791401000	-0.021887000
H	-3.209239000	4.362957000	-0.723623000
O	2.465989000	0.231243000	-3.399197000
H	1.818616000	0.973431000	-3.351014000
H	3.019629000	0.352170000	-2.602309000
O	0.794299000	2.527608000	-3.152439000
H	-0.175281000	2.329862000	-2.962577000
H	0.771500000	3.018791000	-3.988345000
O	4.318152000	0.631221000	-1.113185000
H	4.226057000	-0.156707000	-0.515016000
H	5.188715000	0.543519000	-1.530581000
O	1.595003000	4.310523000	-1.009331000
H	1.355507000	3.716828000	-1.755735000
H	2.334997000	3.862090000	-0.555938000



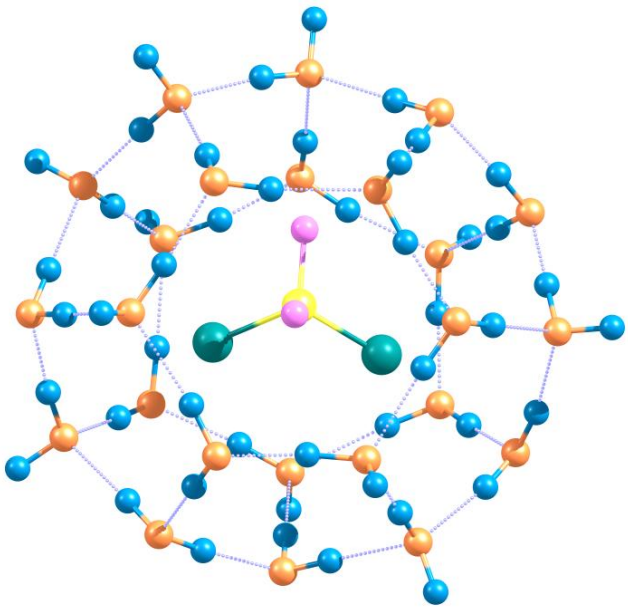
O	3.989014000	-1.545867000	0.497525000
H	4.695565000	-2.203424000	0.586088000
H	3.632699000	-1.403920000	1.423228000
O	-0.584925000	4.263412000	0.760764000
H	-0.367434000	3.617229000	1.467369000
H	0.198561000	4.289469000	0.157046000
O	-1.665255000	-2.692022000	-3.289480000
H	-0.716814000	-2.594358000	-3.500027000
H	-1.682093000	-3.187898000	-2.418401000
O	-3.102654000	-0.464578000	-2.869400000
H	-2.519514000	-1.277263000	-3.009096000
H	-3.671708000	-0.436072000	-3.653760000
O	-1.750459000	-3.923126000	-0.874195000
H	-0.913767000	-4.015775000	-0.375813000
H	-2.344014000	-3.453763000	-0.233775000
O	-4.496997000	-0.437920000	-0.467890000
H	-3.994250000	-0.447703000	-1.323454000
H	-5.352806000	-0.847028000	-0.665264000
O	0.664321000	-4.301289000	0.737900000
H	0.749466000	-5.266260000	0.702586000
H	1.316989000	-3.958351000	0.058733000
O	-4.047297000	1.775407000	1.356339000
H	-3.709455000	2.475987000	0.753877000
H	-4.340913000	1.060539000	0.754337000
O	2.538993000	1.458149000	2.944064000
H	1.593376000	1.745335000	2.982027000
H	2.894712000	1.890859000	2.140405000
O	-1.823463000	-1.793626000	3.383357000
H	-0.916908000	-2.198872000	3.376564000
H	-2.299578000	-2.257316000	4.088840000

O	3.668974000	2.773374000	0.525142000
H	3.991742000	2.063095000	-0.082406000
H	4.434424000	3.338964000	0.708437000
O	-3.276613000	-2.579962000	0.992212000
H	-3.634448000	-1.767240000	0.579096000
H	-2.737499000	-2.277475000	1.752712000
O	3.027346000	-1.143788000	2.994382000
H	2.748799000	-0.168744000	2.966990000
H	3.679813000	-1.183023000	3.711205000
O	0.675482000	-3.066231000	3.314298000
H	1.467032000	-2.492357000	3.322581000
H	0.715073000	-3.549802000	2.455602000
O	-0.064642000	2.507294000	3.005353000
H	-0.879581000	1.932940000	3.172449000
H	-0.079094000	3.149304000	3.732177000
O	-2.274137000	1.106441000	3.541624000
H	-2.107222000	0.142218000	3.470441000
H	-2.931411000	1.311266000	2.835903000
C	-0.049454000	0.054876000	0.006312000
Cl	0.464348000	-1.065738000	1.292534000
Cl	-0.178992000	-0.842121000	-1.515873000
Cl	1.150864000	1.364613000	-0.154780000
Cl	-1.627679000	0.739811000	0.437308000

CF_2Cl_2 within $5^{12}6^2$ clathrate hydrate

O	2.628862000	0.019175000	-3.050321000
H	2.113319000	0.882144000	-3.039847000
H	3.060450000	-0.003841000	-3.918005000

O	-2.974594000	0.285794000	-2.848806000
H	-2.463064000	-0.554543000	-2.842584000
H	-3.549999000	0.247101000	-2.047849000
O	4.522666000	-0.190835000	-0.976682000
H	3.869535000	-0.141261000	-1.715670000
H	4.305828000	0.574575000	-0.406199000
O	-4.559931000	0.179514000	-0.528345000
H	-4.269535000	0.952008000	0.070081000
H	-5.505470000	0.327057000	-0.683016000
O	1.356678000	2.372210000	-3.015073000
H	0.371729000	2.318323000	-3.015064000
H	1.582088000	2.792515000	-2.160643000
O	-1.454623000	2.435677000	-2.854687000
H	-1.996225000	1.578724000	-2.840407000
H	-1.847718000	2.957590000	-3.570948000
O	2.289868000	3.693318000	-0.637153000
H	2.907181000	3.094657000	-0.134804000
H	2.847128000	4.377686000	-1.037741000
O	-2.243908000	3.791203000	-0.503872000
H	-1.963942000	3.300977000	-1.309211000
H	-1.419350000	3.925341000	0.004208000
O	3.912359000	2.032663000	0.766647000
H	4.762174000	2.383122000	1.074522000
H	3.440410000	1.700543000	1.589918000
O	-3.821947000	2.152627000	1.012703000
H	-3.229493000	1.825586000	1.725564000
H	-3.268412000	2.778281000	0.473833000
O	0.964189000	-2.329405000	-3.078354000
H	1.464406000	-1.487390000	-3.044044000
H	1.367576000	-2.902237000	-2.360243000

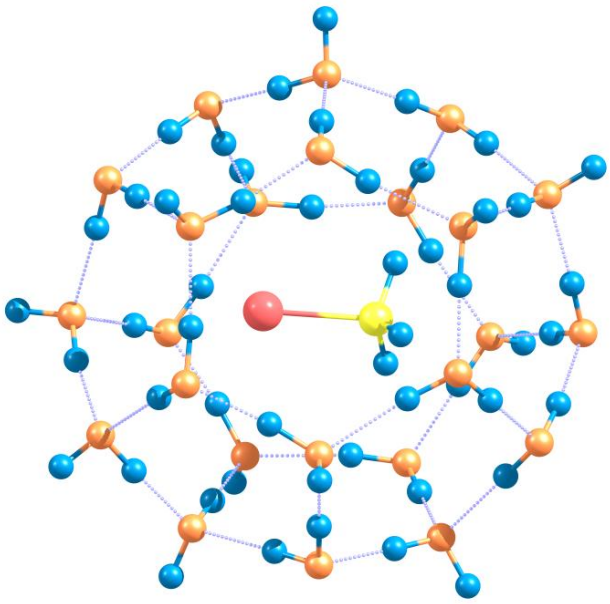


O	-1.609676000	-2.199719000	-2.898074000
H	-0.582195000	-2.191781000	-2.916706000
H	-1.854795000	-2.602154000	-3.745558000
O	2.010869000	-3.812015000	-1.103709000
H	2.636627000	-3.287932000	-0.564515000
H	1.277732000	-4.046197000	-0.475254000
O	-2.439483000	-3.610752000	-0.731903000
H	-2.151670000	-3.106605000	-1.542596000
H	-2.829779000	-4.435992000	-1.056192000
O	3.903404000	-2.314788000	0.518495000
H	4.664978000	-2.912985000	0.551472000
H	4.186623000	-1.542636000	-0.059310000
O	-3.869542000	-2.002291000	1.115944000
H	-4.217928000	-1.266741000	0.562617000
H	-3.440408000	-2.613292000	0.479048000
O	0.353474000	2.389144000	3.090963000
H	-0.508732000	1.899894000	3.117194000
H	0.255553000	3.040817000	2.362761000
O	0.137354000	-2.690267000	2.927293000
H	1.052290000	-2.277575000	2.927118000
H	0.168670000	-3.350312000	3.636722000
O	0.168765000	4.255337000	0.997384000
H	0.939607000	4.139674000	0.388200000
H	0.172301000	5.184943000	1.270137000
O	-0.043133000	-4.334651000	0.625084000
H	-0.875662000	-4.075343000	0.177140000
H	0.019850000	-3.733141000	1.398638000
O	2.619483000	1.160392000	2.938203000
H	1.679106000	1.568403000	2.953238000
H	3.000392000	1.415000000	3.793238000

O	2.632020000	-1.699248000	2.977988000
H	2.601706000	-0.718974000	2.960909000
H	3.114777000	-1.950271000	2.158014000
O	-2.144298000	1.257136000	3.141752000
H	-2.195654000	0.240241000	3.200149000
H	-2.588354000	1.569852000	3.945115000
O	-2.337092000	-1.340141000	3.323448000
H	-1.464449000	-1.762853000	3.160265000
H	-2.916322000	-1.631702000	2.574006000
C	-0.062651000	0.281962000	-0.422501000
Cl	1.427305000	-0.474689000	0.176894000
Cl	-1.493687000	-0.469813000	0.276447000
F	-0.036371000	1.593942000	-0.122572000
F	-0.100584000	0.171044000	-1.756416000

CH_3Br within $5^{12}6^2$ clathrate hydrate

O	-0.114399000	2.334670000	-3.067015000
H	-0.944257000	1.752021000	-3.058589000
H	-0.128930000	2.766309000	-3.935218000
O	0.214942000	-2.931393000	-2.819908000
H	1.011419000	-2.354196000	-2.816953000
H	0.268844000	-3.432189000	-1.968779000
O	-0.238805000	4.273111000	-1.104382000
H	-0.192267000	3.591936000	-1.820170000
H	-0.996576000	3.999576000	-0.546125000
O	0.403845000	-4.226881000	-0.403024000

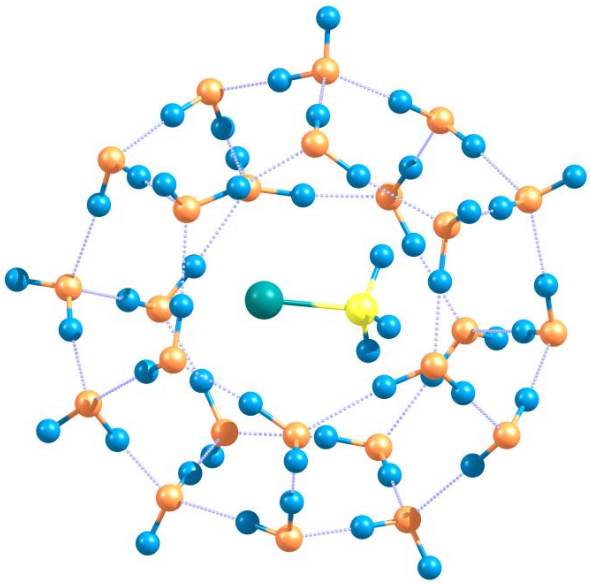


H	-0.432237000	-4.034440000	0.159402000
H	0.434360000	-5.193159000	-0.473258000
O	-2.349334000	0.969477000	-3.140290000
H	-2.203407000	-0.008681000	-3.089754000
H	-2.829918000	1.185980000	-2.315398000
O	-2.109388000	-1.756087000	-2.909104000
H	-1.169081000	-2.135049000	-2.827323000
H	-2.484937000	-2.217368000	-3.674955000
O	-3.887542000	1.798667000	-0.866993000
H	-3.349794000	2.460005000	-0.351050000
H	-4.604665000	2.299793000	-1.284235000
O	-3.500458000	-2.616486000	-0.623539000
H	-3.005779000	-2.316839000	-1.419925000
H	-3.747462000	-1.795516000	-0.153142000
O	-2.405368000	3.535369000	0.568909000
H	-2.819923000	4.352877000	0.883974000
H	-2.025469000	3.085677000	1.387374000
O	-1.692428000	-3.794888000	1.034875000
H	-1.463804000	-3.108501000	1.702153000
H	-2.381068000	-3.384253000	0.445892000
O	2.373967000	1.062808000	-3.031053000
H	1.471080000	1.451635000	-3.025816000
H	2.903606000	1.575078000	-2.345654000
O	2.616143000	-1.478785000	-2.856799000
H	2.489399000	-0.459915000	-2.919142000
H	3.019233000	-1.730880000	-3.701860000
O	3.710332000	2.375041000	-1.151538000
H	3.090508000	2.929966000	-0.633416000
H	4.081055000	1.734679000	-0.488747000
O	4.107235000	-1.913926000	-0.652471000

H	3.598483000	-1.772365000	-1.498821000
H	4.938194000	-2.342952000	-0.904386000
O	1.906143000	3.944026000	0.380704000
H	2.320318000	4.817096000	0.453627000
H	1.087496000	4.082693000	-0.196638000
O	2.496163000	-3.313904000	1.178363000
H	1.763997000	-3.663536000	0.619608000
H	3.098912000	-2.856156000	0.555369000
O	-2.635136000	0.143259000	3.091647000
H	-2.008305000	-0.627663000	3.117555000
H	-3.207918000	-0.031784000	2.312709000
O	2.966232000	0.542343000	2.999280000
H	2.363122000	1.343885000	2.937074000
H	3.531480000	0.700279000	3.770369000
O	-4.276574000	-0.282028000	0.838745000
H	-4.239392000	0.482995000	0.211064000
H	-5.213333000	-0.425741000	1.041160000
O	4.581270000	0.542209000	0.667645000
H	4.438465000	-0.329848000	0.243826000
H	4.033708000	0.527554000	1.482092000
O	-1.418980000	2.365774000	2.730046000
H	-1.849679000	1.431143000	2.828843000
H	-1.641644000	2.818370000	3.558893000
O	1.380303000	2.647876000	2.758336000
H	0.417285000	2.456841000	2.729563000
H	1.575633000	3.150199000	1.930745000
O	-1.015365000	-2.035902000	3.114238000
H	-0.004445000	-1.897570000	3.130605000
H	-1.190210000	-2.591694000	3.889315000
O	1.566038000	-1.880416000	3.268136000

H	2.020731000	-1.011477000	3.208726000
H	1.955478000	-2.430407000	2.535570000
C	0.999900000	0.079920000	0.201421000
H	1.123059000	0.870132000	0.937120000
H	1.393843000	-0.868244000	0.561171000
H	1.415839000	0.364451000	-0.762244000
Br	-0.946890000	-0.174907000	-0.047692000

CH_3Cl within $5^{12}6^2$ clathrate hydrate

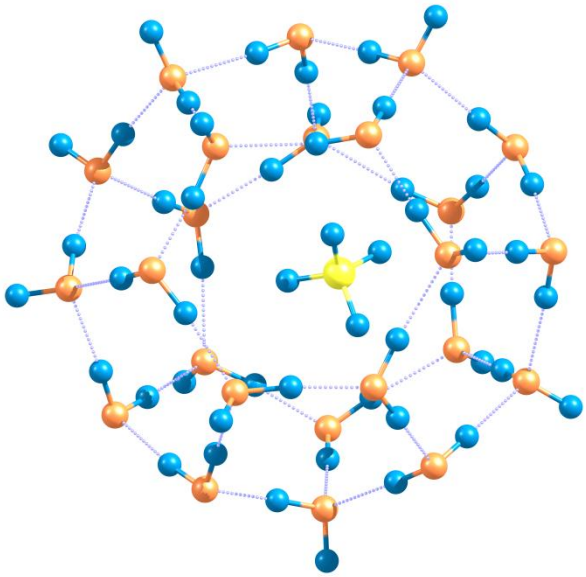


O	-0.352822000	2.317722000	-3.092224000
H	-1.141077000	1.681196000	-3.095834000
H	-0.390880000	2.761704000	-3.953395000
O	0.350203000	-2.936500000	-2.843443000
H	1.097656000	-2.297139000	-2.833861000
H	0.436800000	-3.431196000	-1.991742000
O	-0.621562000	4.198801000	-1.085832000
H	-0.525322000	3.535048000	-1.812987000
H	-1.359546000	3.866182000	-0.533430000
O	0.626319000	-4.219384000	-0.420270000
H	-0.221057000	-4.105586000	0.145777000
H	0.740695000	-5.178785000	-0.498270000
O	-2.489433000	0.789624000	-3.159886000
H	-2.271116000	-0.174137000	-3.097993000
H	-2.991550000	0.980204000	-2.341522000
O	-2.052512000	-1.915971000	-2.909241000
H	-1.090371000	-2.239764000	-2.851800000
H	-2.423226000	-2.401068000	-3.662463000
O	-4.089647000	1.508244000	-0.877572000

H	-3.614800000	2.208735000	-0.352652000
H	-4.851164000	1.946606000	-1.286499000
O	-3.367496000	-2.878010000	-0.612343000
H	-2.888459000	-2.542828000	-1.404033000
H	-3.655311000	-2.074921000	-0.133711000
O	-2.748625000	3.339687000	0.587349000
H	-3.204269000	4.143472000	0.879882000
H	-2.345824000	2.932169000	1.416415000
O	-1.496752000	-3.977362000	1.028471000
H	-1.318978000	-3.293229000	1.713149000
H	-2.211353000	-3.600909000	0.446670000
O	2.229783000	1.227652000	-3.061896000
H	1.299582000	1.545440000	-3.048268000
H	2.717225000	1.767704000	-2.368421000
O	2.633781000	-1.295986000	-2.863387000
H	2.439846000	-0.288568000	-2.932805000
H	3.058719000	-1.524114000	-3.704572000
O	3.452422000	2.606192000	-1.142864000
H	2.794306000	3.116206000	-0.625726000
H	3.861129000	1.991655000	-0.478580000
O	4.145055000	-1.638713000	-0.653360000
H	3.627631000	-1.526470000	-1.498941000
H	5.007842000	-1.996407000	-0.909582000
O	1.540911000	4.030516000	0.402919000
H	1.883855000	4.934151000	0.473567000
H	0.713820000	4.103081000	-0.174235000
O	2.642453000	-3.162362000	1.173882000
H	1.936394000	-3.557989000	0.612132000
H	3.211744000	-2.660675000	0.553368000
O	-2.701420000	-0.070220000	3.078600000

H	-2.026186000	-0.798589000	3.104773000
H	-3.265963000	-0.280979000	2.302029000
O	2.824465000	0.713331000	3.031383000
H	2.171970000	1.475463000	2.976250000
H	3.381491000	0.901318000	3.801704000
O	-4.318773000	-0.598752000	0.839016000
H	-4.327963000	0.158049000	0.201072000
H	-5.245565000	-0.807537000	1.029409000
O	4.428246000	0.834407000	0.688427000
H	4.351912000	-0.045651000	0.263888000
H	3.887409000	0.778633000	1.505451000
O	-1.676790000	2.255234000	2.758143000
H	-2.029531000	1.288176000	2.849855000
H	-1.933253000	2.682436000	3.590585000
O	1.106169000	2.718709000	2.795337000
H	0.157372000	2.466837000	2.764153000
H	1.270517000	3.225026000	1.963457000
O	-0.953403000	-2.155697000	3.109743000
H	0.046791000	-1.952955000	3.134797000
H	-1.103242000	-2.702332000	3.896470000
O	1.611491000	-1.817385000	3.278055000
H	1.994472000	-0.914386000	3.223186000
H	2.040570000	-2.329379000	2.540068000
C	0.979390000	0.156893000	0.210114000
H	1.041318000	0.926254000	0.976795000
H	1.409772000	-0.779563000	0.563189000
H	1.450451000	0.495258000	-0.711055000
Cl	-0.779301000	-0.137495000	-0.134026000

CH_4 within $5^{12}6^2$ clathrate hydrate



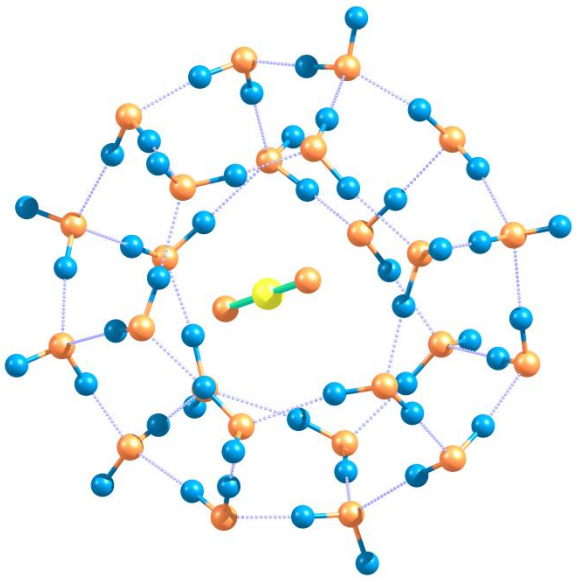
O	0.235327000	-2.460719000	-2.995965000
H	0.979437000	-1.779252000	-3.039355000
H	0.246221000	-2.897790000	-3.861221000
O	-0.694844000	2.808926000	-2.850593000
H	-1.409039000	2.134331000	-2.771783000
H	-0.762288000	3.358492000	-2.030864000
O	0.791173000	-4.287285000	-0.997761000
H	0.591345000	-3.657593000	-1.733406000
H	1.547382000	-3.888559000	-0.520502000
O	-0.822151000	4.256961000	-0.518134000
H	0.066197000	4.215325000	-0.013722000
H	-0.992892000	5.202943000	-0.641155000
O	2.254555000	-0.783050000	-3.145755000
H	2.001525000	0.172800000	-3.095606000
H	2.867705000	-0.924865000	-2.396305000
O	1.725647000	1.896240000	-2.955176000
H	0.751007000	2.196547000	-2.883972000
H	2.045165000	2.324465000	-3.764488000
O	4.155653000	-1.335095000	-1.076407000
H	3.784546000	-2.072802000	-0.517944000
H	4.894768000	-1.715232000	-1.574672000
O	3.235785000	3.069964000	-0.900231000
H	2.686195000	2.670030000	-1.611969000
H	3.600583000	2.305708000	-0.410881000
O	3.020667000	-3.232153000	0.457418000
H	3.524359000	-4.017049000	0.721468000
H	2.675485000	-2.823314000	1.312083000
O	1.412389000	4.181341000	0.792146000

H	1.310594000	3.503277000	1.499273000
H	2.119627000	3.828523000	0.188803000
O	-2.406955000	-1.472364000	-2.876985000
H	-1.464307000	-1.745574000	-2.889502000
H	-2.820160000	-1.985976000	-2.115489000
O	-2.848065000	1.042683000	-2.695878000
H	-2.627589000	0.035863000	-2.745804000
H	-3.359722000	1.218194000	-3.500732000
O	-3.406445000	-2.804138000	-0.810745000
H	-2.668688000	-3.234070000	-0.330409000
H	-3.802539000	-2.178499000	-0.146299000
O	-4.187624000	1.432983000	-0.385811000
H	-3.727431000	1.294323000	-1.259593000
H	-5.063793000	1.787961000	-0.596435000
O	-1.297753000	-4.096528000	0.611116000
H	-1.625296000	-4.998430000	0.746219000
H	-0.508218000	-4.188041000	-0.008717000
O	-2.702148000	3.186954000	1.248096000
H	-2.049932000	3.582632000	0.627125000
H	-3.233426000	2.572202000	0.698472000
O	2.922734000	0.307714000	2.843963000
H	2.210930000	1.002915000	2.876157000
H	3.463758000	0.537924000	2.056838000
O	-2.427940000	-0.706702000	3.071157000
H	-1.747458000	-1.444243000	3.008499000
H	-2.904383000	-0.870322000	3.899112000
O	4.396827000	0.863068000	0.523556000
H	4.403186000	0.079545000	-0.080784000
H	5.322484000	1.122828000	0.643583000
O	-4.353650000	-1.019666000	1.015077000

H	-4.330065000	-0.161923000	0.540560000
H	-3.676150000	-0.923206000	1.719509000
O	2.074074000	-2.101780000	2.654339000
H	2.360640000	-1.111582000	2.701396000
H	2.378404000	-2.483468000	3.492449000
O	-0.681740000	-2.693109000	2.908542000

CO_2 within $5^{12}6^2$ clathrate hydrate

O	-0.648289000	1.883401000	3.173777000
H	0.212260000	1.363351000	3.257544000
H	-0.874979000	2.152181000	4.077303000
O	-0.456814000	-3.414516000	2.249336000
H	-1.277604000	-2.873449000	2.175760000
H	-0.317101000	-3.800513000	1.350758000
O	-0.272802000	4.087638000	1.557458000
H	-0.398939000	3.325105000	2.173961000
H	0.581051000	3.915420000	1.108382000
O	0.009879000	-4.445708000	-0.276710000
H	0.898679000	-4.128210000	-0.666565000
H	0.070187000	-5.412852000	-0.290016000
O	1.642329000	0.612319000	3.360015000
H	1.608165000	-0.357205000	3.164139000
H	2.300106000	0.986886000	2.738580000
O	1.693998000	-2.054996000	2.744480000
H	0.812797000	-2.531322000	2.536304000
H	2.054210000	-2.540062000	3.503045000
O	3.564287000	1.862305000	1.665926000
H	3.080500000	2.561110000	1.144220000



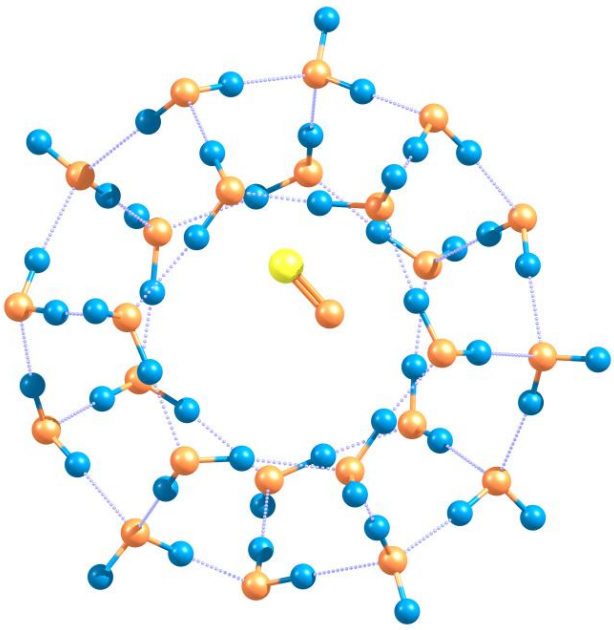
H	4.157316000	2.337249000	2.267686000
O	3.626493000	-2.520901000	0.755513000
H	2.929689000	-2.362087000	1.431452000
H	3.858427000	-1.631721000	0.417729000
O	2.217495000	3.704341000	0.230236000
H	2.592187000	4.593666000	0.139103000
H	2.054551000	3.376131000	-0.708930000
O	2.292180000	-3.715691000	-1.289490000
H	2.182502000	-2.983018000	-1.936402000
H	2.843807000	-3.329717000	-0.557136000
O	-3.026370000	0.422876000	2.665350000
H	-2.142818000	0.835047000	2.768414000
H	-3.465361000	0.950957000	1.932124000
O	-2.914348000	-2.072749000	2.078046000
H	-2.903862000	-1.061218000	2.282626000
H	-3.474426000	-2.452034000	2.772758000
O	-4.085403000	1.872184000	0.681874000
H	-3.389423000	2.484774000	0.366475000
H	-4.280071000	1.300588000	-0.107254000
O	-3.874660000	-2.309963000	-0.422677000
H	-3.542696000	-2.228015000	0.516122000
H	-4.730650000	-2.759419000	-0.364740000
O	-2.142071000	3.757537000	-0.275456000
H	-2.676552000	4.566095000	-0.278603000
H	-1.442688000	3.903687000	0.436703000
O	-1.811911000	-3.295074000	-2.029523000
H	-1.226788000	-3.802487000	-1.420673000
H	-2.590656000	-3.049817000	-1.482326000
O	3.264806000	0.757431000	-2.638680000
H	2.765588000	-0.065127000	-2.877041000

H	3.708565000	0.523313000	-1.793400000
O	-2.221965000	0.854321000	-3.202839000
H	-1.781615000	1.747566000	-3.033121000
H	-2.482678000	0.862127000	-4.135539000
O	4.444642000	0.055570000	-0.184367000
H	4.194833000	0.707876000	0.516769000
H	5.412246000	0.003906000	-0.174312000
O	-4.423864000	0.261135000	-1.500981000
H	-4.198874000	-0.628544000	-1.154780000
H	-3.681154000	0.489629000	-2.100100000
O	1.782907000	2.833380000	-2.235111000
H	2.297646000	1.954999000	-2.372769000
H	2.099077000	3.413340000	-2.945407000
O	-0.995744000	3.129676000	-2.705994000
H	-0.063958000	2.904115000	-2.495134000
H	-1.394353000	3.418222000	-1.849000000
O	1.865026000	-1.553194000	-3.067834000
H	0.918247000	-1.309133000	-2.774005000
H	1.783729000	-1.892878000	-3.971790000
O	-0.471400000	-0.984783000	-2.147307000
H	-1.057229000	-0.349699000	-2.622735000
H	-0.994284000	-1.839422000	-2.095577000
C	0.287501000	0.031095000	0.325245000
O	1.152700000	0.678790000	-0.127296000
O	-0.555176000	-0.589825000	0.839496000

CO within $5^{12}6^2$ clathrate hydrate

O	-0.033193000	-2.562081000	2.900325000

H	-0.844406000	-1.965442000	2.990134000
H	0.048325000	-3.003076000	3.759949000
O	0.454284000	2.719193000	2.806273000
H	1.234915000	2.123750000	2.714705000
H	0.493687000	3.333836000	2.032421000
O	-0.366379000	-4.418018000	0.885401000
H	-0.252774000	-3.783467000	1.635254000
H	-1.155543000	-4.096369000	0.402858000
O	0.508239000	4.350514000	0.595765000
H	-0.366070000	4.217084000	0.087059000
H	0.555758000	5.302856000	0.768957000
O	-2.204182000	-1.102661000	3.158173000
H	-2.026912000	-0.129721000	3.118127000
H	-2.790616000	-1.282726000	2.395199000
O	-1.880370000	1.617856000	2.996947000
H	-0.939891000	2.000999000	2.895693000
H	-2.212234000	2.011601000	3.818583000
O	-3.994672000	-1.776203000	1.027631000
H	-3.543339000	-2.456778000	0.455407000
H	-4.704384000	-2.241855000	1.495314000
O	-3.452218000	2.713057000	0.947707000
H	-2.895196000	2.340108000	1.667992000
H	-3.757419000	1.932171000	0.443572000
O	-2.673183000	-3.515593000	-0.547001000
H	-3.126720000	-4.313735000	-0.858171000
H	-2.347985000	-3.040248000	-1.375415000
O	-1.717365000	4.019013000	-0.693855000
H	-1.591254000	3.408439000	-1.455107000
H	-2.390094000	3.582430000	-0.105907000
O	2.522817000	-1.371934000	2.847110000

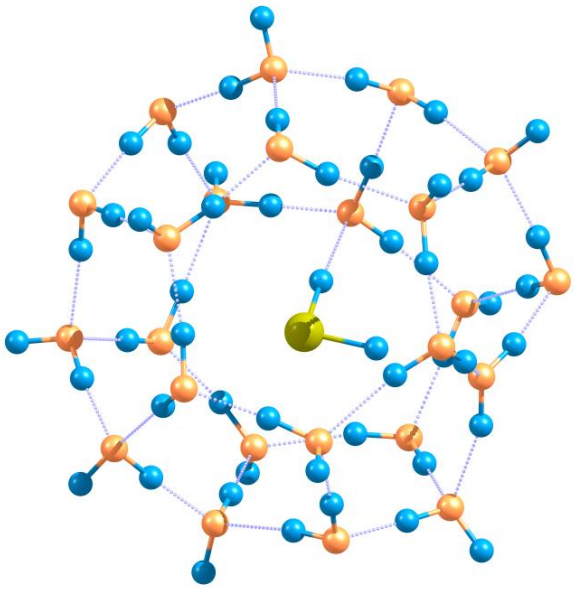


H	1.601150000	-1.705670000	2.800826000
H	3.012141000	-1.841142000	2.102653000
O	2.747110000	1.163153000	2.653651000
H	2.615693000	0.137156000	2.690366000
H	3.225899000	1.369907000	3.471182000
O	3.728945000	-2.592747000	0.816068000
H	3.034925000	-3.065460000	0.311442000
H	4.074227000	-1.911957000	0.178226000
O	4.075464000	1.771908000	0.386883000
H	3.605594000	1.558134000	1.240146000
H	4.912448000	2.188037000	0.641244000
O	1.733041000	-4.006561000	-0.668157000
H	2.141639000	-4.874546000	-0.805428000
H	0.939349000	-4.177842000	-0.070356000
O	2.503136000	3.513747000	-1.193855000
H	1.815838000	3.834137000	-0.567664000
H	3.054177000	2.902765000	-0.658653000
O	-2.898223000	0.082427000	-2.835030000
H	-2.279252000	0.858563000	-2.877684000
H	-3.447057000	0.241465000	-2.035510000
O	2.492288000	-0.489413000	-2.937479000
H	1.908030000	-1.311228000	-2.946788000
H	2.973400000	-0.515806000	-3.778598000
O	-4.417568000	0.442221000	-0.508155000
H	-4.347111000	-0.354842000	0.074278000
H	-5.364124000	0.595092000	-0.647403000
O	4.504987000	-0.675161000	-0.961933000
H	4.408118000	0.181889000	-0.494626000
H	3.802717000	-0.644954000	-1.648021000
O	-1.785692000	-2.220524000	-2.671163000

H	-2.170035000	-1.264246000	-2.703229000
H	-2.025003000	-2.605996000	-3.528564000
O	0.990757000	-2.662812000	-2.965974000
H	0.060291000	-2.408645000	-2.788335000
H	1.267870000	-3.185861000	-2.175362000
O	-1.312049000	2.289992000	-2.868245000
H	-0.298002000	2.129515000	-2.909446000
H	-1.504697000	2.823711000	-3.654590000
O	1.232214000	2.000725000	-3.018849000
H	1.628253000	1.103249000	-2.945657000
H	1.724593000	2.576768000	-2.365981000
C	0.254830000	1.019380000	-0.048405000
O	-0.669175000	0.373862000	-0.215320000

H_2S within $5^{12}6^2$ clathrate hydrate

O	1.093489000	-1.934500000	-3.297341000
H	1.483055000	-0.999506000	-3.274301000
H	1.377110000	-2.299339000	-4.149679000
O	-1.943329000	2.448042000	-2.583997000
H	-2.258238000	1.517081000	-2.529184000
H	-2.175564000	2.848794000	-1.711734000
O	2.306697000	-3.456736000	-1.300281000
H	1.842876000	-2.923910000	-1.991658000
H	2.813612000	-2.806023000	-0.770529000
O	-2.582665000	3.571551000	-0.132107000



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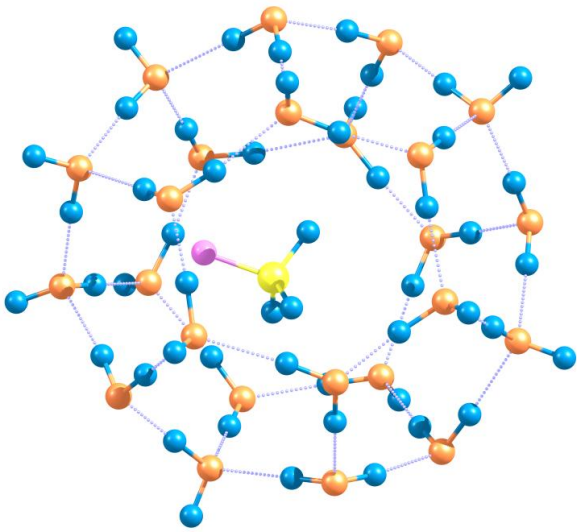
O	2.235220000	0.431845000	-3.283820000
H	1.591354000	1.169897000	-3.139914000
H	2.814618000	0.462018000	-2.495111000
O	0.643567000	2.637778000	-2.858670000
H	-0.352935000	2.491089000	-2.716261000
H	0.690310000	3.219455000	-3.632980000
O	4.144360000	0.495364000	-1.145852000
H	4.073510000	-0.344002000	-0.613050000
H	4.985038000	0.441654000	-1.624776000
O	1.576091000	4.143742000	-0.688898000
H	1.229726000	3.611314000	-1.442018000
H	2.221615000	3.554761000	-0.248304000
O	3.891680000	-1.750443000	0.320479000
H	4.681854000	-2.256311000	0.563264000
H	3.412744000	-1.557296000	1.184383000
O	-0.447957000	4.380836000	1.103703000
H	-0.199687000	3.753408000	1.817894000
H	0.305782000	4.348460000	0.452463000
O	-1.704766000	-2.179999000	-3.168674000
H	-0.745278000	-1.985453000	-3.270363000
H	-1.737175000	-2.669572000	-2.304963000
O	-3.116010000	-0.093687000	-2.580948000
H	-2.500210000	-0.885099000	-2.801282000
H	-3.698863000	-0.021150000	-3.352472000
O	-1.600101000	-3.077626000	-0.648888000
H	-0.950345000	-3.721717000	-0.293882000
H	-2.366997000	-3.053064000	-0.011314000
O	-4.448154000	-0.416331000	-0.247516000

H	-3.947928000	-0.329752000	-1.107255000
H	-5.379962000	-0.507458000	-0.496077000
O	0.556095000	-4.437678000	0.404865000
H	0.675341000	-5.398730000	0.406308000
H	1.229548000	-4.076773000	-0.257483000
O	-3.830053000	1.700932000	1.501204000
H	-3.458441000	2.410595000	0.925582000
H	-4.111600000	0.999690000	0.873502000
O	2.645148000	1.345380000	2.953700000
H	1.753088000	1.752049000	3.088716000
H	2.987633000	1.776767000	2.139175000
O	-1.870211000	-1.920511000	3.177434000
H	-0.969185000	-2.345377000	2.998286000
H	-2.118733000	-2.219222000	4.064808000
O	3.563617000	2.519431000	0.581154000
H	3.824562000	1.825596000	-0.076519000
H	4.324436000	3.113737000	0.662920000
O	-3.601993000	-2.750413000	1.117121000
H	-3.940004000	-1.920241000	0.716094000
H	-3.066935000	-2.457220000	1.888260000
O	2.680646000	-1.222852000	2.629319000
H	2.574014000	-0.208897000	2.717661000
H	3.169168000	-1.484286000	3.425340000
O	0.499361000	-3.006490000	2.799952000
H	1.159391000	-2.292245000	2.662955000
H	0.526565000	-3.539880000	1.971587000
O	0.169548000	2.516799000	3.153675000
H	-0.520697000	1.799723000	2.967381000
H	-0.074593000	2.906591000	4.006406000
O	-1.549740000	0.711253000	2.453774000

H	-1.698773000	-0.177811000	2.851747000
H	-2.439467000	1.060966000	2.145665000
S	0.267842000	-0.302514000	-0.180961000
H	-0.512886000	-1.406294000	-0.366191000
H	-0.481078000	0.167323000	0.855801000

CH_3F within $5^{12}6^2$ clathrate hydrate



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O	2.401596000	-2.006985000	-2.762821000
H	2.531016000	-1.030386000	-2.766412000
H	2.824649000	-2.314584000	-1.923264000
O	-3.267796000	2.618893000	-1.082520000
H	-2.749689000	2.188510000	-1.805678000
H	-3.599042000	1.878847000	-0.532274000
O	3.497282000	-2.766454000	-0.356323000
H	2.786437000	-3.255774000	0.194259000
H	4.221905000	-3.404442000	-0.443549000
O	-2.284691000	-1.159562000	-3.042407000
H	-1.453948000	-1.685531000	-2.938269000
H	-2.785022000	-1.307123000	-2.213347000
O	-0.077057000	-2.787978000	-2.771014000
H	0.873814000	-2.421742000	-2.746334000
H	-0.085836000	-3.374829000	-3.542845000
O	-4.043022000	-1.651585000	-0.845128000
H	-4.202847000	-0.813588000	-0.332696000
H	-4.884378000	-1.882304000	-1.266282000

O	-0.416757000	-4.468102000	-0.554846000
H	-0.277526000	-3.888127000	-1.337761000
H	-1.185064000	-4.073397000	-0.094358000
O	-4.389995000	0.614800000	0.587161000
H	-5.256624000	0.929469000	0.884952000
H	-3.798950000	0.608647000	1.398544000
O	1.721559000	-4.007016000	1.056054000
H	1.382696000	-3.372381000	1.727993000
H	0.939403000	-4.234404000	0.483464000
O	0.847305000	2.260972000	-2.978398000
H	-0.070280000	1.913718000	-3.030939000
H	0.827856000	3.019990000	-2.317333000
O	2.884400000	0.737245000	-2.773560000
H	2.029785000	1.309921000	-2.826627000
H	3.343531000	0.915025000	-3.608988000
O	0.802237000	4.209208000	-1.182324000
H	-0.014657000	4.145522000	-0.644389000
H	1.542037000	4.073835000	-0.532218000
O	4.213076000	1.538943000	-0.563035000
H	3.756194000	1.253824000	-1.402172000
H	5.094088000	1.841264000	-0.829330000
O	-1.572833000	4.009073000	0.366944000
H	-1.924371000	4.911548000	0.399000000
H	-2.230739000	3.483921000	-0.193964000
O	4.389076000	-0.637799000	1.239135000
H	4.095105000	-1.400292000	0.690950000
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O	-1.844471000	-1.758864000	2.954166000
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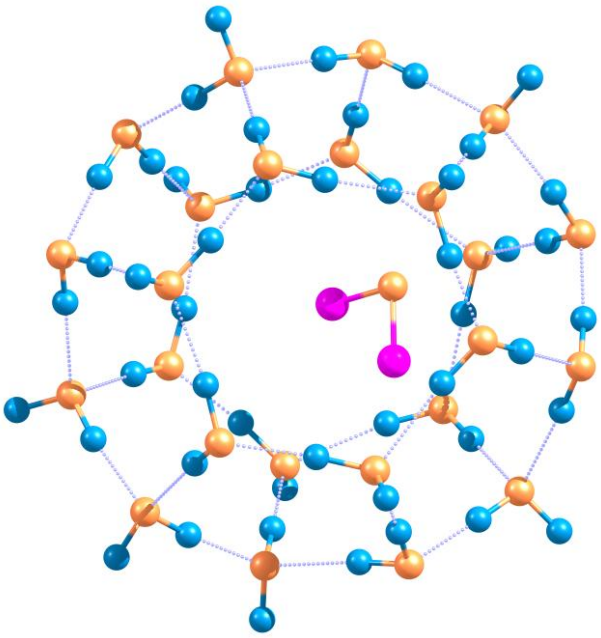
H	-2.112752000	-2.312332000	2.186406000

O	1.573645000	2.345274000	2.819896000
H	0.577845000	2.487906000	2.822328000
H	1.898337000	2.802853000	3.610392000
O	-2.658715000	-3.321630000	0.792270000
H	-3.189379000	-2.760561000	0.170792000
H	-3.242420000	-4.044765000	1.066418000
O	2.772710000	3.670261000	0.626327000
H	3.301711000	2.954712000	0.214240000
H	2.340076000	3.233707000	1.392171000
O	-2.819839000	0.601989000	2.744006000
H	-2.363324000	-0.319807000	2.784120000
H	-3.286642000	0.672186000	3.591461000
O	-1.035461000	2.782881000	2.773674000
H	-1.620515000	1.994033000	2.774013000
H	-1.255174000	3.268071000	1.941483000
O	0.837164000	-2.204180000	3.011450000
H	1.482860000	-1.403536000	3.033033000
H	1.031949000	-2.686972000	3.829818000
O	2.522367000	-0.272994000	3.151015000
H	2.155816000	0.626208000	2.997884000
H	3.246961000	-0.394464000	2.473619000
C	-0.405188000	0.402006000	0.066107000
H	-0.434328000	1.076356000	0.924863000
H	0.238701000	-0.455963000	0.282444000
H	-0.042537000	0.939579000	-0.814107000
F	-1.706029000	-0.062388000	-0.181904000

N_2O within $5^{12}6^2$ clathrate hydrate



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O	-0.482957000	-2.657014000	-3.057447000
H	0.405747000	-2.240253000	-2.968644000
H	-0.559636000	-3.265284000	-2.280876000
O	0.595387000	4.349677000	-0.731913000
H	0.526784000	3.769510000	-1.529008000
H	-0.216039000	4.163602000	-0.216482000
O	-0.681303000	-4.255155000	-0.827616000
H	-1.485687000	-3.968706000	-0.262217000
H	-0.849432000	-5.186730000	-1.036352000
O	-2.127248000	1.739465000	-3.031794000
H	-2.178849000	0.751371000	-3.035548000
H	-2.602799000	2.009789000	-2.219947000
O	-2.469510000	-0.989377000	-2.981317000
H	-1.653249000	-1.602069000	-2.982203000
H	-2.949441000	-1.234189000	-3.787598000
O	-3.572697000	2.674397000	-0.739004000
H	-2.935565000	3.191922000	-0.172118000
H	-4.179193000	3.323049000	-1.127110000
O	-4.154984000	-1.806970000	-0.886839000
H	-3.552015000	-1.537058000	-1.616234000
H	-4.237432000	-1.006829000	-0.329919000
O	-1.780135000	3.949102000	0.808230000
H	-1.990484000	4.826395000	1.162401000
H	-1.545918000	3.376249000	1.604676000
O	-2.717150000	-3.570024000	0.613387000

H	-2.382807000	-3.033329000	1.368519000
H	-3.290815000	-2.956391000	0.080683000
O	2.493528000	0.878334000	-2.930631000
H	1.697338000	1.451777000	-2.884595000
H	3.091074000	1.181594000	-2.181293000
O	2.101314000	-1.636405000	-2.871724000
H	2.212950000	-0.605815000	-2.854724000
H	2.489588000	-1.899599000	-3.720598000
O	4.020699000	1.633083000	-0.891036000
H	3.571941000	2.298687000	-0.329186000
H	4.212432000	0.869602000	-0.285637000
O	3.375531000	-2.687051000	-0.741330000
H	2.928339000	-2.314733000	-1.552106000
H	4.080431000	-3.265875000	-1.067753000
O	2.631622000	3.507795000	0.728485000
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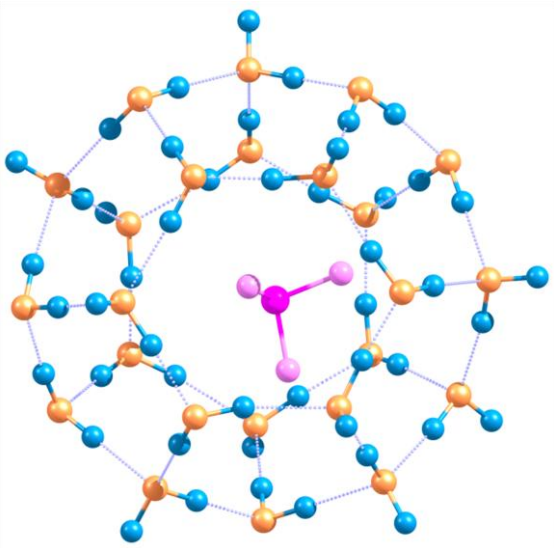
H	1.871896000	3.838030000	0.154443000
O	1.542152000	-4.119944000	0.872935000
H	0.755946000	-4.195494000	0.286041000
H	2.201107000	-3.633357000	0.333473000
O	-2.745507000	0.392268000	2.973703000
H	-2.315905000	-0.503144000	2.941619000
H	-3.351168000	0.409378000	2.200271000
O	2.675779000	-0.464375000	2.937743000
H	2.259323000	0.450172000	2.890477000
H	3.180691000	-0.475229000	3.764796000
O	-4.431380000	0.540641000	0.733693000
H	-4.201509000	1.328733000	0.180461000
H	-5.372442000	0.624588000	0.948311000
O	4.432082000	-0.522020000	0.732101000

H	4.113904000	-1.300781000	0.228587000
H	3.864676000	-0.504356000	1.533095000
O	-1.145475000	2.392286000	2.842626000
H	-1.740934000	1.551546000	2.864900000
H	-1.215219000	2.769170000	3.733358000
O	1.631644000	1.952270000	2.777707000
H	0.655333000	2.011265000	2.704138000
H	2.000383000	2.516268000	2.056442000
O	-1.739030000	-2.128544000	2.812172000
H	-0.720705000	-2.237606000	2.829151000
H	-2.045807000	-2.646628000	3.572415000
O	0.800050000	-2.562066000	2.949706000
H	1.421847000	-1.801434000	2.955001000
H	1.103775000	-3.160040000	2.210051000
O	1.184346000	-0.248826000	0.245636000
N	0.973627000	0.975263000	-0.101486000
N	0.135764000	-0.137835000	0.993628000

NF_3 within $5^{12}6^2$ clathrate hydrate

O	-0.249001000	-2.542443000	2.895920000
H	-0.988920000	-1.856310000	2.922409000
H	-0.258308000	-2.958111000	3.771777000
O	0.652943000	2.748980000	2.917421000
H	1.360015000	2.067858000	2.825490000
H	0.756154000	3.337584000	2.128778000
O	-0.692367000	-4.357437000	0.863806000
H	-0.555455000	-3.741505000	1.624714000

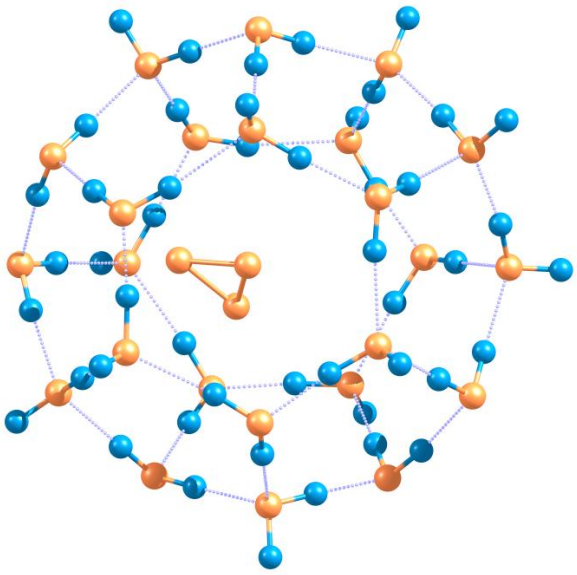
H	-1.458317000	-3.992817000	0.375481000
O	0.896557000	4.283267000	0.654291000
H	0.015664000	4.249569000	0.134039000
H	1.042614000	5.225272000	0.829921000
O	-2.253119000	-0.844810000	2.980200000
H	-2.025032000	0.118203000	3.007856000
H	-2.818073000	-0.954086000	2.188697000
O	-1.771311000	1.846352000	2.975927000
H	-0.798135000	2.153607000	2.919078000
H	-2.096140000	2.236664000	3.801992000
O	-4.088989000	-1.373444000	0.868744000
H	-3.695300000	-2.108581000	0.321835000
H	-4.795281000	-1.774175000	1.397593000
O	-3.212641000	3.087158000	0.913807000
H	-2.702495000	2.654405000	1.635305000
H	-3.605228000	2.348451000	0.407751000
O	-2.903166000	-3.276811000	-0.619753000
H	-3.435200000	-4.009219000	-0.966515000
H	-2.505058000	-2.816742000	-1.423962000
O	-1.315375000	4.213200000	-0.685316000
H	-1.186467000	3.558433000	-1.409674000
H	-2.042728000	3.843897000	-0.116631000
O	2.383820000	-1.534025000	2.908396000
H	1.446038000	-1.816260000	2.843144000
H	2.863184000	-2.033028000	2.176831000
O	2.784446000	0.977548000	2.733656000
H	2.575498000	-0.036914000	2.758465000
H	3.259513000	1.138677000	3.563656000
O	3.559036000	-2.827248000	0.906361000
H	2.840505000	-3.245936000	0.388364000



H	3.967395000	-2.173221000	0.278261000
O	4.249831000	1.500193000	0.530381000
H	3.733134000	1.317074000	1.363856000
H	5.110961000	1.836407000	0.819859000
O	1.480489000	-4.061313000	-0.614635000
H	1.810424000	-4.959113000	-0.770254000
H	0.654073000	-4.177368000	-0.049272000
O	2.899057000	3.385635000	-1.098116000
H	2.200306000	3.725380000	-0.494848000
H	3.390114000	2.731491000	-0.556152000
O	-2.708764000	0.408494000	-2.827880000
H	-1.999368000	1.105041000	-2.822326000
H	-3.292933000	0.630702000	-2.069873000
O	2.632188000	-0.585947000	-2.891426000
H	1.959185000	-1.336398000	-2.880092000
H	3.120739000	-0.701967000	-3.720611000
O	-4.338585000	0.913186000	-0.599642000
H	-4.339956000	0.092409000	-0.047292000
H	-5.265998000	1.108777000	-0.800781000
O	4.530534000	-0.963566000	-0.835859000
H	4.487563000	-0.106307000	-0.361666000
H	3.868983000	-0.863322000	-1.555322000
O	-1.832734000	-1.992847000	-2.663739000
H	-2.136996000	-1.009081000	-2.686451000
H	-2.030180000	-2.330832000	-3.551194000
O	0.909113000	-2.589171000	-2.879025000
H	0.004566000	-2.258711000	-2.695312000
H	1.134392000	-3.152577000	-2.099961000
O	-0.895721000	2.423111000	-2.791327000
H	0.109384000	2.207856000	-2.851108000

H	-1.062962000	2.975801000	-3.570546000
O	1.626504000	2.024492000	-3.052350000
H	1.941777000	1.096764000	-2.966381000
H	2.128241000	2.543855000	-2.361983000
N	-0.281703000	-0.082823000	0.190240000
F	-0.728338000	-1.399939000	0.124353000
F	-1.473834000	0.619114000	0.083324000
F	0.262622000	0.090573000	-1.064050000

O_3 within $5^{12}6^2$ clathrate hydrate

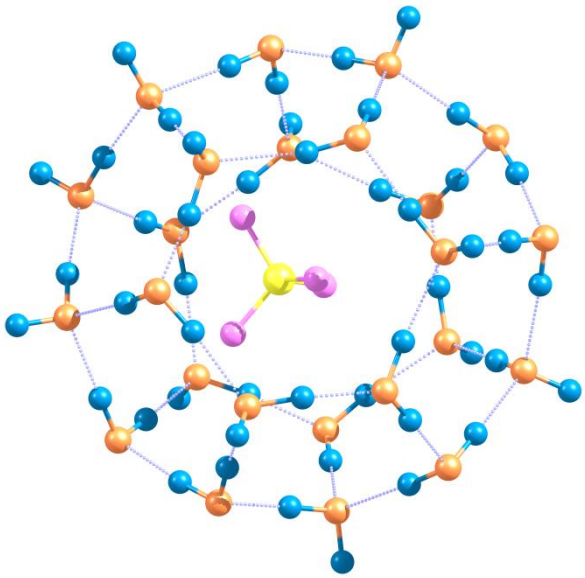


O	0.136376000	2.543332000	2.922541000
H	0.937180000	1.929515000	2.987471000
H	0.100657000	2.999186000	3.777594000
O	-0.396500000	-2.797325000	2.853791000
H	-1.157799000	-2.177798000	2.759467000
H	-0.424072000	-3.366960000	2.045546000
O	0.491494000	4.373792000	0.883693000
H	0.363451000	3.742119000	1.633455000
H	1.278543000	4.040980000	0.405400000
O	-0.426314000	-4.303234000	0.553447000
H	0.459914000	-4.200912000	0.055209000
H	-0.512287000	-5.256088000	0.708687000
O	2.275790000	1.033508000	3.109487000
H	2.084926000	0.062579000	3.067775000
H	2.863362000	1.209174000	2.346683000
O	1.931640000	-1.676739000	2.943551000
H	0.985774000	-2.061153000	2.873068000
H	2.280072000	-2.060475000	3.763242000

O	4.093896000	1.697354000	0.997746000
H	3.655831000	2.391106000	0.430728000
H	4.796325000	2.150327000	1.488338000
O	3.542359000	-2.786139000	0.933199000
H	2.962218000	-2.409132000	1.633416000
H	3.853465000	-2.009464000	0.426557000
O	2.791321000	3.466145000	-0.555826000
H	3.246330000	4.266559000	-0.858835000
H	2.458637000	3.003062000	-1.388392000
O	1.813770000	-4.076915000	-0.733144000
H	1.668234000	-3.427611000	-1.458806000
H	2.489927000	-3.658331000	-0.136302000
O	-2.412299000	1.333585000	2.876816000
H	-1.496570000	1.685576000	2.873815000
H	-2.878222000	1.806500000	2.122375000
O	-2.671623000	-1.207323000	2.673647000
H	-2.518016000	-0.189075000	2.716715000
H	-3.163538000	-1.409327000	3.484470000
O	-3.546555000	2.548356000	0.800462000
H	-2.868502000	3.037520000	0.289614000
H	-3.916692000	1.888151000	0.156468000
O	-3.991012000	-1.769315000	0.383939000
H	-3.521876000	-1.562811000	1.239498000
H	-4.821875000	-2.200096000	0.633882000
O	-1.600352000	3.996540000	-0.688374000
H	-1.994403000	4.871360000	-0.823991000
H	-0.806873000	4.151818000	-0.086295000
O	-2.433182000	-3.494461000	-1.227505000
H	-1.728049000	-3.795988000	-0.611077000
H	-2.982876000	-2.886853000	-0.687323000

O	2.997720000	-0.116040000	-2.868140000
H	2.355077000	-0.874718000	-2.886831000
H	3.559047000	-0.283895000	-2.079255000
O	-2.438672000	0.467931000	-3.005693000
H	-1.833939000	1.275469000	-2.980205000
H	-2.907662000	0.534440000	-3.851509000
O	4.513973000	-0.517443000	-0.540879000
H	4.453905000	0.280151000	0.042127000
H	5.458602000	-0.683142000	-0.678991000
O	-4.392519000	0.667857000	-0.979179000
H	-4.304920000	-0.192405000	-0.515963000
H	-3.731355000	0.619420000	-1.703662000
O	1.889068000	2.189690000	-2.683297000
H	2.282541000	1.238246000	-2.729427000
H	2.104777000	2.585381000	-3.542206000
O	-0.893654000	2.608052000	-2.971442000
H	0.031850000	2.341375000	-2.787724000
H	-1.165413000	3.135061000	-2.181704000
O	1.359903000	-2.278960000	-2.839302000
H	0.346090000	-2.120489000	-2.902698000
H	1.560872000	-2.820668000	-3.618345000
O	-1.180795000	-2.025746000	-3.101270000
H	-1.579777000	-1.128244000	-3.051063000
H	-1.676451000	-2.585735000	-2.437313000
O	-0.250001000	0.114501000	0.726578000
O	-1.485116000	0.368868000	0.032230000
O	-0.549525000	-0.595335000	-0.492539000

CF_4 within $5^{12}6^2$ clathrate hydrate



O	0.460127000	-2.413094000	-2.925318000
H	1.161152000	-1.688100000	-2.963324000
H	0.500061000	-2.847078000	-3.791400000
O	-0.822735000	2.709283000	-2.838574000
H	-1.487371000	1.983480000	-2.783444000
H	-0.972516000	3.259180000	-2.029927000
O	1.045461000	-4.218151000	-0.921829000
H	0.855051000	-3.590218000	-1.661490000
H	1.772920000	-3.802693000	-0.415234000
O	-1.191202000	4.156788000	-0.533468000
H	-0.315155000	4.184858000	-0.005443000
H	-1.409599000	5.087292000	-0.694963000
O	2.380895000	-0.619930000	-3.041109000
H	2.084872000	0.324526000	-3.019772000
H	2.967058000	-0.726952000	-2.264999000
O	1.672823000	2.024158000	-2.913810000
H	0.674401000	2.230766000	-2.848858000
H	1.951743000	2.462438000	-3.732658000
O	4.218168000	-1.076536000	-0.889224000
H	3.881307000	-1.839616000	-0.343920000
H	5.002177000	-1.401272000	-1.357278000
O	2.991750000	3.340863000	-0.806415000
H	2.520499000	2.903018000	-1.550630000
H	3.415956000	2.605452000	-0.321228000
O	3.184819000	-3.073311000	0.604287000
H	3.739658000	-3.809627000	0.903238000
H	2.753781000	-2.693131000	1.431302000
O	1.006865000	4.254736000	0.827787000

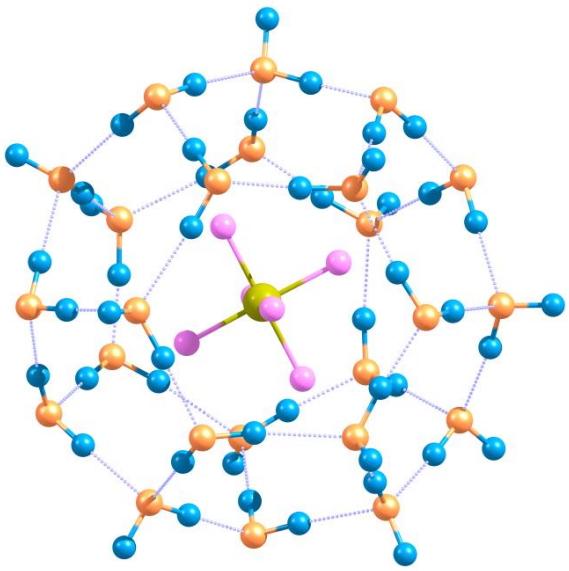
H	0.930644000	3.578231000	1.539071000
H	1.764303000	3.963672000	0.253350000
O	-2.259688000	-1.655057000	-2.962795000
H	-1.297883000	-1.834106000	-2.887590000
H	-2.685860000	-2.197654000	-2.229666000
O	-2.860520000	0.815335000	-2.742352000
H	-2.584103000	-0.181413000	-2.796665000
H	-3.351080000	0.972686000	-3.563912000
O	-3.297920000	-3.065225000	-0.960770000
H	-2.547236000	-3.432512000	-0.449636000
H	-3.760402000	-2.463987000	-0.317614000
O	-4.326227000	1.157653000	-0.504305000
H	-3.806739000	1.039816000	-1.348007000
H	-5.215379000	1.429593000	-0.775984000
O	-1.143858000	-4.169005000	0.556772000
H	-1.412100000	-5.094159000	0.663034000
H	-0.308046000	-4.197844000	-0.006619000
O	-3.135371000	3.091097000	1.187323000
H	-2.456995000	3.492873000	0.599200000
H	-3.571523000	2.415604000	0.624951000
O	2.612610000	0.482628000	2.842029000
H	1.868058000	1.139836000	2.891430000
H	3.166280000	0.771086000	2.083394000
O	-2.569990000	-0.878992000	2.922039000
H	-1.845980000	-1.579260000	2.910111000
H	-3.069511000	-1.051336000	3.734711000
O	4.207925000	1.179797000	0.647776000
H	4.291991000	0.382912000	0.066870000
H	5.110367000	1.432406000	0.894062000
O	-4.415541000	-1.335720000	0.829448000

H	-4.428997000	-0.468831000	0.371148000
H	-3.764818000	-1.207213000	1.554194000
O	1.997017000	-2.005438000	2.717303000
H	2.192245000	-0.996901000	2.744164000
H	2.262854000	-2.332770000	3.590754000
O	-0.723308000	-2.776710000	2.906372000
H	0.174322000	-2.405552000	2.774884000
H	-0.891908000	-3.316197000	2.096909000
O	0.699412000	2.397823000	2.905361000
H	-0.289057000	2.111325000	2.954694000
H	0.825477000	2.940343000	3.699263000
O	-1.786704000	1.806181000	3.142652000
H	-2.015649000	0.855879000	3.033658000
H	-2.321011000	2.292410000	2.452717000
C	0.384864000	0.010760000	-0.001985000
F	1.113679000	1.121877000	0.000121000
F	-0.455605000	0.029812000	-1.027610000
F	-0.292320000	-0.084030000	1.134452000
F	1.198034000	-1.045348000	-0.116782000

SF_6 within $5^{12}6^2$ clathrate hydrate

O	-1.128534000	-2.269838000	3.038584000
H	-1.601344000	-1.382313000	3.111541000
H	-1.306455000	-2.722330000	3.877238000
O	1.513003000	2.426681000	2.900630000
H	1.958550000	1.550064000	2.851466000
H	1.782679000	2.900328000	2.075369000

O	-2.146506000	-3.757486000	0.931547000
H	-1.797775000	-3.231931000	1.692386000
H	-2.726561000	-3.144833000	0.435562000
O	2.216515000	3.709402000	0.559920000
H	1.371344000	3.944026000	0.035875000
H	2.644317000	4.563220000	0.726686000
O	-2.485195000	-0.004293000	3.201652000
H	-1.933391000	0.816068000	3.187948000
H	-3.041346000	0.052964000	2.398564000
O	-1.089728000	2.380503000	3.059884000
H	-0.075463000	2.343984000	2.979302000
H	-1.249482000	2.912476000	3.854643000
O	-4.312417000	0.066503000	0.984281000
H	-4.204042000	-0.742092000	0.412253000
H	-5.158017000	-0.039254000	1.445994000
O	-2.019297000	3.946153000	0.905929000
H	-1.682967000	3.402257000	1.653465000
H	-2.622593000	3.352161000	0.416258000
O	-3.896076000	-2.078582000	-0.598113000
H	-4.633812000	-2.646408000	-0.867528000
H	-3.424802000	-1.810410000	-1.446552000
O	0.090459000	4.348770000	-0.777236000
H	-0.036847000	3.708677000	-1.513862000
H	-0.699756000	4.246419000	-0.183237000
O	1.723183000	-2.233866000	2.961567000
H	0.744427000	-2.177165000	2.959742000
H	1.955052000	-2.845448000	2.198120000
O	2.943888000	0.014609000	2.768173000
H	2.414202000	-0.869759000	2.814741000
H	3.496047000	0.004670000	3.565215000

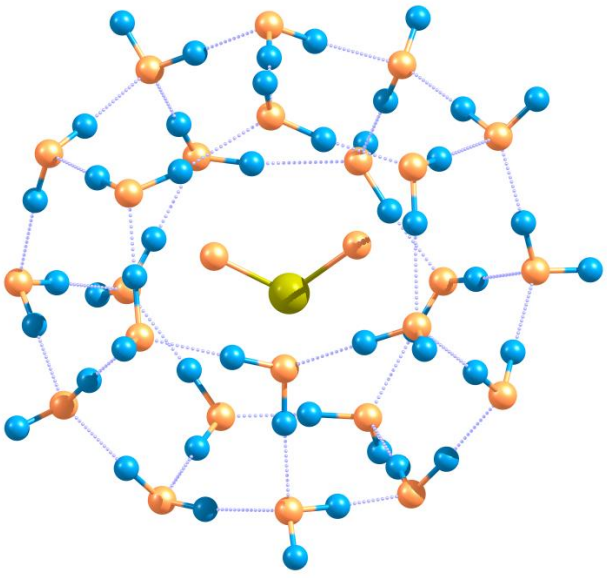


O	2.289565000	-3.812906000	0.884583000
H	1.468872000	-3.997410000	0.382838000
H	2.865201000	-3.332025000	0.232610000
O	4.371824000	0.013465000	0.466644000
H	3.864872000	0.024079000	1.324946000
H	5.307965000	-0.028166000	0.712214000
O	-0.083952000	-4.295126000	-0.636136000
H	-0.110147000	-5.253871000	-0.775527000
H	-0.864982000	-4.094916000	-0.032012000
O	3.745379000	2.192618000	-1.243298000
H	3.235273000	2.771153000	-0.633273000
H	3.999134000	1.428245000	-0.684151000
O	-2.560010000	1.242432000	-2.916059000
H	-1.668439000	1.674296000	-2.977663000
H	-2.970920000	1.626489000	-2.110558000
O	2.104319000	-1.449768000	-3.053057000
H	1.228547000	-1.944684000	-3.038650000
H	2.560101000	-1.766671000	-3.847583000
O	-3.774469000	2.236496000	-0.582137000
H	-4.038086000	1.485265000	0.006383000
H	-4.583124000	2.741452000	-0.755706000
O	3.735401000	-2.365044000	-0.923033000
H	3.971816000	-1.536309000	-0.455214000
H	3.144425000	-2.070328000	-1.649801000
O	-2.602314000	-1.334364000	-2.794872000
H	-2.522823000	-0.311339000	-2.823474000
H	-3.012102000	-1.572840000	-3.640921000
O	-0.168699000	-2.827342000	-2.992407000
H	-0.950092000	-2.246163000	-2.885278000
H	-0.138466000	-3.371586000	-2.169548000

O	-0.182766000	2.594922000	-2.963429000
H	0.695466000	2.069576000	-3.039518000
H	-0.160709000	3.207379000	-3.714953000
O	2.078130000	1.373125000	-3.221631000
H	2.045259000	0.393701000	-3.149913000
H	2.720464000	1.673360000	-2.519771000
S	0.020916000	-0.008742000	-0.002567000
F	-0.108058000	-0.067306000	-1.596794000
F	0.829651000	-1.385152000	-0.013147000
F	1.383991000	0.810229000	-0.129806000
F	0.124262000	0.045105000	1.593415000
F	-1.363476000	-0.827987000	0.126357000
F	-0.809453000	1.363922000	0.009808000

SO_2 within $5^{12}6^2$ clathrate hydrate

O	-0.088941000	2.675191000	2.709914000
H	0.812268000	2.230840000	2.804833000
H	-0.168351000	3.240770000	3.493253000
O	-0.022935000	-1.711470000	2.135011000
H	-0.924282000	-1.485225000	2.494458000
H	-0.062169000	-2.658505000	1.830186000
O	-0.046935000	4.293459000	0.475923000
H	-0.071065000	3.717528000	1.279425000
H	0.740879000	3.992259000	-0.022351000
O	-0.039806000	-4.172565000	1.061171000
H	0.813929000	-4.119524000	0.489237000
H	0.036425000	-4.993863000	1.569208000
O	2.342407000	1.687807000	3.022073000



H	2.340198000	0.709801000	3.141505000
H	2.813788000	1.822324000	2.173153000
O	2.305918000	-1.085373000	3.187973000
H	1.382643000	-1.324068000	2.877459000
H	2.413729000	-1.495445000	4.059008000
O	3.867239000	2.198955000	0.663548000
H	3.276407000	2.710420000	0.045997000
H	4.560937000	2.814736000	0.944083000
O	3.760061000	-2.313448000	1.085547000
H	3.295154000	-1.904496000	1.846958000
H	3.972270000	-1.560502000	0.495335000
O	2.248725000	3.540871000	-1.028063000
H	2.564120000	4.350639000	-1.456908000
H	1.942778000	2.934598000	-1.769818000
O	2.111210000	-3.949768000	-0.322820000
H	1.902603000	-3.458937000	-1.151031000
H	2.742493000	-3.372159000	0.187218000
O	-2.611216000	1.431690000	2.822627000
H	-1.702627000	1.776932000	2.679066000
H	-3.147771000	1.735449000	2.019357000
O	-2.520409000	-1.077147000	2.910746000
H	-2.566774000	-0.024278000	2.840948000
H	-2.802522000	-1.281753000	3.815193000
O	-3.970031000	2.209506000	0.696835000
H	-3.326233000	2.673027000	0.120304000
H	-4.241752000	1.415384000	0.163220000
O	-3.885880000	-2.177114000	0.862601000
H	-3.427657000	-1.774202000	1.649697000
H	-4.716374000	-2.548688000	1.194522000
O	-2.153033000	3.627837000	-0.967028000

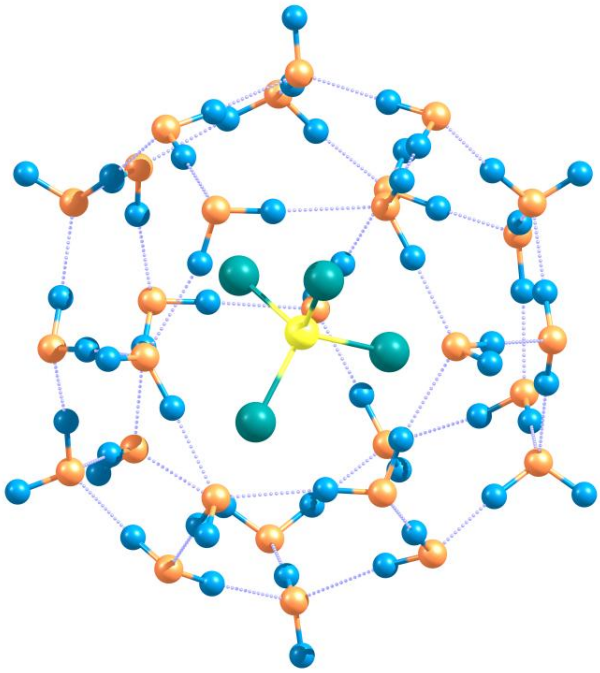
H	-2.599471000	4.465839000	-1.160105000
H	-1.354288000	3.876051000	-0.402272000
O	-2.235431000	-3.880505000	-0.668289000
H	-1.490237000	-4.075577000	-0.059936000
H	-2.837589000	-3.306378000	-0.147481000
O	2.830209000	-0.233000000	-2.914026000
H	2.298909000	-1.067522000	-2.852981000
H	3.397493000	-0.230196000	-2.110000000
O	-2.704379000	-0.161026000	-2.913726000
H	-2.194424000	0.706675000	-2.982764000
H	-3.216901000	-0.218490000	-3.734256000
O	4.431249000	-0.147505000	-0.623318000
H	4.250660000	0.690762000	-0.126474000
H	5.386690000	-0.163930000	-0.783623000
O	-4.588744000	0.011251000	-0.807060000
H	-4.341744000	-0.751098000	-0.243089000
H	-3.921429000	-0.008441000	-1.527439000
O	1.429821000	1.921820000	-2.963275000
H	1.943656000	1.033251000	-2.912432000
H	1.576454000	2.239813000	-3.867840000
O	-1.386937000	2.113197000	-3.132886000
H	-0.433042000	1.952633000	-2.976607000
H	-1.679350000	2.679060000	-2.376510000
O	1.418085000	-2.556935000	-2.646899000
H	0.397238000	-2.461869000	-2.642674000
H	1.603946000	-3.152050000	-3.389606000
O	-1.146755000	-2.440495000	-2.670488000
H	-1.668322000	-1.608744000	-2.754582000
H	-1.586109000	-2.981222000	-1.955813000
S	0.119314000	-0.377399000	-0.124396000

O	-1.162983000	0.317925000	0.026225000
O	1.332715000	0.413937000	0.145597000

Table S5. Cartesian coordinates for optimized geometries of the Greenhouse gases encapsulated within $5^{12}6^4$ clathrate hydrate computes at B3LYP/6-31G(d) level of theory and basis set.

CCl_4 within $5^{12}6^4$ clathrate hydrate

O	2.397120000	-2.199202000	-3.195348000
H	1.429646000	-2.334345000	-3.305665000
H	2.603065000	-2.517130000	-2.286901000
O	-2.468923000	-0.942612000	-3.897123000
H	-2.098115000	-0.037821000	-4.019918000
H	-1.699302000	-1.548359000	-3.871743000
O	-1.485214000	1.673547000	-4.048812000
H	-1.678759000	2.116629000	-4.889079000
H	-0.486529000	1.815616000	-3.911346000
O	1.046008000	2.235090000	-3.777356000
H	1.159905000	2.875925000	-3.026093000
H	1.699899000	1.521979000	-3.614958000
O	-2.798968000	3.082888000	-2.034800000
H	-3.328633000	2.412920000	-1.540246000
H	-2.321817000	2.576854000	-2.736092000
O	-4.324342000	1.255487000	-0.595475000
H	-4.120205000	1.390777000	0.387631000
H	-5.251803000	1.522437000	-0.688360000
O	-1.216383000	4.397785000	-0.453531000



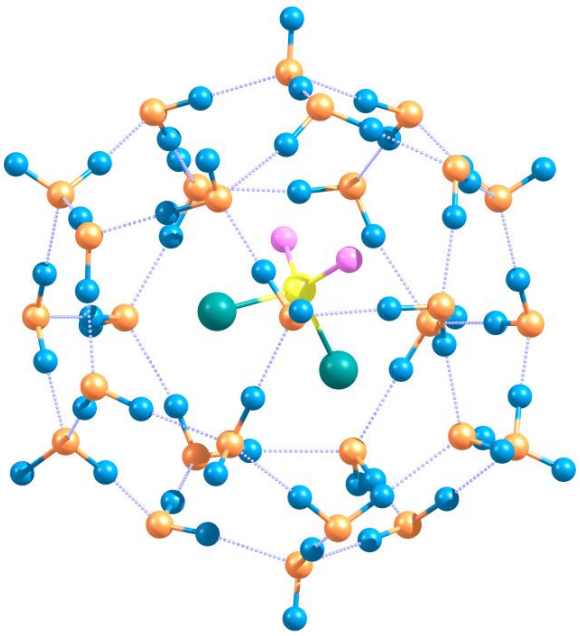
H	-1.343458000	5.308624000	-0.762013000
H	-1.820311000	3.840089000	-1.062597000
O	2.789317000	2.411417000	2.510386000
H	3.380995000	2.888872000	3.111726000
H	3.028765000	2.724004000	1.596572000
O	3.498218000	3.149325000	-0.011801000
H	4.138761000	3.866122000	-0.136605000
H	3.912046000	2.341787000	-0.459361000
O	1.322841000	3.973869000	-1.685736000
H	0.490377000	4.026883000	-1.169584000
H	2.004406000	3.647455000	-1.062094000
O	-1.899597000	3.806422000	2.100531000
H	-1.654807000	4.094866000	1.176706000
H	-2.279073000	4.585409000	2.534496000
O	4.594178000	1.047886000	-1.163114000
H	4.606714000	0.251623000	-0.583109000
H	4.131064000	0.776735000	-1.993477000
O	4.515173000	-1.171589000	0.562603000
H	4.062125000	-0.839295000	1.420203000
H	5.407358000	-1.423564000	0.847455000
O	3.140136000	0.327177000	-3.413285000
H	3.642156000	0.351475000	-4.242161000
H	2.820875000	-0.627196000	-3.326887000
O	-2.725026000	-2.772978000	2.548620000
H	-2.829411000	-2.793861000	1.573818000
H	-1.813411000	-3.130123000	2.717539000
O	-3.212195000	-3.129254000	-0.245457000
H	-3.564691000	-2.360732000	-0.828561000
H	-3.973153000	-3.720909000	-0.138203000
O	-4.192374000	-1.286752000	-1.771203000

H	-4.206920000	-0.412451000	-1.317080000
H	-3.614874000	-1.155236000	-2.566569000
O	-3.901806000	1.755742000	1.952318000
H	-3.531882000	0.987661000	2.452761000
H	-3.219480000	2.457420000	2.024010000
O	-1.086311000	-4.268054000	-1.385657000
H	-1.884492000	-3.838225000	-0.950833000
H	-1.353561000	-5.184024000	-1.557887000
O	-0.333879000	-2.835591000	-3.596127000
H	-0.616798000	-3.357115000	-2.798062000
H	-0.317814000	-3.473071000	-4.326466000
O	0.983856000	-4.634341000	0.612658000
H	0.265469000	-4.477516000	-0.034143000
H	1.703438000	-4.048325000	0.298447000
O	3.094589000	-3.154045000	-0.641444000
H	3.595647000	-2.441921000	-0.157412000
H	3.738469000	-3.862610000	-0.793762000
O	-0.160215000	-3.663091000	2.953649000
H	0.450999000	-3.000580000	3.343757000
H	0.314402000	-4.068003000	2.186543000
O	1.433160000	-1.559846000	4.039419000
H	1.727434000	-1.791798000	4.934063000
H	0.740729000	-0.827668000	4.192328000
O	3.536349000	-0.283315000	2.785261000
H	2.780583000	-0.780753000	3.189356000
H	3.218262000	0.641818000	2.679027000
O	-0.337258000	0.284024000	4.570862000
H	-0.119989000	1.216067000	4.313736000
H	-1.202914000	0.086352000	4.146228000
O	0.281742000	2.871926000	3.795192000

H	1.068756000	2.747260000	3.225150000
H	-0.418501000	3.210958000	3.201423000
O	-2.846420000	-0.321965000	3.463778000
H	-2.785247000	-1.254582000	3.062365000
H	-3.416353000	-0.433713000	4.240247000
C	0.021430000	-0.017958000	0.019533000
Cl	-0.989821000	-0.291770000	-1.427122000
Cl	1.696147000	0.369298000	-0.487509000
Cl	-0.633002000	1.354078000	0.958099000
Cl	0.017922000	-1.480756000	1.036086000

CF_2Cl_2 within $5^{12}6^4$ clathrate hydrate

O	0.866520000	0.182238000	-4.493298000
H	-0.095727000	0.119882000	-4.299355000
H	1.269235000	-0.612465000	-4.073204000
O	-3.541646000	1.590982000	-2.421390000
H	-3.030567000	2.373579000	-2.110017000
H	-2.926630000	1.082639000	-2.989506000
O	-2.137583000	3.786448000	-1.454305000
H	-2.497815000	4.605559000	-1.827097000
H	-1.132583000	3.848551000	-1.626791000
O	0.397464000	4.116568000	-1.893159000
H	0.891777000	4.201462000	-1.033416000
H	0.857596000	3.399212000	-2.381257000
O	-2.595829000	3.737697000	1.260119000
H	-3.110318000	2.912436000	1.433466000
H	-2.454312000	3.761346000	0.281622000
O	-4.024465000	1.419543000	1.803030000



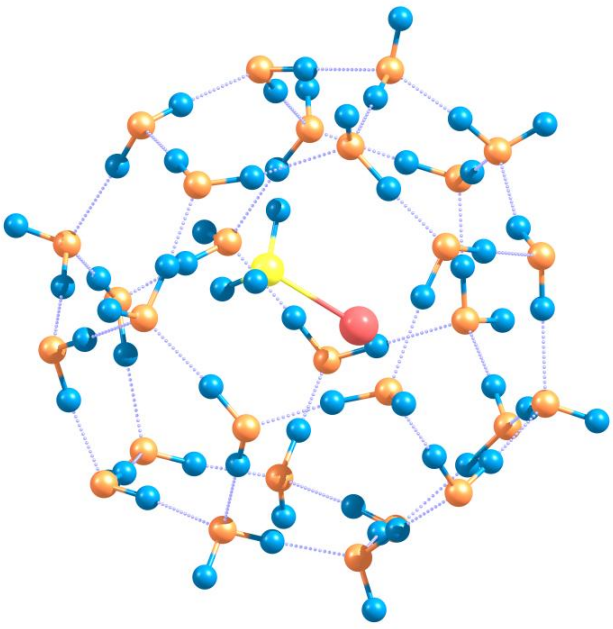
H	-3.469519000	0.900086000	2.478784000
H	-4.823448000	1.674762000	2.289472000
O	-0.300498000	3.734707000	2.432838000
H	-0.292742000	4.603006000	2.864857000
H	-1.206518000	3.700138000	1.950153000
O	4.063633000	0.351352000	2.205794000
H	4.826996000	0.435023000	2.796957000
H	4.045553000	1.183858000	1.659038000
O	3.958595000	2.525260000	0.596378000
H	4.677748000	3.174060000	0.642412000
H	4.013052000	2.135190000	-0.340545000
O	1.683783000	4.254301000	0.498768000
H	1.020610000	3.971775000	1.165361000
H	2.411748000	3.600750000	0.559061000
O	-0.249994000	1.625633000	4.095247000
H	-0.232538000	2.424489000	3.496547000
H	-0.277039000	1.974051000	4.999201000
O	4.102026000	1.515521000	-1.799724000
H	4.155812000	0.532411000	-1.841408000
H	3.340403000	1.776373000	-2.374514000
O	4.183008000	-1.267549000	-1.842615000
H	4.154541000	-1.558266000	-0.855436000
H	5.037051000	-1.588649000	-2.170825000
O	1.952706000	2.272974000	-3.342039000
H	2.252259000	2.814809000	-4.088129000
H	1.498134000	1.473020000	-3.766320000
O	-2.370444000	-3.641909000	1.185123000
H	-2.753051000	-3.063722000	0.493289000
H	-1.553934000	-4.060614000	0.781868000
O	-3.846193000	-2.280006000	-0.813391000

H	-4.201672000	-1.324877000	-0.667167000
H	-4.618530000	-2.857818000	-0.714686000
O	-4.802811000	0.093066000	-0.529270000
H	-4.532958000	0.513618000	0.320456000
H	-4.405551000	0.670523000	-1.233770000
O	-2.641007000	0.219424000	3.658438000
H	-2.355567000	-0.710570000	3.479822000
H	-1.800487000	0.708486000	3.802476000
O	-2.484092000	-2.484893000	-3.069379000
H	-3.031309000	-2.413964000	-2.226557000
H	-2.940975000	-3.131660000	-3.628107000
O	-1.909568000	-0.039043000	-4.086367000
H	-2.136669000	-0.945726000	-3.745144000
H	-2.312393000	0.014390000	-4.966639000
O	-0.026409000	-3.822247000	-2.479589000
H	-0.863285000	-3.337160000	-2.630252000
H	0.668837000	-3.135782000	-2.539926000
O	2.013443000	-2.040255000	-3.260960000
H	2.812653000	-1.797891000	-2.716988000
H	2.324360000	-2.685517000	-3.914051000
O	-0.134591000	-4.691252000	0.140867000
H	0.636041000	-4.246493000	0.554923000
H	-0.076901000	-4.450252000	-0.816042000
O	2.115843000	-3.519876000	1.436811000
H	2.521226000	-4.333150000	1.777069000
H	1.697483000	-3.093807000	2.268410000
O	4.221883000	-1.964744000	0.631744000
H	3.442343000	-2.520288000	0.895915000
H	4.170262000	-1.159344000	1.194831000
O	1.078001000	-2.551630000	3.599683000

H	1.429081000	-1.653858000	3.841611000
H	0.105942000	-2.437701000	3.488205000
O	2.027015000	-0.051164000	4.139954000
H	2.634672000	0.149338000	3.398287000
H	1.261634000	0.552049000	4.030423000
O	-1.688438000	-2.332565000	3.305004000
H	-1.950442000	-2.818181000	2.443229000
H	-2.044602000	-2.890618000	4.013389000
C	-0.021244000	-0.391213000	0.350645000
Cl	-1.451137000	0.344463000	-0.410729000
Cl	1.488705000	0.304650000	-0.303972000
F	-0.060448000	-0.187175000	1.670856000
F	-0.030990000	-1.707804000	0.127761000

CH_3Br within $5^{12}6^4$ clathrate hydrate

O	4.106623000	-1.945974000	0.694377000
H	3.354883000	-2.429247000	1.106836000
H	4.081151000	-1.052146000	1.102788000
O	-0.263541000	-4.444810000	0.879835000
H	-0.352404000	-4.303623000	-0.091472000
H	0.510586000	-3.904988000	1.141722000
O	-0.513353000	-4.062292000	-1.855660000
H	-0.437583000	-4.918033000	-2.304534000
H	0.246625000	-3.504907000	-2.239232000
O	1.382408000	-2.735961000	-3.018247000
H	1.005550000	-1.975369000	-3.540555000
H	2.182103000	-2.389546000	-2.565121000
O	-2.931619000	-2.875986000	-2.407951000



H	-3.305407000	-2.675633000	-1.515596000
H	-2.065939000	-3.318919000	-2.225675000
O	-3.971001000	-2.276868000	0.084720000
H	-4.235751000	-1.295363000	0.080567000
H	-4.809988000	-2.754233000	0.175290000
O	-2.479453000	-0.681133000	-3.676878000
H	-2.816867000	-0.881138000	-4.563838000
H	-2.640916000	-1.543979000	-3.141851000
O	0.437067000	3.709724000	-2.493303000
H	0.514647000	4.494617000	-3.056422000
H	0.866629000	2.963768000	-3.002553000
O	1.666109000	1.697087000	-3.751512000
H	2.004265000	1.861992000	-4.645115000
H	2.487102000	1.417991000	-3.209174000
O	0.256510000	-0.663852000	-4.330942000
H	-0.667195000	-0.620320000	-4.000303000
H	0.684284000	0.159276000	-4.011714000
O	-3.729156000	1.312282000	-2.391030000
H	-3.251680000	0.594721000	-2.898166000
H	-4.463643000	1.589754000	-2.959130000
O	3.804728000	1.030373000	-2.454320000
H	3.807086000	1.484752000	-1.581399000
H	3.763039000	0.063699000	-2.247053000
O	3.856289000	2.431298000	-0.031442000
H	3.029884000	3.034421000	-0.026443000
H	4.603432000	3.044295000	-0.109442000
O	3.709971000	-1.663444000	-1.885229000
H	4.478883000	-2.115720000	-2.264984000
H	3.808244000	-1.778825000	-0.884022000
O	-2.268014000	0.950675000	3.653712000

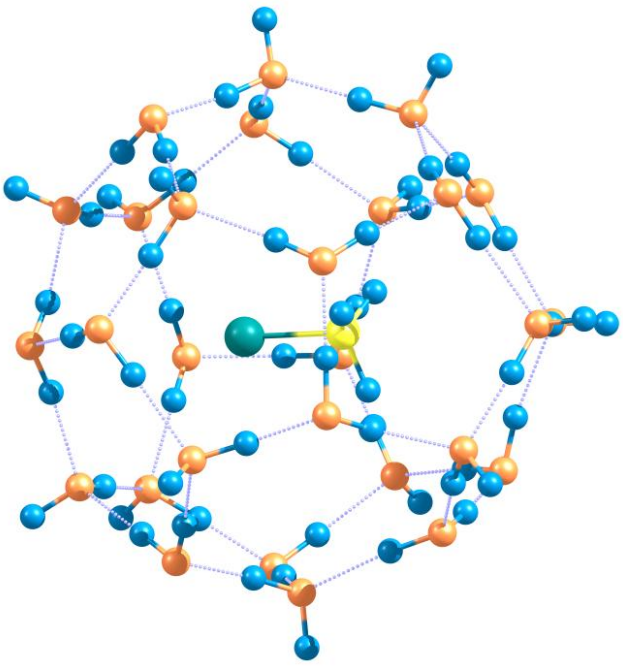
H	-1.972916000	0.018071000	3.582562000
H	-1.441743000	1.494317000	3.809574000
O	-1.488194000	-1.738870000	3.815995000
H	-1.855386000	-2.385400000	3.087929000
H	-2.012817000	-1.934745000	4.607751000
O	-2.403376000	-3.381279000	2.106244000
H	-2.918032000	-2.927504000	1.399065000
H	-1.634980000	-3.821257000	1.639650000
O	-4.777035000	0.200768000	-0.043182000
H	-4.428203000	0.792727000	0.667600000
H	-4.426581000	0.591364000	-0.875350000
O	1.123760000	-1.961248000	4.126871000
H	0.121665000	-1.891902000	4.034086000
H	1.285220000	-2.286900000	5.025168000
O	2.074674000	-3.347382000	1.996664000
H	1.760481000	-2.872775000	2.810295000
H	2.389210000	-4.212404000	2.300610000
O	2.112718000	0.695563000	3.950770000
H	1.790150000	-0.227269000	4.013283000
H	2.781642000	0.688838000	3.234598000
O	4.069385000	0.584391000	1.915591000
H	3.978626000	1.301696000	1.228636000
H	4.926039000	0.737197000	2.342292000
O	-0.058352000	2.417076000	3.975159000
H	0.014926000	3.023117000	3.206473000
H	0.757663000	1.863550000	3.965953000
O	-0.018225000	4.215250000	1.804568000
H	0.003442000	5.082152000	2.238672000
H	-0.952952000	4.165513000	1.383356000
O	1.865451000	4.061501000	-0.149292000

H	1.201098000	4.127777000	0.584879000
H	1.343592000	3.957468000	-0.978602000
O	-2.390312000	4.152716000	0.787555000
H	-2.392958000	4.039739000	-0.201214000
H	-2.887564000	3.378124000	1.138988000
O	-2.329316000	3.722332000	-1.900930000
H	-1.382444000	3.598968000	-2.120348000
H	-2.752193000	2.851390000	-2.060542000
O	-3.773346000	1.959365000	1.819702000
H	-3.167181000	1.527918000	2.519472000
H	-4.507710000	2.334381000	2.329778000
C	0.316265000	0.755432000	0.838479000
H	0.917764000	0.521680000	1.714358000
H	0.583996000	1.728140000	0.431154000
H	-0.744829000	0.701168000	1.073771000
Br	0.707805000	-0.589584000	-0.556084000

CH_3Cl within $5^{12}6^4$ clathrate hydrate

O	0.587330000	2.575380000	-3.529876000
H	1.308103000	1.908407000	-3.569082000
H	0.774536000	3.139084000	-2.744795000
O	1.961206000	-2.077583000	-3.557180000
H	0.988631000	-2.239917000	-3.543982000
H	2.072852000	-1.105887000	-3.587362000
O	-0.738203000	-2.721456000	-3.537114000

H	-0.879803000	-3.242107000	-4.342652000
H	-1.457474000	-1.994152000	-3.575847000
O	-2.631233000	-0.968279000	-3.716349000
H	-3.259728000	-1.085297000	-2.950769000
H	-2.310493000	-0.043156000	-3.641164000
O	-1.235539000	-4.368885000	-1.384648000
H	-0.397647000	-4.351725000	-0.861407000
H	-1.059630000	-3.786578000	-2.164570000
O	1.104070000	-4.294092000	0.088087000
H	0.879749000	-4.047680000	1.053413000
H	1.450961000	-5.197921000	0.140590000
O	-3.143631000	-3.335424000	0.011507000
H	-3.851179000	-3.992156000	-0.081815000
H	-2.367771000	-3.717833000	-0.541223000
O	-3.559691000	1.593574000	2.309138000
H	-4.323955000	1.849386000	2.847017000
H	-3.913106000	1.425350000	1.391395000
O	-4.437822000	1.231838000	-0.209833000
H	-5.381719000	1.392678000	-0.363396000
H	-3.961700000	1.942467000	-0.766537000
O	-4.234676000	-1.257976000	-1.551889000
H	-3.805124000	-1.919092000	-0.965876000
H	-4.211374000	-0.415594000	-1.049555000
O	-2.208273000	-3.021803000	2.517916000
H	-2.582918000	-3.121295000	1.597878000
H	-2.713476000	-3.632026000	3.075879000
O	-3.284650000	3.076605000	-1.631657000
H	-2.588166000	3.524148000	-1.097003000
H	-2.796357000	2.617416000	-2.357690000
O	-1.330239000	4.380482000	-0.116284000



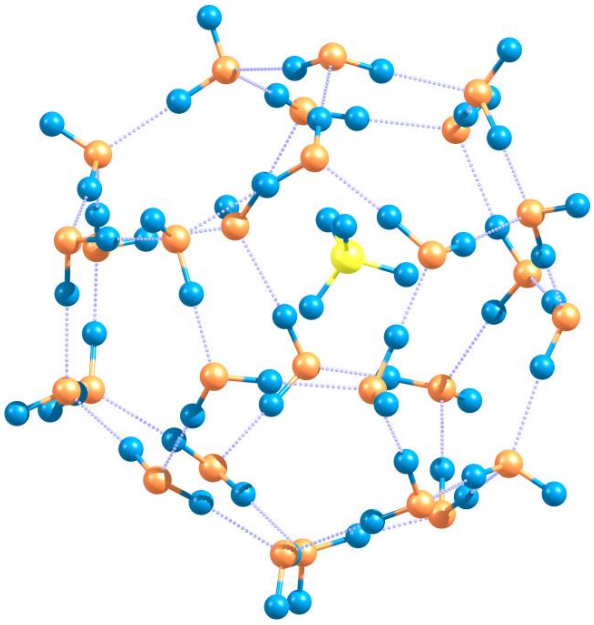
H	-1.409025000	4.021810000	0.850993000
H	-1.632912000	5.299688000	-0.051372000
O	-1.903584000	1.747757000	-3.618832000
H	-2.194360000	2.073866000	-4.484223000
H	-0.929889000	2.004528000	-3.561516000
O	3.835119000	-0.524882000	2.544478000
H	4.002693000	-0.762785000	1.608776000
H	3.622135000	0.449329000	2.519462000
O	4.504796000	-1.083046000	-0.156901000
H	3.896283000	-1.805835000	-0.572347000
H	5.371318000	-1.506956000	-0.058914000
O	3.057207000	-2.873955000	-1.243047000
H	2.353589000	-3.326027000	-0.719919000
H	2.648807000	-2.623202000	-2.119507000
O	0.480533000	-3.793414000	2.553613000
H	0.988888000	-3.032900000	2.930643000
H	-0.457941000	-3.497281000	2.557171000
O	4.410683000	1.078105000	-1.681157000
H	4.488659000	0.259377000	-1.098619000
H	5.319525000	1.349162000	-1.881109000
O	2.630379000	0.681779000	-3.679962000
H	3.334012000	0.819132000	-2.990347000
H	3.083605000	0.731139000	-4.535313000
O	3.467783000	3.254943000	-0.061423000
H	3.755666000	2.506088000	-0.621686000
H	2.587940000	3.507791000	-0.410313000
O	1.069415000	4.133777000	-1.286610000
H	0.205446000	4.230390000	-0.791067000
H	1.328397000	5.033618000	-1.536982000
O	3.128796000	2.056627000	2.393022000

H	2.215489000	2.257379000	2.695568000
H	3.266201000	2.554361000	1.551133000
O	0.585401000	2.550281000	3.452996000
H	0.798234000	3.091283000	4.229599000
H	0.343167000	1.634839000	3.851446000
O	-1.643303000	3.611052000	2.299608000
H	-0.822050000	3.220589000	2.699778000
H	-2.310771000	2.886545000	2.317733000
O	0.023148000	0.289172000	4.561990000
H	-0.891269000	-0.020319000	4.321725000
H	0.633147000	-0.401430000	4.214491000
O	-2.468175000	-0.531092000	3.824097000
H	-2.809242000	0.147470000	3.205383000
H	-2.371698000	-1.350085000	3.293510000
O	1.813628000	-1.681996000	3.697649000
H	2.580560000	-1.248059000	3.185873000
H	2.218314000	-1.985119000	4.524791000
C	1.075457000	0.297625000	-0.209757000
H	0.850462000	0.947501000	-1.056852000
H	1.742298000	0.792742000	0.497399000
H	1.503047000	-0.644674000	-0.555335000
Cl	-0.476381000	-0.066245000	0.648020000

CH_4 within $5^{12}6^4$ clathrate hydrate

O	0.294231000	2.572265000	-3.607449000
H	1.155565000	2.107339000	-3.509434000
H	0.216888000	3.165562000	-2.825519000
O	2.888780000	-1.548134000	-3.128669000

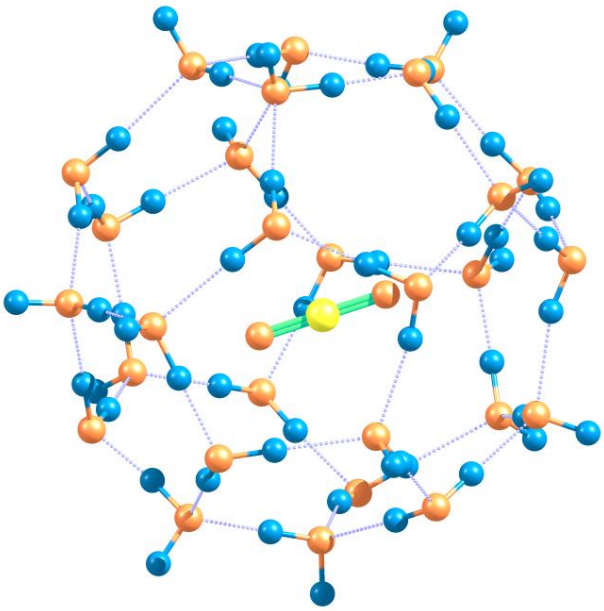
H	2.002845000	-1.972631000	-3.201311000
H	2.731295000	-0.584684000	-3.204014000
O	0.479210000	-2.925740000	-3.372475000
H	0.600225000	-3.472735000	-4.163761000
H	-0.390184000	-2.417085000	-3.545615000
O	-1.766167000	-1.740118000	-3.886905000
H	-2.440055000	-2.005427000	-3.203218000
H	-1.716677000	-0.760740000	-3.829061000
O	0.159032000	-4.580909000	-1.200033000
H	0.900185000	-4.332223000	-0.595115000
H	0.275195000	-4.003208000	-1.995181000
O	2.210274000	-3.848445000	0.498923000
H	1.816064000	-3.638803000	1.414422000
H	2.772504000	-4.624444000	0.646449000
O	-2.109002000	-4.058018000	-0.100720000
H	-2.602854000	-4.882444000	-0.232082000
H	-1.194579000	-4.238002000	-0.536489000
O	-4.147121000	0.600996000	1.847423000
H	-5.013596000	0.649591000	2.278699000
H	-4.325035000	0.319993000	0.906227000
O	-4.551589000	-0.051839000	-0.732089000
H	-5.476461000	-0.165967000	-1.000761000
H	-4.222039000	0.747073000	-1.278987000
O	-3.511087000	-2.412712000	-1.916877000
H	-3.003593000	-2.919057000	-1.245598000
H	-3.795076000	-1.592029000	-1.460919000
O	-1.618520000	-3.440187000	2.472818000
H	-1.838705000	-3.670026000	1.526038000
H	-1.990801000	-4.155496000	3.010343000
O	-3.774020000	1.987569000	-2.130203000



H	-3.317127000	2.645222000	-1.555312000
H	-3.084331000	1.675022000	-2.766280000
O	-2.494659000	3.850299000	-0.493308000
H	-2.601293000	3.522720000	0.478577000
H	-3.033417000	4.655798000	-0.532387000
O	-1.838936000	1.069959000	-3.864649000
H	-2.116078000	1.262803000	-4.773525000
H	-0.986488000	1.599116000	-3.738696000
O	3.358224000	0.624227000	2.992129000
H	3.681733000	0.408149000	2.092124000
H	2.918808000	1.518419000	2.902331000
O	4.541088000	0.149294000	0.465453000
H	4.265887000	-0.736313000	0.011891000
H	5.461186000	0.016719000	0.741003000
O	3.943989000	-2.040869000	-0.704065000
H	3.295487000	-2.618627000	-0.238958000
H	3.573058000	-1.892716000	-1.619118000
O	1.163302000	-3.453618000	2.846663000
H	1.380527000	-2.569961000	3.236427000
H	0.186867000	-3.440769000	2.731084000
O	4.090802000	2.165431000	-1.190735000
H	4.289150000	1.407046000	-0.557882000
H	4.923429000	2.650898000	-1.291971000
O	2.758025000	1.278327000	-3.375912000
H	3.283232000	1.612435000	-2.599801000
H	3.310426000	1.438160000	-4.156151000
O	2.389882000	4.017549000	0.178806000
H	2.942839000	3.359782000	-0.290281000
H	1.525995000	3.990122000	-0.281587000
O	0.026883000	4.212099000	-1.379209000

H	-0.884714000	4.089313000	-0.992394000
H	0.091192000	5.152158000	-1.605940000
O	2.084215000	2.959346000	2.704335000
H	1.117959000	2.849734000	2.836137000
H	2.192277000	3.392874000	1.822650000
O	-0.642305000	2.682494000	3.376782000
H	-0.643939000	3.296120000	4.128122000
H	-0.683702000	1.757770000	3.816318000
O	-2.906818000	3.099645000	1.923213000
H	-2.072440000	2.962930000	2.445245000
H	-3.350909000	2.220959000	1.914704000
O	-0.716866000	0.393731000	4.580697000
H	-1.476474000	-0.173348000	4.282048000
H	0.097529000	-0.111701000	4.351867000
O	-2.775428000	-1.128997000	3.627348000
H	-3.191362000	-0.578417000	2.931914000
H	-2.374176000	-1.889336000	3.155535000
O	1.628118000	-1.008712000	4.001804000
H	2.294373000	-0.381912000	3.541765000
H	2.014191000	-1.161823000	4.877989000
C	0.921246000	0.512606000	-0.271699000
H	0.050049000	0.005062000	0.152411000
H	0.613394000	1.083439000	-1.152830000
H	1.664736000	-0.234403000	-0.564377000
H	1.345239000	1.186902000	0.477675000

CO_2 within $5^{12}6^4$ clathrate hydrate

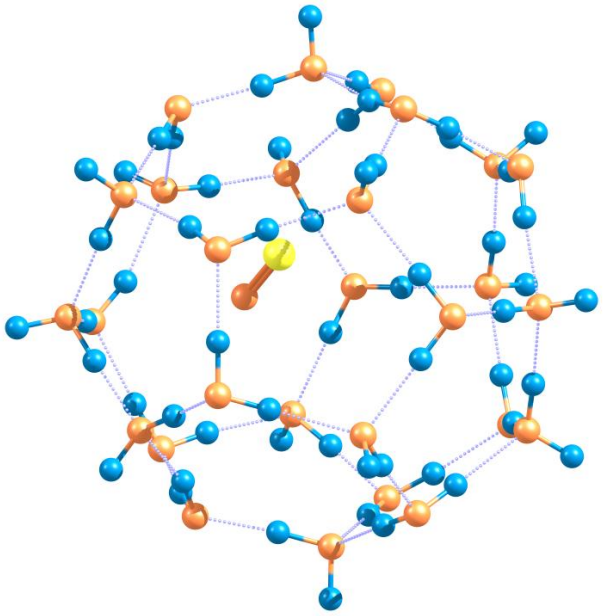


O	-1.434119000	-2.422328000	-3.534817000
H	-0.449937000	-2.394517000	-3.518677000
H	-1.717912000	-1.483195000	-3.622811000
O	3.084999000	-3.089743000	-1.419638000
H	2.617975000	-3.446069000	-0.629149000
H	2.374918000	-2.787640000	-2.021878000
O	1.821895000	-4.129239000	0.844009000
H	2.128830000	-5.038609000	0.980390000
H	0.811300000	-4.208665000	0.754855000
O	-0.765213000	-4.434874000	0.739226000
H	-1.136337000	-3.891155000	1.482803000
H	-1.215791000	-4.080884000	-0.057473000
O	2.499296000	-2.582437000	3.017248000
H	3.062610000	-1.861015000	2.644071000
H	2.252031000	-3.146493000	2.242400000
O	4.031914000	-0.527881000	1.991295000
H	3.671594000	0.361859000	2.328681000
H	4.921448000	-0.590321000	2.371861000
O	0.400390000	-1.571825000	4.100325000
H	0.326381000	-2.068384000	4.930210000
H	1.235098000	-1.965370000	3.641784000
O	-3.578631000	1.475450000	2.332427000
H	-4.309706000	1.813450000	2.871355000
H	-3.703171000	0.487132000	2.292891000
O	-3.933017000	-1.190238000	2.112886000
H	-4.672807000	-1.601582000	2.585574000
H	-4.105786000	-1.389887000	1.126084000
O	-1.688804000	-2.790227000	2.681179000

H	-0.999737000	-2.264569000	3.140760000
H	-2.436377000	-2.182649000	2.496121000
O	0.778426000	1.075793000	4.355761000
H	0.618506000	0.091666000	4.298920000
H	0.891524000	1.271805000	5.298057000
O	-4.407521000	-1.726662000	-0.384344000
H	-4.310939000	-0.900678000	-0.913792000
H	-3.690308000	-2.322223000	-0.709642000
O	-4.127277000	0.612010000	-1.881172000
H	-3.932741000	1.379956000	-1.220734000
H	-4.996107000	0.830392000	-2.252683000
O	-2.403801000	-3.416440000	-1.320185000
H	-2.872769000	-4.218980000	-1.596853000
H	-2.004451000	-3.041015000	-2.173554000
O	2.792888000	3.486039000	-1.205114000
H	3.023859000	2.571549000	-1.472222000
H	1.965635000	3.714913000	-1.723446000
O	3.747463000	1.032108000	-2.226142000
H	4.012291000	0.254426000	-1.592938000
H	4.590820000	1.418747000	-2.508509000
O	4.489839000	-0.894776000	-0.731064000
H	4.275112000	-0.729167000	0.215880000
H	4.002315000	-1.732955000	-0.973699000
O	3.157805000	1.705243000	3.008740000
H	2.901460000	2.404474000	2.356944000
H	2.326082000	1.504105000	3.492898000
O	2.202001000	0.171958000	-4.179732000
H	2.817824000	0.507474000	-3.454086000
H	2.681307000	0.297063000	-5.012716000
O	1.350114000	-2.316735000	-3.530948000

H	1.676953000	-1.418782000	-3.807560000
H	1.720463000	-2.938894000	-4.175587000
O	-0.021609000	1.967881000	-4.280983000
H	0.748928000	1.365275000	-4.237335000
H	-0.763648000	1.433825000	-3.931053000
O	-2.207969000	0.244442000	-3.725126000
H	-2.913834000	0.434487000	-3.044084000
H	-2.625308000	0.404873000	-4.585271000
O	0.518932000	4.027869000	-2.509056000
H	-0.206845000	3.964362000	-1.851097000
H	0.315630000	3.333332000	-3.182360000
O	-1.568069000	4.074184000	-0.596101000
H	-1.883741000	4.970659000	-0.790917000
H	-1.093753000	4.174001000	0.305904000
O	-3.800915000	2.543434000	-0.229911000
H	-2.978563000	3.077165000	-0.386591000
H	-3.703085000	2.176372000	0.678757000
O	-0.365456000	4.427086000	1.670074000
H	-0.736837000	3.854040000	2.392293000
H	0.575185000	4.151958000	1.569778000
O	-1.372832000	2.745938000	3.574645000
H	-2.057297000	2.209964000	3.122747000
H	-0.651691000	2.120129000	3.797477000
O	2.312491000	3.704260000	1.324768000
H	2.486829000	3.577843000	0.323197000
H	2.803954000	4.508483000	1.552600000
C	-0.629078000	-0.942454000	0.012295000
O	0.349921000	-1.530577000	-0.233379000
O	-1.599753000	-0.333134000	0.244837000

CO within $5^{12}6^4$ clathrate hydrate



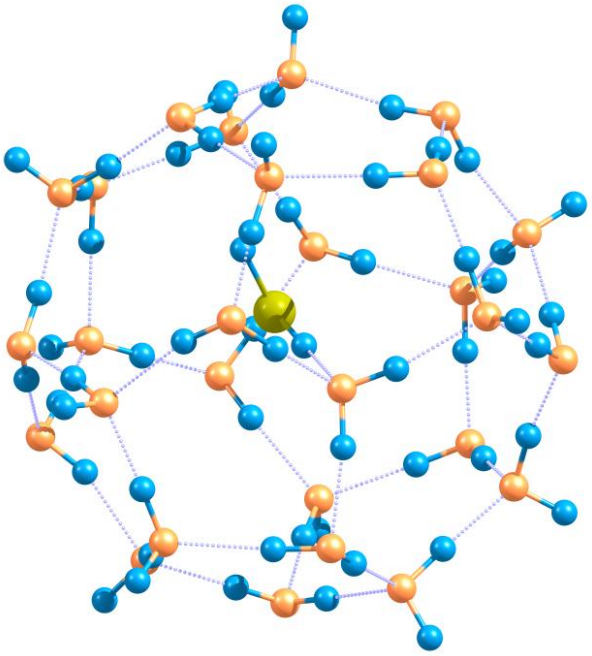
O	0.754672000	1.217387000	-4.244087000
H	1.636467000	1.037590000	-3.848593000
H	0.376825000	1.964837000	-3.725933000
O	3.813870000	-1.704968000	-1.730855000
H	3.081295000	-2.359262000	-1.811389000
H	3.543186000	-0.920390000	-2.248420000
O	1.863664000	-3.678093000	-1.829458000
H	2.245004000	-4.423826000	-2.317873000
H	0.991659000	-3.468952000	-2.320398000
O	-0.349980000	-3.289810000	-3.113235000
H	-1.120672000	-3.476802000	-2.511332000
H	-0.482469000	-2.365782000	-3.418033000
O	1.269823000	-4.499983000	0.726920000
H	1.775175000	-3.880975000	1.308086000
H	1.491366000	-4.222604000	-0.197157000
O	2.648413000	-2.734614000	2.346611000
H	2.002519000	-2.320225000	3.015931000
H	3.268270000	-3.245240000	2.889826000
O	-1.258122000	-4.236307000	1.135417000
H	-1.551670000	-5.154154000	1.245795000
H	-0.246880000	-4.312251000	0.963425000
O	-4.544096000	0.099966000	0.751680000
H	-5.488777000	0.066126000	0.965163000
H	-4.416793000	-0.513551000	-0.025537000
O	-4.134647000	-1.459290000	-1.403420000
H	-4.919160000	-1.902644000	-1.762027000
H	-3.824320000	-0.838628000	-2.154935000

O	-2.408085000	-3.712562000	-1.388458000
H	-2.012316000	-3.815753000	-0.495698000
H	-2.945202000	-2.893423000	-1.339444000
O	-1.569450000	-2.681459000	3.310213000
H	-1.491622000	-3.267230000	2.504872000
H	-1.927359000	-3.245915000	4.012009000
O	-3.403133000	0.111467000	-3.329880000
H	-3.244079000	1.020280000	-2.983278000
H	-2.526340000	-0.195780000	-3.669128000
O	-2.950560000	2.673768000	-2.324789000
H	-3.243855000	2.682435000	-1.336308000
H	-3.578024000	3.266537000	-2.766783000
O	-0.952001000	-0.777814000	-4.222182000
H	-1.025104000	-1.016399000	-5.159099000
H	-0.262247000	-0.039613000	-4.195552000
O	2.221047000	2.476859000	3.066010000
H	2.709551000	2.028619000	2.343859000
H	1.681047000	3.191600000	2.615104000
O	3.994424000	1.421125000	1.142834000
H	4.080026000	0.396264000	1.031815000
H	4.773916000	1.681022000	1.657986000
O	4.320477000	-1.092925000	0.848506000
H	3.686432000	-1.629968000	1.377865000
H	4.161466000	-1.347497000	-0.102347000
O	0.976611000	-1.824746000	4.120279000
H	0.914419000	-0.838836000	4.182423000
H	0.076770000	-2.113759000	3.848801000
O	3.754030000	2.589394000	-1.208531000
H	3.875939000	2.148488000	-0.309312000
H	4.497987000	3.202961000	-1.305571000

O	3.276873000	0.730782000	-3.116382000
H	3.498209000	1.427471000	-2.440093000
H	3.973766000	0.783667000	-3.787988000
O	1.471156000	4.285279000	-0.858186000
H	2.241499000	3.688129000	-0.948953000
H	0.766093000	3.844755000	-1.374860000
O	-0.364543000	3.289849000	-2.764503000
H	-1.322998000	3.098087000	-2.564541000
H	-0.361987000	4.117920000	-3.268253000
O	0.714248000	4.294503000	1.805919000
H	-0.198765000	3.934969000	1.789624000
H	0.988068000	4.343147000	0.857073000
O	-1.980179000	3.422312000	1.973849000
H	-2.312461000	4.222855000	2.409716000
H	-1.982016000	2.720387000	2.719652000
O	-3.815625000	2.709708000	0.088065000
H	-3.133498000	2.979229000	0.758499000
H	-4.083188000	1.797215000	0.343296000
O	-1.992578000	1.726387000	3.930642000
H	-2.527873000	0.912108000	3.736049000
H	-1.070865000	1.408603000	4.073893000
O	-3.402338000	-0.521831000	3.272556000
H	-3.716495000	-0.363612000	2.358252000
H	-2.755408000	-1.255618000	3.204613000
O	0.637306000	0.890889000	4.350590000
H	1.258923000	1.494039000	3.802661000
H	0.821189000	1.132739000	5.271391000
C	0.904497000	-0.324411000	-1.160278000
O	1.149771000	0.622610000	-0.578271000

H_2S within $5^{12}6^4$ clathrate hydrate

O	1.462620000	-4.434160000	-0.818654000
H	0.545481000	-4.382171000	-0.464778000
H	2.028798000	-4.060153000	-0.107031000
O	-3.355567000	-2.970623000	-0.943272000
H	-3.145309000	-2.426525000	-1.738259000
H	-2.487544000	-3.276832000	-0.610117000
O	-2.825552000	-1.457395000	-3.221094000
H	-3.323822000	-1.854071000	-3.951946000
H	-1.853366000	-1.476448000	-3.537004000
O	-0.418148000	-1.502684000	-4.176119000
H	-0.092905000	-0.565116000	-4.267912000
H	0.243911000	-1.945774000	-3.602287000
O	-3.609592000	1.140205000	-2.830723000
H	-3.900223000	1.158730000	-1.887879000
H	-3.335567000	0.202206000	-2.992310000
O	-4.367367000	1.206634000	-0.164544000
H	-3.802161000	1.922913000	0.270879000
H	-5.279458000	1.526364000	-0.091960000
O	-1.584697000	2.688151000	-3.216344000
H	-1.828697000	3.163536000	-4.025535000
H	-2.377671000	2.060882000	-3.036330000
O	3.447144000	2.788966000	-0.924963000
H	4.086064000	3.463704000	-1.199775000
H	3.245918000	2.255556000	-1.744903000
O	2.985758000	1.263096000	-3.090661000
H	3.499682000	1.479321000	-3.883975000
H	3.283355000	0.319458000	-2.840165000



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O	-1.182445000	4.181146000	-1.025760000
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H	-1.402006000	5.095050000	-1.261466000
O	3.810545000	-1.124933000	-2.486734000
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H	4.355135000	-0.301832000	0.625407000
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O	1.700085000	-2.843069000	-2.899518000
H	1.922140000	-3.451981000	-3.620506000
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O	-1.445788000	0.545695000	4.167305000
H	-2.054526000	-0.094528000	3.736667000
H	-0.550825000	0.255341000	3.839659000
O	-2.952186000	-1.576212000	3.077841000
H	-3.473242000	-1.450227000	2.187690000
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H	-4.299062000	-0.438188000	0.577739000
H	-4.010407000	-1.952944000	0.240693000
O	-2.958000000	3.158324000	0.848716000
H	-2.451596000	3.062967000	1.692501000
H	-2.329734000	3.551973000	0.201299000
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H	-1.862584000	-2.807121000	2.927863000
H	-1.518443000	-4.246859000	3.461541000

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O	1.428380000	-2.752679000	3.474231000
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H	1.970532000	-2.984199000	2.689332000
O	3.038108000	-3.339647000	1.229680000
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H	3.720276000	-3.966064000	1.514920000
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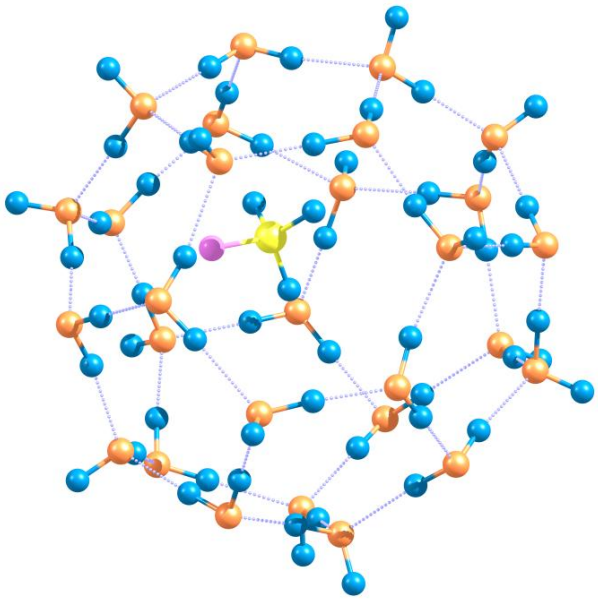
CH_3F within $5^{12}6^4$ clathrate hydrate



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O	4.297768000	0.479666000	1.661189000
H	5.164747000	0.653276000	2.057986000
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O	4.383588000	1.248783000	-0.912007000
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O	1.517678000	-2.450045000	3.286382000
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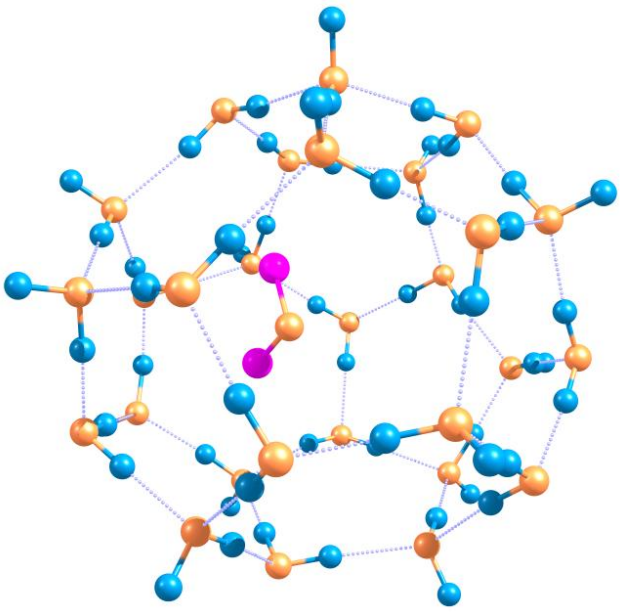
N_2O within $5^{12}6^4$ clathrate hydrate



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O	1.116078000	4.340525000	-1.576051000
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O	-1.207268000	3.590507000	2.247473000
H	-1.414725000	4.406409000	2.729626000
H	-0.955892000	2.927917000	2.987294000
O	-3.534483000	2.756564000	1.093899000
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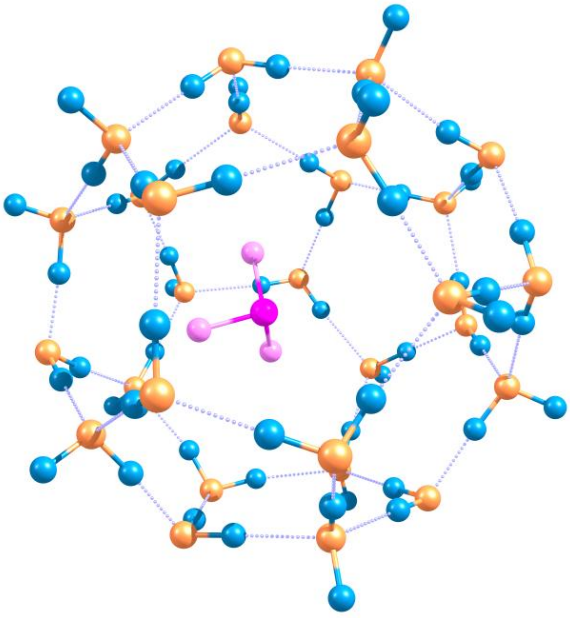
NF_3 within $5^{12}6^4$ clathrate hydrate



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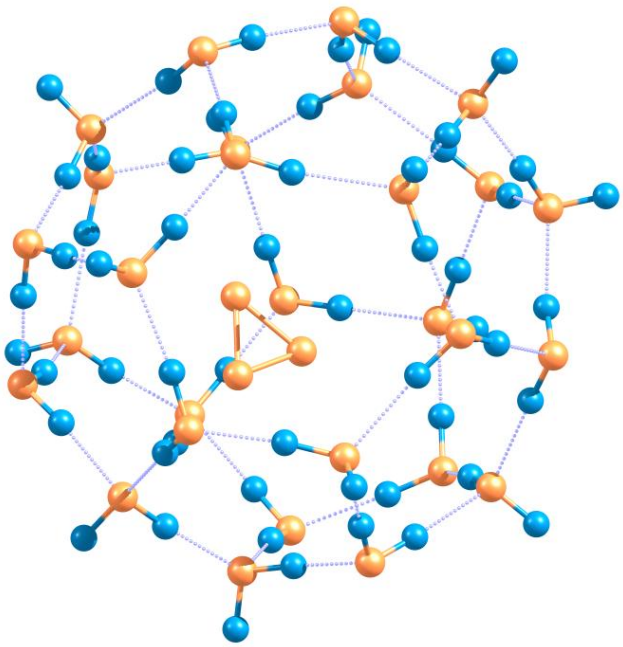
H	-0.137755000	-0.837651000	-4.283937000
O	-2.275427000	1.364881000	-3.693791000
H	-2.797533000	1.155209000	-2.891899000
H	-1.559226000	1.963642000	-3.394505000
O	1.647283000	-0.590233000	-4.144350000

H	2.040004000	-1.347782000	-3.577612000
H	1.986067000	-0.759057000	-5.037051000
N	-0.634339000	0.379210000	-0.081661000
F	-1.118068000	0.528020000	1.208505000
F	-1.464680000	-0.606468000	-0.582846000
F	-1.133104000	1.515278000	-0.702715000

O_3 within $5^{12}6^4$ clathrate hydrate



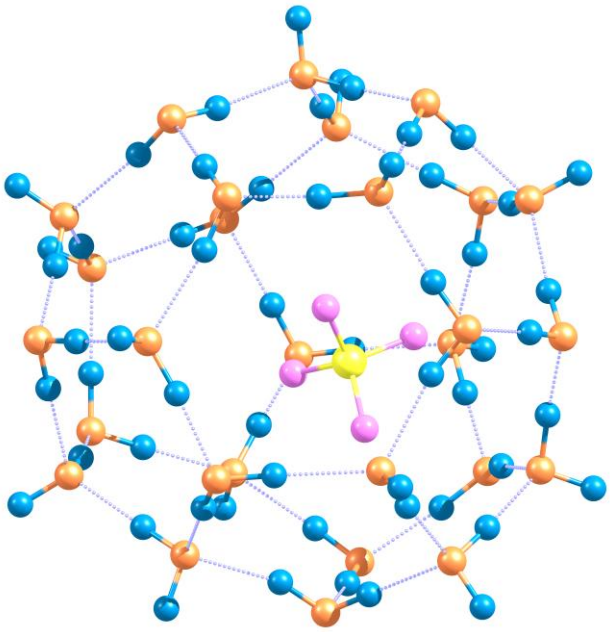
O	-0.396074000	2.184130000	-4.034729000
H	0.528866000	1.872031000	-3.909166000
H	-0.558076000	2.808791000	-3.290803000
O	3.196150000	-1.273931000	-3.199274000
H	2.444390000	-1.906748000	-3.132188000
H	2.780260000	-0.396823000	-3.328674000
O	1.126279000	-3.135764000	-3.016938000
H	1.263790000	-3.751267000	-3.753278000
H	0.169767000	-2.803006000	-3.142792000
O	-1.337657000	-2.449381000	-3.415879000
H	-1.927606000	-2.763604000	-2.677567000
H	-1.537313000	-1.495117000	-3.532244000
O	1.275496000	-4.501389000	-0.638477000
H	1.980922000	-4.025046000	-0.135883000
H	1.229115000	-4.036400000	-1.510966000
O	3.225810000	-3.125134000	0.753247000
H	2.845929000	-2.844905000	1.654650000
H	3.940981000	-3.742165000	0.972032000
O	-0.993250000	-4.317098000	0.560195000
H	-1.303947000	-5.235966000	0.570046000

H	-0.086013000	-4.360310000	0.076329000
O	-3.977415000	-0.017812000	2.078857000
H	-4.801885000	-0.099178000	2.581572000
H	-4.144301000	-0.461951000	1.200378000
O	-4.398023000	-1.111966000	-0.347284000
H	-5.301714000	-1.415785000	-0.524631000
H	-4.246788000	-0.353228000	-1.013350000
O	-2.833642000	-3.268864000	-1.311143000
H	-2.202717000	-3.556745000	-0.616465000
H	-3.321916000	-2.509658000	-0.925799000
O	-0.489450000	-3.245187000	2.970596000
H	-0.712456000	-3.666605000	2.092731000
H	-0.646971000	-3.927897000	3.640301000
O	-4.108879000	0.829191000	-2.047338000
H	-3.790315000	1.646581000	-1.598691000
H	-3.407577000	0.608303000	-2.707678000
O	-3.190663000	3.138138000	-0.781324000
H	-3.161508000	2.934261000	0.229341000
H	-3.896860000	3.796345000	-0.874310000
O	-2.112591000	0.212522000	-3.851057000
H	-2.498202000	0.176147000	-4.739885000
H	-1.419848000	0.951096000	-3.900620000
O	3.366780000	1.835515000	2.593509000
H	3.596417000	1.536614000	1.688635000
H	2.760227000	2.623659000	2.467796000
O	4.402038000	1.180027000	0.048430000
H	4.395759000	0.201436000	-0.290789000
H	5.319900000	1.342301000	0.315964000
O	4.492997000	-1.214048000	-0.831412000
H	4.006658000	-1.845942000	-0.252709000

H	4.046040000	-1.268535000	-1.722783000
O	2.235733000	-2.583679000	3.100306000
H	2.260086000	-1.633370000	3.375652000
H	1.278493000	-2.803763000	3.059276000
O	3.463351000	2.830172000	-1.783239000
H	3.849667000	2.211089000	-1.086834000
H	4.180887000	3.434106000	-2.027366000
O	2.261958000	1.362637000	-3.715750000
H	2.723537000	1.924396000	-3.035888000
H	2.738510000	1.516963000	-4.545809000
O	1.533807000	4.485180000	-0.464882000
H	2.194471000	3.904862000	-0.894919000
H	0.677308000	4.182822000	-0.829892000
O	-0.855947000	3.903436000	-1.887807000
H	-1.706501000	3.649522000	-1.432627000
H	-0.983059000	4.814926000	-2.191944000
O	1.654651000	3.863680000	2.233444000
H	0.761471000	3.510104000	2.434352000
H	1.614071000	4.139276000	1.285046000
O	-0.896307000	2.963037000	3.051615000
H	-1.037127000	3.661309000	3.710314000
H	-0.712121000	2.127386000	3.616423000
O	-3.255204000	2.650261000	1.729715000
H	-2.385702000	2.768673000	2.196158000
H	-3.509238000	1.709925000	1.874110000
O	-0.423453000	0.909920000	4.549978000
H	-1.045697000	0.158815000	4.358494000
H	0.477428000	0.569167000	4.341283000
O	-2.113901000	-1.130245000	3.894615000
H	-2.702126000	-0.800253000	3.184172000

H	-1.576412000	-1.842928000	3.488680000
O	2.151178000	0.019881000	3.972870000
H	2.613509000	0.723857000	3.389324000
H	2.625246000	0.060490000	4.817678000
O	-0.996299000	-1.039051000	0.481021000
O	-1.249883000	-0.548955000	-0.847361000
O	-1.342553000	0.342517000	0.281223000

CF_4 within $5^{12}6^4$ clathrate hydrate



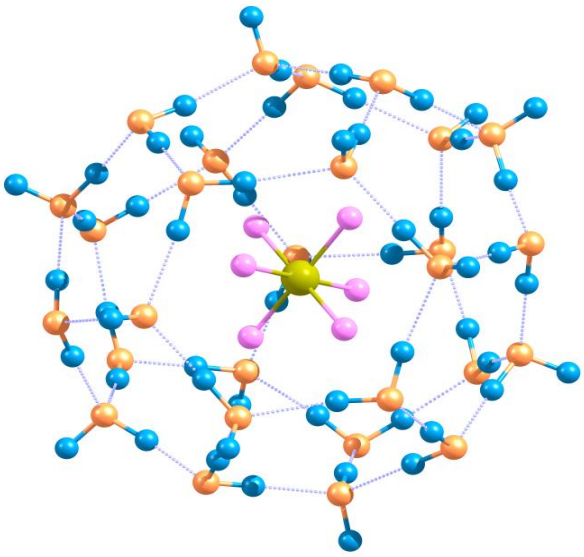
O	0.559574000	-3.286571000	-3.173920000
H	-0.358552000	-2.933732000	-3.153428000
H	0.703127000	-3.665004000	-2.275966000
O	-2.776264000	0.386365000	-3.404448000
H	-1.997270000	0.976092000	-3.530735000
H	-2.409969000	-0.508553000	-3.251207000
O	-0.675918000	2.146676000	-3.839467000
H	-0.828858000	2.498359000	-4.729901000
H	0.273617000	1.768691000	-3.873821000
O	1.753848000	1.284336000	-4.026533000
H	2.328770000	1.791723000	-3.390671000
H	1.870963000	0.339177000	-3.785372000
O	-0.826129000	4.181926000	-2.007326000
H	-1.561818000	3.909174000	-1.405959000
H	-0.776603000	3.466064000	-2.688986000
O	-2.863302000	3.394416000	-0.316273000
H	-2.499573000	3.413378000	0.634090000
	-3.545870000	4.082847000	-0.332349000
O	1.419741000	4.275853000	-0.757675000

H	1.774377000	5.137580000	-1.027013000
H	0.516595000	4.209048000	-1.246715000
O	4.143709000	0.537043000	2.060388000
H	4.968889000	0.731965000	2.529656000
H	4.341376000	0.668872000	1.090951000
O	4.616528000	0.771501000	-0.578069000
H	5.521431000	1.011424000	-0.831318000
H	4.473718000	-0.156974000	-0.983763000
O	3.218836000	2.637287000	-2.188614000
H	2.579407000	3.137717000	-1.636243000
H	3.633160000	1.986653000	-1.582504000
O	0.850438000	4.045655000	1.857251000
H	1.101899000	4.149483000	0.895829000
H	1.032589000	4.902659000	2.271550000
O	4.319191000	-1.585471000	-1.610670000
H	3.966668000	-2.213101000	-0.937112000
H	3.622057000	-1.539922000	-2.310772000
O	3.294095000	-3.332589000	0.301614000
H	3.271827000	-2.822298000	1.197844000
H	3.951550000	-4.032173000	0.438644000
O	2.352220000	-1.409660000	-3.532768000
H	2.738873000	-1.644612000	-4.390361000
H	1.624104000	-2.098952000	-3.382494000
O	-3.294163000	-0.744771000	2.880869000
H	-3.574758000	-0.752726000	1.941749000
H	-2.716115000	-1.555259000	2.995579000
O	-4.376820000	-0.922179000	0.276367000
H	-4.261229000	-0.082133000	-0.316159000
H	-5.313128000	-0.922245000	0.528392000
O	-4.189736000	1.124179000	-1.238176000

H	-3.691391000	1.880564000	-0.851465000
H	-3.698762000	0.882023000	-2.073065000
O	-1.910308000	3.590712000	2.096301000
H	-1.993242000	2.764722000	2.635111000
H	-0.941656000	3.741667000	2.022351000
O	-3.501186000	-3.087683000	-0.966110000
H	-3.867826000	-2.274718000	-0.497520000
H	-4.239159000	-3.710827000	-1.042587000
O	-2.072394000	-2.336364000	-3.141794000
H	-2.616383000	-2.647284000	-2.369461000
H	-2.540369000	-2.646094000	-3.932303000
O	-1.556206000	-4.256464000	0.774009000
H	-2.223186000	-3.843963000	0.188028000
H	-0.695391000	-4.050486000	0.356095000
O	0.915810000	-4.235957000	-0.587649000
H	1.777096000	-3.912124000	-0.202478000
H	0.949086000	-5.203077000	-0.532887000
O	-1.648782000	-2.833364000	3.136385000
H	-0.738371000	-2.479397000	3.231319000
H	-1.627547000	-3.392609000	2.321300000
O	0.932905000	-1.872959000	3.740183000
H	0.984298000	-2.347702000	4.584887000
H	0.783277000	-0.898042000	4.018679000
O	3.365779000	-2.096575000	2.544167000
H	2.471398000	-2.028969000	2.972313000
H	3.648932000	-1.165608000	2.393636000
O	0.528121000	0.546359000	4.552555000
H	1.195612000	1.189460000	4.193703000
H	-0.345957000	0.848475000	4.212381000
O	2.350983000	2.247560000	3.440383000

H	2.907659000	1.678407000	2.869550000
H	1.849120000	2.825821000	2.827499000
O	-1.992749000	1.343334000	3.664183000
H	-2.489142000	0.527227000	3.295996000
H	-2.460241000	1.555551000	4.486734000
C	-0.722083000	-0.109013000	0.044658000
F	-1.596485000	0.726372000	0.594204000
F	0.212201000	-0.425418000	0.933841000
F	-1.349876000	-1.216551000	-0.348574000
F	-0.156860000	0.471938000	-1.010420000

SF_6 within $5^{12}6^4$ clathrate hydrate



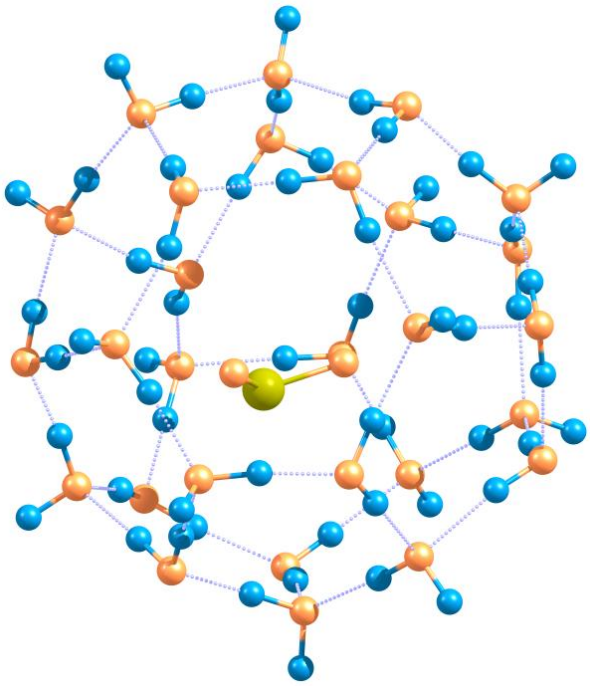
O	-1.30591300	-2.21714000	3.05773300
H	-1.71491200	-1.29758500	3.11466300
H	-1.50857000	-2.63641600	3.90794800
O	1.72340000	2.32186500	2.92566100
H	2.10738100	1.41774000	2.85708500
H	2.01603500	2.79302100	2.10745000
O	-2.42731500	-3.64204200	0.94937000
H	-2.02900000	-3.16447100	1.71710500
H	-2.92638200	-2.95770100	0.45816100
O	2.49842200	3.58917700	0.59107000
H	1.68717500	3.90841300	0.05991600
H	3.03279900	4.38498400	0.73449800
O	-2.47563400	0.15378000	3.20594900
H	-1.85052400	0.91913200	3.18907800
H	-3.04620000	0.27932700	2.42092200
O	-0.87914200	2.41158800	3.05470100

H	0.13316900	2.32160300	2.99184500
H	-1.02469400	2.97988700	3.82664600
O	-4.32296400	0.41170100	1.01165700
H	-4.23237200	-0.40241200	0.44433300
H	-5.18219300	0.33803100	1.45412500
O	-1.69781000	3.99988400	0.88025600
H	-1.39320100	3.43128500	1.62306100
H	-2.32396000	3.44321000	0.37541500
O	-3.96891800	-1.75791300	-0.55538400
H	-4.74240800	-2.27512600	-0.82700100
H	-3.48607000	-1.51813100	-1.40619000
O	0.43609400	4.38965300	-0.76935600
H	0.27866900	3.77033300	-1.51761700
H	-0.35990500	4.30082200	-0.18026600
O	1.54014600	-2.33178400	2.93903200
H	0.56650300	-2.21793600	2.96138200
H	1.71765200	-2.94036200	2.15835700
O	2.95331100	-0.19837100	2.76369700
H	2.34046300	-1.02755100	2.80511100
H	3.49359700	-0.26192100	3.56645300
O	1.96478000	-3.89927900	0.82846200
H	1.13378500	-4.02051400	0.32444400
H	2.59017500	-3.48374500	0.17768800
O	4.38701300	-0.34667500	0.47065800
H	3.88570800	-0.30246900	1.33118800
H	5.32571300	-0.36956100	0.70840900
O	-0.43366300	-4.32315900	-0.66055300
H	-0.46353600	-5.28511400	-0.77288300
H	-1.19386500	-4.09796300	-0.04039300
O	3.82324700	1.87370100	-1.19631900

H	3.37290600	2.49713200	-0.58367200
H	4.01936300	1.08835700	-0.64265900
O	-2.47504500	1.45748600	-2.94202400
H	-1.55666500	1.83277300	-2.97755300
H	-2.88354000	1.86192200	-2.14566000
O	1.99867000	-1.60646600	-3.07985500
H	1.09274900	-2.04211100	-3.04583500
H	2.40910400	-1.94451900	-3.89021700
O	-3.63860700	2.50625100	-0.60457600
H	-3.97310000	1.79720000	-0.00074700
H	-4.36553100	3.13689400	-0.71715500
O	3.59172100	-2.64922700	-0.97550800
H	3.91756900	-1.85767100	-0.49810400
H	3.03327200	-2.28711400	-1.69766400
O	-2.66795400	-1.10826800	-2.77626300
H	-2.52731300	-0.09179200	-2.82571500
H	-3.11074900	-1.33668300	-3.60829900
O	-0.37387500	-2.80869300	-2.99331100
H	-1.09715500	-2.15873900	-2.87546500
H	-0.40208700	-3.37334400	-2.18494000
O	-0.00582300	2.64334000	-2.95021700
H	0.81608600	2.03455700	-3.02487300
H	0.06036100	3.22880500	-3.72047400
O	2.13338800	1.21622900	-3.20397100
H	2.03507900	0.23978500	-3.15524800
H	2.78594300	1.45603100	-2.48791300
S	0.01646400	-0.01114600	-0.00412400
F	-0.12747400	-0.05749100	-1.59713400
F	-0.59087700	-1.49276100	0.08834200
F	1.48917700	-0.61301700	-0.10997700

F	0.13814200	0.03452500	1.59028400
F	-1.47719800	0.58683200	0.10149100
F	0.59701100	1.47334900	-0.09412000

SO_2 within $5^{12}6^4$ clathrate hydrate



O	-0.542452000	4.181657000	-1.944977000
H	-0.199395000	3.588352000	-2.646772000
H	0.157787000	4.168054000	-1.249343000
O	-0.724567000	0.071497000	-2.837634000
H	-1.660995000	-0.096170000	-3.115124000
H	-0.440158000	0.930612000	-3.226663000
O	-3.311111000	-0.595732000	-3.134532000
H	-3.860198000	-0.598273000	-3.932444000
H	-3.758876000	0.055625000	-2.482017000
O	-4.354759000	1.065251000	-1.460226000
H	-4.412178000	0.601200000	-0.580311000
H	-3.751361000	1.826242000	-1.308911000
O	-2.951912000	-3.114420000	-1.965192000
H	-2.000881000	-3.348168000	-2.101176000
H	-3.084622000	-2.244804000	-2.408018000
O	-0.318337000	-3.901595000	-2.322038000
H	0.104589000	-4.075838000	-1.407747000
H	-0.343447000	-4.772138000	-2.747678000
O	-3.435760000	-2.884548000	0.570027000
H	-4.227816000	-3.435335000	0.669919000
H	-3.208607000	-2.946794000	-0.425419000
O	-0.953307000	0.243796000	4.376260000
H	-1.204094000	0.195274000	5.310866000

H	-1.768399000	0.541584000	3.887001000
O	-3.090328000	1.130965000	2.979245000
H	-3.856455000	1.386513000	3.516474000
H	-2.785633000	2.001907000	2.532124000
O	-4.371791000	-0.268130000	0.891007000
H	-4.002693000	-1.176568000	0.814923000
H	-3.885382000	0.161161000	1.626828000
O	-1.248502000	-3.815853000	1.880932000
H	-2.044580000	-3.430204000	1.424356000
H	-1.558579000	-4.628887000	2.307144000
O	-2.339537000	3.340487000	1.881669000
H	-1.373369000	3.484306000	2.028075000
H	-2.462035000	3.313863000	0.901878000
O	0.342085000	3.789639000	2.374636000
H	0.710750000	3.022644000	2.954627000
H	0.402204000	4.570210000	2.946744000
O	-2.761719000	3.310732000	-0.854980000
H	-3.355613000	4.060368000	-1.015929000
H	-1.889266000	3.579333000	-1.298325000
O	4.371943000	-1.698131000	-0.671794000
H	3.870095000	-1.440954000	-1.472377000
H	4.540920000	-0.840121000	-0.179926000
O	3.191226000	-1.039183000	-3.173217000
H	2.274885000	-1.451592000	-3.388711000
H	3.821868000	-1.493760000	-3.752261000
O	0.865918000	-1.930368000	-3.821631000
H	0.548612000	-2.704951000	-3.295582000
H	0.271307000	-1.199796000	-3.517063000
O	0.682592000	-4.509595000	-0.013486000
H	1.512812000	-4.026088000	0.223912000

H	0.026554000	-4.227594000	0.663612000
O	2.969282000	1.585779000	-3.443425000
H	3.083659000	0.588325000	-3.375999000
H	3.716104000	1.911838000	-3.967291000
O	0.426254000	2.360627000	-3.872510000
H	1.384890000	2.115507000	-3.752243000
H	0.316333000	2.555288000	-4.814950000
O	3.736849000	2.670288000	-0.894665000
H	3.432404000	2.243656000	-1.719832000
H	2.918256000	3.044909000	-0.506867000
O	1.478914000	4.142980000	-0.043879000
H	1.097055000	3.953591000	0.857296000
H	1.918876000	5.002925000	0.035795000
O	4.716813000	0.596023000	0.666537000
H	4.119724000	0.557848000	1.445144000
H	4.394738000	1.363074000	0.132671000
O	3.223013000	0.413967000	3.061393000
H	3.969453000	0.506069000	3.673865000
H	2.952794000	-0.569588000	3.150331000
O	1.196731000	1.983763000	3.983448000
H	1.937645000	1.429647000	3.620355000
H	0.457744000	1.353731000	4.139867000
O	2.640271000	-2.095751000	3.335337000
H	1.692447000	-2.237468000	3.598514000
H	2.731936000	-2.516479000	2.448863000
O	-0.001490000	-2.397902000	3.978803000
H	-0.348020000	-1.482484000	4.007410000
H	-0.435129000	-2.811352000	3.202115000
O	2.992445000	-3.289423000	0.838556000
H	3.491649000	-2.634390000	0.232204000

H	3.634790000	-3.995595000	1.007349000
S	-1.062237000	0.250808000	-0.226313000
O	-0.666153000	-1.127883000	0.083181000
O	-0.085026000	1.313416000	0.046871000

Table S6. Global Chemical indices of Greenhouse gases within 5^{12} hydrate clathrates. All values in eV.

Energy gap (E_g) $= E_{LUMO} - E_{HOMO}$ Chemical potential (μ) $= \frac{E_{HOMO}+E_{LUMO}}{2}$ Chemical Hardness (η) $= \frac{E_{LUMO}-E_{HOMO}}{2}$ Electronegativity (χ) $= \frac{-(E_{HOMO}+E_{LUMO})}{2}$ Electrophilicity (ω) $= = \frac{-\eta^2}{2\chi}$

Molecules	**HOMO**	**LUMO**	E_g	μ	η	χ	ω
CCl_4	-7.04	-1.67	5.38	-4.36	2.69	4.36	0.02
CF_2Cl_2	-6.8	-0.24	6.56	-3.52	3.28	3.52	0.03
CH_3Br	-7.01	0.04	7.05	-3.49	3.53	3.49	0.03
CH_3Cl	-6.75	0.458	7.21	-3.15	3.6	3.15	0.03
CH_4	-6.7	0.237	6.94	-3.23	3.47	3.23	0.03
CO_2	-6.64	0.303	6.95	-3.17	3.47	3.17	0.03
CO	-6.7	-0.45	6.25	-3.58	3.13	3.58	0.02
H_2S	-5.92	0.466	6.38	-2.73	3.19	2.73	0.02
CH_3F	-6.94	0.502	7.44	-3.22	3.72	3.22	0.03
N_2O	-6.59	-3.86	2.72	-5.23	1.36	5.23	0.01
NF_3	-6.71	-0.02	6.69	-3.36	3.35	3.36	0.03
O_3	-6.71	-4.55	2.16	-5.63	1.08	5.63	0.00
CF_4	-6.71	0.312	7.03	-3.20	3.51	3.20	0.03
SF_6	-6.86	-2.24	4.61	-4.55	2.31	4.55	0.02
SO_2	-6.75	-1.73	5.03	-4.24	2.51	4.24	0.02

Table S7. Global Chemical indices of Greenhouse gases within $5^{12}6^2$ hydrate clathrates. All values in eV.

Molecules	HOMO	LUMO	E_g	μ	η	χ	ω
CCl_4	-6.93	-1.59	5.34	-4.26	2.67	4.26	0.02
CF_2Cl_2	-6.76	-0.53	6.23	-3.64	3.12	3.64	0.02
CH_3Br	-6.88	0.038	6.92	-3.42	3.46	3.42	0.03
CH_3Cl	-6.73	0.136	6.86	-3.29	3.43	3.29	0.03
CH_4	-6.72	0.135	6.85	-3.29	3.43	3.29	0.03
CO_2	-7.02	0.183	7.20	-3.42	3.6	3.42	0.03
CO	-7.13	-0.47	6.65	-3.8	3.33	3.8	0.03
H_2S	-6.65	0.189	6.84	-3.23	3.42	3.23	0.03
CH_3F	-6.99	0.014	7.00	-3.49	3.5	3.49	0.03
N_2O	-7.09	-2.65	4.44	-4.87	2.22	4.87	0.02
NF_3	-6.69	-0.05	6.64	-3.37	3.32	3.37	0.03
O_3	-7.04	-5.03	2.01	-6.03	1.01	6.03	0.00
CF_4	-7.35	0.258	7.61	-3.55	3.81	3.55	0.03
SF_6	-6.91	-2.58	4.33	-4.75	2.17	4.75	0.02
SO_2	-7.16	-2.41	4.75	-4.78	2.38	4.78	0.02

Table S8. Global Chemical indices of Greenhouse gases within $5^{12}6^4$ hydrate clathrates. All values in eV.

Molecules	HOMO	LUMO	E_g	μ	η	χ	ω
CCl_4	-6.91	-1.78	5.13	-4.35	2.57	4.35	0.02
CF_2Cl_2	-7.1	-0.60	6.50	-3.85	3.25	3.85	0.03
CH_3Br	-6.87	-0.12	6.75	-3.5	3.38	3.50	0.03
CH_3Cl	-6.89	0.17	7.06	-3.36	3.53	3.36	0.03
CH_4	-6.85	0.20	7.05	-3.33	3.53	3.33	0.03
CO_2	-6.79	0.24	7.03	-3.28	3.52	3.28	0.03
CO	-6.86	-1.02	5.84	-3.94	2.92	3.94	0.02
H_2S	-6.91	0.24	7.15	-3.33	3.57	3.33	0.03
CH_3F	-6.97	0.13	7.11	-3.42	3.55	3.42	0.03
N_2O	-6.75	-2.54	4.21	-4.64	2.11	4.64	0.01
NF_3	-7.41	-0.52	6.89	-3.96	3.45	3.96	0.03
O_3	-6.95	-4.70	2.25	-5.83	1.13	5.83	0.00
CF_4	-6.9	0.27	7.17	-3.31	3.58	3.31	0.03
SF_6	-6.89	-2.79	4.09	-4.84	2.05	4.84	0.01
SO_2	-7.28	-2.08	5.21	-4.68	2.60	4.68	0.02

Table S9. Bonding and anti-bonding occupancies and their *s*- and *p*-orbital contribution of their Greenhouse gases

Guest Molecule	Bond	Occupancy		Contribution in %	
		σ (Bonding)	σ* (Anti Bonding)	*s*-orbital	*p*-orbital
CCl_4	C-Cl	1.98925	0.10883	25.00	74.82
				14.43	85.02
CF_2Cl_2	C-Cl	1.98678	0.12333	25.53	74.24
				14.41	85.07
	C-F	1.99549	0.12319	24.53	75.05
				29.78	70.13
CH_3Br	C-H	1.99824	0.00881	27.73	72.21
				100.0	-
	C-Br	1.99824	0.00177	16.81	83.08
				11.38	87.90
CH_3Cl	C-H	1.99757	0.01165	27.10	72.83
				100.0	-
	C-Cl	1.99820	0.00167	18.69	81.13
				15.22	84.33
CH_4	C-H	1.99926	0.00046	25.00	74.94
				100.0	-
CO_2	C-O	1.99891	0.37901	-	99.74
				-	99.62
CO	C-O	2.0000	0	-	99.57
				-	99.58
H_2S	S-H	1.99888	0.00094	15.47	83.78
				100.0	-
CH_3F	C-H	1.99859	0.01852	26.70	72.83
				100.0	-
	C-F	1.99927	0.00259	19.95	79.87
				26.16	73.68
	C-F	1.99825	0.00425	19.03	80.8
				25.81	74.05
N_2O	O-N	1.98936	0.01572	22.23	77.27
				14.20	85.58
NF_3	N-F	1.99187	0.09659	12.18	87.46
				14.50	85.34

O_3	O-O	1.98839	0.00897	6.680	92.98
				6.680	92.98
CF_4	C-F	1.99380	0.12620	25.00	74.65
				27.63	72.19
SF_6	S-F	1.88535	0.17710	16.67	50.00
				15.94	83.89
SO_2	S-O	1.99455	0.10899	16.18	81.93
				24.37	74.94

Table S10. Bonding and anti-bonding occupancies and their *s*- and *p*-orbital contribution of their Greenhouse gases after encapsulated in 5^{12}.

Guest Molecule	Bond	Occupancy		Contribution in %	
		σ (Bonding)	σ* (Anti Bonding)	*s*-orbital	*p*-orbital
CCl_4	C-Cl	1.9887	0.11261	24.73	75.08
				14.64	84.84
CF_2Cl_2	C-Cl	1.98679	0.12932	26.24	73.54
				14.57	84.89
	C-F	1.99490	0.13355	23.67	75.91
				29.51	70.41
CH_3Br	C-H	1.99648	0.01876	28.46	71.48
				100.0	-
	C-Br	1.99652	0.01706	14.59	85.28
				12.28	87.45
CH_3Cl	C-H	1.99625	0.01995	27.49	72.45
				100.0	-
	C-Cl	1.99713	0.01148	17.04	82.77
				16.12	83.49
CH_4	C-H	1.99796	0.00867	25.37	74.57
				100.0	-
CO_2	C-O	1.99815	0.36670	49.88	50.09
				37.32	62.25
CO	C-O	1.99806	0.00751	5.050	94.55
				9.750	89.76
H_2S	S-H	1.99763	0.05235	18.63	80.76
				100.0	-
	C-F	1.99927	0.00259	19.95	79.87
				26.16	73.68
CH_3F	C-H	1.99757	0.01983	27.26	72.66
				100.0	-
	C-F	1.99783	0.00685	17.60	82.24
				25.30	74.57
N_2O	O-N	1.98098	0.05114	19.40	80.10
				13.71	86.07
NF_3	N-F	1.99079	0.10352	11.39	88.25
				14.26	85.58

O_3	O-O	1.99493	0.06199	13.82	85.93
				22.03	77.81
CF_4	C-F	1.99343	0.12596	24.85	74.63
				27.64	72.27
SF_6	S-F	1.88446	0.18078	16.52	49.98
				16.24	83.60
SO_2	S-O	1.99251	0.11352	16.08	82.12
				26.00	73.42

Table S11. Bonding and anti-bonding occupancies and their *s*- and *p*-orbital contribution of their Greenhouse gases after encapsulated in $5^{12}6^2$.

Guest Molecule	Bond	Occupancy		Contribution in %	
		σ (Bonding)	σ* (Anti Bonding)	*s*-orbital	*p*-orbital
CCl_4	C-Cl	1.98902	0.12283	24.65	75.17
				14.76	84.72
CF_2Cl_2	C-Cl	1.98642	0.12391	25.44	74.33
				14.82	84.67
	C-F	1.99486	0.13183	23.79	75.80
				29.41	70.50
CH_3Br	C-H	1.99727	0.01487	28.26	71.67
				100.0	-
	C-Br	1.99742	0.00835	15.30	84.58
				11.97	87.77
CH_3Cl	C-H	1.99658	0.01803	27.40	72.54
				100.0	-
	C-Cl	1.99776	0.00605	17.20	82.61
				15.74	83.86
CH_4	C-H	1.99818	0.00744	25.30	74.65
				100.0	-
CO_2	C-O	1.99795	0.02065	49.91	50.06
				37.10	62.47
CO	C-O	1.9979	0.00566	7.380	92.24
				13.69	85.80
H_2S	S-H	1.99795	0.04156	17.92	81.45
				100.0	-
CH_3F	C-H	1.99763	0.02193	27.27	72.65
				100.0	-
	C-F	1.99798	0.00469	18.59	81.24
				25.85	74.01
N_2O	O-N	1.98682	0.02711	20.41	79.09
				14.58	85.2
NF_3	N-F	1.99087	0.09799	11.90	87.74
				14.32	85.52
O_3	O-O	1.98785	0.01543	6.640	93.03

				6.410	93.25
CF_4	C-F	1.99355	0.12449	25.06	74.42
				27.55	72.36
SF_6	S-F	1.88369	0.18043	16.64	50.00
				15.95	83.88
SO_2	S-O	1.99235	0.11747	15.63	82.45
				25.10	74.32

Table S12. Bonding and anti-bonding occupancies and their *s*- and *p*-orbital contribution of their Greenhouse gases after encapsulated in $5^{12}6^4$.

Guest Molecule	Bond	Occupancy		Contribution in %	
		σ (Bonding)	σ* (Anti Bonding)	*s*-orbital	*p*-orbital
CCl_4	C-Cl	1.989	0.11954	25.15	74.67
				14.37	85.09
CF_2Cl_2	C-Cl	1.98639	0.12583	25.97	73.80
				14.26	85.21
	C-F	1.99512	0.12469	24.39	75.19
				29.60	70.31
CH_3Br	C-H	1.9974	0.01328	27.83	72.10
				100.0	-
	C-Br	1.99766	0.01307	16.24	83.64
				11.46	88.25
CH_3Cl	C-H	1.99714	0.01440	26.93	73.00
				100.0	-
	C-Cl	1.99795	0.00359	17.98	81.84
				15.43	84.15
CH_4	C-H	1.99853	0.00618	25.35	74.60
				100.0	-
CO_2	C-O	1.99765	0.37329	0.750	98.99
				0.250	99.38
CO	C-O	1.99935	0.0047	0.010	99.57
				0.010	99.57
H_2S	S-H	1.9986	0.00997	15.95	83.33
				100.0	-
CH_3F	C-H	1.9982	0.01695	26.63	73.29
				100.0	-
	C-F	1.99825	0.00425	19.03	80.80
				25.81	74.05
N_2O	O-N	1.98182	0.04882	18.92	80.57
				14.04	85.74
NF_3	N-F	1.99107	0.09589	12.18	87.46
				14.40	85.43

O_3	O-O	1.98796	0.01031	6.680	92.98
				6.720	92.94
CF_4	C-F	1.99365	0.12382	25.11	74.52
				27.63	72.19
SF_6	S-F	1.88373	0.17904	16.77	50.00
				15.70	84.12
SO_2	S-O	1.9936	0.1126	16.10	82.04
				25.36	74.03

Electron localization function (ELF)

The electron localization function (ELF) has proven to be highly significant across a wide range of applications. This provides a chemically insightful measure of interactions between molecules and effectively identifies regions of electron delocalization.[i] It has been observed that ELF calculations produce distinct types of basins around attractors associated with either core or valence groups. The ELF determined through [ii]

$$ELF(r) = \frac{1}{1 + [D(r)/D_0(r)]^2} \tag{6}$$

Where,

$$D(r) = \frac{1}{2}\sum_i \eta_i |\nabla\varphi_i|^2 - \frac{1}{8}\left[\frac{|\nabla\rho_\alpha(r)|^2}{\rho_\alpha(r)} + \frac{|\nabla\rho_\beta(r)|^2}{\rho_\beta(r)}\right] \tag{7}$$

$$D_0(r) = \frac{3}{10}(6\pi^2)^{2/3}\left[\rho_\alpha(r)^{5/3} + \rho_\beta(r)^{5/3}\right] \tag{8}$$

The initial term of *D(r)* represents the exact kinetic energy density of a non-interacting electron system, while the second term corresponds to the Weizsäcker kinetic energy density *(T_w)*. Therefore, *$D(r) = T_s(r) - T_w(r)$* highlights the additional kinetic energy density resulting from Pauli repulsion, known as the Pauli kinetic energy density. The *$D_0(r)$* term can be understood as the Thomas-Fermi kinetic energy density (*T_{TF}*), which is the exact kinetic energy density of a uniform, non-interacting electron gas. Since *$D_0(r)$* is used as the reference in ELF, the ELF essentially indicates the degree of relative electron localization.[iii] Figure 8 illustrates the colored ELF map, which was generated using Multiwfn software. High and low ELF values correspond to regions of high and low electron density, respectively, and are indicative of covalent and non-covalent interactions.

These ELF changes have significant implications. Enhanced polarization or localization, as seen in polar molecules, often strengthens interactions with the clathrate cage, stabilizing the encapsulated molecule. Conversely, dispersed electron density, typical in weakly polarized molecules, correlates with bond weakening, as reflected in shifts in vibrational frequencies. ELF analysis aids in understanding the stability of within clathrate cages. Molecules such as CO_2, CH_4, and SF_6 trapped in clathrates may exhibit reduced reactivity or mobility, contributing to greenhouse gas sequestration and mitigating environmental harm. Thus, ELF provides a comprehensive understanding of the electronic environment changes induced by clathrate encapsulation, essential for predicting guest molecule behaviour. The ELF analysis offers qualitative insights by graphically representing areas of electron localization.

The Pauli exclusion principle underpins many chemical concepts, including ELF, which provides insights based on this principle.[iv] As Paulis reported, ELF is instrumental in understanding the exchange repulsive effect and chemical bonding between interacting molecules, addressing questions raised by Lewis.[v] Based on the ELF color scale and values (refer to Table 5), ELF values between 0.5 and 1 (Red/Blue) signify regions of localized bonding and non-bonding electrons, where the electron density distribution approaches homogeneity. Conversely, ELF values below 0.5 (Red) indicate delocalized electrons, often reflecting metallic characteristics.[vi] Here, the chemical bonding nature was explored through the topological analysis of ELF. The results show minor changes in electron density following the formation of the complex. The electron density of both the guest and host molecules undergoes changes upon encapsulation within all the three types of hydrate clathrate cages. The Electron Localization Function (ELF) images aid in understanding the transitions occurring between the guest and host. These transitions result in alterations in the electron density of the atoms within the hydrate clathrate cages. According to Bader et al.,**Error! Bookmark not defined.** ELF and the negative L aplacian of the electron density convey equivalent information. The Electron Localization Function (ELF) provides insights into the spatial distribution of electron density and bonding characteristics in molecules. When are encased within clathrate hydrate cages, their electronic structure, particularly bond electron density, is influenced by interactions with the hydrate framework. For weakly polarized molecules like CCl_4, CF_2Cl_2 and CF_4 ELF analysis shows that before encapsulation, electron density is highly localized around covalent bonds with minimal delocalization, maintaining symmetry. After encapsulation, the clathrate environment perturbs the outer electron cloud, slightly redistributing electron density. Highly electronegative atoms (e.g., F, Cl) experience enhanced polarization of electron density due to interactions with the polar water framework of the cage, weakening bond localization.

Polar molecules such as CH_3Br, CH_3Cl, H_2S and SO_2 display significant ELF asymmetry even before encapsulation due to their dipole moments. After encapsulation, the cage interactions amplify this polarization, with increased electron localization near electronegative atoms. This stabilization of high electron density regions can slightly shift bond lengths and angles, as seen in SO_2, where sulphur shows increased electron localization, and in H_2S, where lone pair regions become more localized. Strongly bonded molecules like CO, CO_2, and N_2O) exhibit highly localized ELF distributions along their bonding axes (e.g., C≡O in CO, or C=O in CO_2). While these molecules maintain rigid bonding frameworks, the clathrate cage can distort ELF distributions slightly, particularly near lone pairs. For CO, the anisotropic interactions of its C≡O bond with the cage lead to inconsistent ELF changes, while for N_2O, ELF redistribution occurs near terminal atoms, reflecting weak stabilization. Highly polarizable molecules like SF_6 and CF_4 display highly localized ELF near electronegative atoms. Upon encapsulation, the hydrate cage induces stronger polarization in bonds due to its electric field, as evidenced by more localized electron density around F atoms and slightly reduced density near central atoms (S or C). In SF_6, subtle ELF changes around sulphur highlight these interactions.

Table 13. Topological parameters of Greenhouse gases

Molecule	***Bond***	***ρ(r)***	***G(r)***	***V(r)***	$-G(r)/V(r)$	***H(r)***	$\nabla^2\rho(r)$	***ELF***	***LOL***	***ε***
CCl_4	C-Cl	0.1885	0.06301	-0.1823	0.34564	-0.1193	-0.2253	0.8886	0.7385	0
CF_2Cl_2	C-Cl	0.1944	0.06239	-0.1893	0.32958	-0.127	-0.2584	0.9002	0.7502	0.02153
	C-F	0.2856	0.3637	-0.7928	0.45875	-0.429	-0.2611	0.4886	0.4943	0.07251
CH_3Br	C-H	0.2786	0.03418	-0.314	0.10885	-0.2799	-0.9829	0.99	0.9089	0.01932
	C-Br	0.1427	0.04489	-0.1257	0.35712	-0.08082	-0.1437	0.8614	0.7138	0
CH_3Cl	C-H	0.2784	0.03363	-0.3123	0.10768	-0.2786	-0.9802	0.9903	0.9101	0.02658
	C-Cl	0.1741	0.05655	-0.1652	0.34231	-0.1086	-0.2085	0.8836	0.7337	0
CH_4	C-H	0.2686	0.03928	-0.2999	0.13098	-0.2606	-0.8854	0.9852	0.8909	0
CO_2	C-O	0.4421	0.8823	-1.641	0.53766	-0.7593	0.4916	0.4107	0.455	0
CO	C-O	0.4712	0.1108	-0.1878	0.58999	-0.7701	1.354	0.3531	0.4249	0
H_2S	S-H	0.2028	0.04193	-0.204	0.20554	-0.1621	-0.4807	0.9582	0.8274	0.09614
CH_3F	C-H	0.2784	0.03242	-0.3085	0.10509	-0.276	-0.9746	0.991	0.9131	0.04937
	C-F	0.2376	0.3263	-0.6528	0.49985	-0.3265	-0.7241	0.3914	0.445	0
N_2O	N-O	0.397	0.3421	-0.8705	0.39299	-0.5284	-0.745	0.7641	0.6428	0.32364
NF_3	N-F	0.3158	0.2265	-0.5036	0.44976	-0.277	-0.2018	0.775	0.6498	0.07923
O_3	O-O	0.2842	0.2415	-0.48	0.50313	-0.2385	0.01199	0.6807	0.5935	0.0403
CF_4	C-F	0.2954	0.352	-0.8082	0.43554	-0.4561	-0.416	0.5331	0.5165	0
SF_6	S-F	0.2074	0.245	-0.4804	0.50999	-0.2353	0.03895	0.4204	0.4599	0
SO_2	S-O	0.2746	0.6105	-0.9068	0.67325	-0.2962	1.256	0.2294	0.353	0.15083

Table S14. Topological parameters of Greenhouse gases within 5^{12} hydrate

Molecule	*Bond*	*ρ(r)*	*G(r)*	*V(r)*	$-G(r)/V(r)$	*H(r)*	$\nabla^2\rho(r)$	*ELF*	*LOL*	*ε*
CCl_4	C-Cl	0.1897	0.06381	-0.1848	0.34529	-0.121	-0.2289	0.8882	0.7381	0.00089
CF_2Cl_2	C-Cl	0.2056	0.06736	-0.2086	0.32291	-0.1413	-0.2958	0.903	0.7532	0.02034
	C-F	0.2872	0.371	-0.8038	0.46156	-0.4327	-0.2465	0.4835	0.4917	0.09038
CH_3Br	C-H	0.2841	0.03316	-0.3251	0.102	-0.292	-1.035	0.9912	0.914	0.02307
	C-Br	0.1398	0.04415	-0.1223	0.361	-0.07816	-0.136	0.857	0.7101	0.00446
CH_3Cl	C-H	0.2824	0.03231	-0.3201	0.10094	-0.2878	-1.022	0.9914	0.9152	0.02815
	C-Cl	0.1703	0.05768	-0.1645	0.35064	-0.1068	-0.1966	0.8715	0.7226	0.00164
CH_4	C-H	0.2701	0.03831	-0.302	0.12685	-0.2637	-0.9015	0.9862	0.8943	0.00118
CO_2	C-O	0.4401	0.8692	-1.625	0.53489	-0.7558	0.4537	0.4143	0.4568	0.00385
CO	C-O	0.4704	1.098	-1.869	0.58748	-0.7711	1.308	0.3561	0.4265	0.00082
H_2S	S-H	0.1968	0.0344	-0.1811	0.18995	-0.1467	-0.4492	0.9686	0.8475	0.06595
CH_3F	C-H	0.2836	0.03157	-0.3186	0.09909	-0.287	-1.022	0.9919	0.9175	0.05238
	C-F	0.2132	0.2931	-0.5723	0.51214	-0.2791	0.05616	0.3572	0.4271	0.01329
N_2O	N-O	0.4098	0.3522	-0.9118	-0.3863	-0.5596	-0.8298	0.7727	0.6483	0.29696
NF_3	N-F	0.3184	0.2283	-0.5107	0.44703	-0.2824	-0.2162	0.777	0.6512	0.07749
O_3	O-O	0.2796	0.2393	-0.47063	-0.5087	-0.2312	0.03267	0.6728	0.5891	0.03845
CF_4	C-F	0.297	0.3581	-0.8179	0.43783	-0.4598	-0.4068	0.5291	0.5145	0.00177
SF_6	S-F	0.2065	0.2421	-0.476	0.50861	-0.2338	0.03318	0.4226	0.461	0.00207
SO_2	S-O	0.2705	0.5785	-0.8732	0.66251	-0.2947	1.135	0.2398	0.3597	0.13289

Table S15. Topological parameters of Greenhouse gases within $5^{12}6^2$ hydrate cage.

Molecule	***Bond***	***ρ(r)***	***G(r)***	***V(r)***	$-G(r)/V(r)$	***H(r)***	$\nabla^2\rho(r)$	***ELF***	***LOL***	***ε***
CCl_4	C-Cl	0.1967	0.06697	-0.1969	0.34012	-0.1299	-0.252	0.8906	0.7405	0.00414
CF_2Cl_2	C-Cl	0.1989	0.06433	-0.1971	0.32638	-0.1328	-0.274	0.9015	0.7516	0.02141
	C-F	0.281	0.354	-0.7735	0.45766	-0.4195	-0.262	0.4888	0.4944	0.08961
CH_3Br	C-H	0.2809	0.03375	-0.3184	0.106	-0.2847	-1.003	0.9905	0.9111	0.02343
	C-Br	0.1378	0.04269	-0.1183	0.36086	-0.07563	-0.1317	0.8594	0.712	0.00076
CH_3Cl	C-H	0.28	0.03231	-0.3151	0.10254	-0.2828	-1.002	0.9912	0.9141	0.02947
	C-Cl	0.1673	0.05595	-0.1587	0.35255	-0.1028	-0.1873	0.8716	0.7227	0.00073
CH_4	C-H	0.2694	0.03862	-0.3008	0.12839	-0.2621	-0.8942	0.9858	0.8931	0.00241
CO_2	C-O	0.4452	0.8969	-1.663	0.53933	-0.7662	0.5227	0.4085	0.4538	0.00359
CO	C-O	0.4694	1.096	-1.864	0.58798	-0.768	1.313	0.3554	0.4261	0.00111
H_2S	S-H	0.1978	0.03524	-0.1839	0.19163	-0.1487	-0.4538	0.9676	0.8454	0.06567
CH_3F	C-H	0.28	0.03174	-0.3115	0.10189	-0.2797	-0.9922	0.9915	0.9155	0.05256
	C-F	0.2218	0.3032	-0.5989	0.50626	-0.2957	0.02979	0.3721	0.435	0.01023
N_2O	N-O	0.3966	0.3388	-0.8634	-0.3924	-0.5245	-0.7428	0.7669	0.6446	0.31623
NF_3	N-F	0.3127	0.2248	-0.4961	0.45313	-0.2712	-0.1854	0.7719	0.6479	0.07885
O_3	O-O	0.4299	0.4033	-0.8732	-0.4619	-0.4698	0.2533	0.7523	0.6354	0.06811
CF_4	C-F	0.298	0.3572	-0.8194	0.43593	-0.4621	-0.4198	0.5332	0.5166	0.00264
SF_6	S-F	0.2064	0.2372	-0.4714	0.50318	-0.2342	0.0118	0.4323	0.466	0.00077
SO_2	S-O	0.2738	0.5991	-0.8968	0.66804	-0.2977	1.205	0.2344	0.3562	0.14501

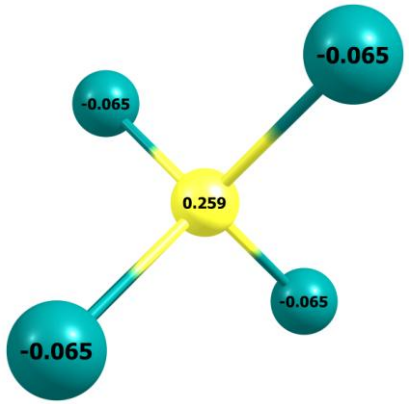
Table S16. Topological parameters of Greenhouse gases within $5^{12}6^4$ hydrate cage.

Molecule	***Bond***	***ρ(r)***	***G(r)***	***V(r)***	$-G(r)/V(r)$	***H(r)***	$\nabla^2\rho(r)$	***ELF***	***LOL***	ε
CCl_4	C-Cl	0.1905	0.06393	-0.186	0.34371	-0.1221	-0.2328	0.8893	0.7392	0.00211
CF_2Cl_2	C-Cl	0.1942	0.06234	-0.189	0.32984	-0.1266	-0.2573	0.8999	0.75	0.02148
	C-F	0.2846	0.3589	-0.7861	0.45656	-0.4272	-0.2733	0.4925	0.4962	0.07735
CH_3Br	C-H	0.2799	0.03357	-0.3168	0.10597	-0.2832	-0.9986	0.9905	0.911	0.02186
	C-Br	0.1395	0.04325	-0.1206	0.35862	-0.07734	-0.1363	0.8612	0.7136	0.00107
CH_3Cl	C-H	0.2785	0.03316	-0.3123	0.10618	-0.2791	-0.984	0.9906	0.9113	0.02778
	C-Cl	0.1706	0.05607	-0.1616	0.34697	-0.1055	-0.1978	0.8784	0.7289	0.00343
CH_4	C-H	0.2687	0.03928	-0.3	0.13093	-0.2607	-0.8857	0.9852	0.891	0.00093
CO_2	C-O	0.4431	0.8866	-0.1648	5.37985	-0.762	0.4984	0.4103	0.4547	0.00081
CO	C-O	0.4711	1.104	-1.876	0.58849	-0.772	1.328	0.355	0.4259	0.00034
H_2S	S-H	0.1974	0.0337	-0.1813	0.18588	-0.1476	-0.4557	0.9701	0.8508	0.07076
CH_3F	C-H	0.2795	0.03246	-0.3105	0.10454	-0.2781	-0.9826	0.9911	0.9135	0.05124
	C-F	0.2282	0.3111	-0.6195	0.50218	-0.3083	0.01119	0.3823	0.4403	0.01283
N_2O	N-O	0.3971	0.3411	-0.8684	-0.3928	-0.5273	-0.7446	0.7653	0.6436	0.32207
NF_3	N-F	0.3142	0.2259	-0.4998	0.45198	-0.2739	-0.1922	0.7732	0.6486	0.07898
O_3	O-O	0.3896	0.3582	-0.7587	-0.4721	-0.4005	0.242	0.7351	0.6249	0.05935
CF_4	C-F	0.2967	0.354	-0.8131	0.43537	-0.4591	-0.4201	0.5339	0.517	0.00069
SF_6	S-F	0.2052	0.2345	-0.4667	0.50246	-0.2321	0.00971	0.4331	0.4664	0.00027
SO_2	S-O	0.2719	0.5909	-0.8857	0.66716	-0.2947	1.184	0.2352	0.3567	0.14091

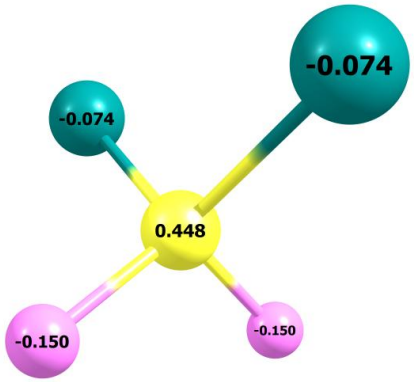
Table S17. Electron density ($\rho(r)$) and Laplacian electron density ($\nabla^2\rho(r)$) of the bond critical point between guest and host molecules.

Greenhouse gases	Bond	5^{12}		$5^{12}6^2$		$5^{12}6^4$	
		$\rho(r)$	$\nabla^2\rho(r)$	$\rho(r)$	$\nabla^2\rho(r)$	$\rho(r)$	$\nabla^2\rho(r)$
CCl_4	Cl-O	0.0123	0.0437	0.0162	0.0582	0.006	0.0238
CF_2Cl_2	F-O	0.0126	0.0546	0.0081	0.038	0.006	0.0302
CH_3Br	H-O	0.0118	0.0363	0.0091	0.028	0.0095	0.0291
CH_3Cl	H-O	0.0095	0.0303	0.0086	0.0272	0.0072	0.0229
CH_4	H-O	0.0056	0.019	0.0067	0.0225	0.0043	0.0155
CO	O-O	0.0047	0.0174	0.0024	0.0134	0.0013	0.0083
CO_2	O-O	0.0138	0.0488	0.0053	0.0232	0.0042	0.0199
H_2S	H-O	0.0322	0.0778	0.0288	0.0719	0.0302	0.0766
CH_3F	H-O	0.0097	0.0304	0.0086	0.0274	0.0078	0.0242
N_2O	O-O	0.0055	0.0205	0.0036	0.017	0.0038	0.0178
NF_3	F-O	0.0078	0.0366	0.005	0.0271	0.0067	0.0318
O_3	O-O	0.0019	0.0115	0.0033	0.0165	0.0052	0.0225
CF_4	F-O	0.0091	0.0429	0.0054	0.0284	0.0058	0.0304
SF_6	F-O	0.0122	0.0483	0.0065	0.0309	0.0045	0.024
SO_2	S-O	0.0184	0.052	0.0287	0.0761	0.0276	0.0751

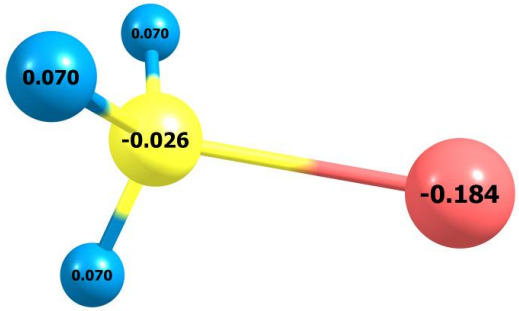
Figure S1. Mulliken charges of the Greenhouse gases monomers before encapsulation in clathrate hydrate computes at B3LYP/6-31G(d) level of theory and basis set.



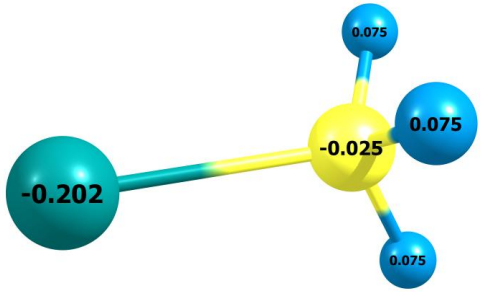
CCl_4



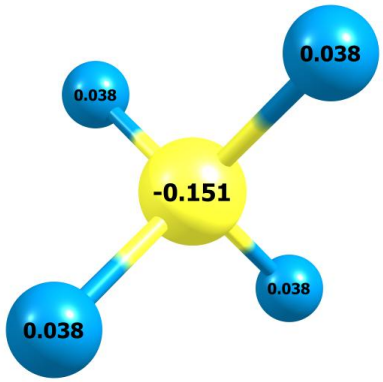
CCl_2F_2



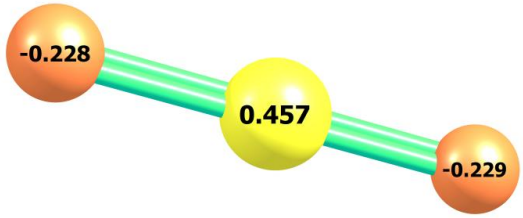
CH_3Br



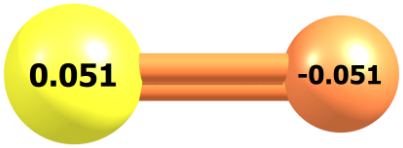
CH_3Cl



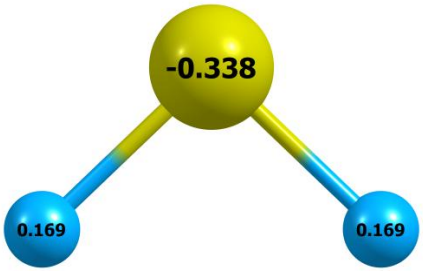
CH_4



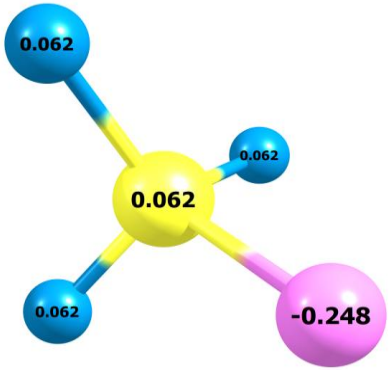
CO_2



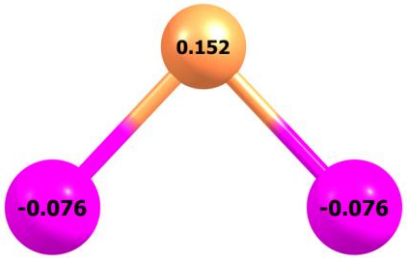
CO



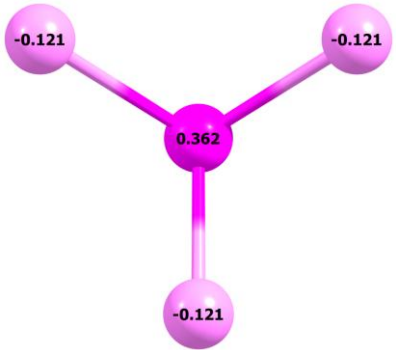
H_2S



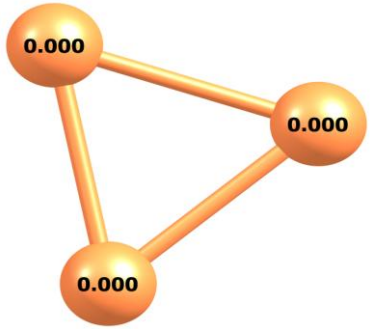
CH_3F



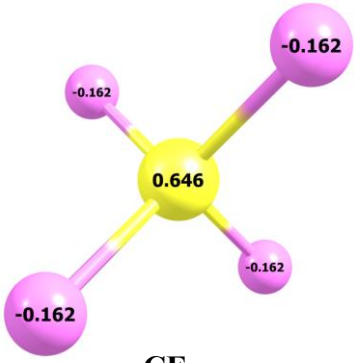
N_2O



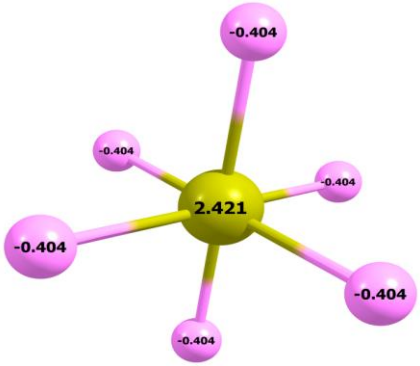
NF_3



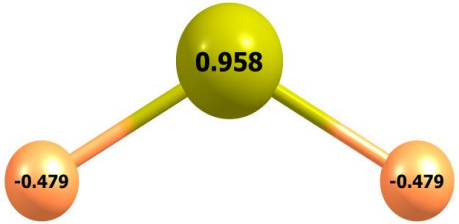
O_3



CF_4



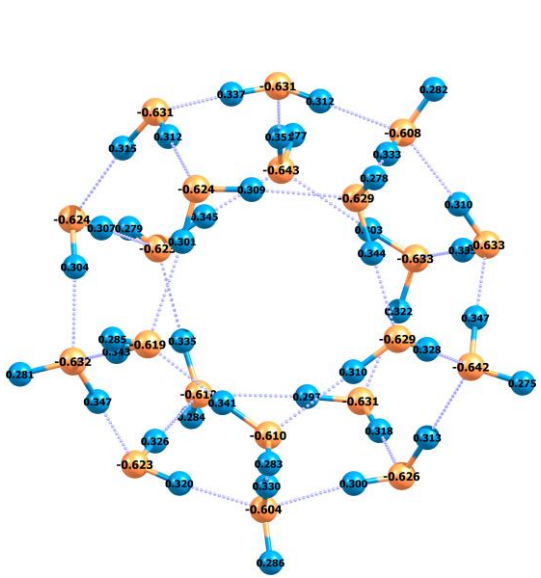
SF_6



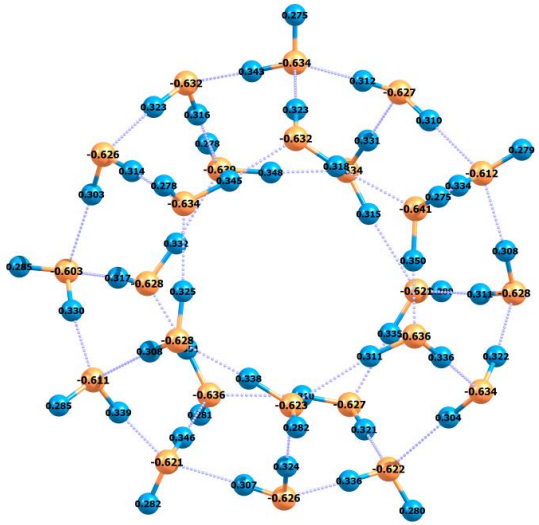
SO_2

S162

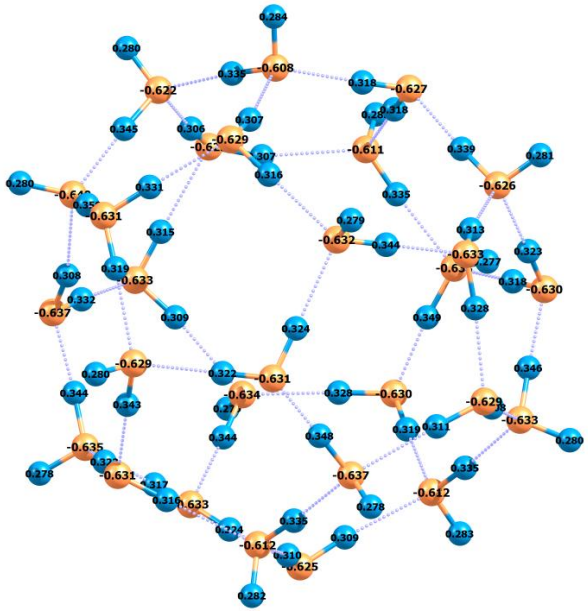
Figure S2. Mulliken charges of the empty 5^{12}, $5^{12}6^2$ and $5^{12}6^4$ clathrate hydrate monomers computes at B3LYP/6-31G(d) level of theory and basis set.



5^{12}

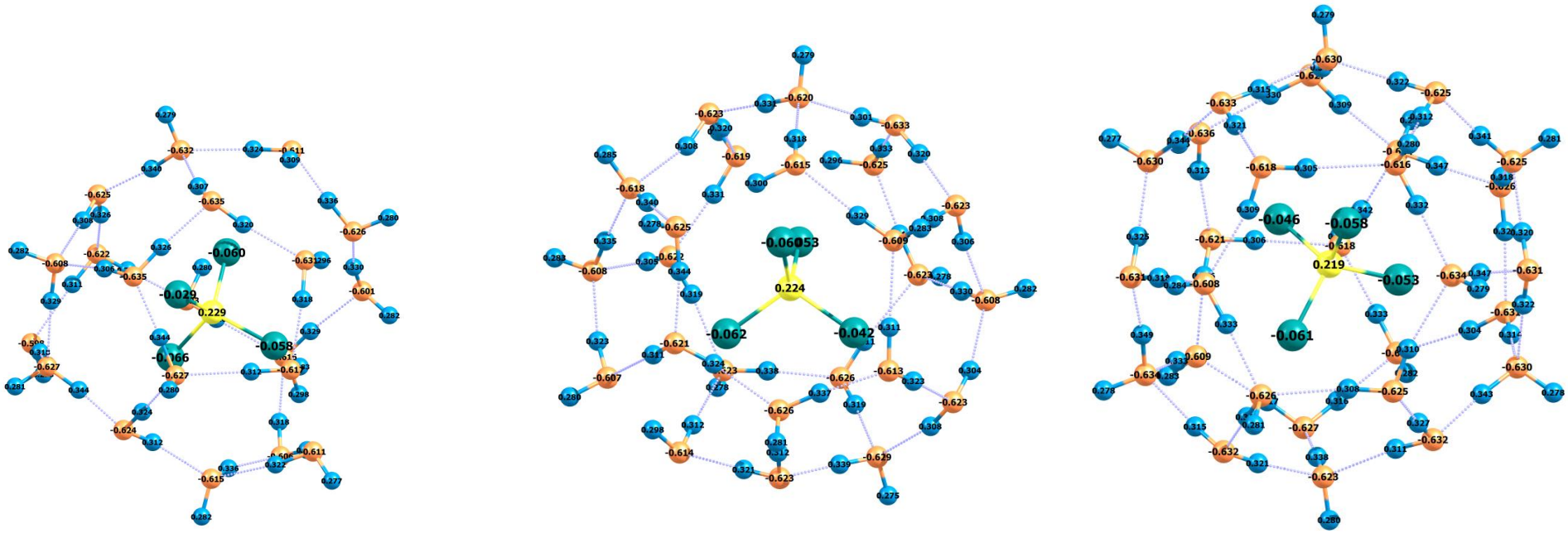


$5^{12}6^2$



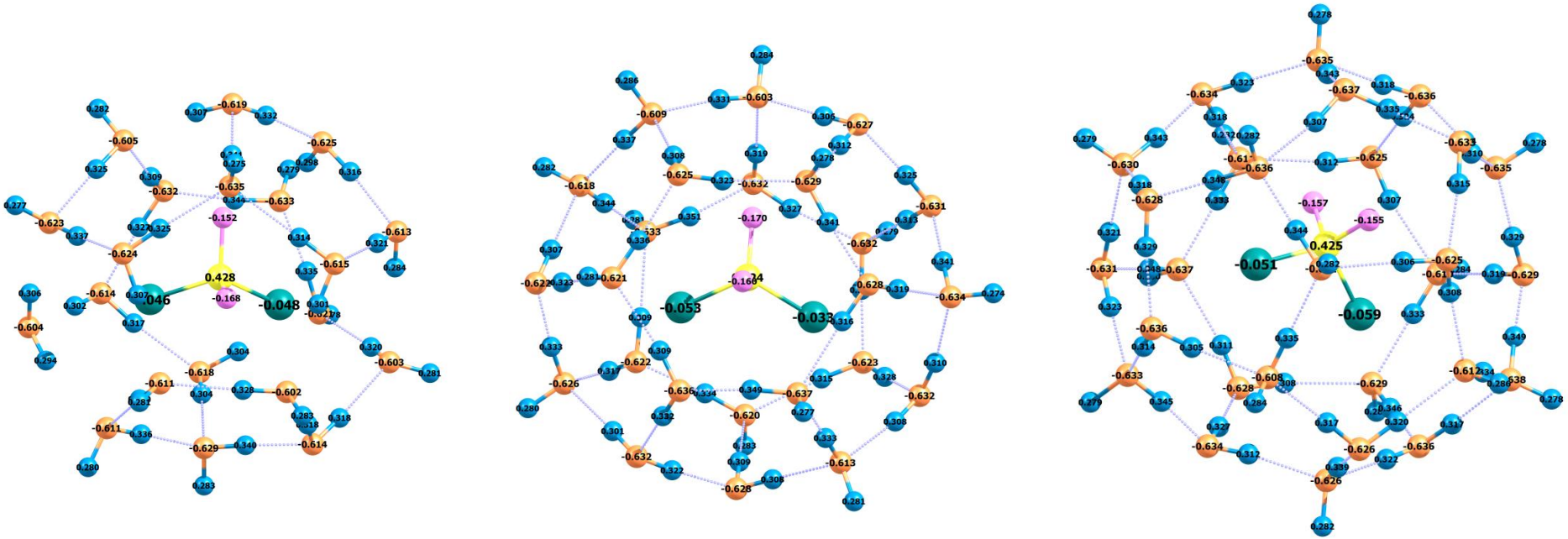
$5^{12}6^4$

Figure S3. Mulliken charges of the CCl_4 molecule within 5^{12}, $5^{12}6^2$ and $5^{12}6^4$ clathrate hydrates computes at B3LYP/6-31G(d) level of theory and basis set.



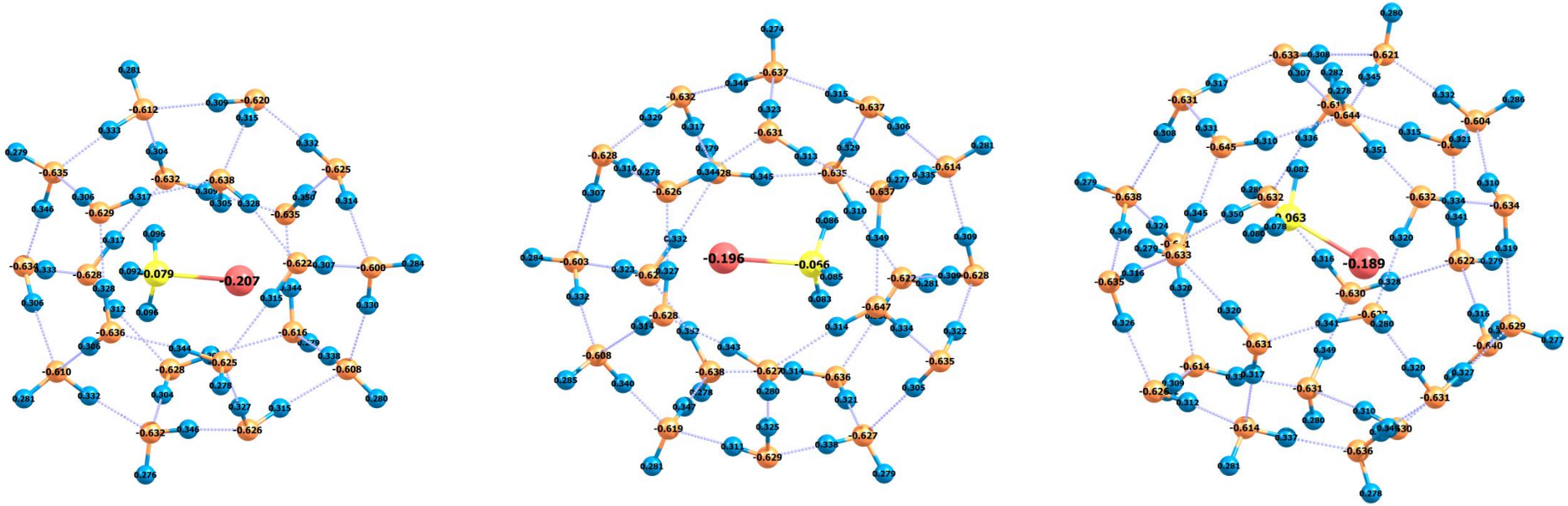
5^{12} **$5^{12}6^2$** **$5^{12}6^4$**

Figure S4. Mulliken charges of the CF_2Cl_2 molecule within 5^{12}, $5^{12}6^2$ and $5^{12}6^4$ clathrate hydrates computes at B3LYP/6-31G(d) level of theory and basis set.



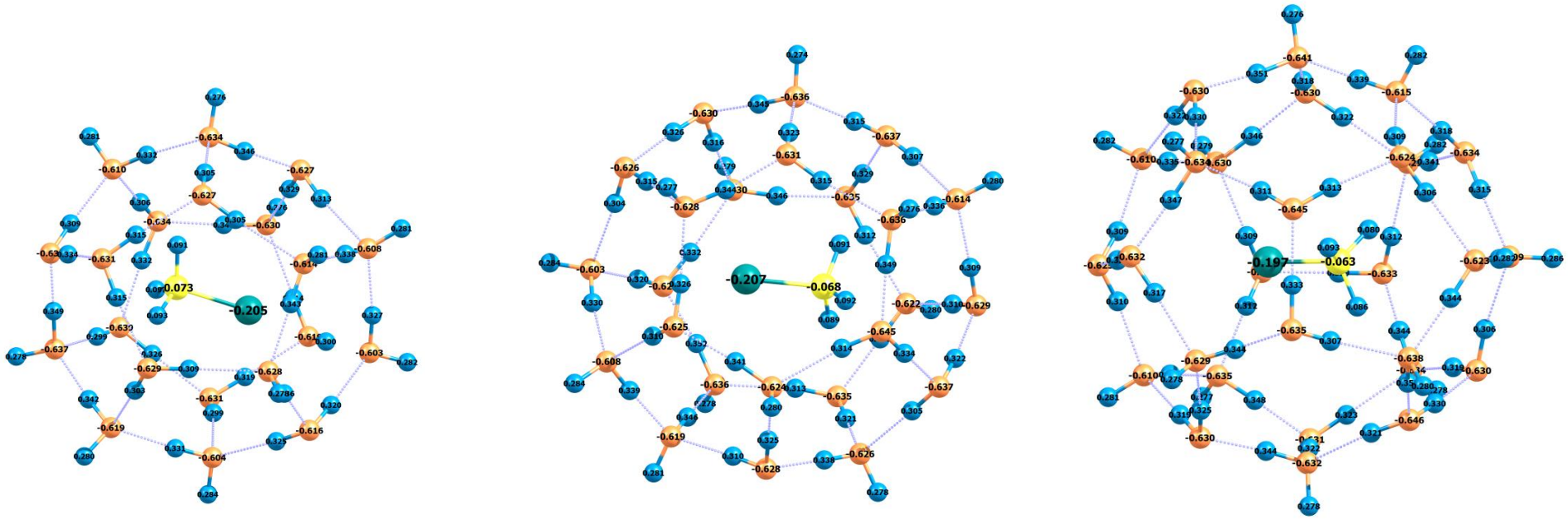
5^{12} **$5^{12}6^2$** **$5^{12}6^4$**

Figure S5. Mulliken charges of the CH_3Br molecule within 5^{12}, $5^{12}6^2$ and $5^{12}6^4$ clathrate hydrates computes at B3LYP/6-31G(d) level of theory and basis set.



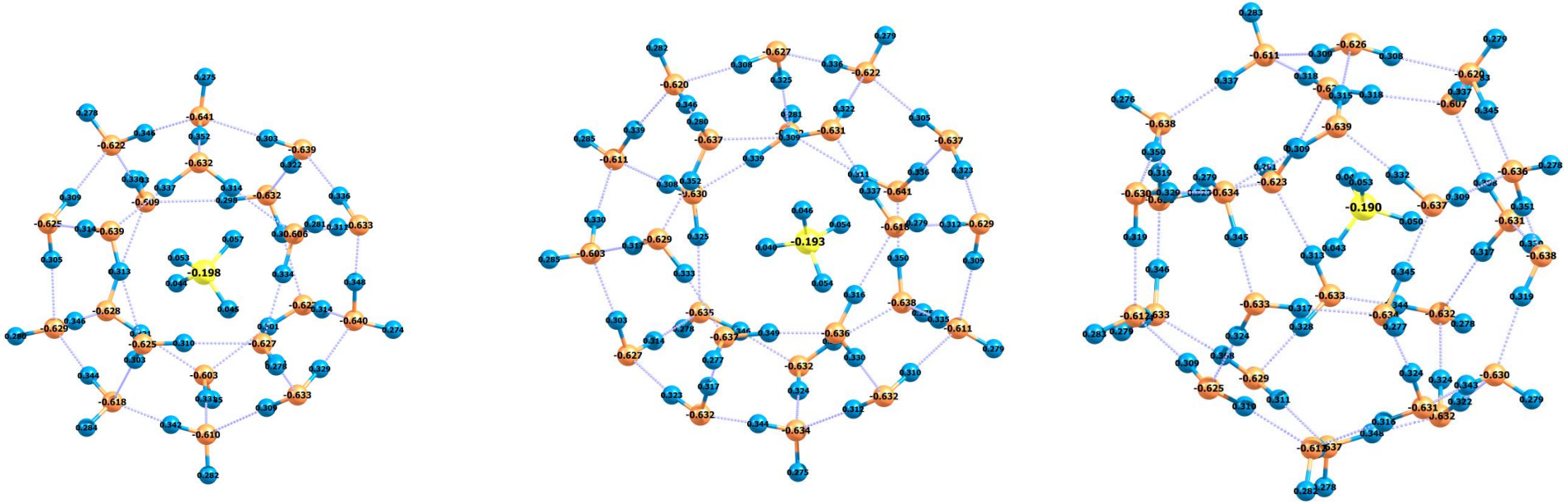
5^{12} **$5^{12}6^2$** **$5^{12}6^4$**

Figure S6. Mulliken charges of the CH_3Cl molecule within 5^{12}, $5^{12}6^2$ and $5^{12}6^4$ clathrate hydrates computes at B3LYP/6-31G(d) level of theory and basis set.



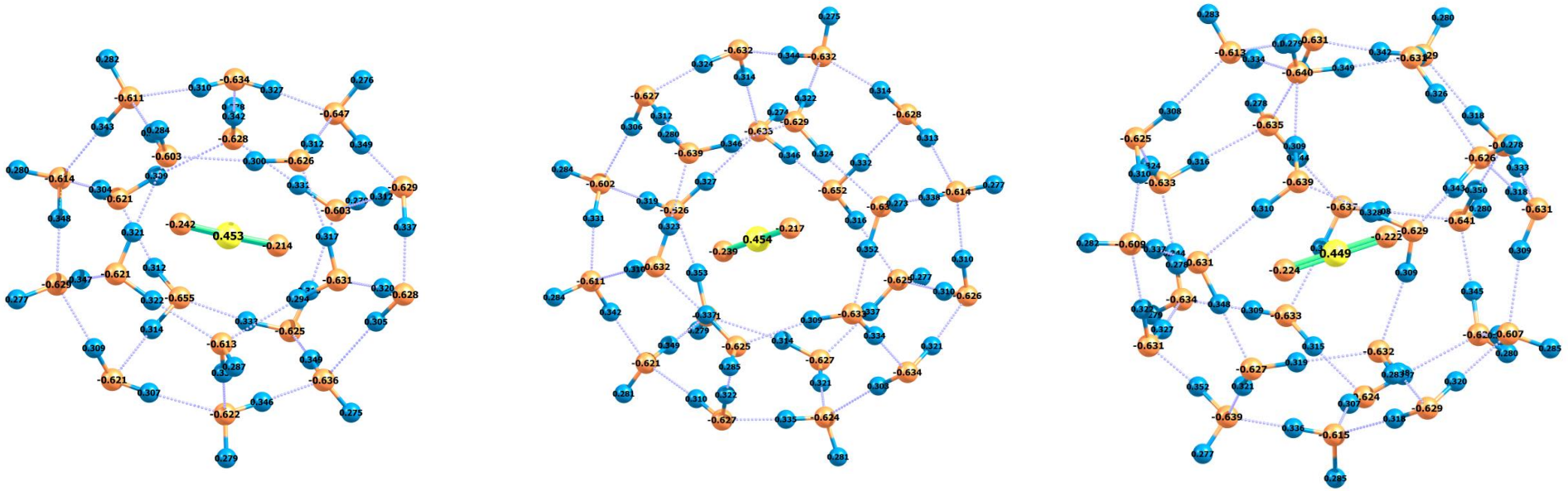
5^{12} **$5^{12}6^2$** **$5^{12}6^4$**

Figure S7. Mulliken charges of the CH_4 molecule within 5^{12}, $5^{12}6^2$ and $5^{12}6^4$ clathrate hydrates computes at B3LYP/6-31G(d) level of theory and basis set.



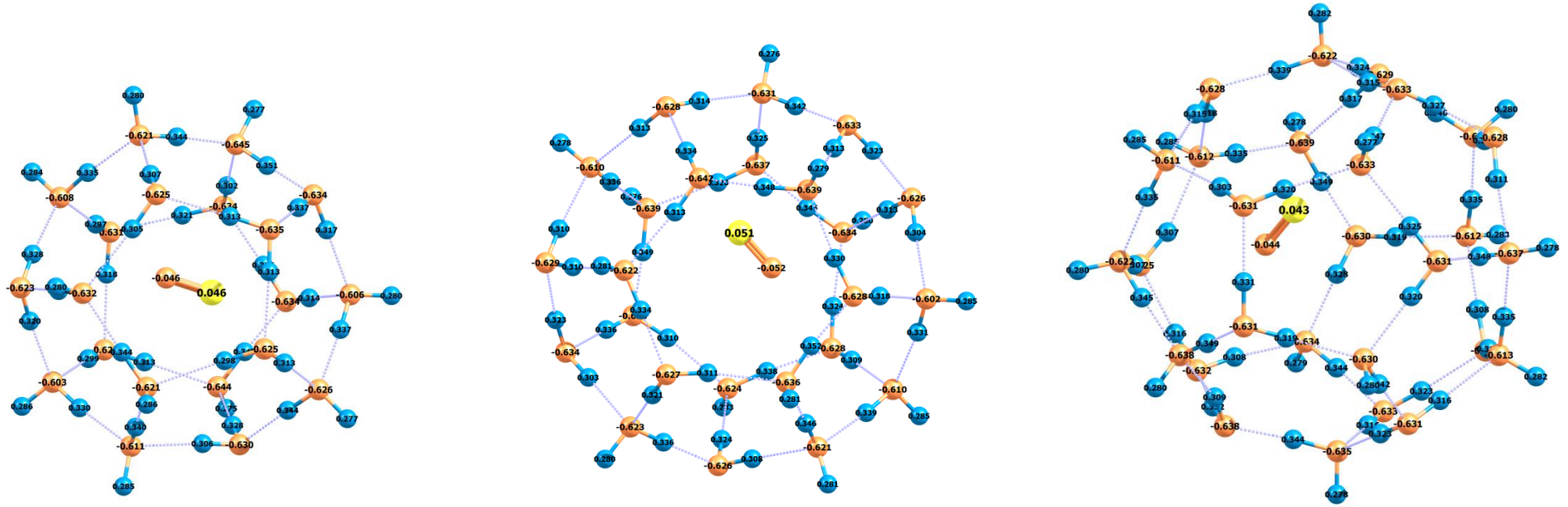
5^{12} **$5^{12}6^2$** **$5^{12}6^4$**

Figure S8. Mulliken charges of the CO_2 molecule within 5^{12}, $5^{12}6^2$ and $5^{12}6^4$ clathrate hydrates computes at B3LYP/6-31G(d) level of theory and basis set.



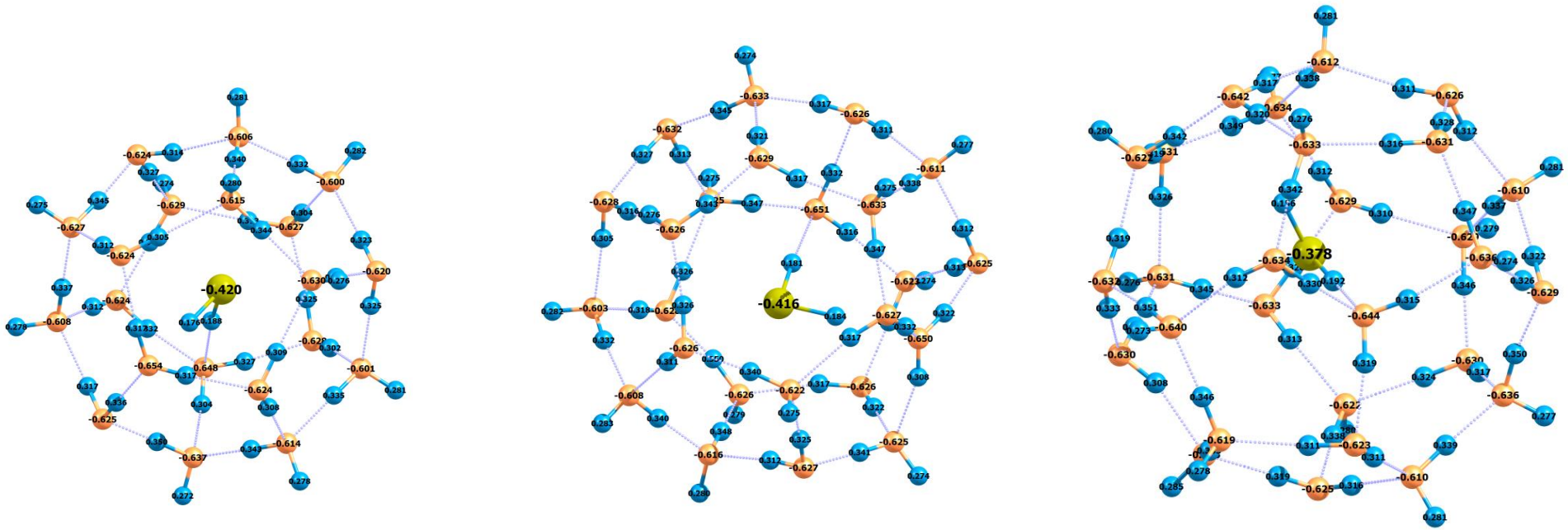
5^{12} **$5^{12}6^2$** **$5^{12}6^4$**

Figure S9. Mulliken charges of the CO molecule within 5^{12}, $5^{12}6^2$ and $5^{12}6^4$ clathrate hydrates computes at B3LYP/6-31G(d) level of theory and basis set.



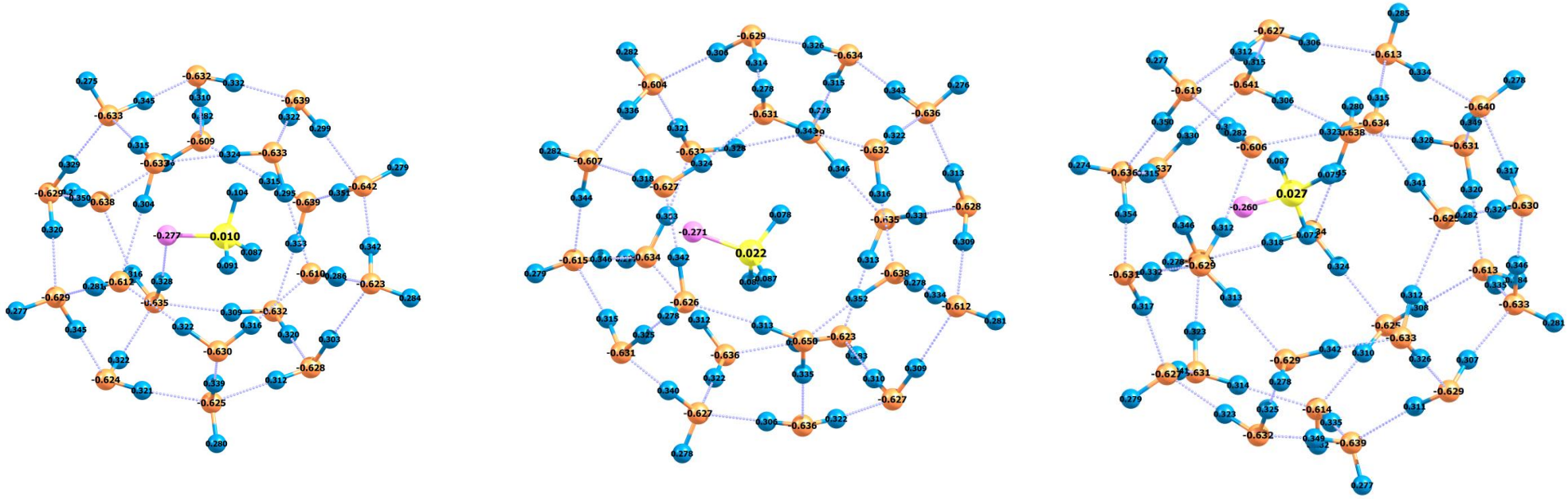
5^{12} **$5^{12}6^2$** **$5^{12}6^4$**

Figure S10. Mulliken charges of the H_2S molecule within 5^{12}, $5^{12}6^2$ and $5^{12}6^4$ clathrate hydrates computes at B3LYP/6-31G(d) level of theory and basis set.



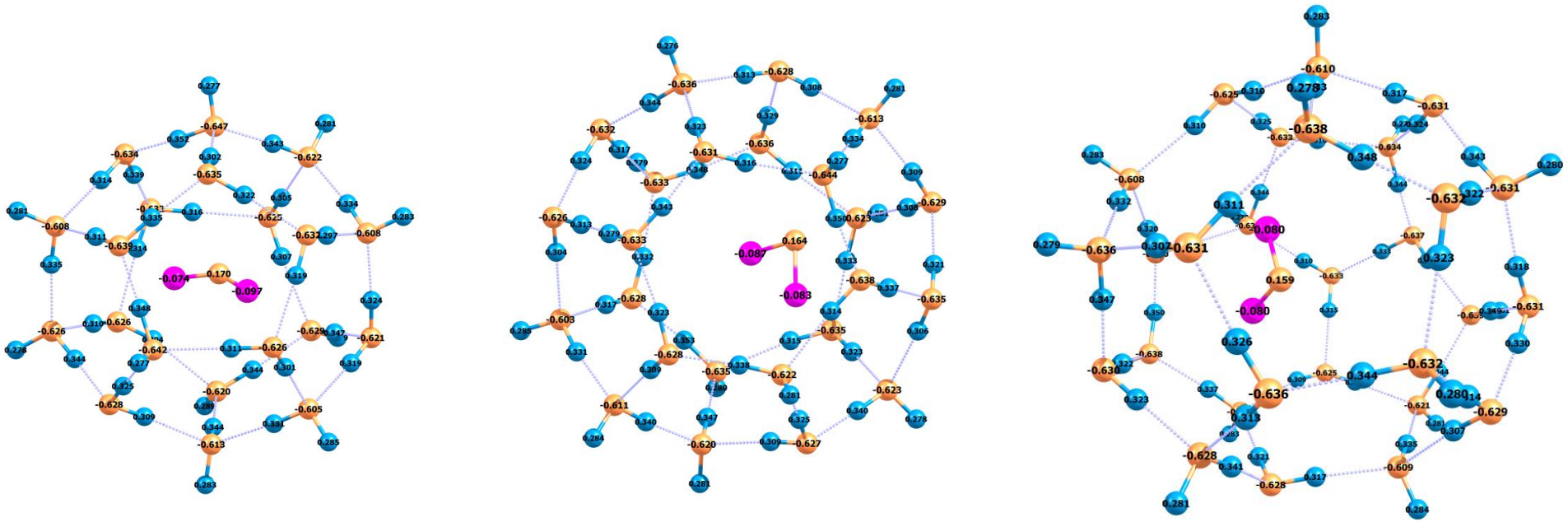
5^{12} **$5^{12}6^2$** **$5^{12}6^4$**

Figure S11. Mulliken charges of the CH_3F molecule within 5^{12}, $5^{12}6^2$ and $5^{12}6^4$ clathrate hydrates computes at B3LYP/6-31G(d) level of theory and basis set.



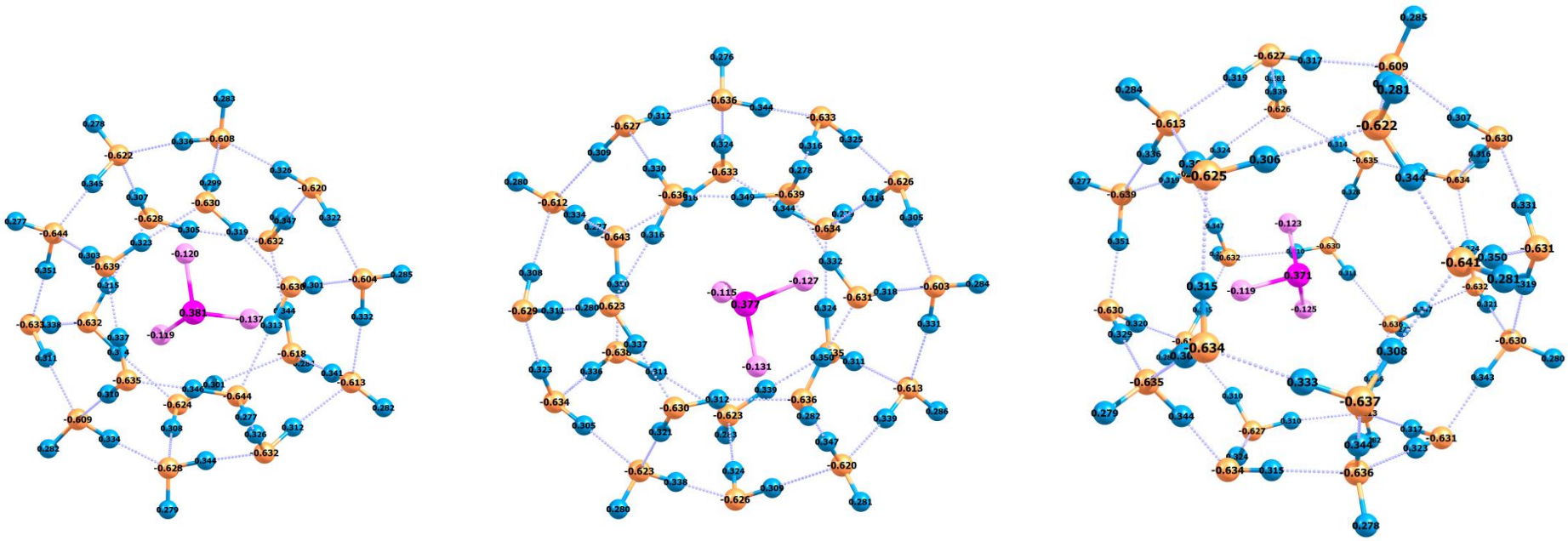
5^{12} **$5^{12}6^2$** **$5^{12}6^4$**

Figure S12. Mulliken charges of the N_2O molecule within 5^{12}, $5^{12}6^2$ and $5^{12}6^4$ clathrate hydrates computes at B3LYP/6-31G(d) level of theory and basis set.



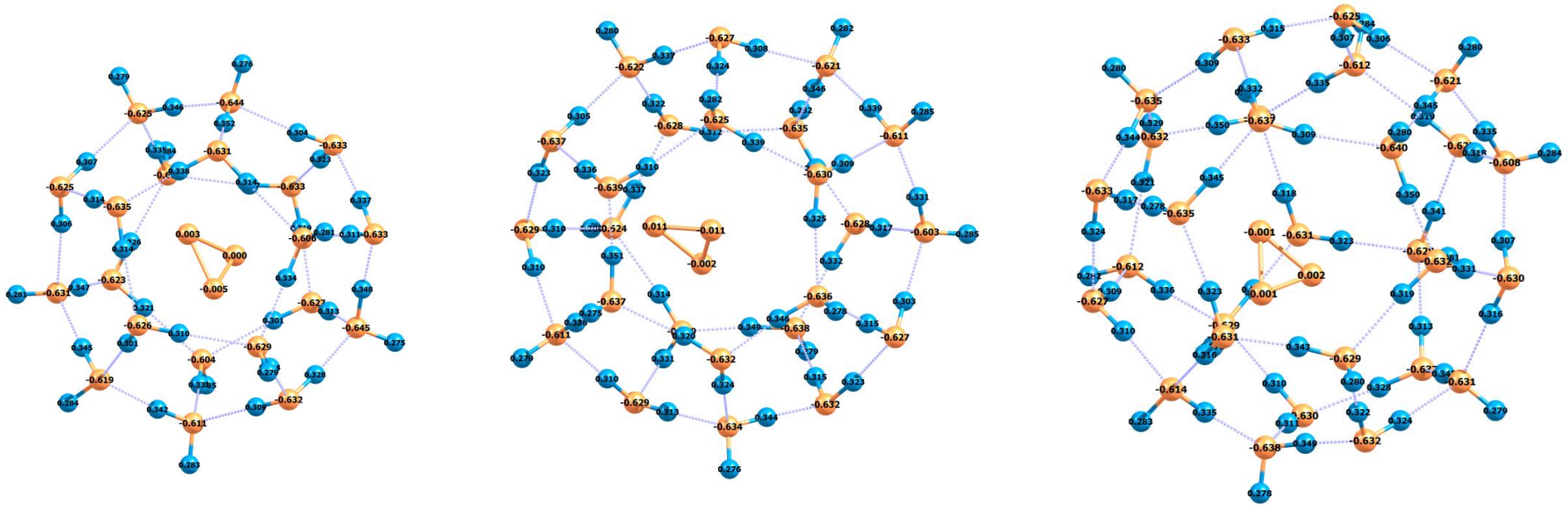
5^{12} **$5^{12}6^2$** **$5^{12}6^4$**

Figure S13. Mulliken charges of the NF_3 molecule within 5^{12}, $5^{12}6^2$ and $5^{12}6^4$ clathrate hydrates computes at B3LYP/6-31G(d) level of theory and basis set.



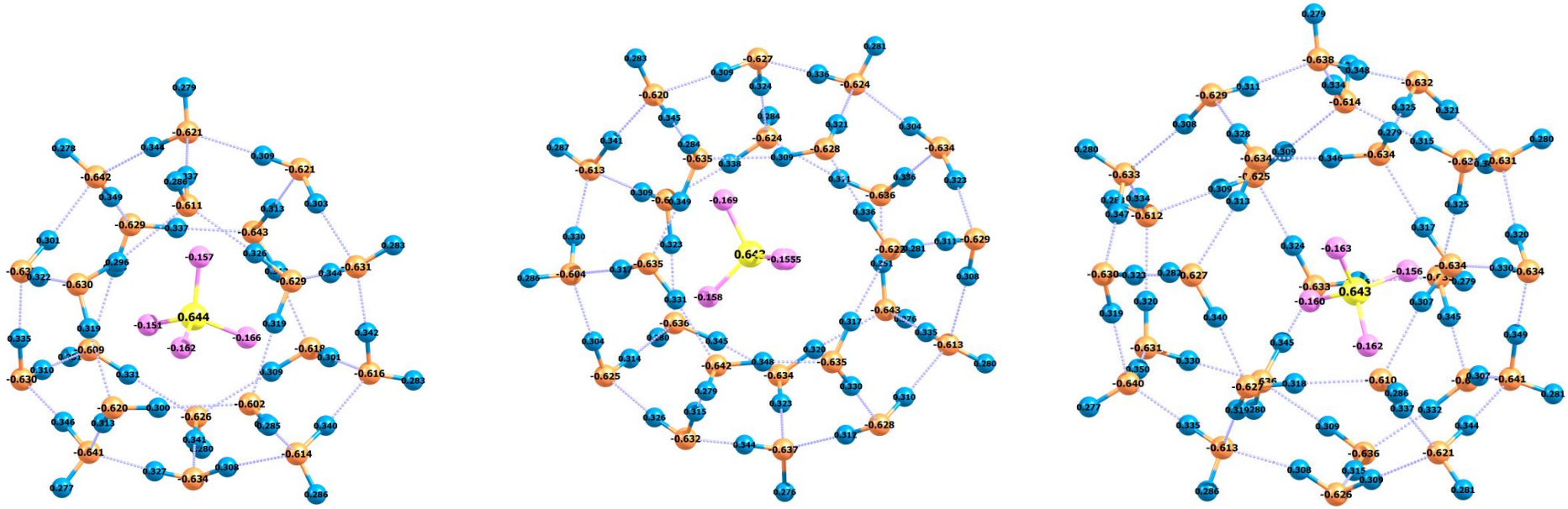
5^{12} **$5^{12}6^2$** **$5^{12}6^4$**

Figure S14. Mulliken charges of the O_3 molecule within 5^{12}, $5^{12}6^2$ and $5^{12}6^4$ clathrate hydrates computes at B3LYP/6-31G(d) level of theory and basis set.



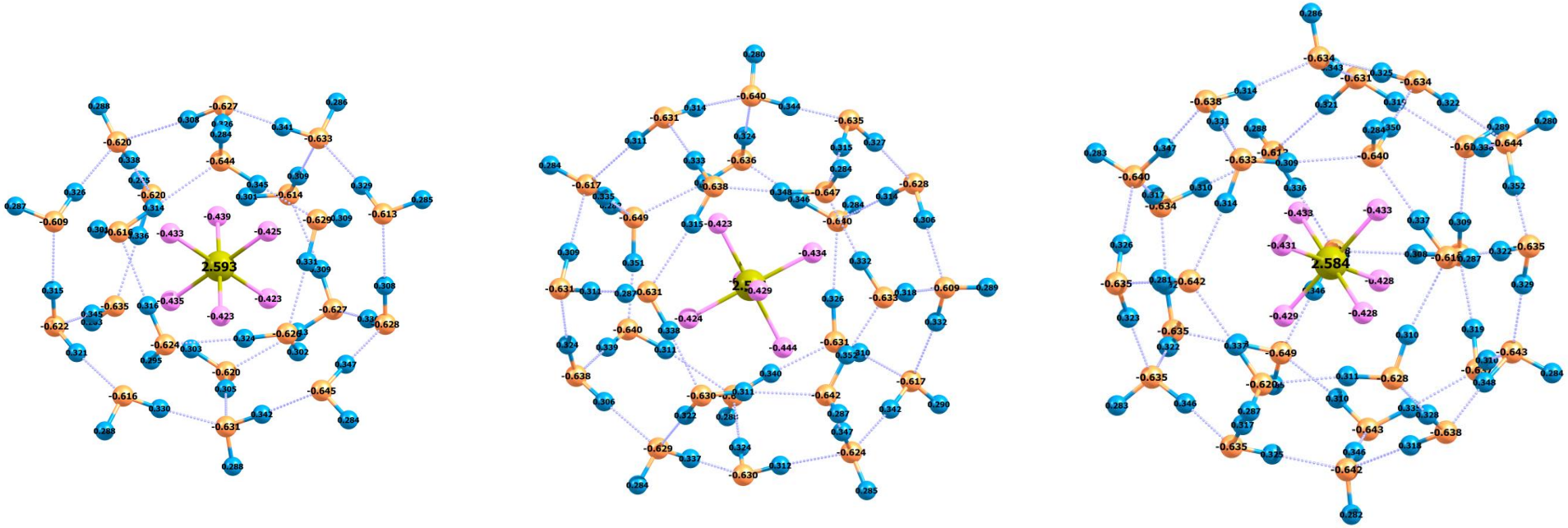
5^{12} **$5^{12}6^2$** **$5^{12}6^4$**

Figure S15. Mulliken charges of the CF_4 molecule within 5^{12}, $5^{12}6^2$ and $5^{12}6^4$ clathrate hydrates computes at B3LYP/6-31G(d) level of theory and basis set.



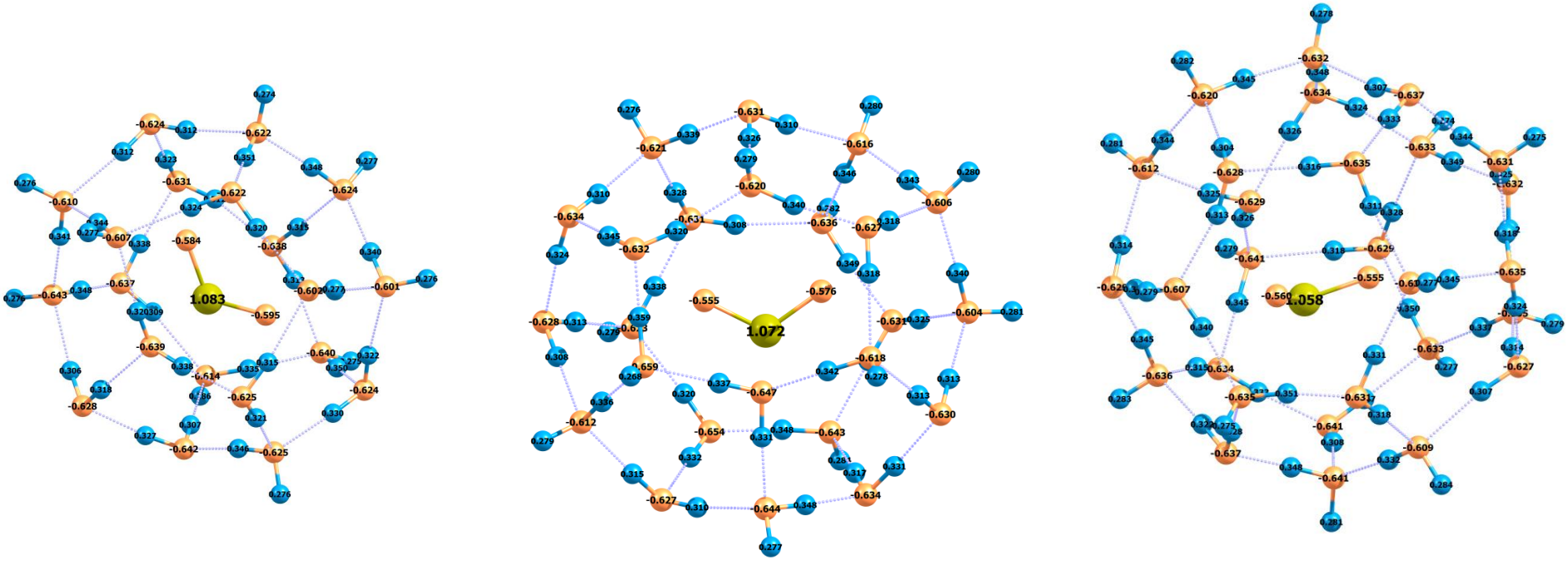
5^{12} **$5^{12}6^2$** **$5^{12}6^4$**

Figure S16. Mulliken charges of the SF_6 molecule within 5^{12}, $5^{12}6^2$ and $5^{12}6^4$ clathrate hydrates computes at B3LYP/6-31G(d) level of theory and basis set.



5^{12} **$5^{12}6^2$** **$5^{12}6^4$**

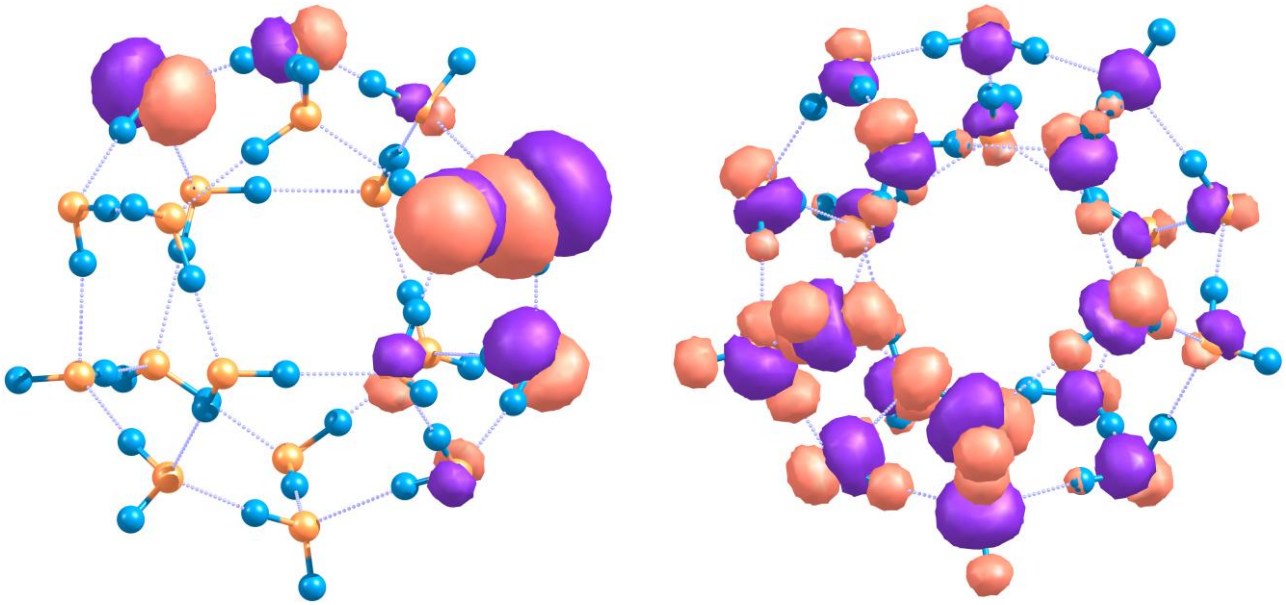
Figure S17. Mulliken charges of the SO_2 molecule within 5^{12}, $5^{12}6^2$ and $5^{12}6^4$ clathrate hydrates computes at B3LYP/6-31G(d) level of theory and basis set.



5^{12} **$5^{12}6^2$** **$5^{12}6^4$**

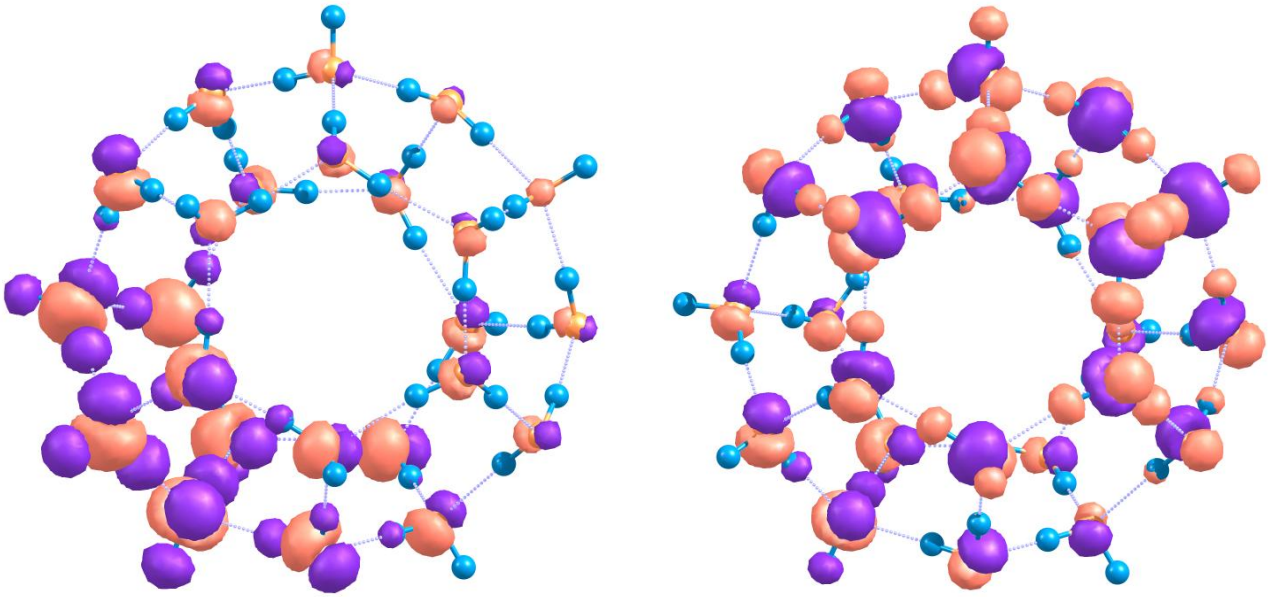
Figure S18. Frontier molecular orbital of the empty 5^{12}, $5^{12}6^2$ and $5^{12}6^4$ clathrate hydrates computes at B3LYP/6-31G(d) level of theory and basis set.

HOMO **LUMO**



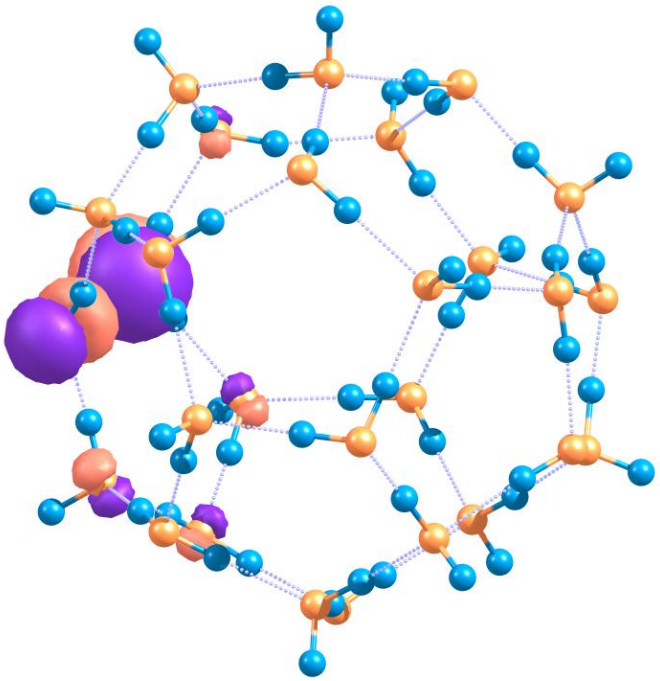
5^{12}

HOMO **LUMO**

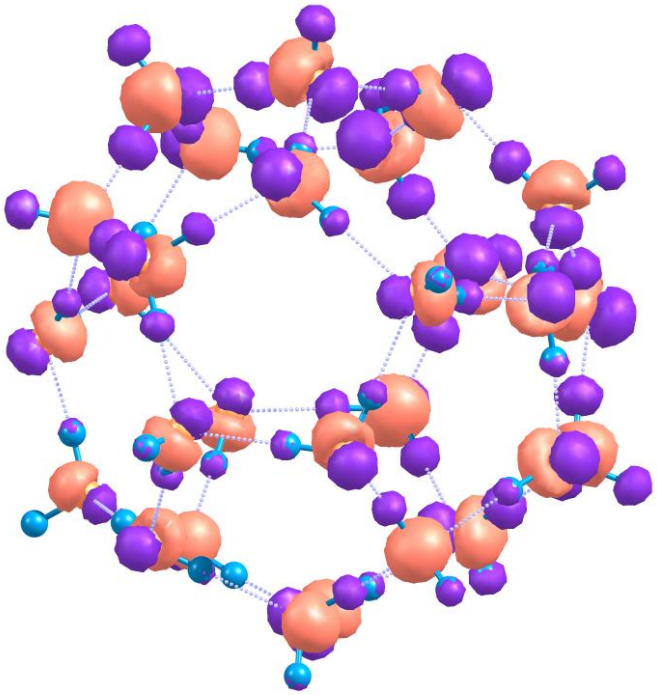


$5^{12}6^2$

HOMO



LUMO



$5^{12}6^{4}$

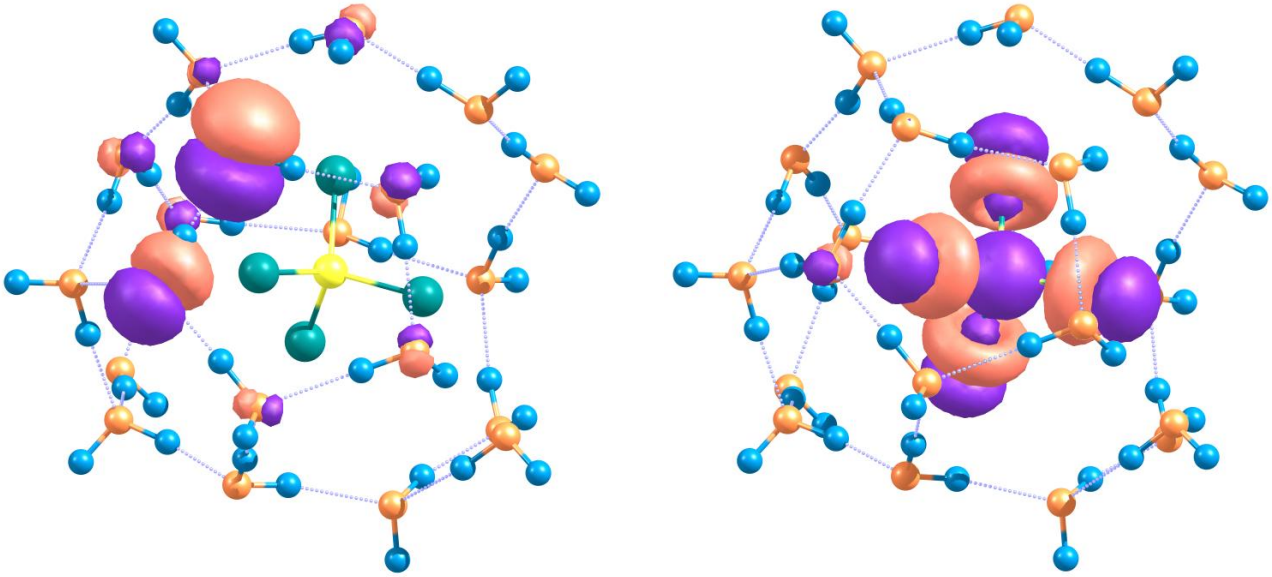
Figure S19. Frontier molecular orbital of the CCl_4 molecule before and after encapsulation in 5^{12}, $5^{12}6^2$ and $5^{12}6^4$ clathrate hydrates computes at B3LYP/6-31G(d) level of theory and basis set.

Before Encapsulation

HOMO **LUMO**

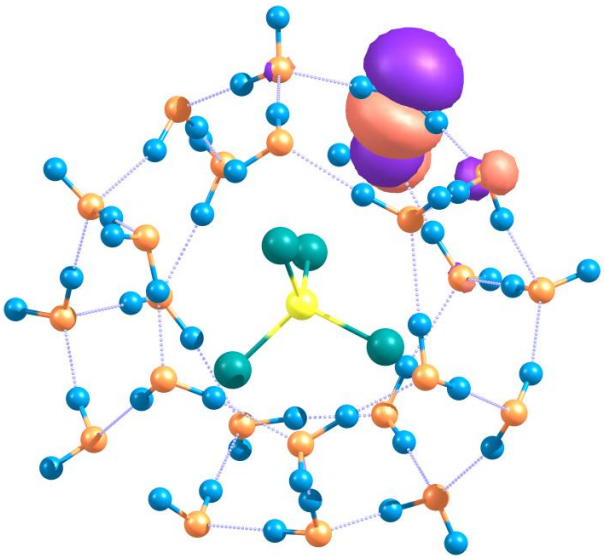
After Encapsulation

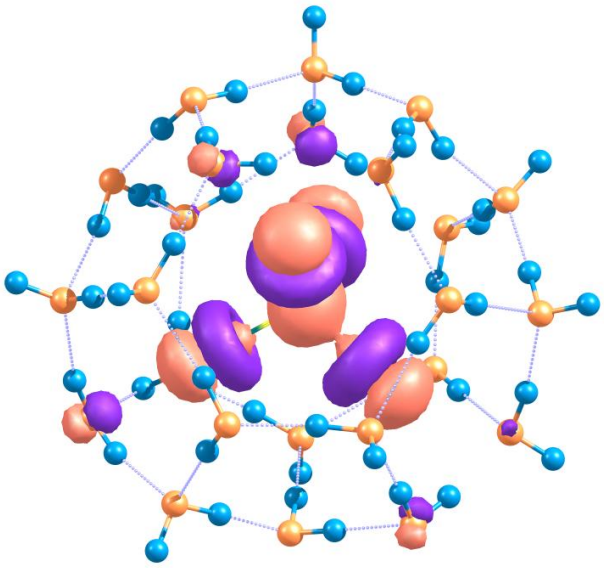
HOMO **LUMO**



5^{12}

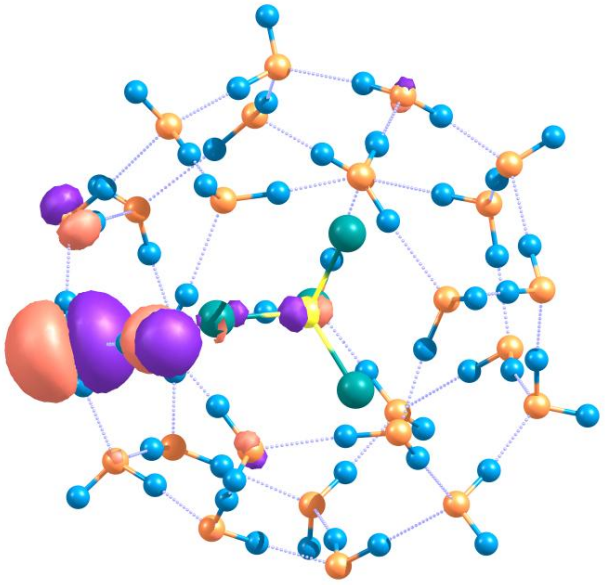
HOMO **LUMO**

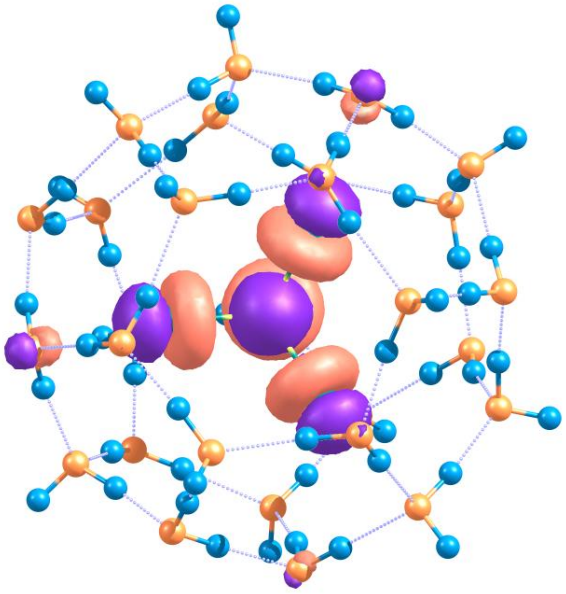




$5^{12}6^{2}$

HOMO **LUMO**



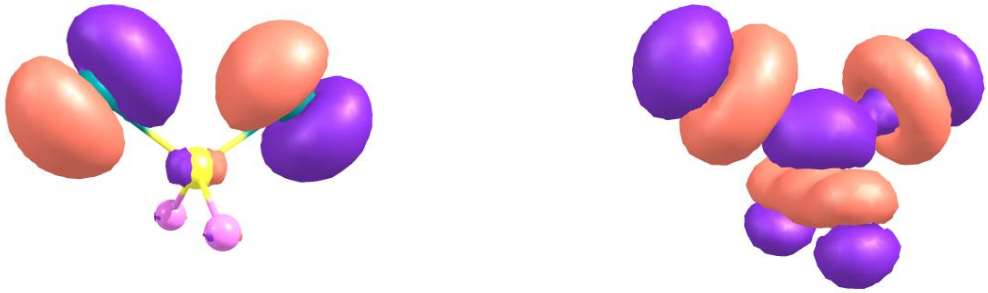


$5^{12}6^{4}$

Figure S20. Frontier molecular orbital of the CF_2Cl_2 molecule before and after encapsulation in 5^{12}, $5^{12}6^2$ and $5^{12}6^4$ clathrate hydrates computes at B3LYP/6-31G(d) level of theory and basis set.

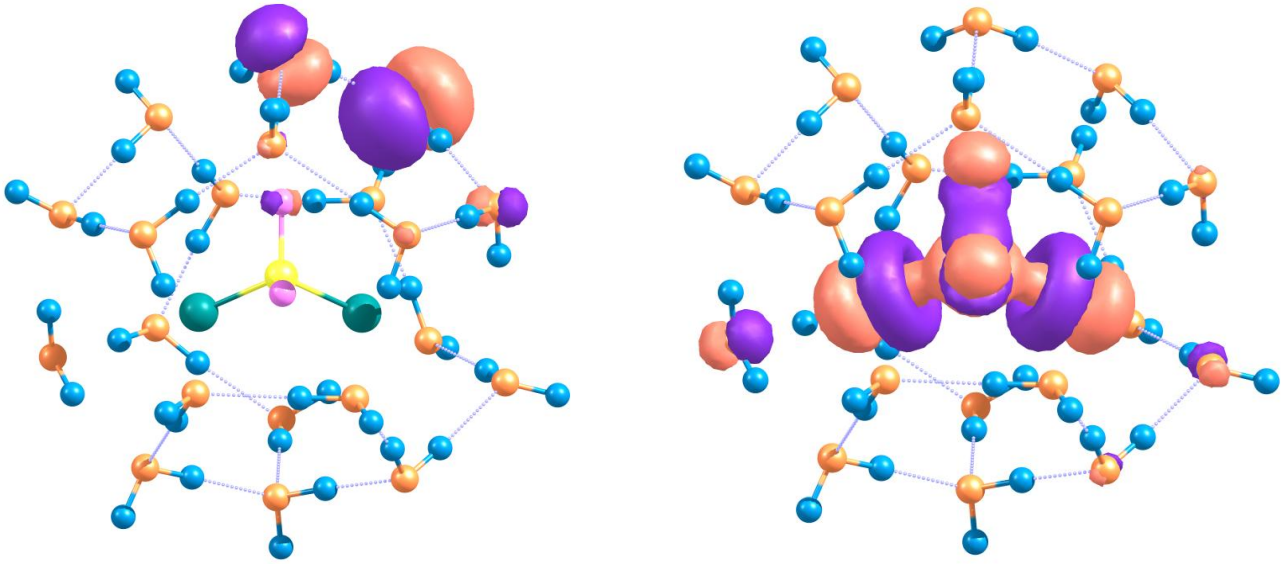
Before Encapsulation

HOMO **LUMO**



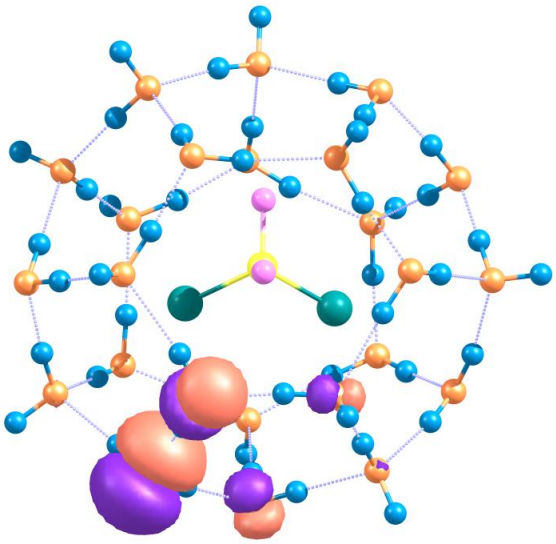
After Encapsulation

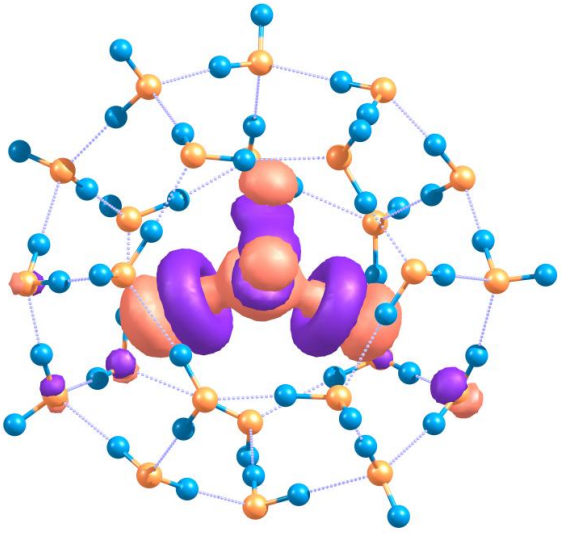
HOMO **LUMO**



5^{12}

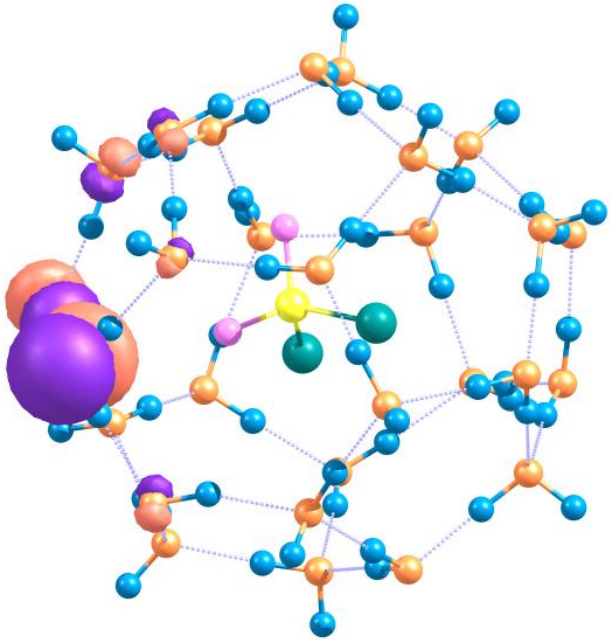
HOMO **LUMO**

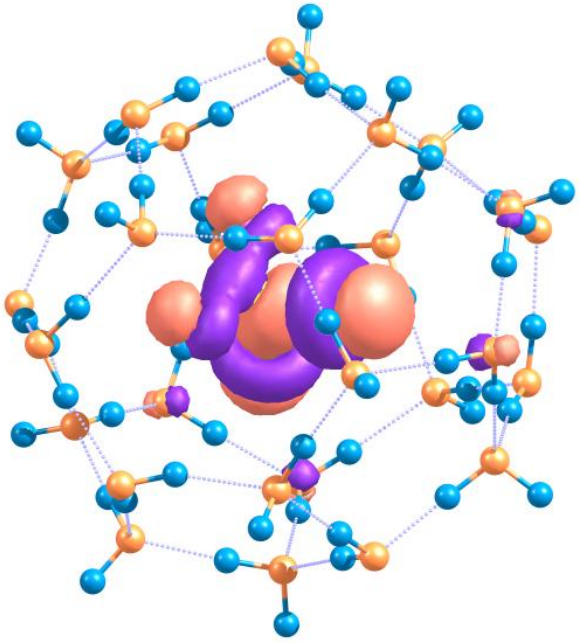




$5^{12}6^{2}$

HOMO **LUMO**





$5^{12}6^{4}$

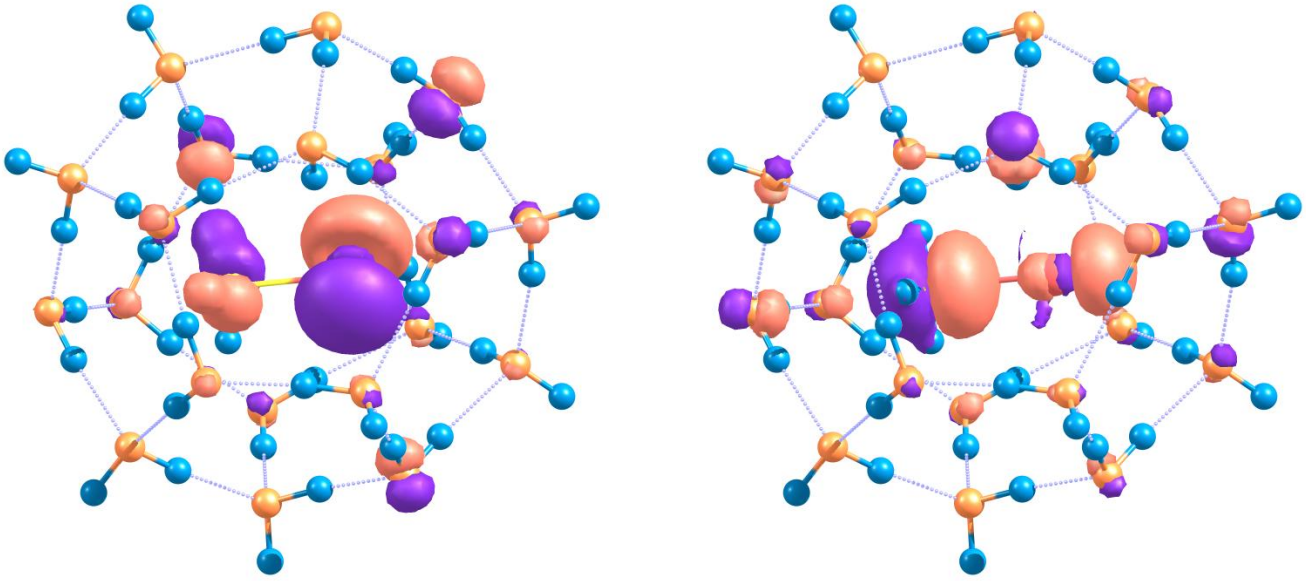
Figure S21. Frontier molecular orbital of the CH_3Br molecule before and after encapsulation in 5^{12}, $5^{12}6^2$ and $5^{12}6^4$ clathrate hydrates computes at B3LYP/6-31G(d) level of theory and basis set.

Before Encapsulation

HOMO **LUMO**

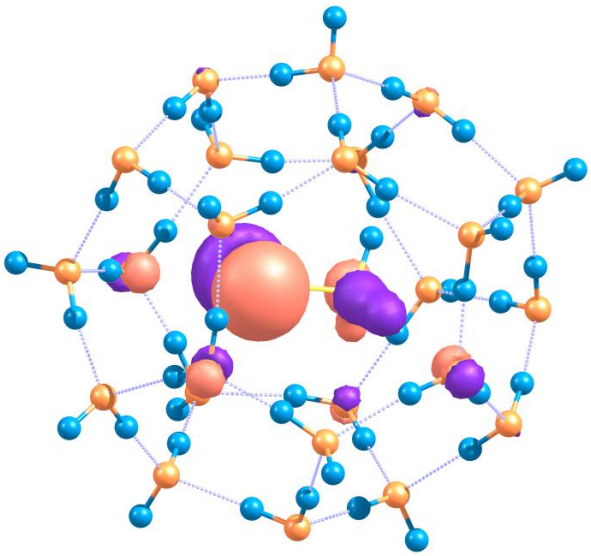
After Encapsulation

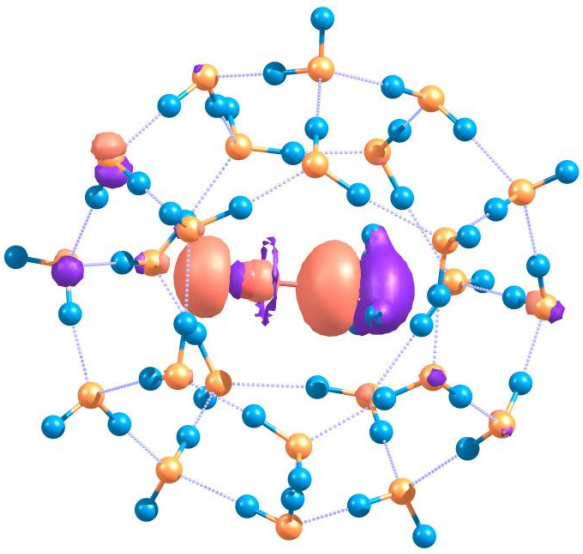
HOMO **LUMO**



5^{12}

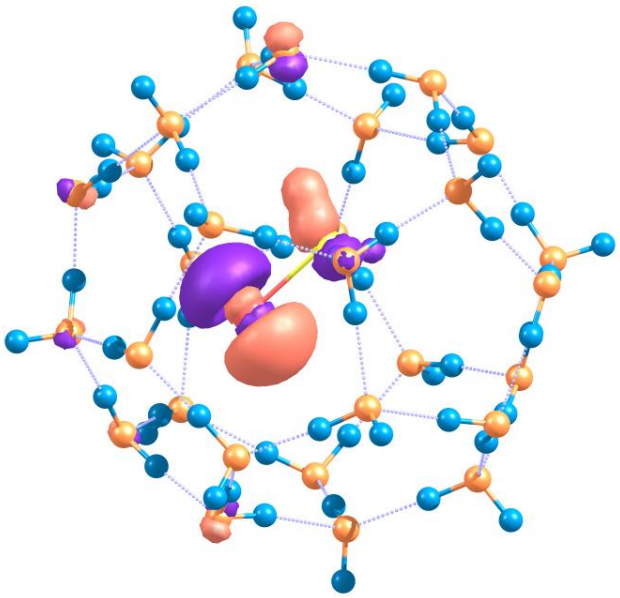
HOMO **LUMO**

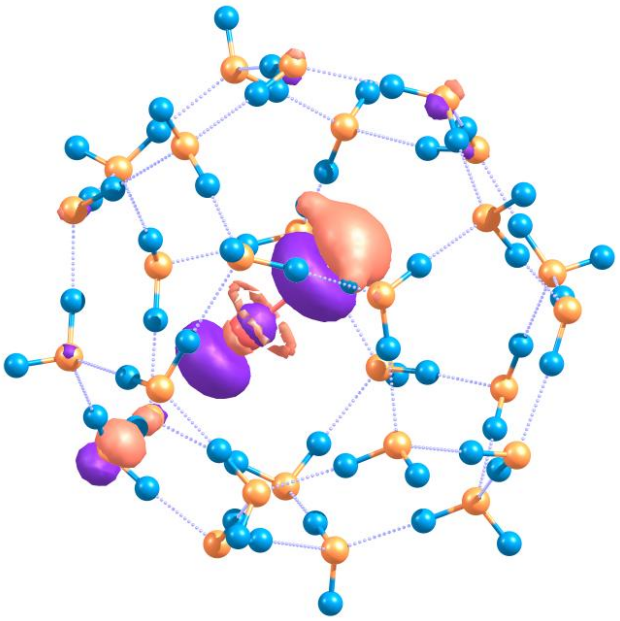




$5^{12}6^{2}$

HOMO **LUMO**



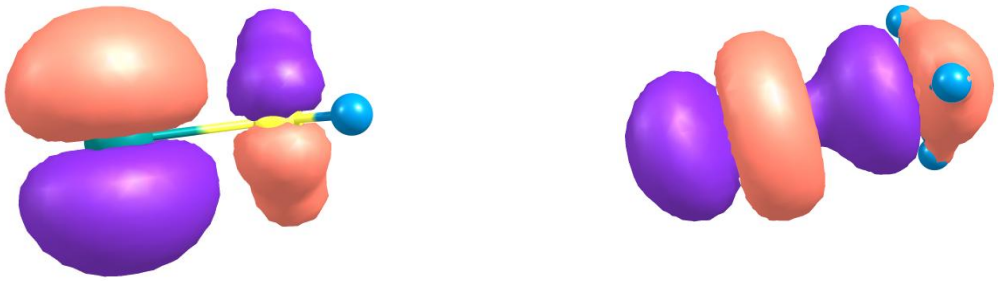


$5^{12}6^{4}$

Figure S22. Frontier molecular orbital of the CH_3Cl molecule before and after encapsulation in 5^{12}, $5^{12}6^2$ and $5^{12}6^4$ clathrate hydrates computes at B3LYP/6-31G(d) level of theory and basis set.

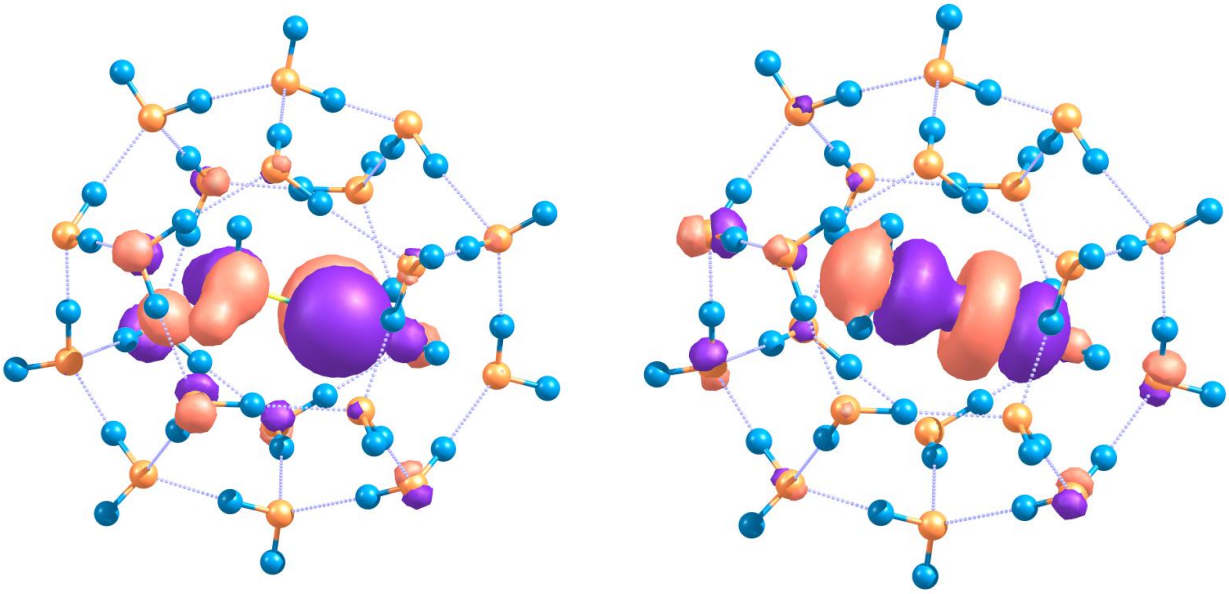
Before Encapsulation

HOMO **LUMO**



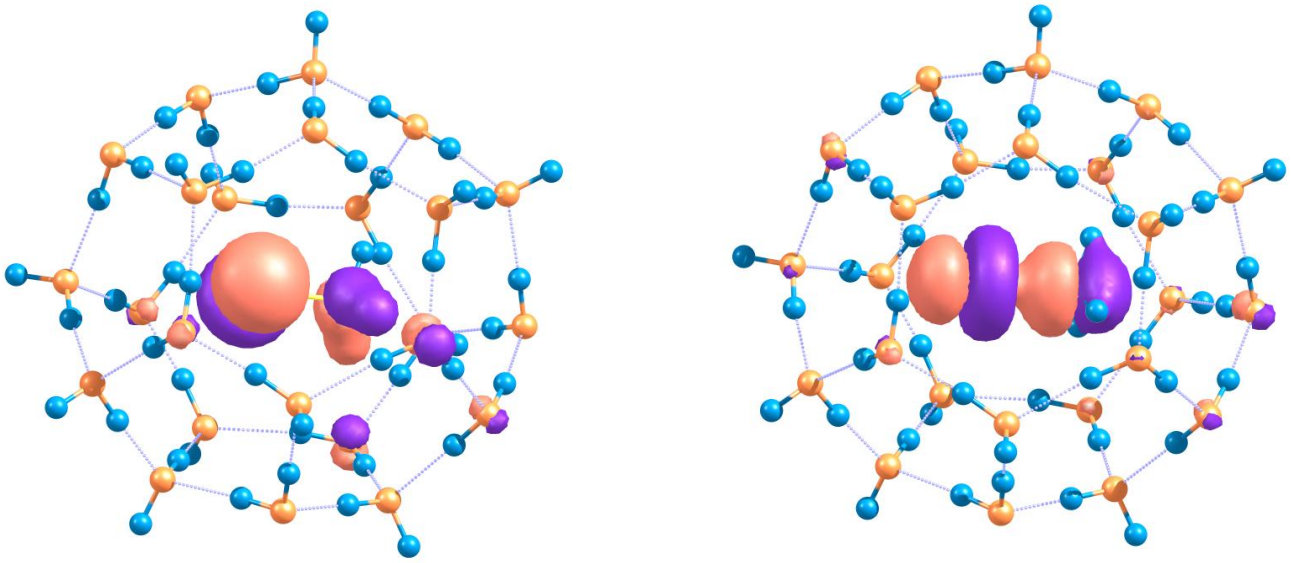
After Encapsulation

HOMO **LUMO**



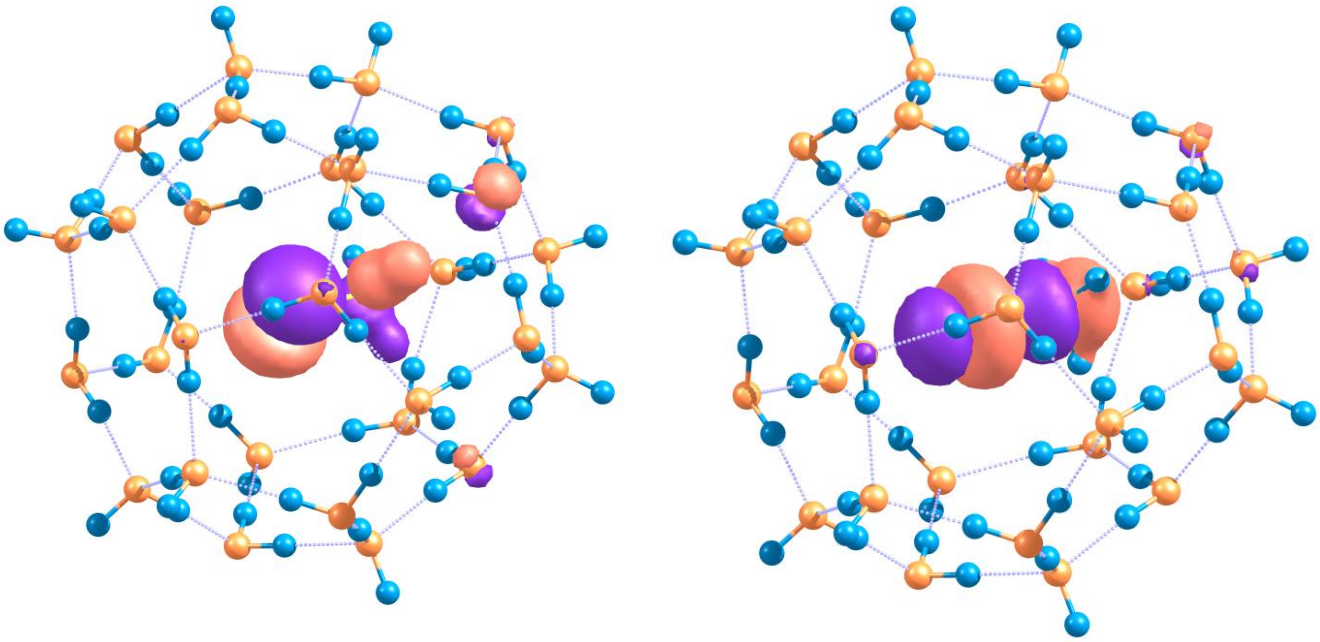
5^{12}

HOMO **LUMO**



$5^{12}6^{2}$

HOMO **LUMO**



$5^{12}6^{4}$

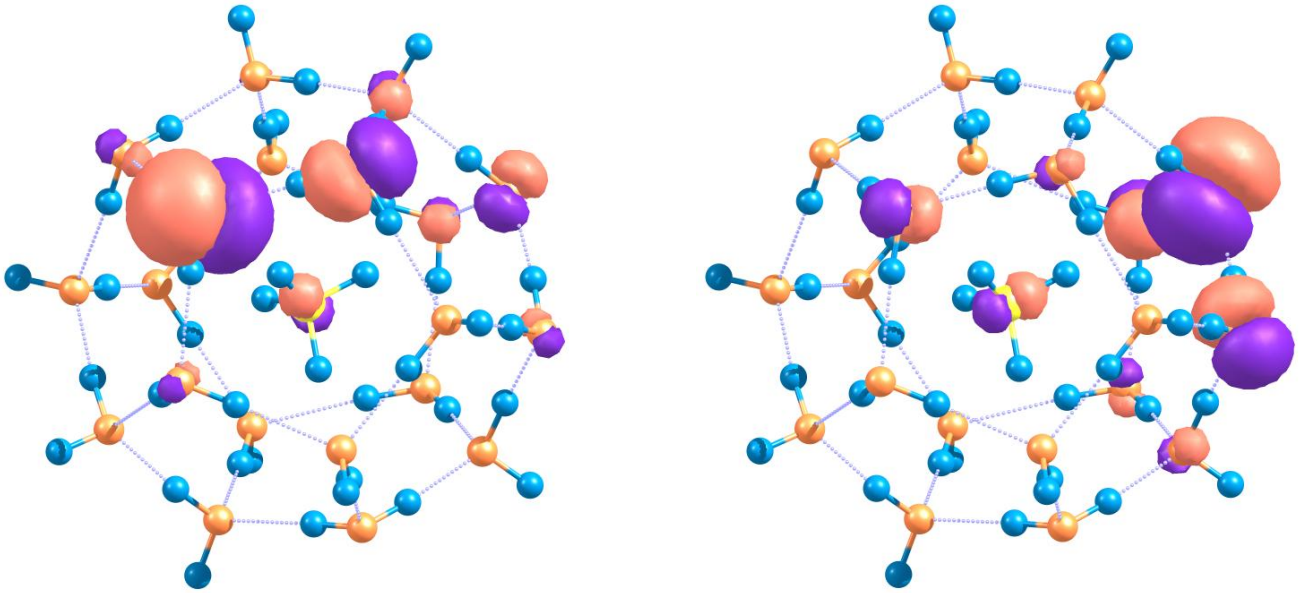
Figure S23. Frontier molecular orbital of the CH_4 molecule before and after encapsulation in 5^{12}, $5^{12}6^2$ and $5^{12}6^4$ clathrate hydrates computes at B3LYP/6-31G(d) level of theory and basis set.

Before Encapsulation

HOMO **LUMO**

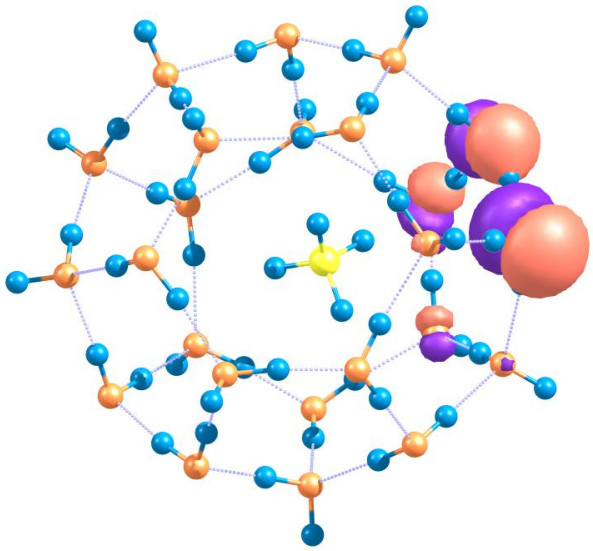
After Encapsulation

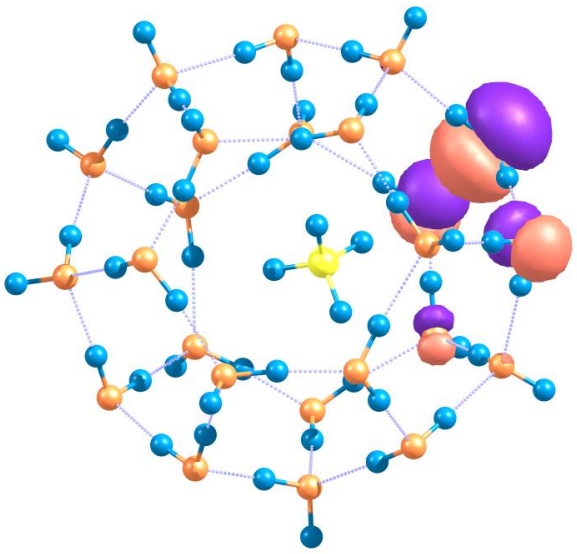
HOMO **LUMO**



5^{12}

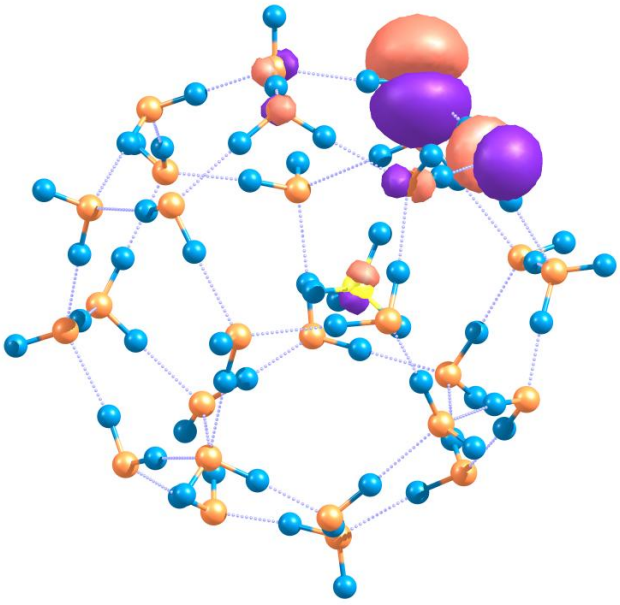
HOMO **LUMO**

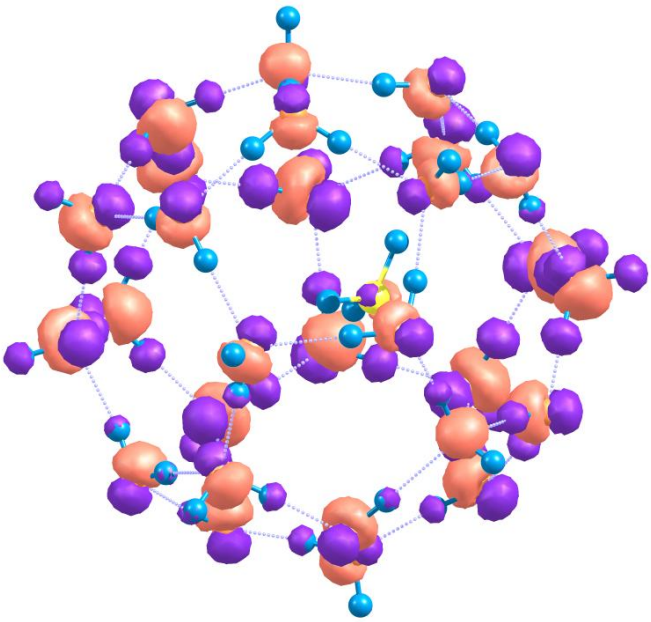




$5^{12}6^{2}$

HOMO **LUMO**





$5^{12}6^{4}$

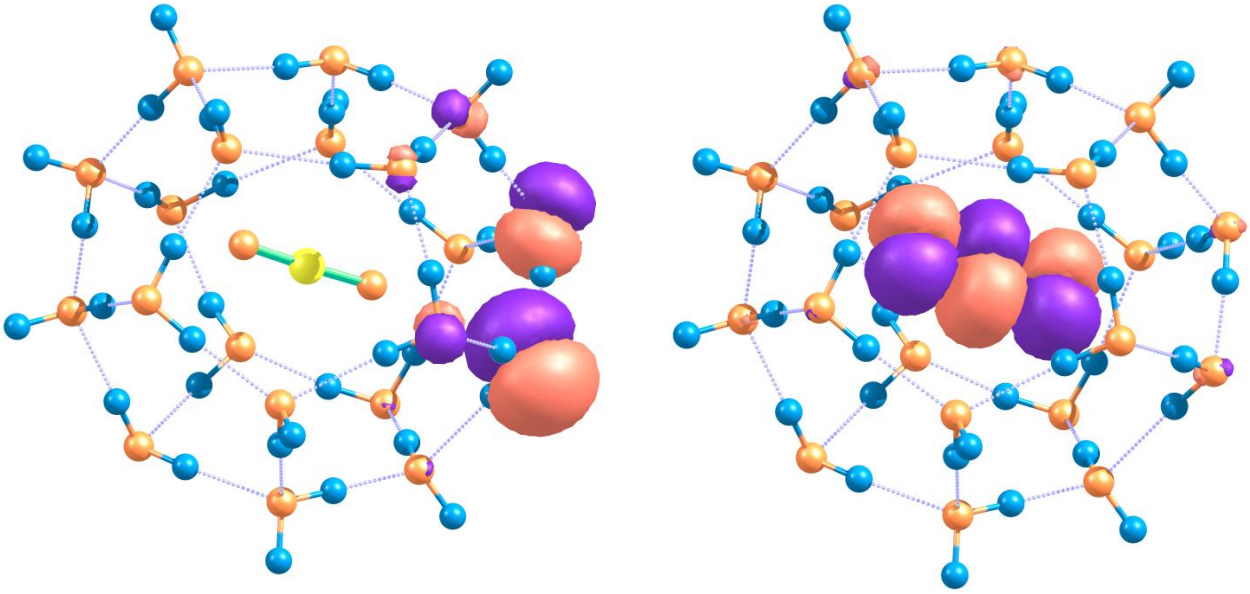
Figure S24. Frontier molecular orbital of the CO_2 molecule before and after encapsulation in 5^{12}, $5^{12}6^2$ and $5^{12}6^4$ clathrate hydrates computes at B3LYP/6-31G(d) level of theory and basis set.

Before Encapsulation

HOMO **LUMO**

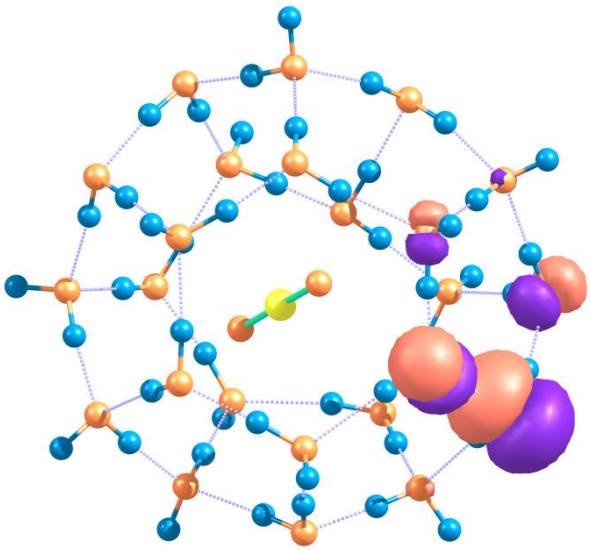
After Encapsulation

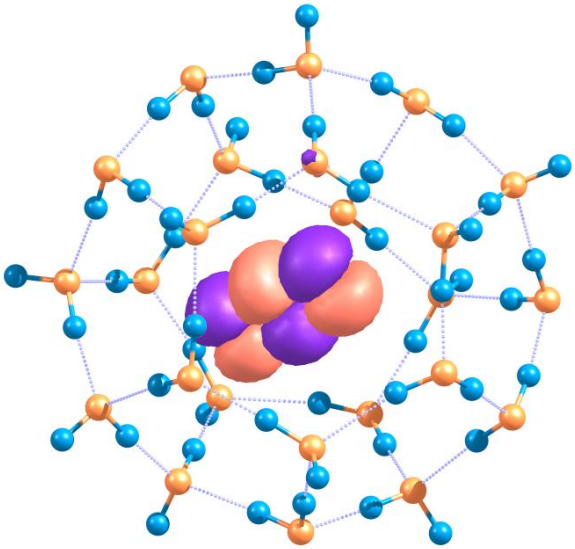
HOMO **LUMO**



5^{12}

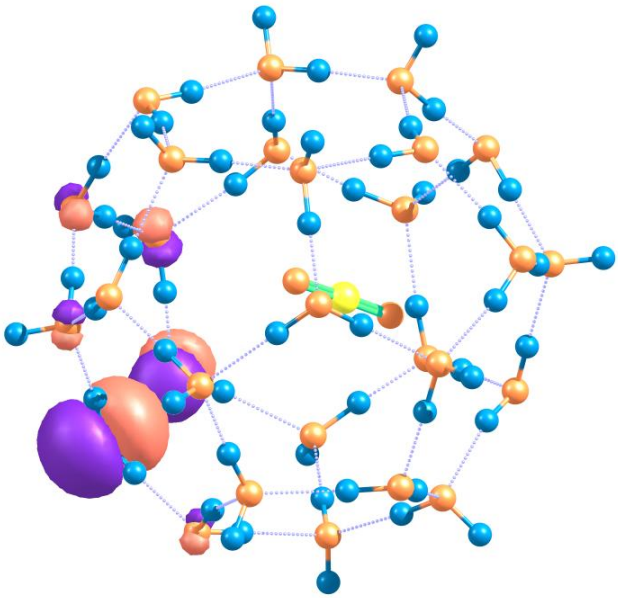
HOMO **LUMO**

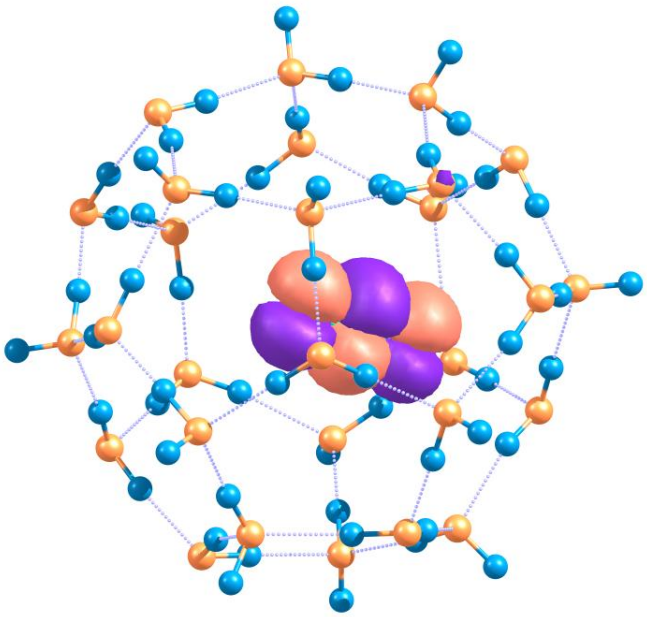




$5^{12}6^{2}$

HOMO **LUMO**





$5^{12}6^{4}$

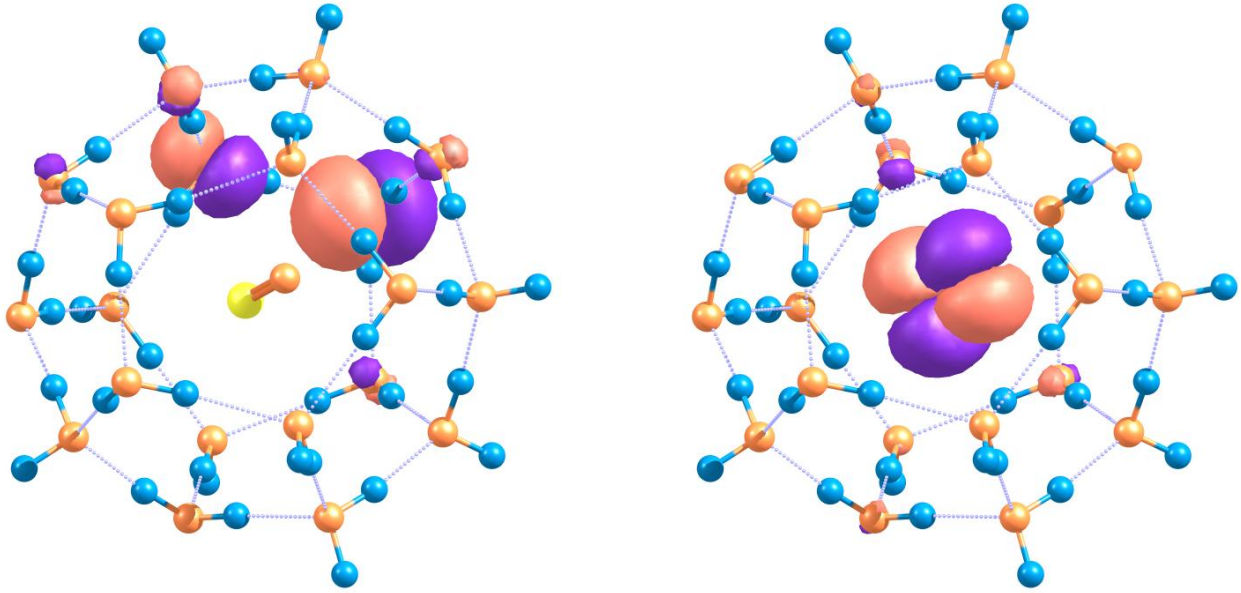
Figure S25. Frontier molecular orbital of the CO molecule before and after encapsulation in 5^{12}, $5^{12}6^2$ and $5^{12}6^4$ clathrate hydrates computes at B3LYP/6-31G(d) level of theory and basis set.

Before Encapsulation

HOMO **LUMO**

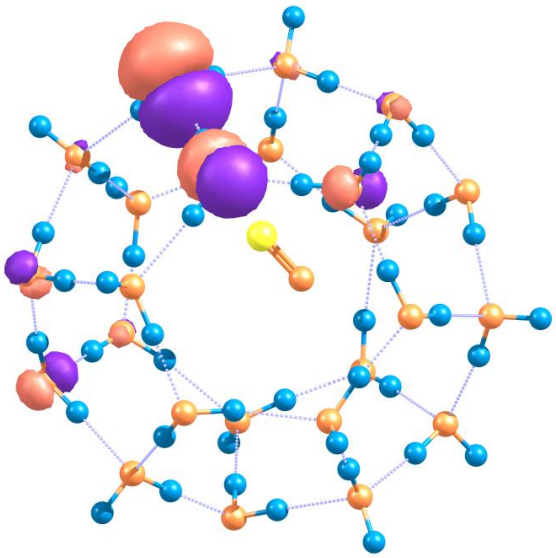
After Encapsulation

HOMO **LUMO**

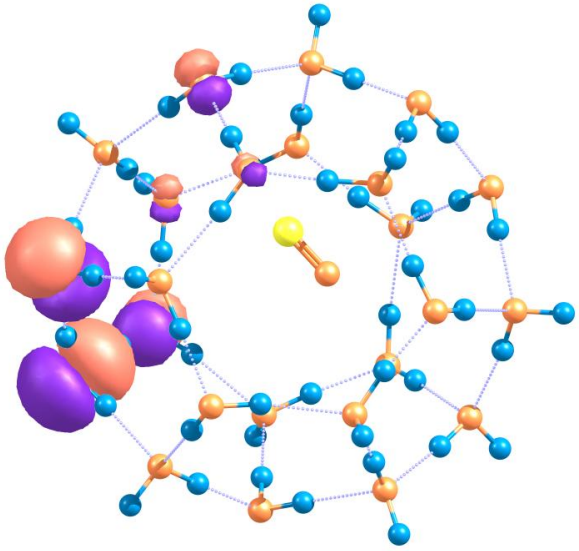


5^{12}

HOMO

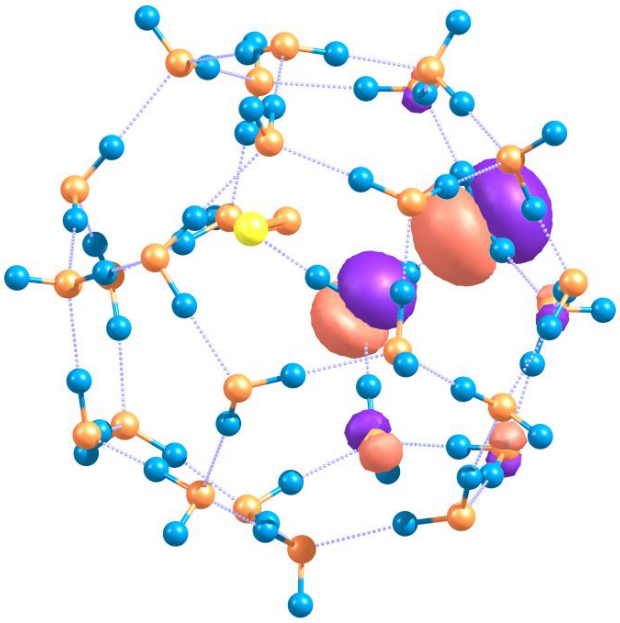


LUMO

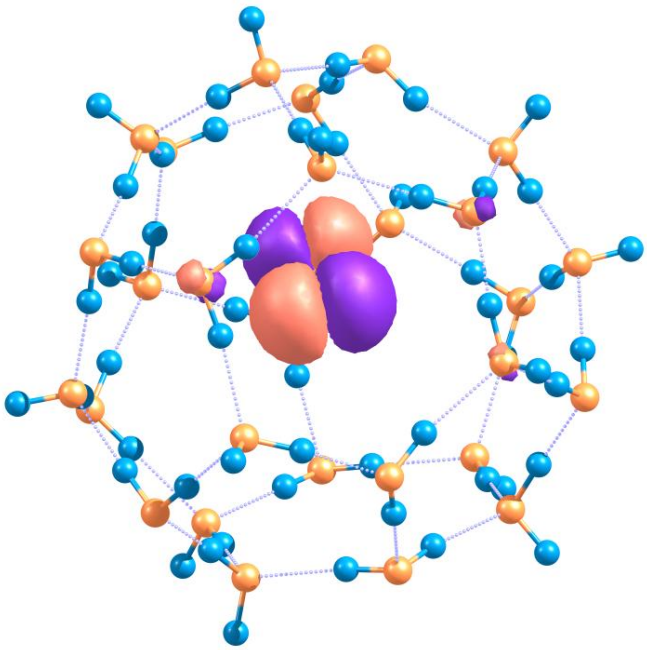


$5^{12}6^{2}$

HOMO



LUMO



$5^{12}6^{4}$

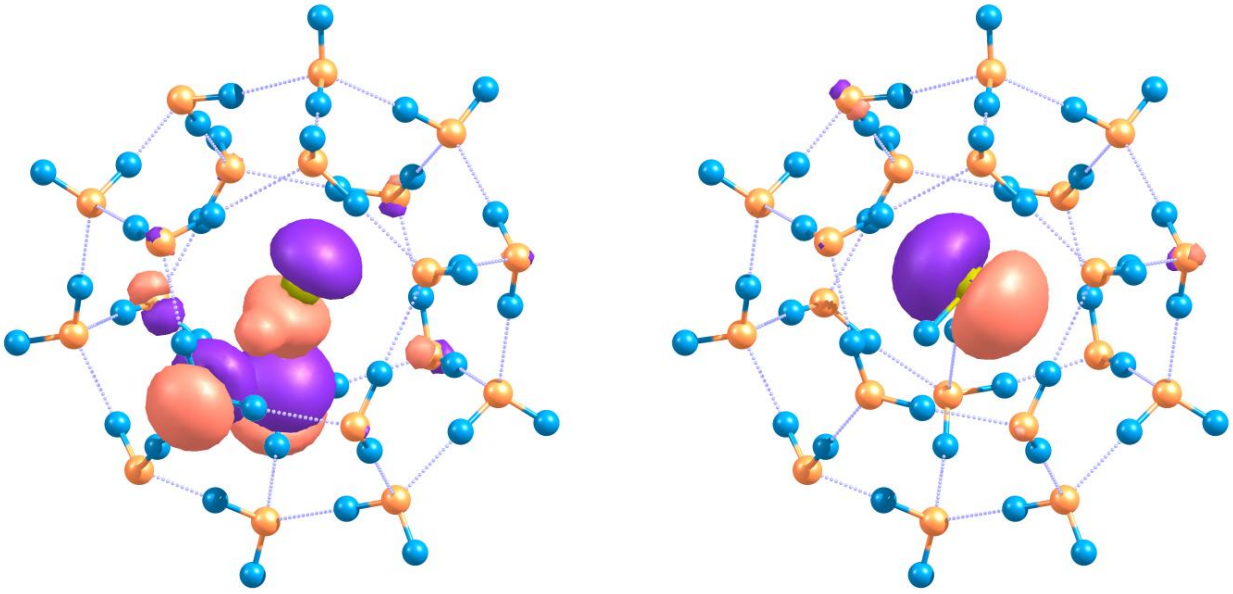
Figure S26. Frontier molecular orbital of the H_2S molecule before and after encapsulation in 5^{12}, $5^{12}6^2$ and $5^{12}6^4$ clathrate hydrates computes at B3LYP/6-31G(d) level of theory and basis set.

Before Encapsulation

HOMO **LUMO**

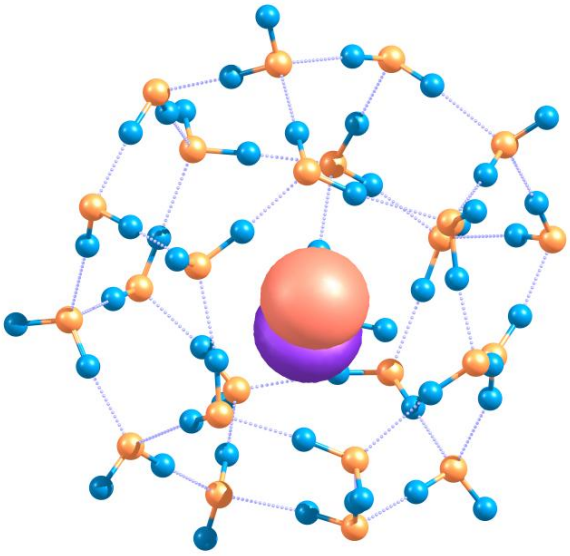
After Encapsulation

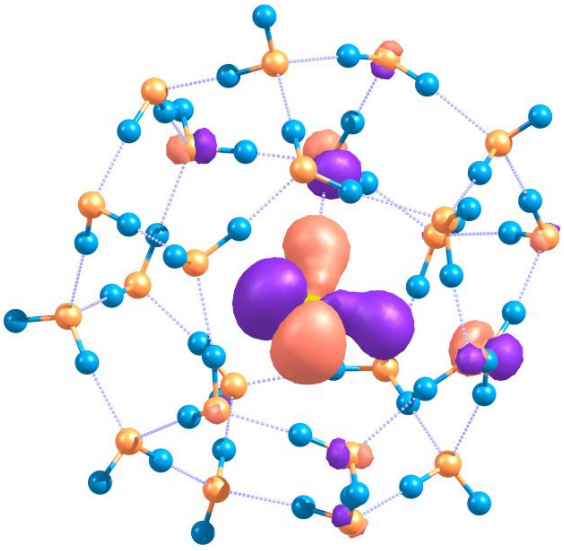
HOMO **LUMO**



5^{12}

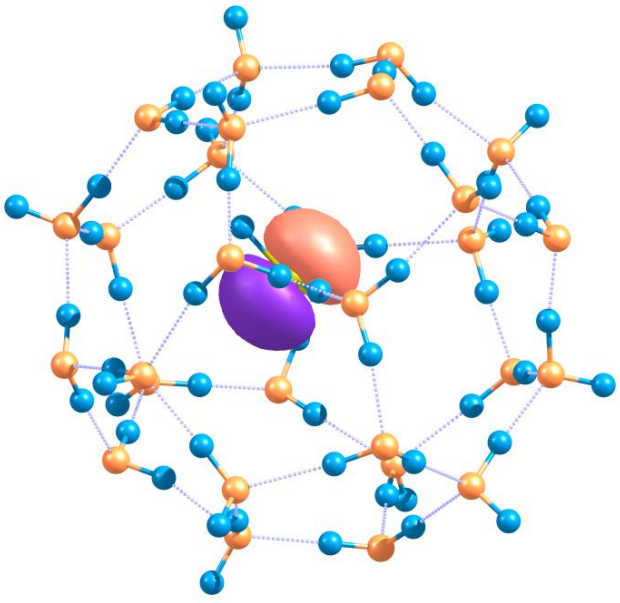
HOMO **LUMO**

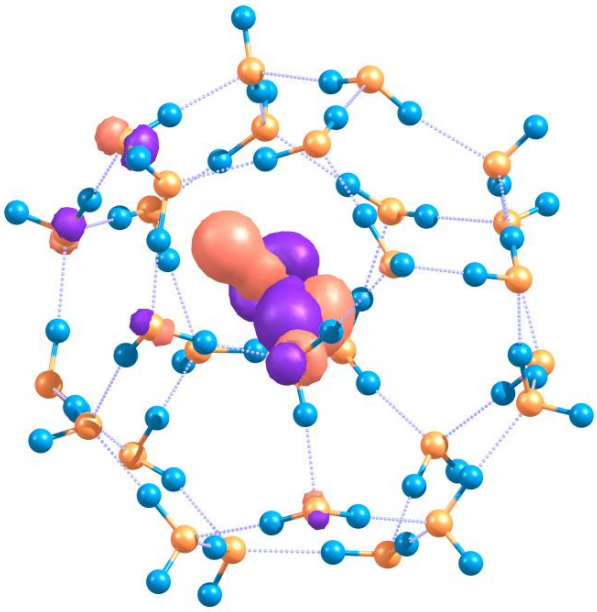




$5^{12}6^{2}$

HOMO **LUMO**





$5^{12}6^{4}$

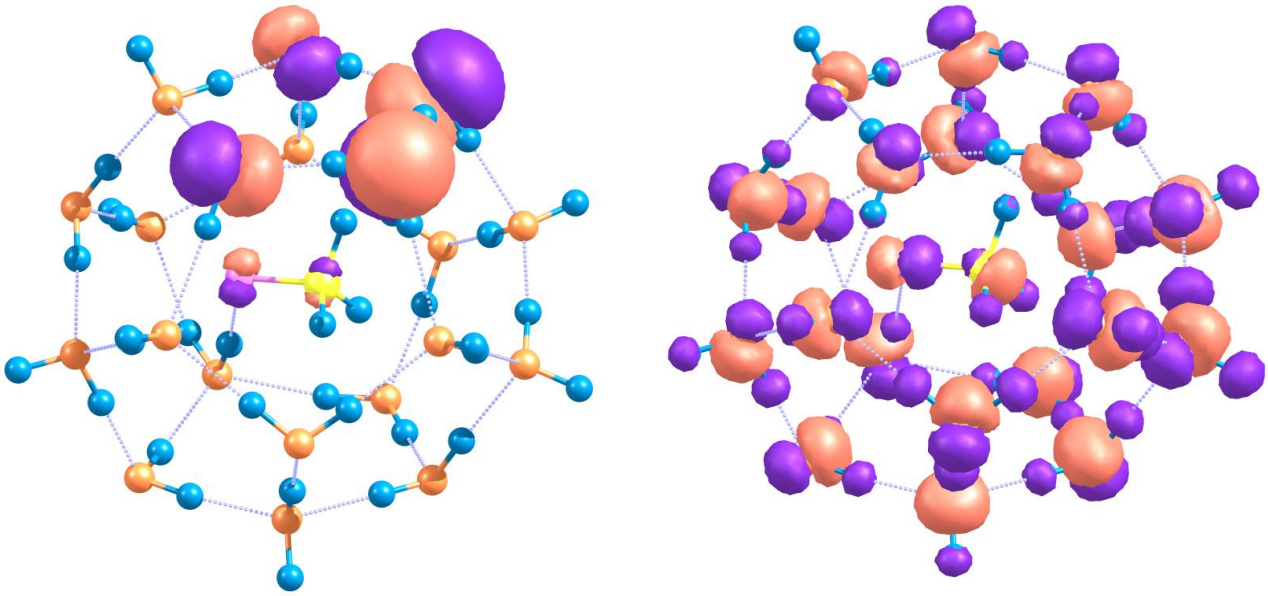
Figure S27. Frontier molecular orbital of the CH_3F molecule before and after encapsulation in 5^{12}, $5^{12}6^2$ and $5^{12}6^4$ clathrate hydrates computes at B3LYP/6-31G(d) level of theory and basis set.

Before Encapsulation

HOMO **LUMO**

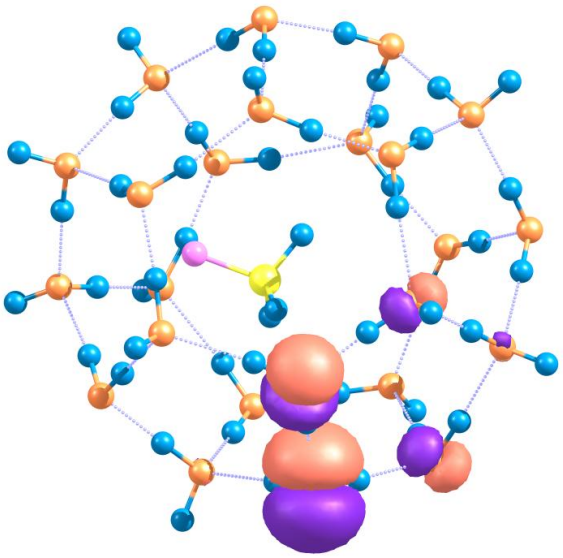
After Encapsulation

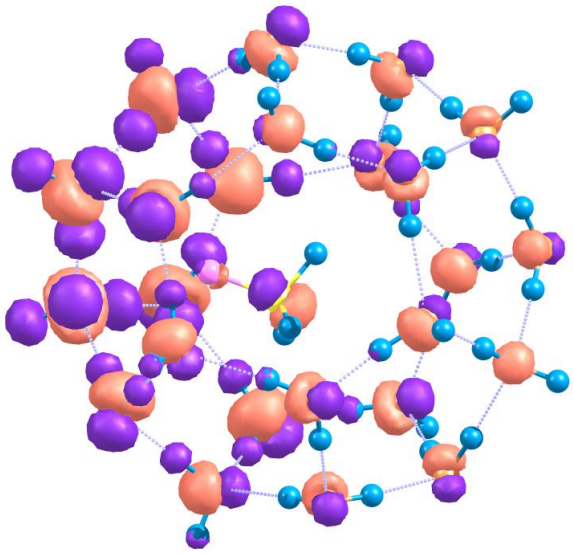
HOMO **LUMO**



5^{12}

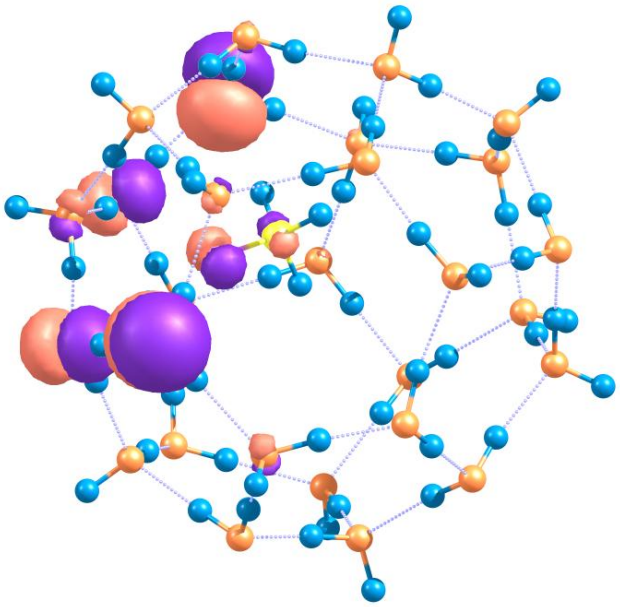
HOMO **LUMO**

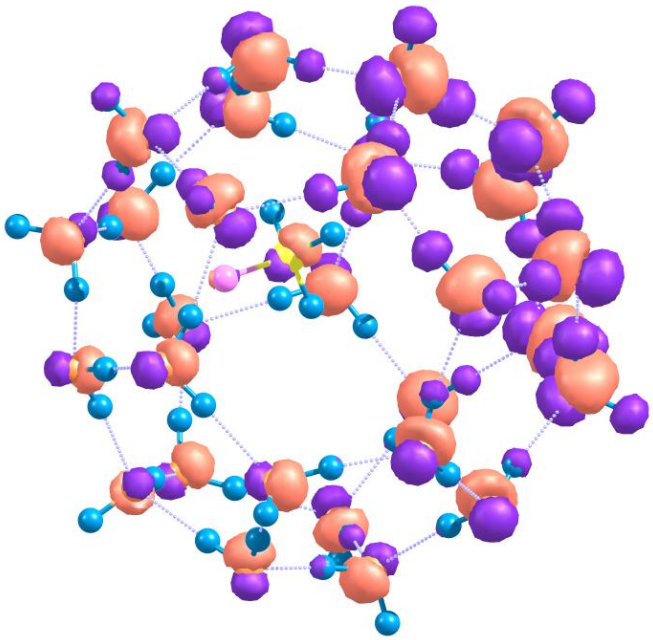




$5^{12}6^{2}$

HOMO **LUMO**





$5^{12}6^{4}$

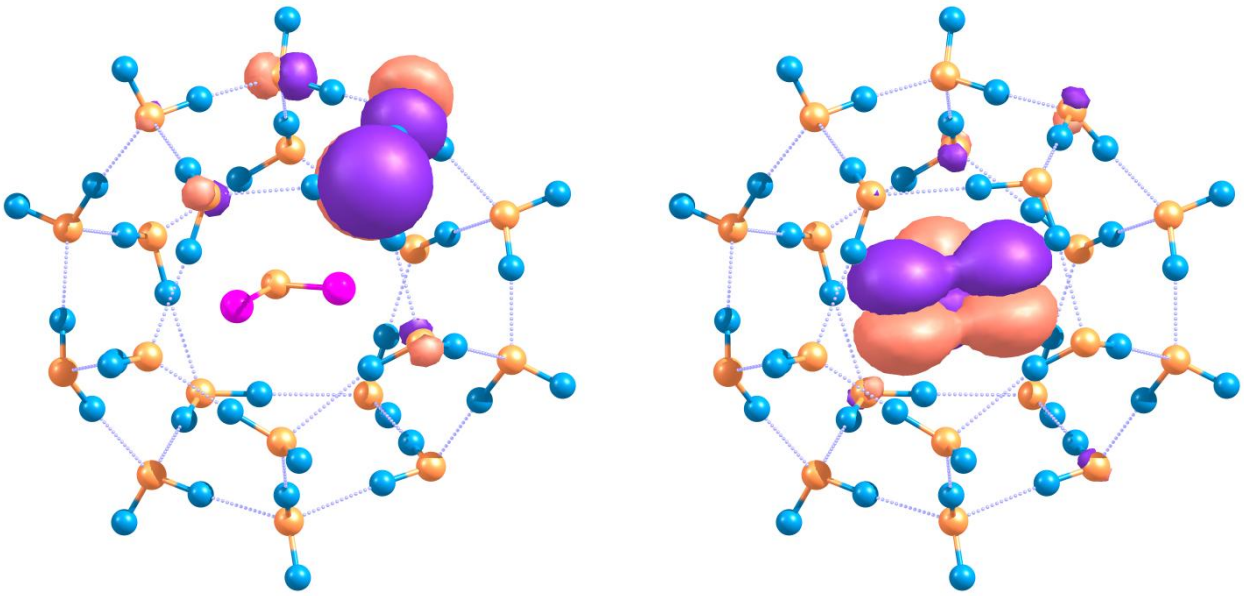
Figure S28. Frontier molecular orbital of the N_2O molecule before and after encapsulation in 5^{12}, $5^{12}6^2$ and $5^{12}6^4$ clathrate hydrates computes at B3LYP/6-31G(d) level of theory and basis set.

Before Encapsulation

HOMO **LUMO**

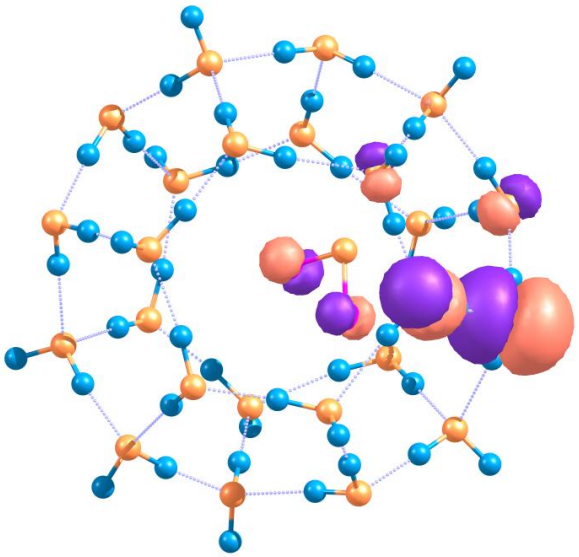
After Encapsulation

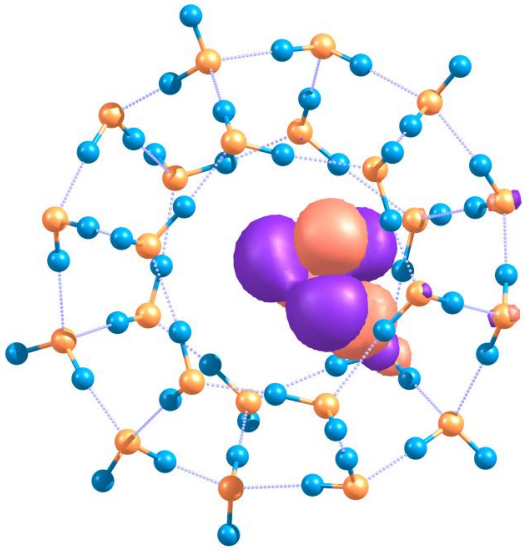
HOMO **LUMO**



5^{12}

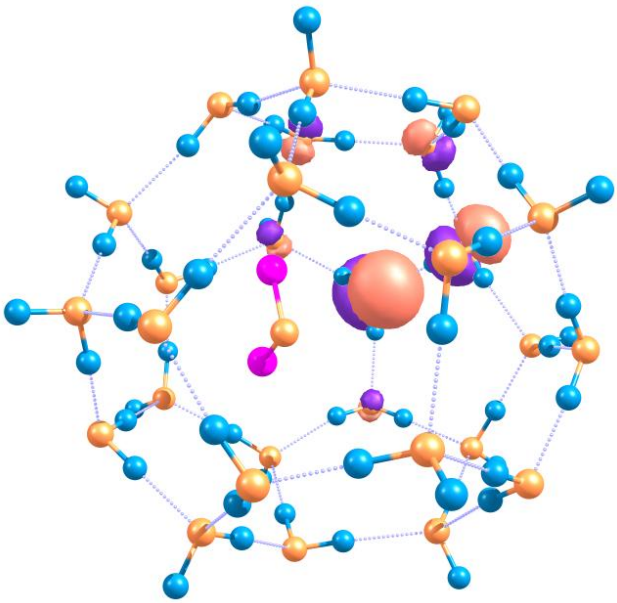
HOMO **LUMO**

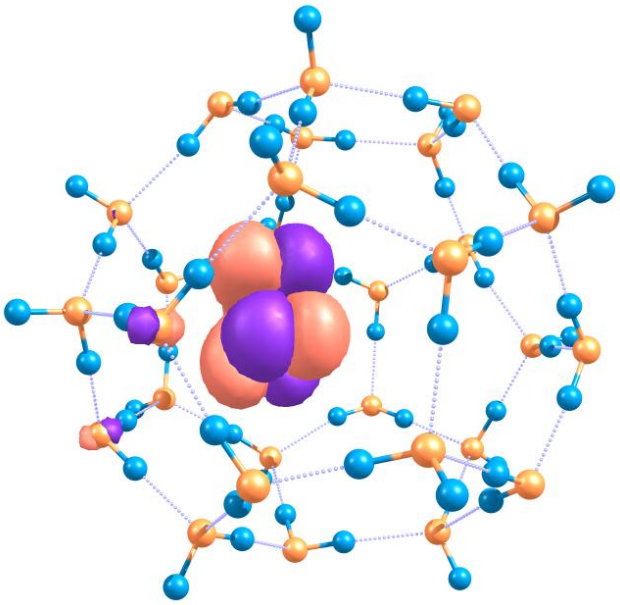




$5^{12}6^{2}$

HOMO **LUMO**





$5^{12}6^{4}$

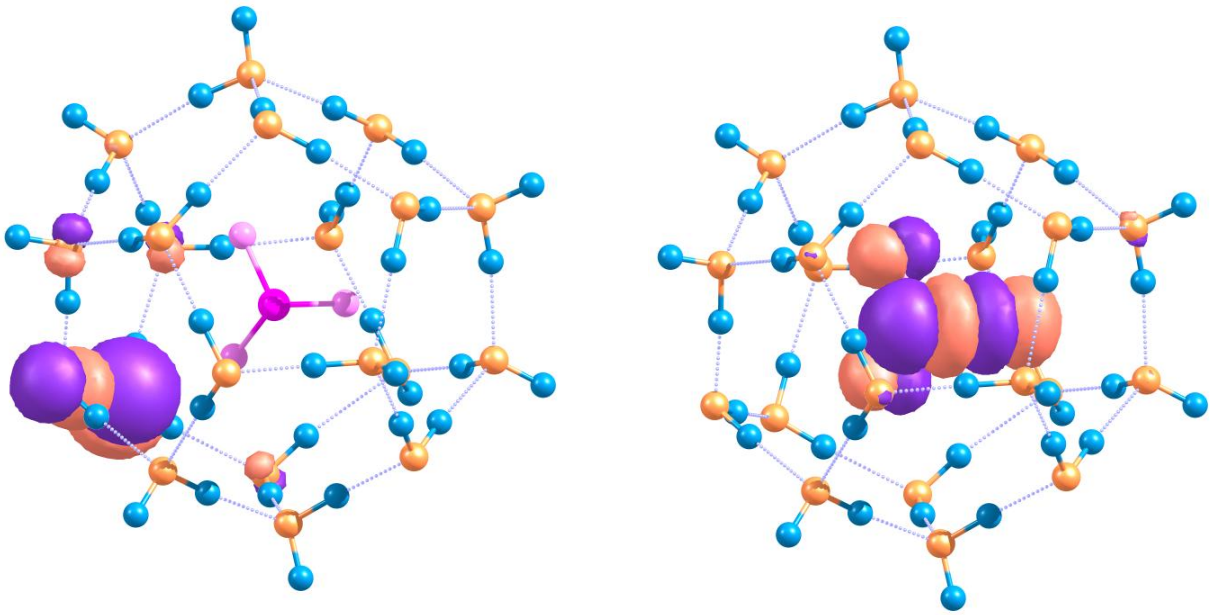
Figure S29. Frontier molecular orbital of the NF_3 molecule before and after encapsulation in 5^{12}, $5^{12}6^2$ and $5^{12}6^4$ clathrate hydrates computes at B3LYP/6-31G(d) level of theory and basis set.

Before Encapsulation

HOMO **LUMO**

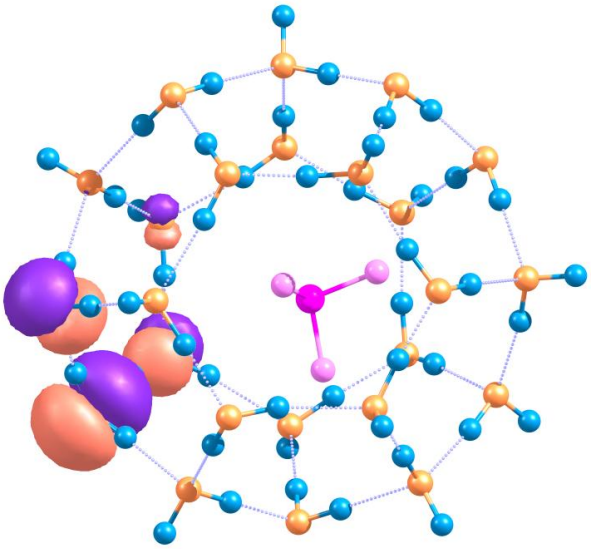
After Encapsulation

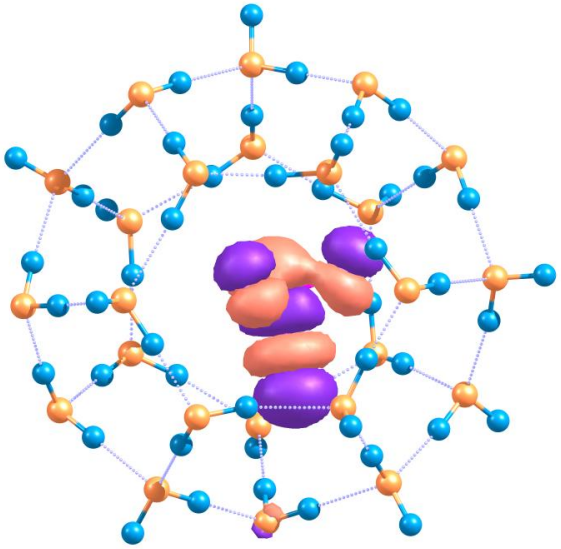
HOMO **LUMO**



5^{12}

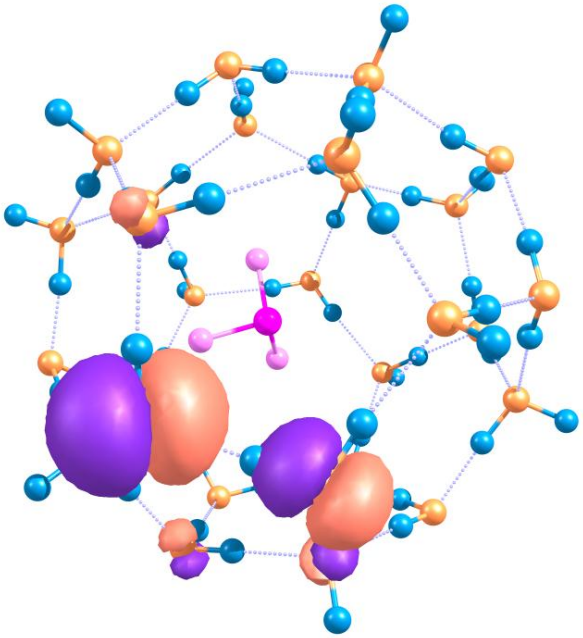
HOMO **LUMO**

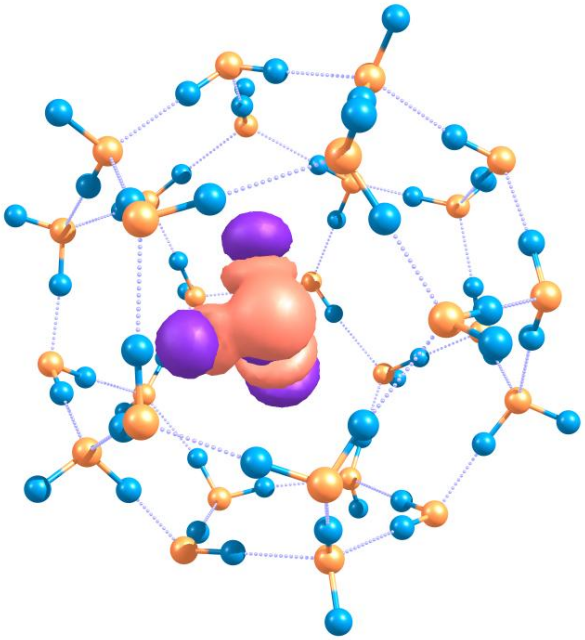




$5^{12}6^{2}$

HOMO **LUMO**





$5^{12}6^{4}$

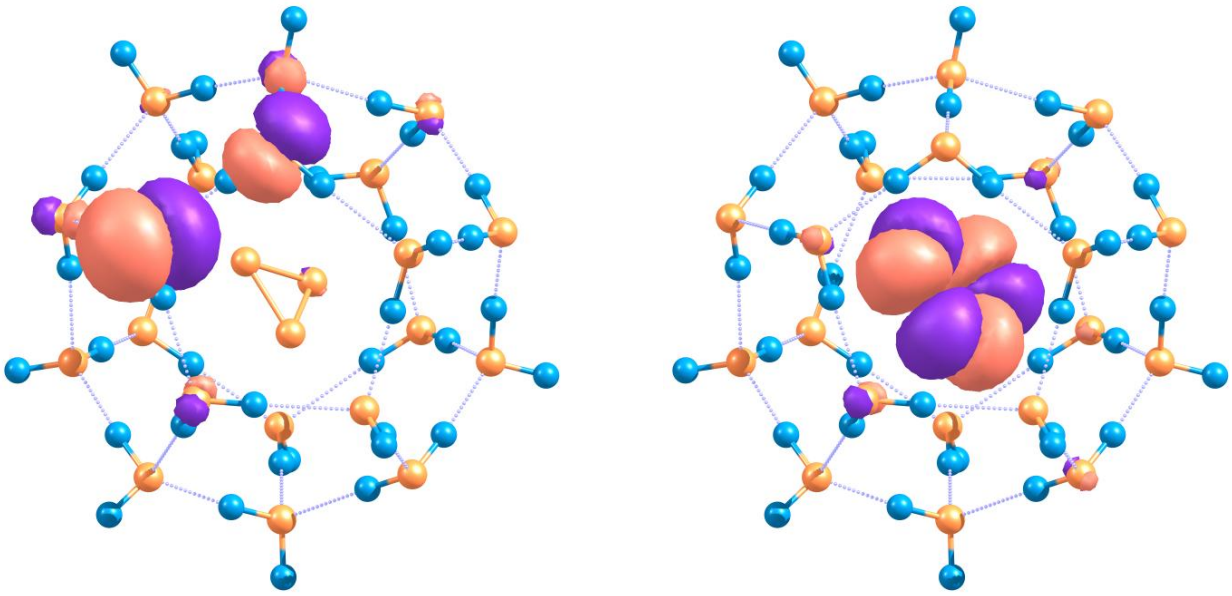
Figure S30. Frontier molecular orbital of the O_3 molecule before and after encapsulation in 5^{12}, $5^{12}6^2$ and $5^{12}6^4$ clathrate hydrates computes at B3LYP/6-31G(d) level of theory and basis set.

Before Encapsulation

HOMO **LUMO**

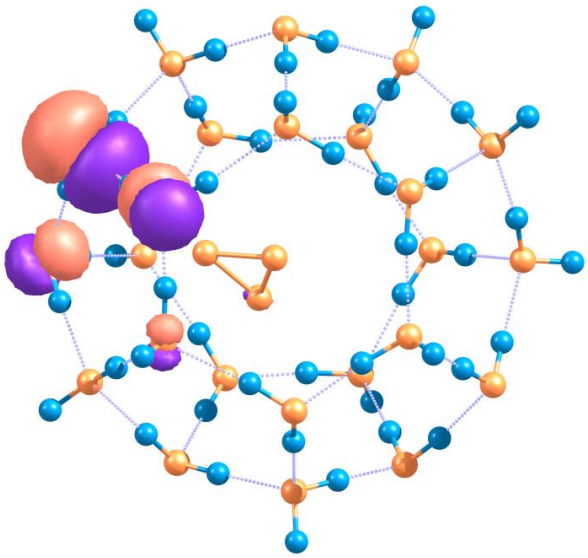
After Encapsulation

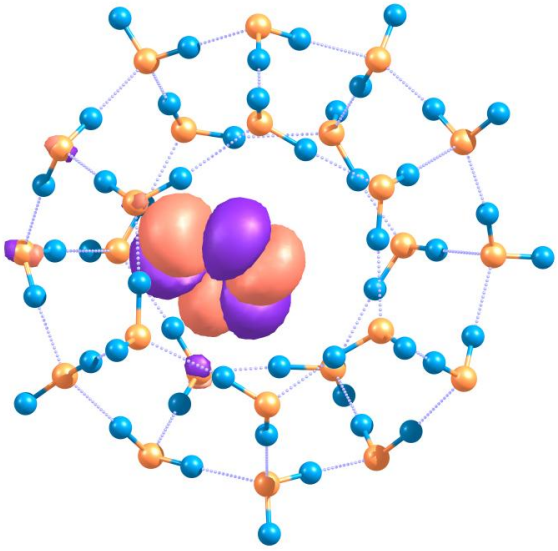
HOMO **LUMO**



5^{12}

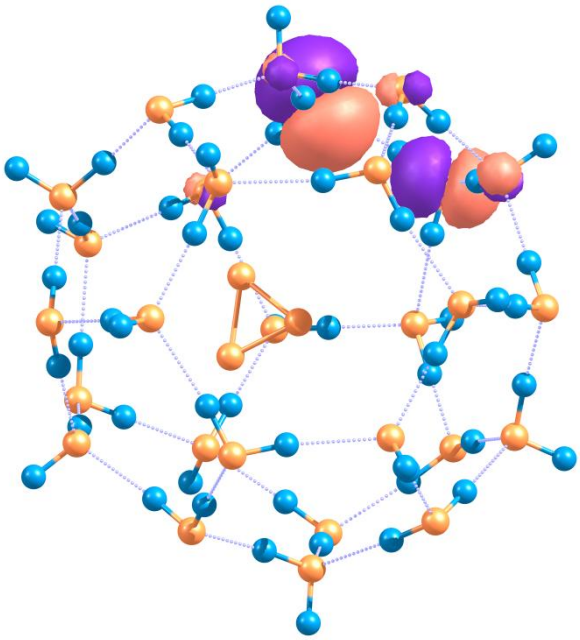
HOMO **LUMO**

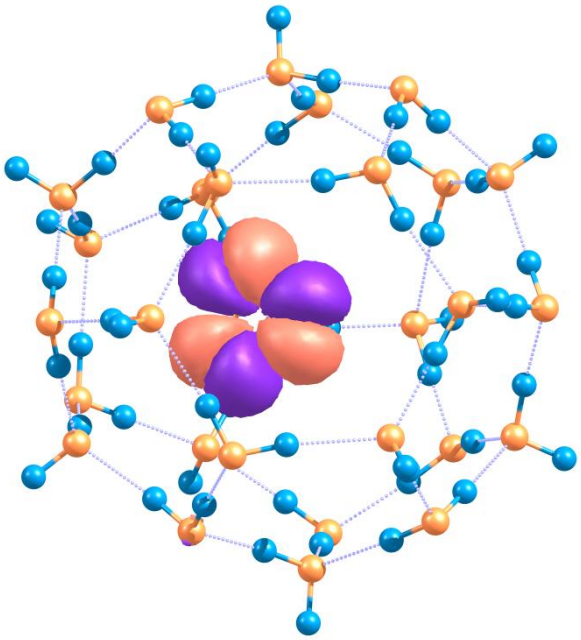




$5^{12}6^{2}$

HOMO **LUMO**





$5^{12}6^{4}$

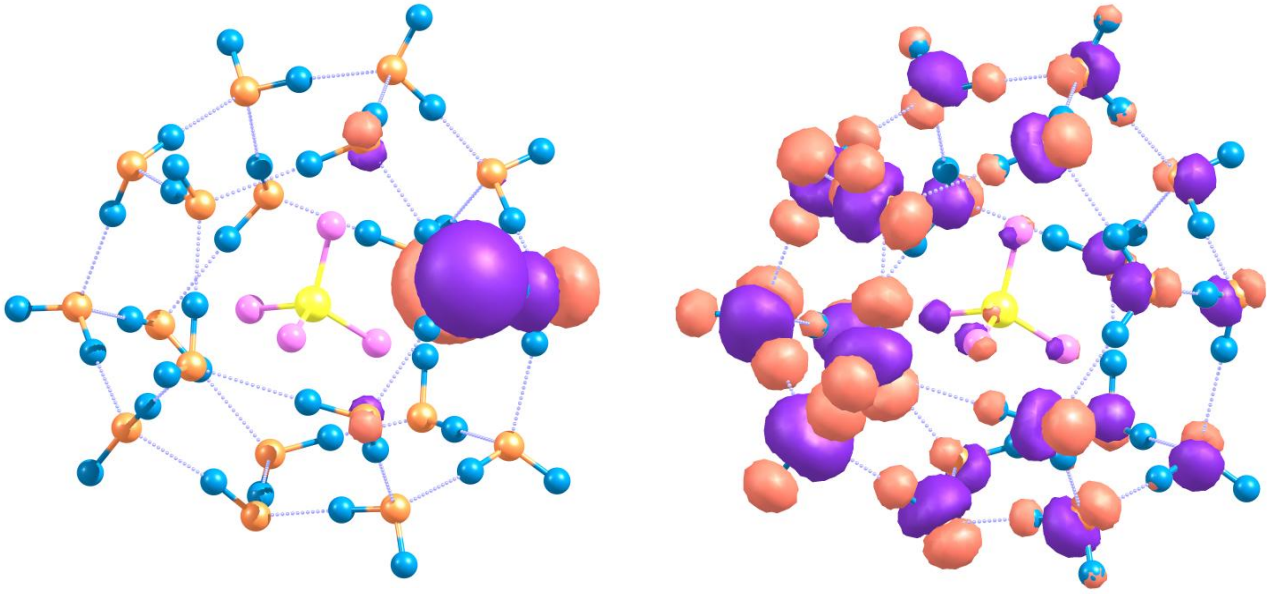
Figure S31. Frontier molecular orbital of the CF_4 molecule before and after encapsulation in 5^{12}, $5^{12}6^2$ and $5^{12}6^4$ clathrate hydrates computes at B3LYP/6-31G(d) level of theory and basis set.

Before Encapsulation

HOMO **LUMO**

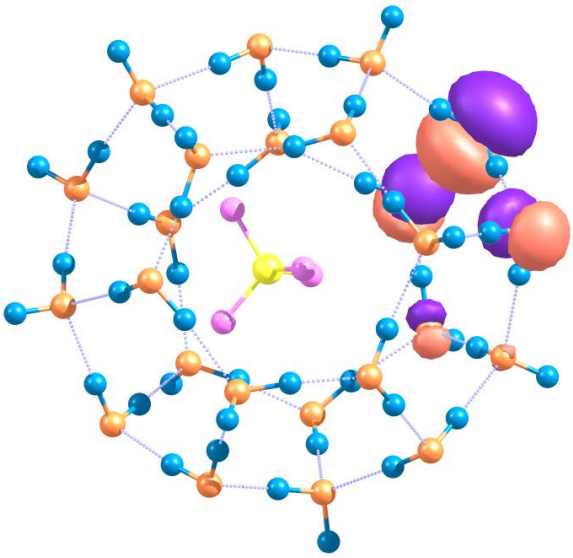
After Encapsulation

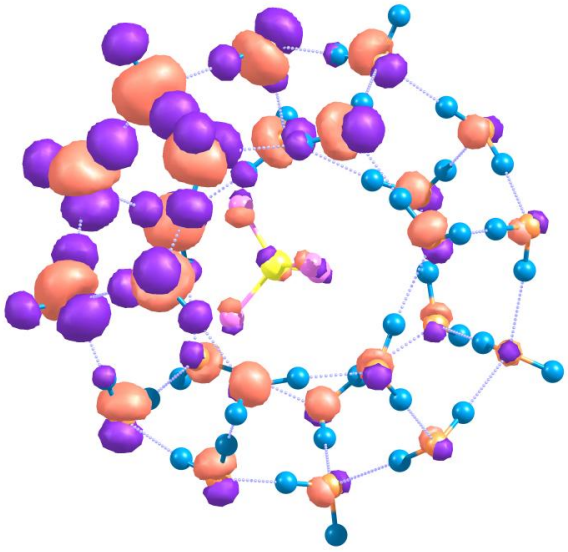
HOMO **LUMO**



5^{12}

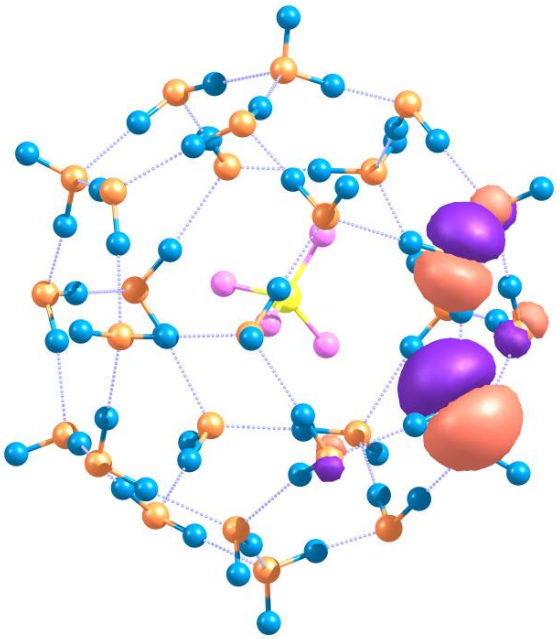
HOMO **LUMO**

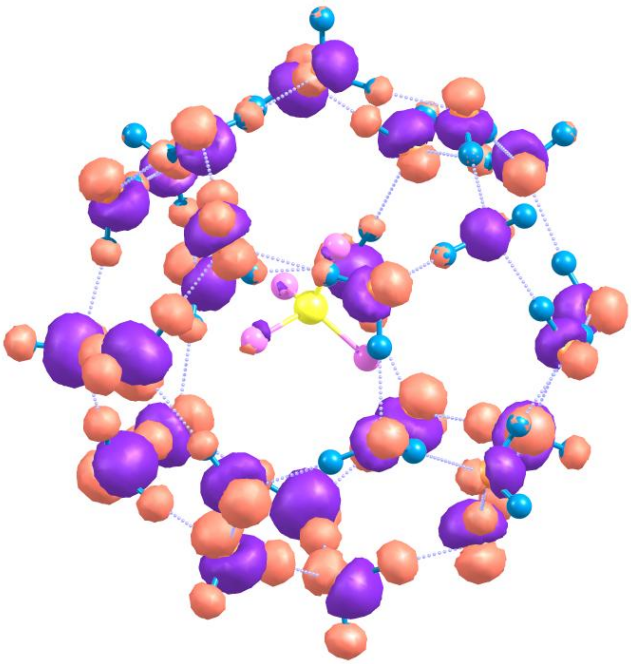




$5^{12}6^{2}$

HOMO **LUMO**



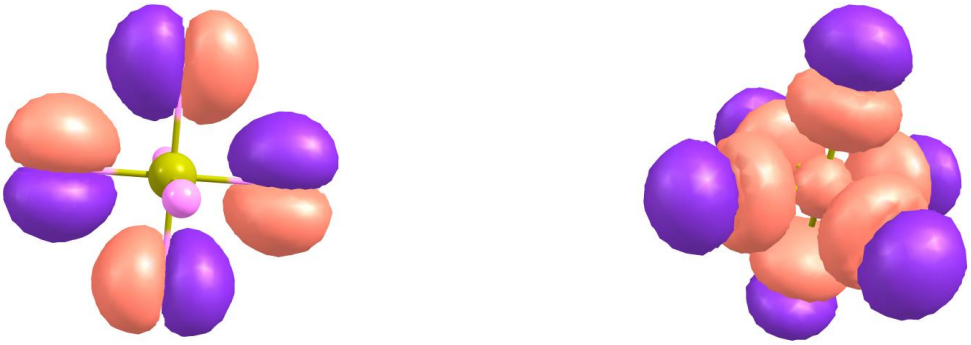


$5^{12}6^{4}$

Figure S32. Frontier molecular orbital of the SF_6 molecule before and after encapsulation in 5^{12}, $5^{12}6^2$ and $5^{12}6^4$ clathrate hydrates computes at B3LYP/6-31G(d) level of theory and basis set.

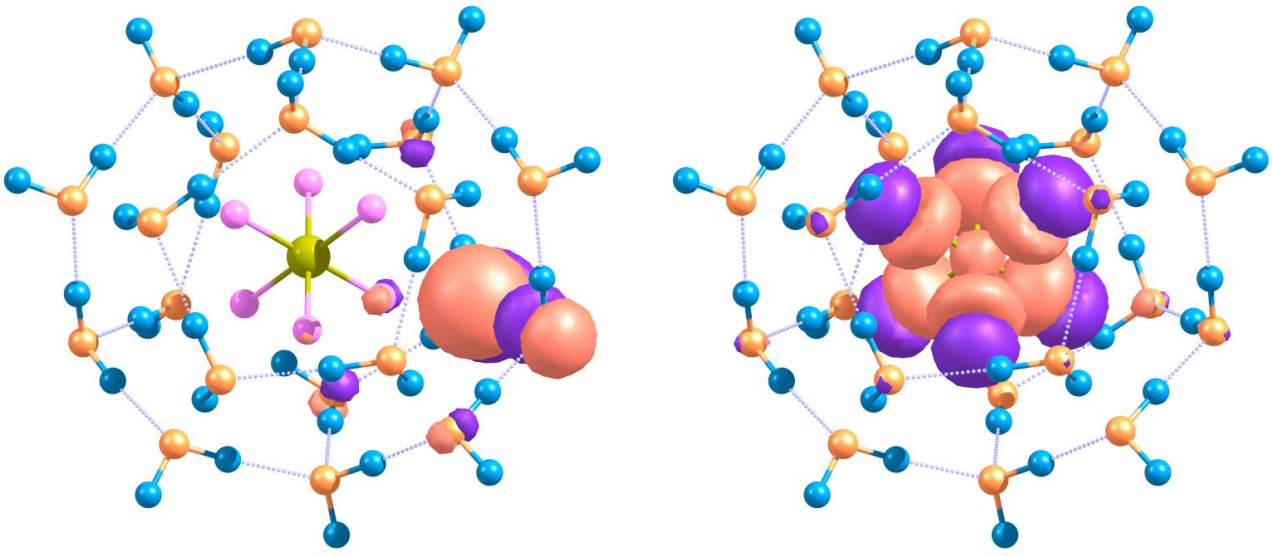
Before Encapsulation

HOMO **LUMO**



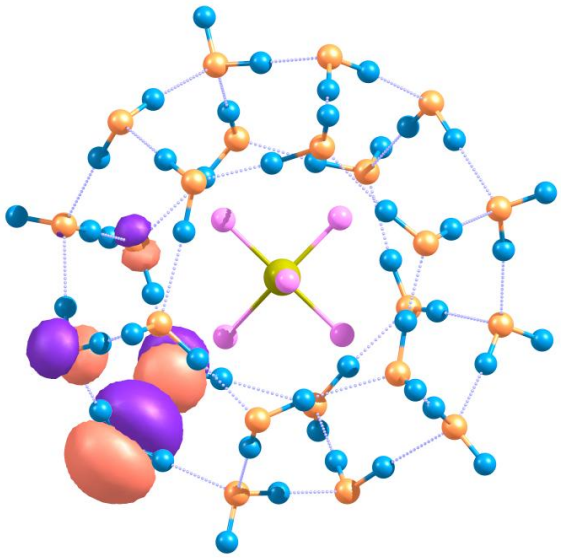
After Encapsulation

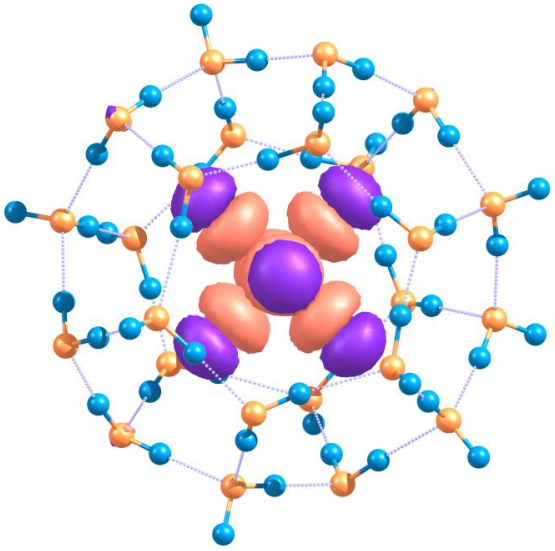
HOMO **LUMO**



5^{12}

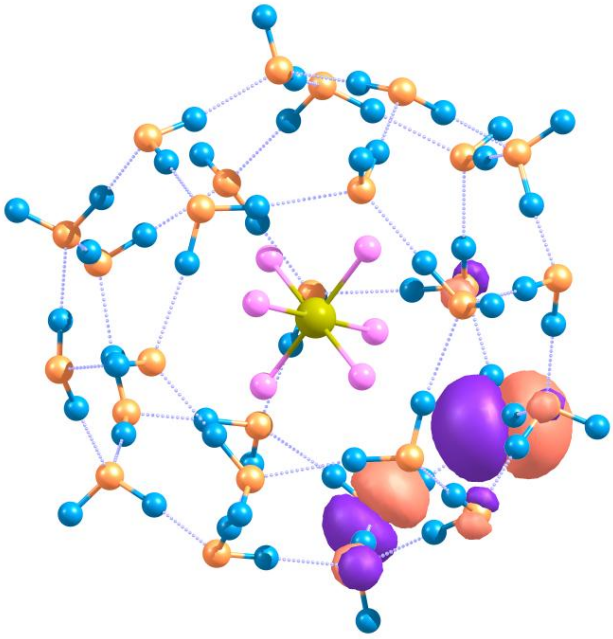
HOMO **LUMO**

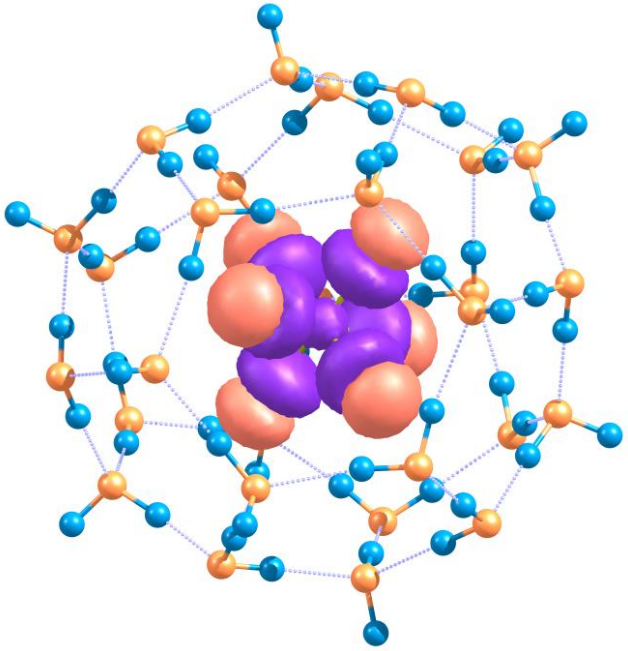




$5^{12}6^{2}$

HOMO **LUMO**





$5^{12}6^{4}$

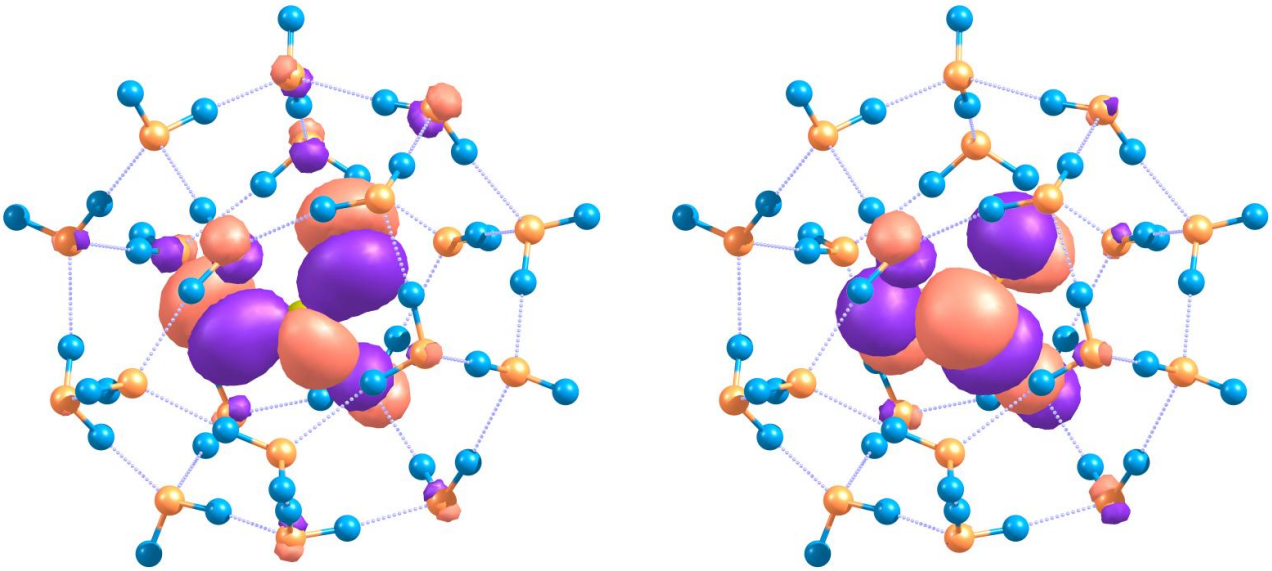
Figure S33. Frontier molecular orbital of the SO_2 molecule before and after encapsulation in 5^{12}, $5^{12}6^2$ and $5^{12}6^4$ clathrate hydrates computes at B3LYP/6-31G(d) level of theory and basis set.

Before Encapsulation

HOMO **LUMO**

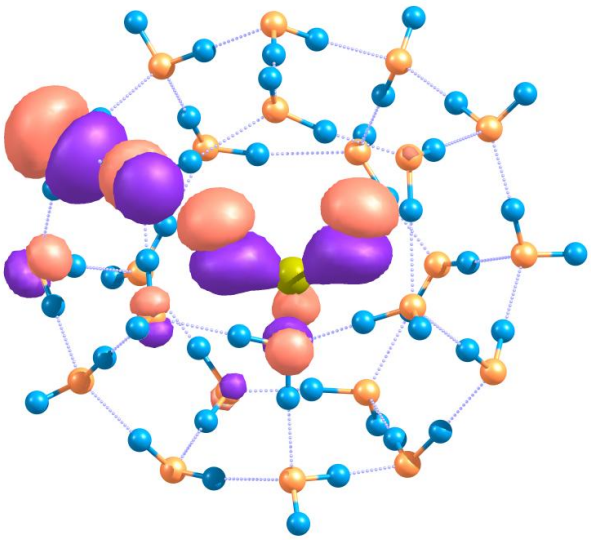
After Encapsulation

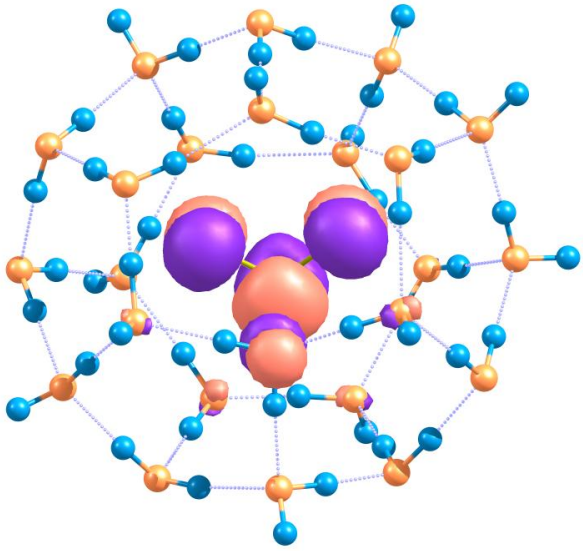
HOMO **LUMO**



5^{12}

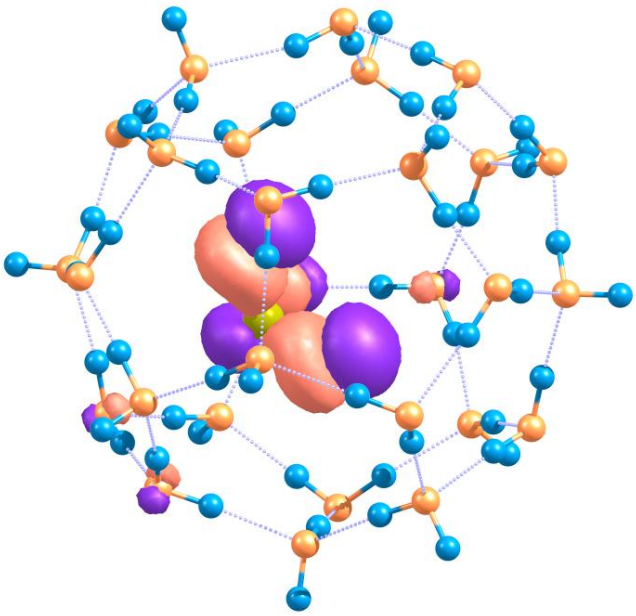
HOMO **LUMO**

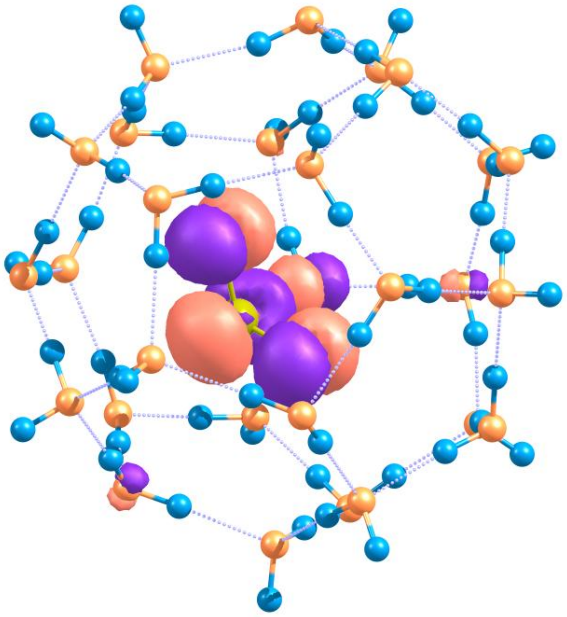




$5^{12}6^{2}$

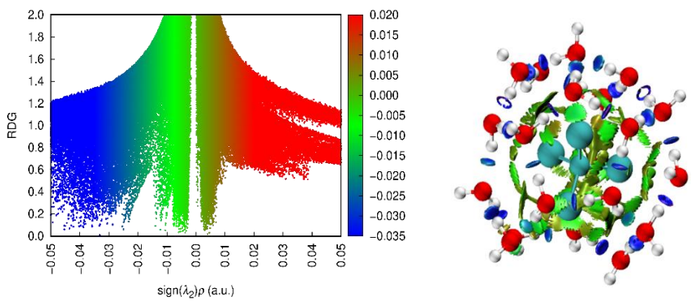
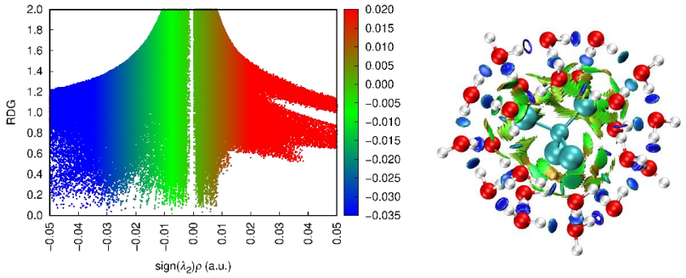
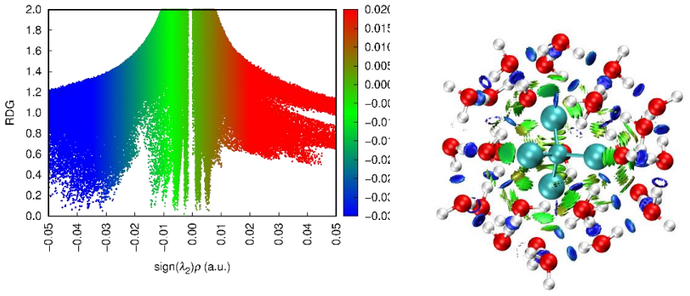
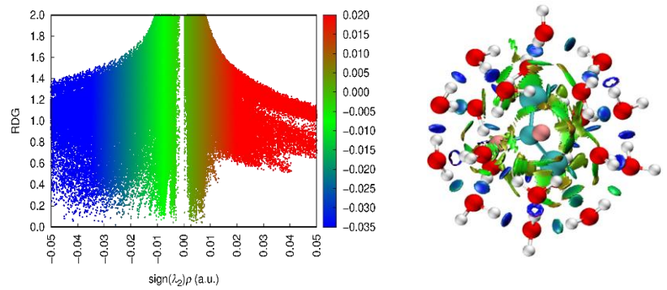
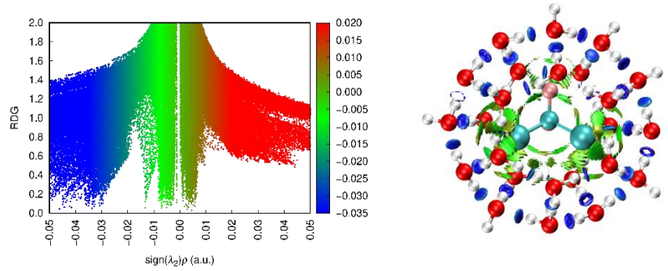
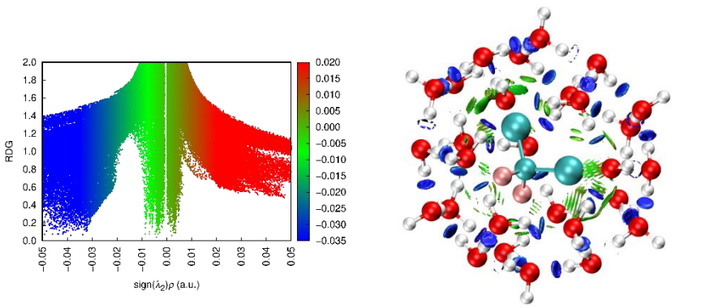
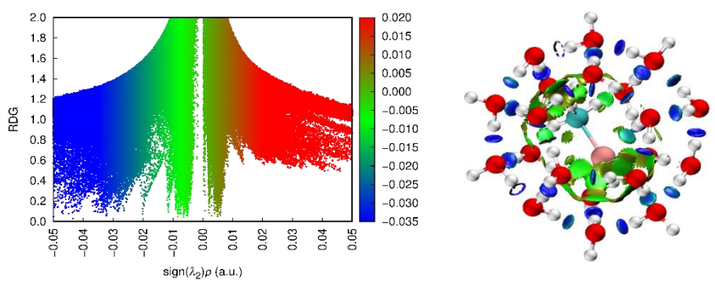
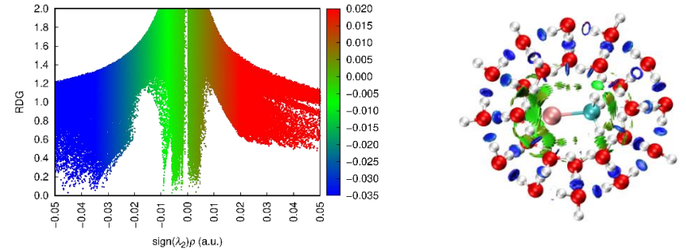
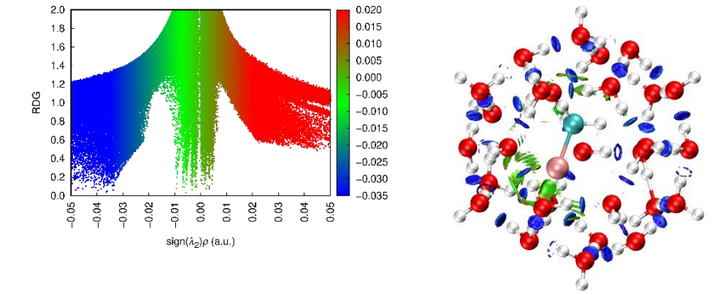
HOMO **LUMO**

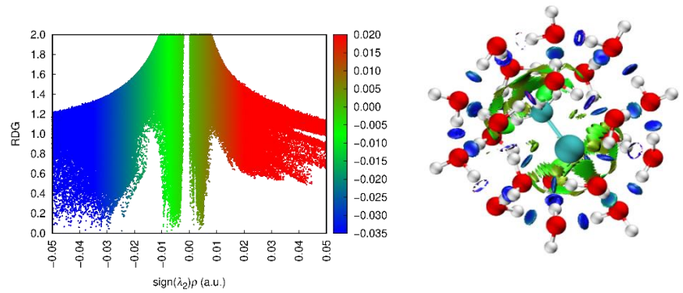
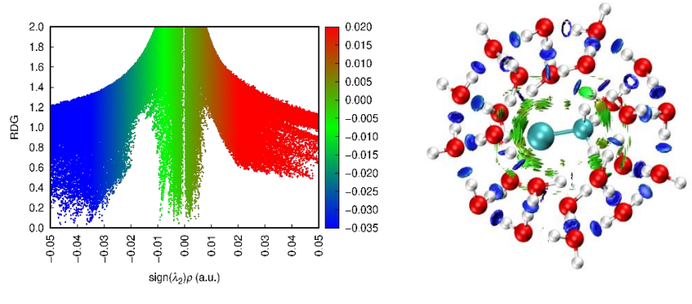
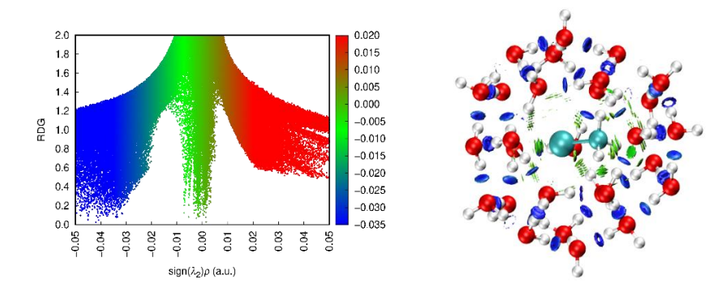
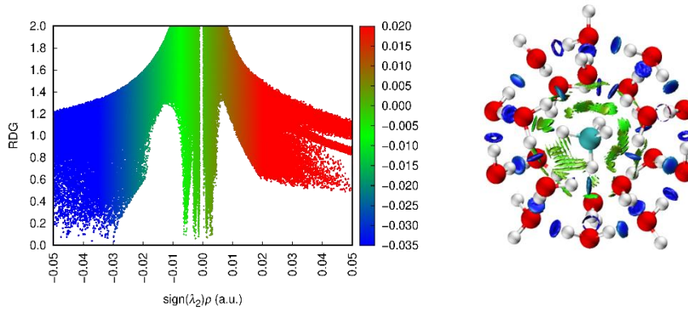
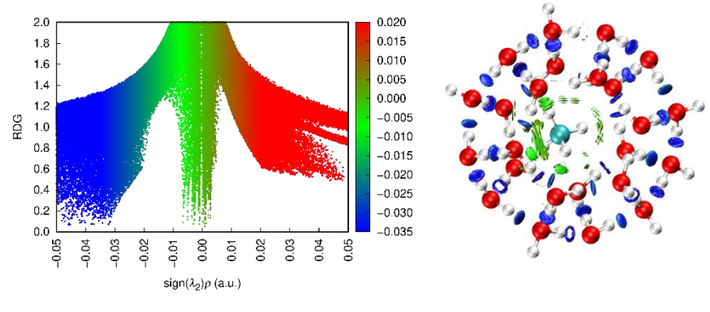
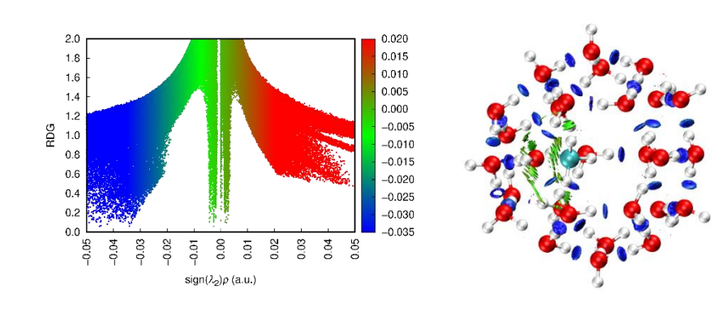
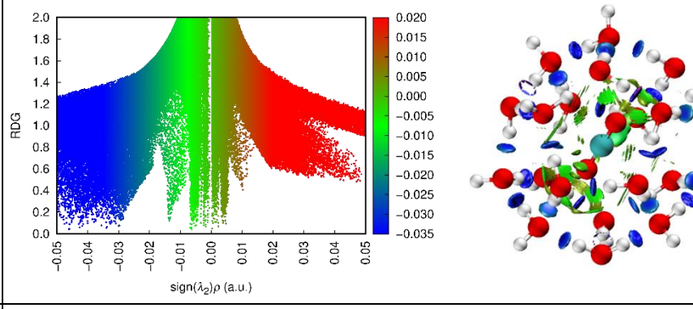
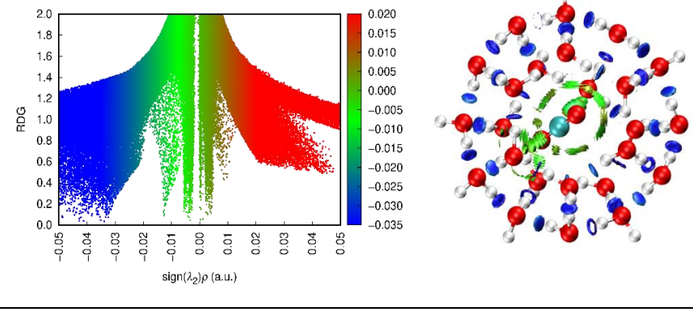
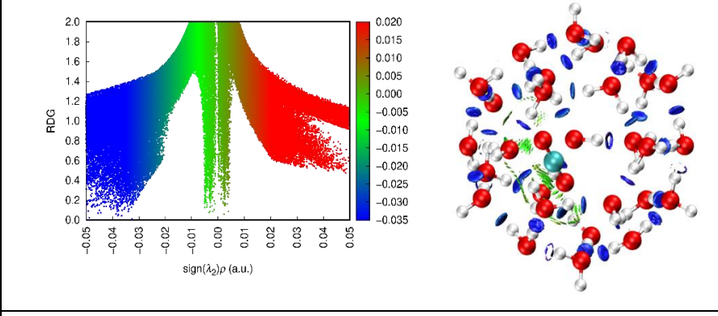
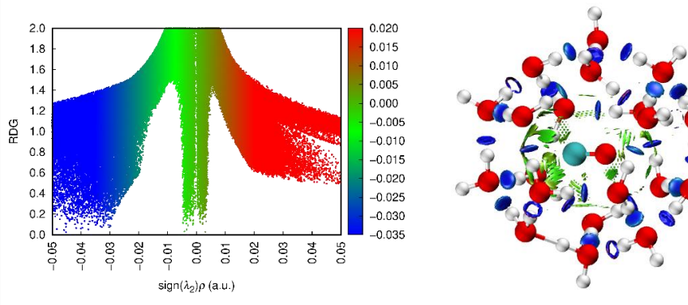
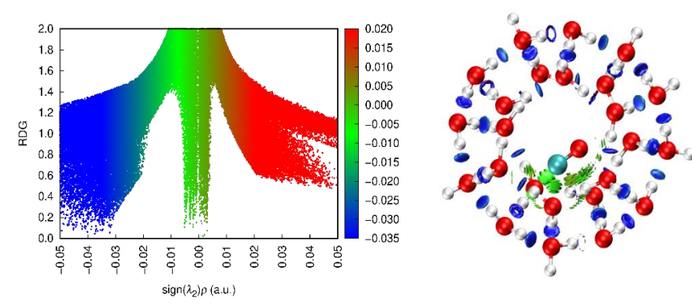
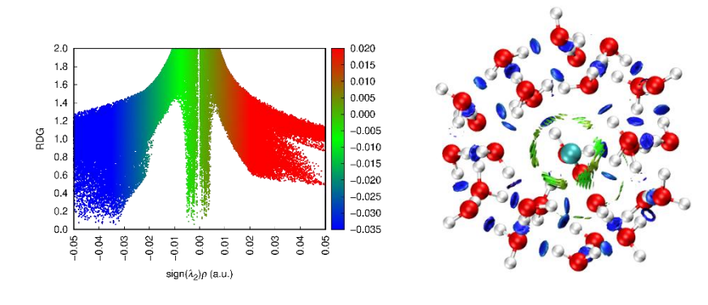


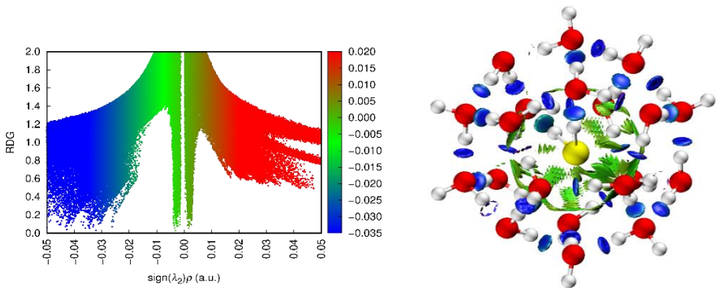
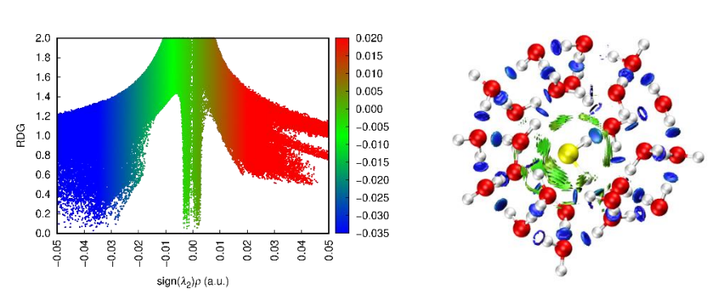
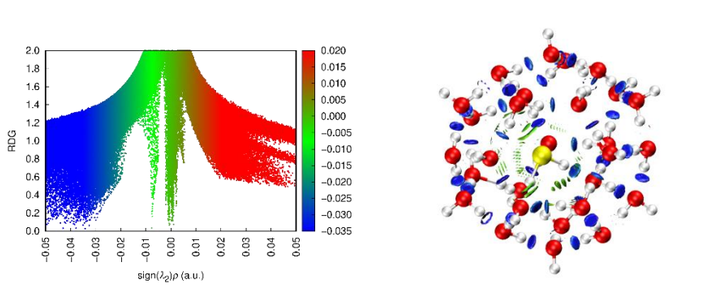
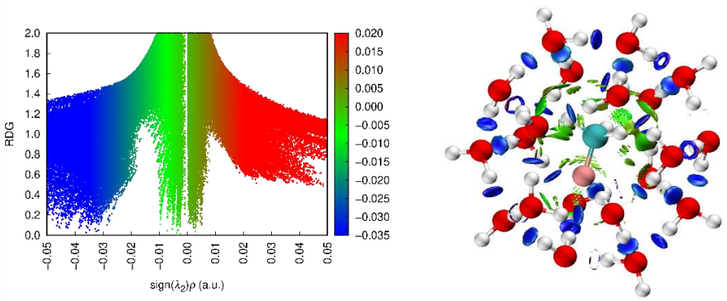
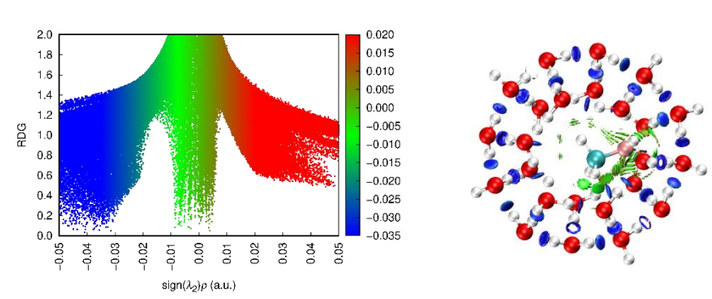
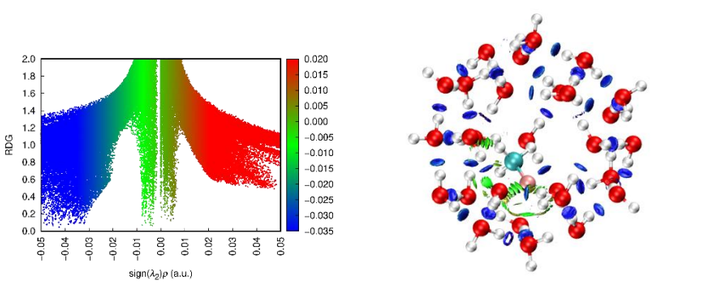
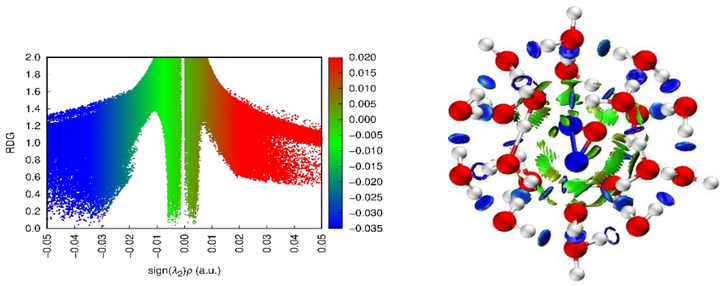
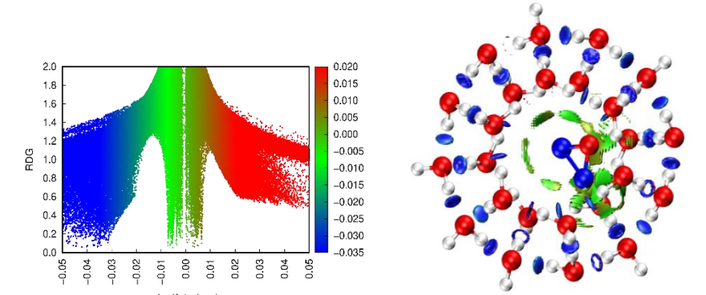
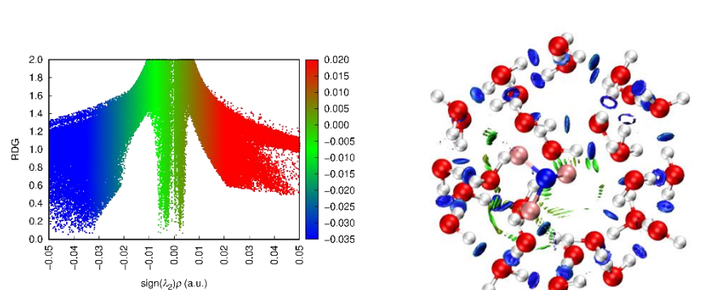
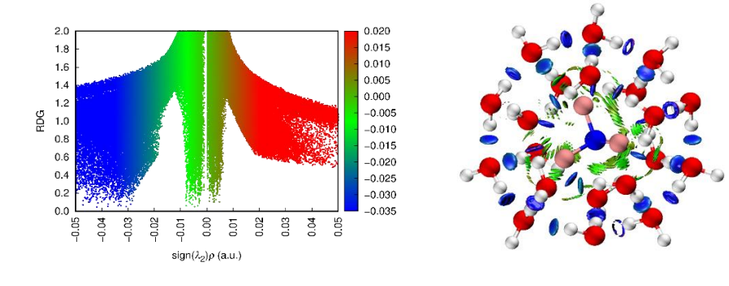
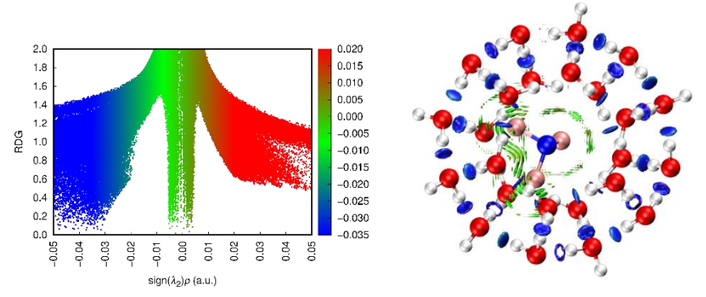
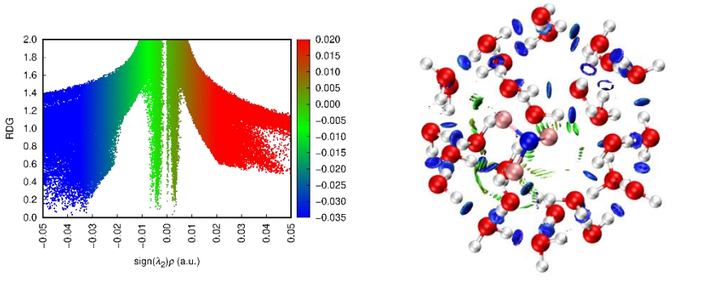


$5^{12}6^{4}$

Figure S34. RDG plot and their iso-surface from Non-covalent Interaction (NCI) analysis.

	5^{12}	$5^{12}6^{2}$	$5^{12}6^{4}$
CCl_4			
CF_2Cl_2			
CH_3Br			

CH_3Cl			
CH_4			
CO_2			
CO			

H_2S			
CH_3F			
N_2O			
NF_3			

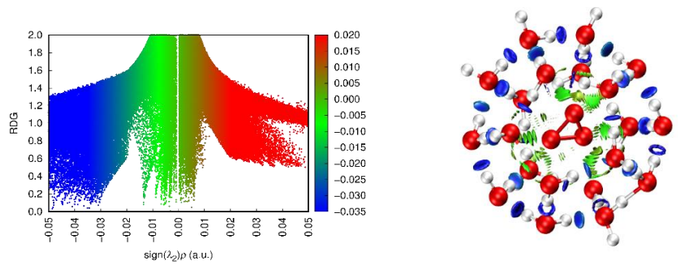
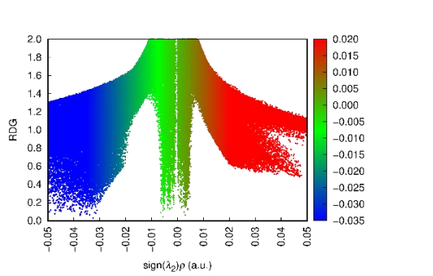
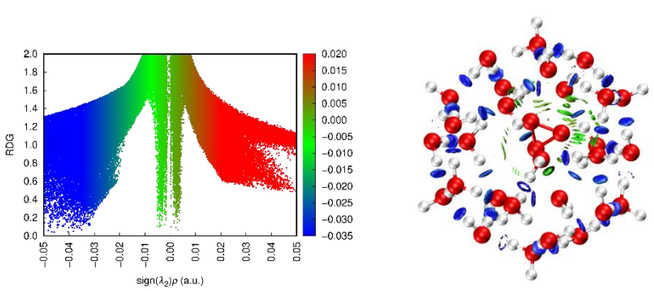
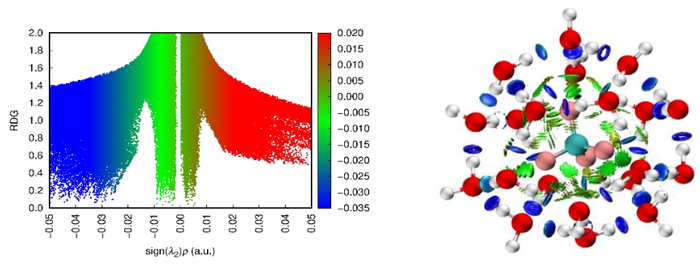
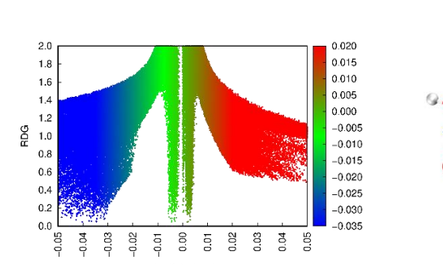
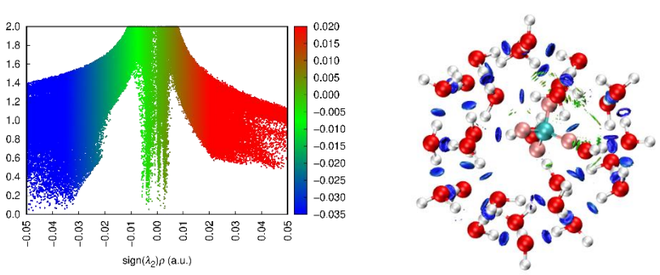
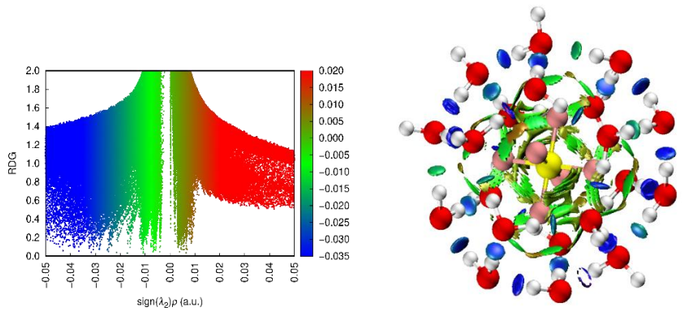
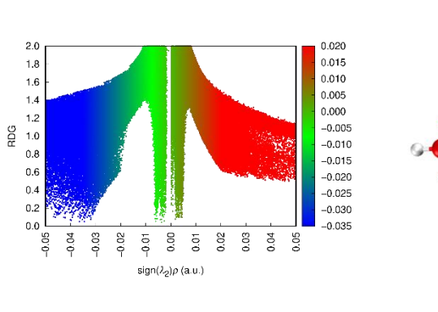
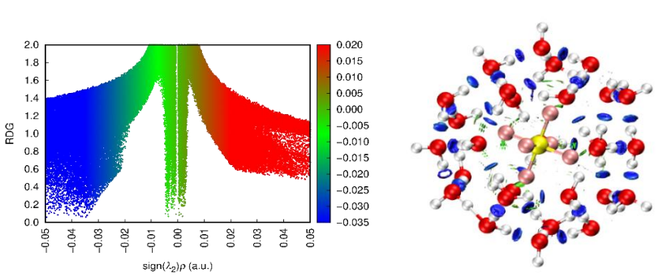
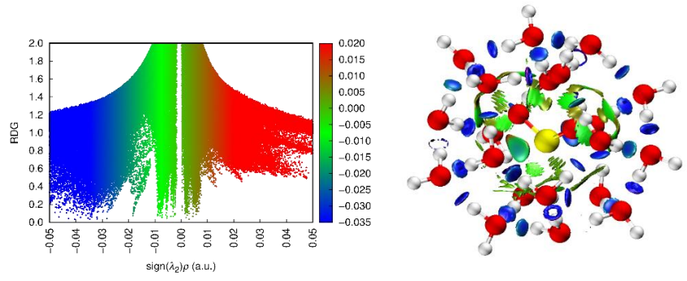
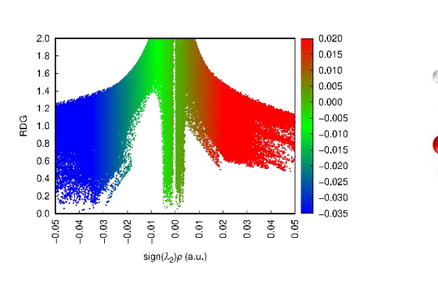
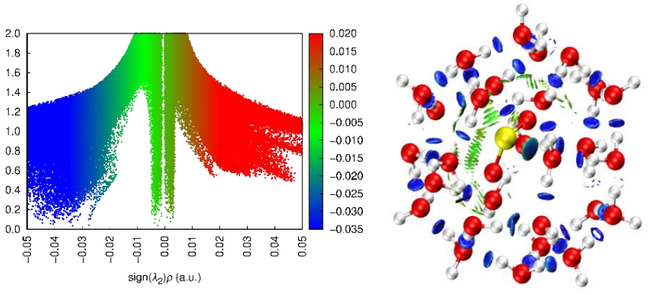
O_3			
CF_4			
SF_6			
SO_2			

Figure S35. Electron Localized function (ELF) Mapping of greenhouse gases encased within 5^{12} clathrate hydrate.

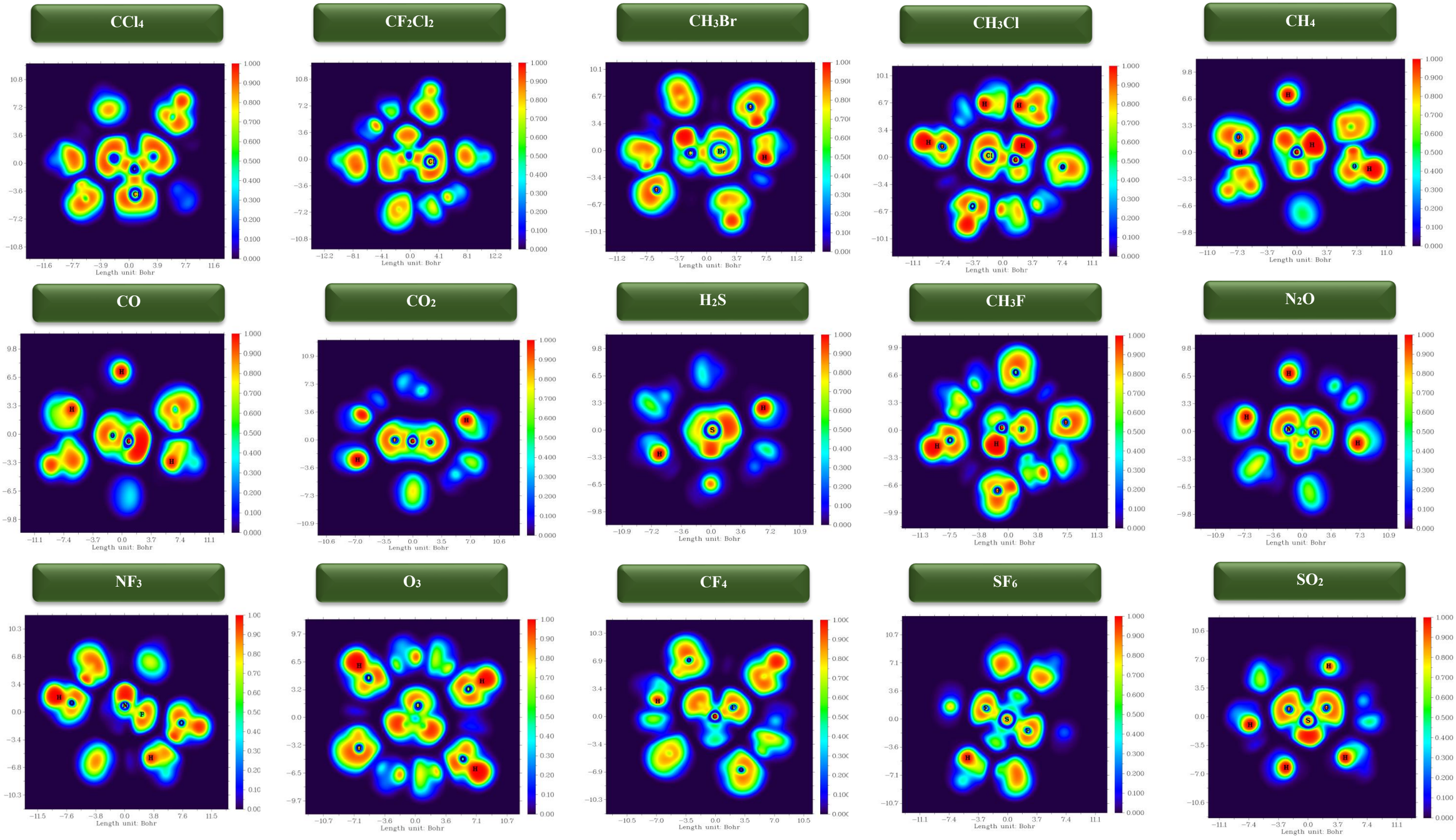


Figure S36. Electron Localized Function (ELF) Mapping of Greenhouse gases encased within $5^{12}6^2$ clathrate hydrate.

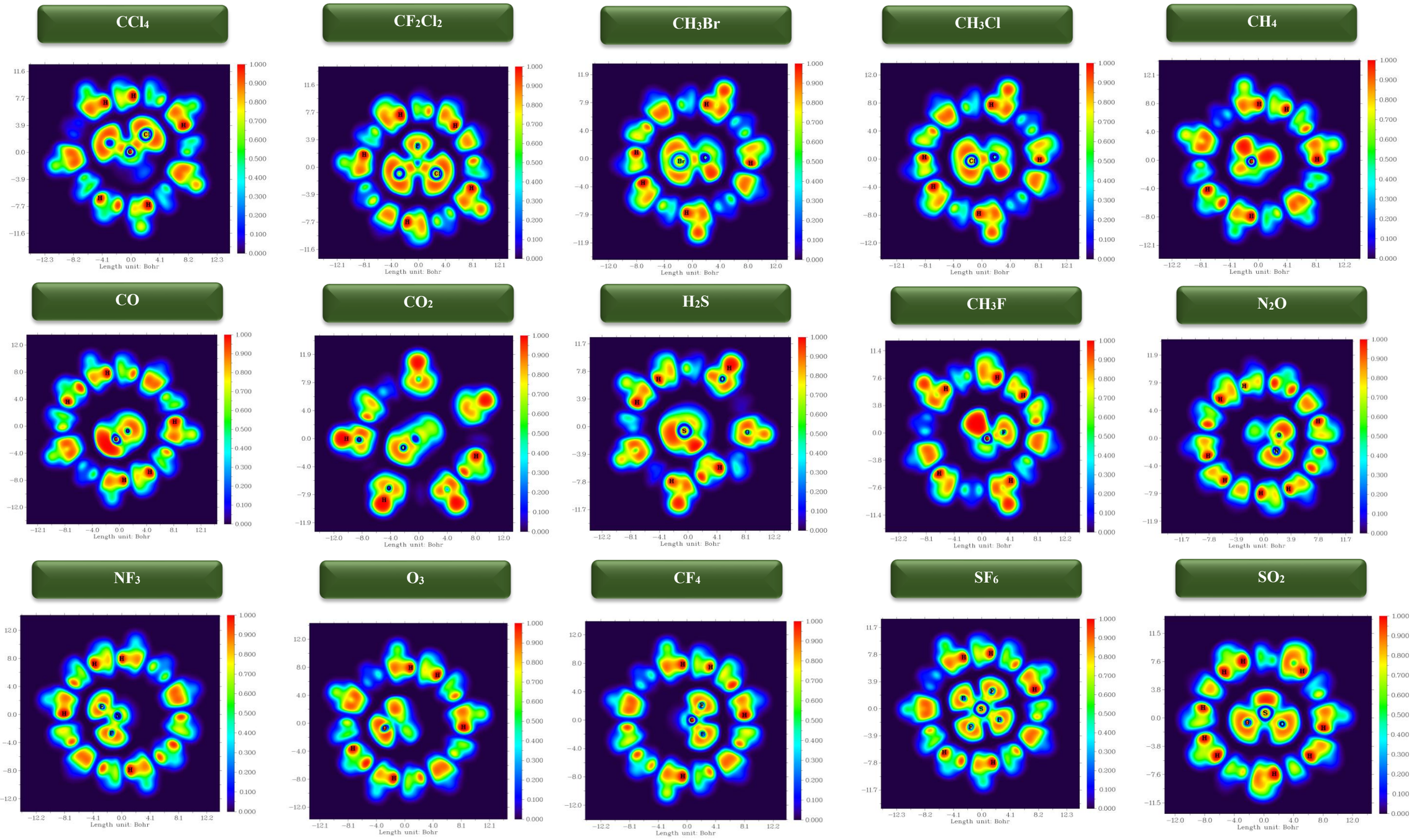


Figure S37. Electron Localized Function (ELF) Mapping of Greenhouse gases encased within $5^{12}6^4$ clathrate hydrate.

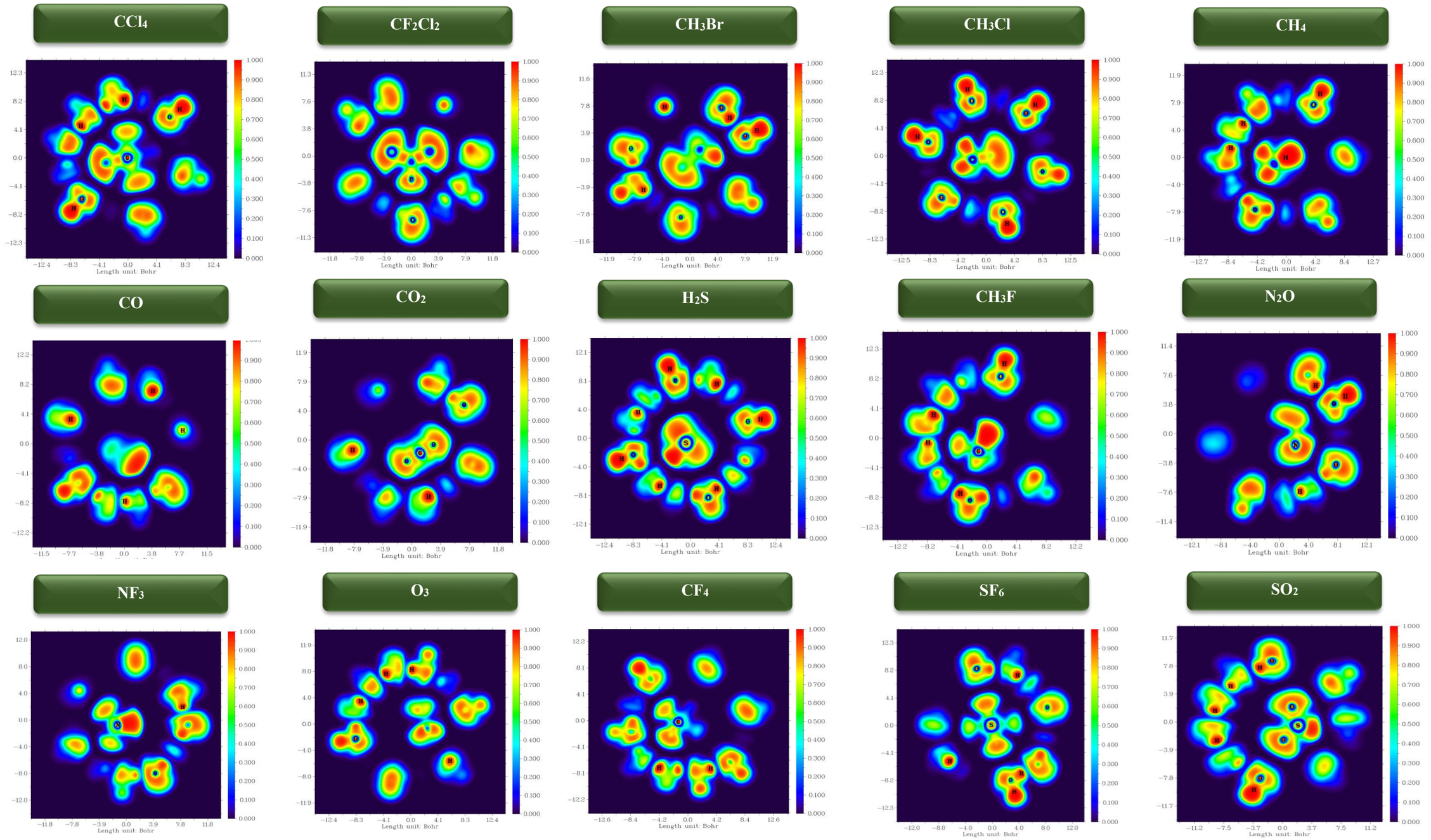


Figure S38. Bar plot for the energy gap among the Greenhouse gasess encapsulation in 5^{12}, $5^{12}6^2$ and $5^{12}6^4$ clathrate hydrates.

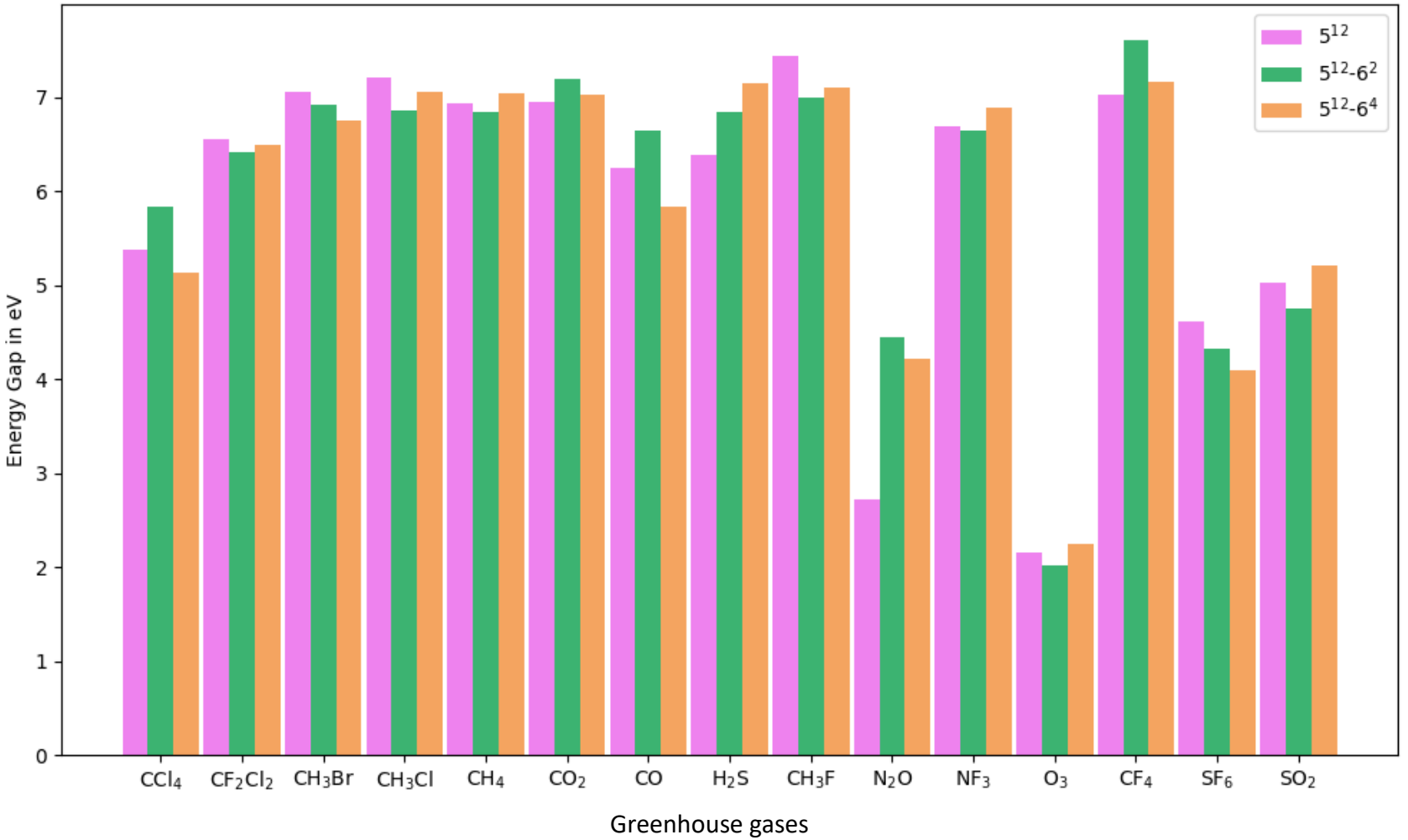


Figure S39. Bar plot for the chemical potential among the Greenhouse gases encapsulation in 5^{12}, $5^{12}6^2$ and $5^{12}6^4$ clathrate hydrates.

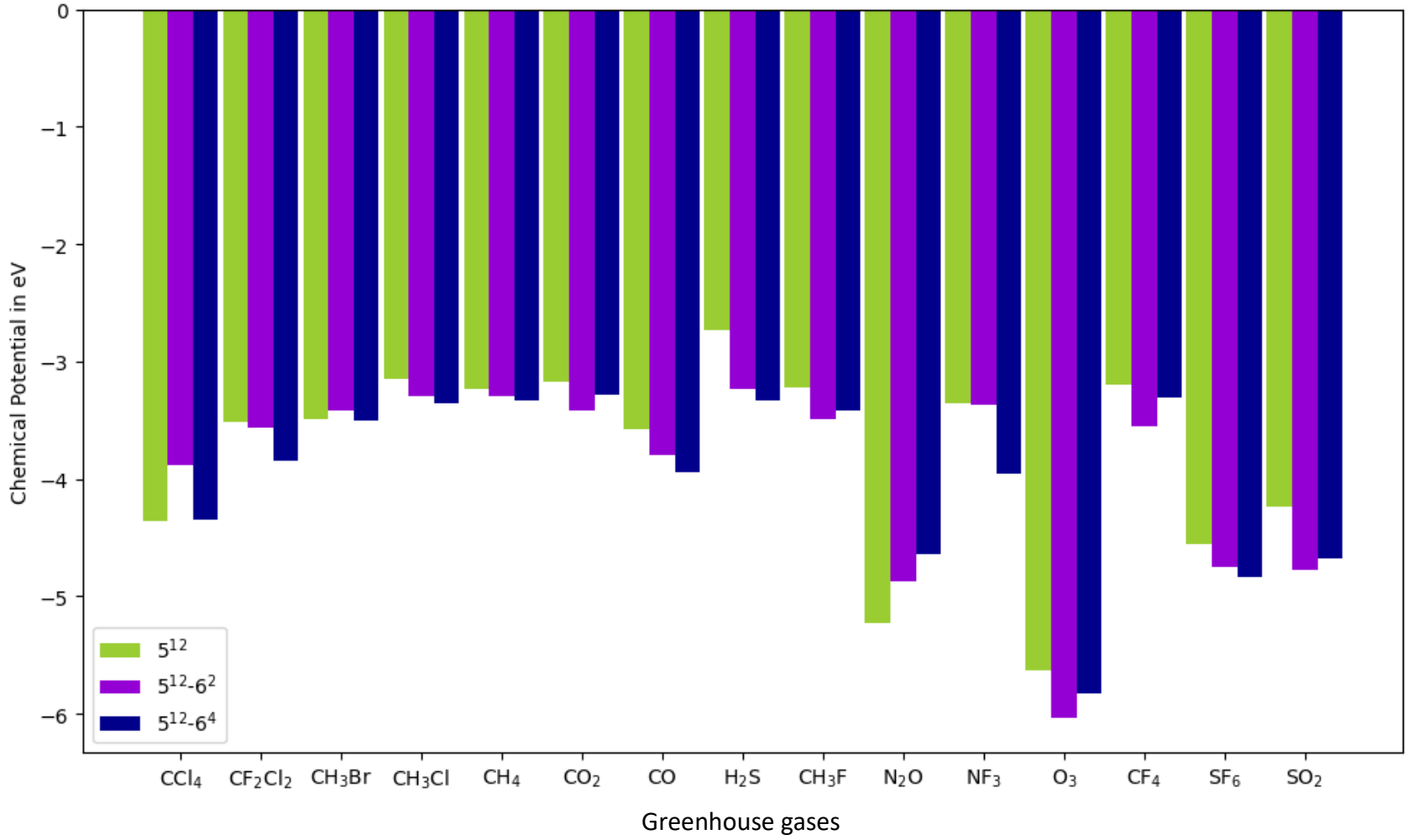


Figure S40. Bar plot for the chemical hardness among the Greenhouse gases encapsulation in 5^{12}, $5^{12}6^2$ and $5^{12}6^4$ clathrate hydrates.

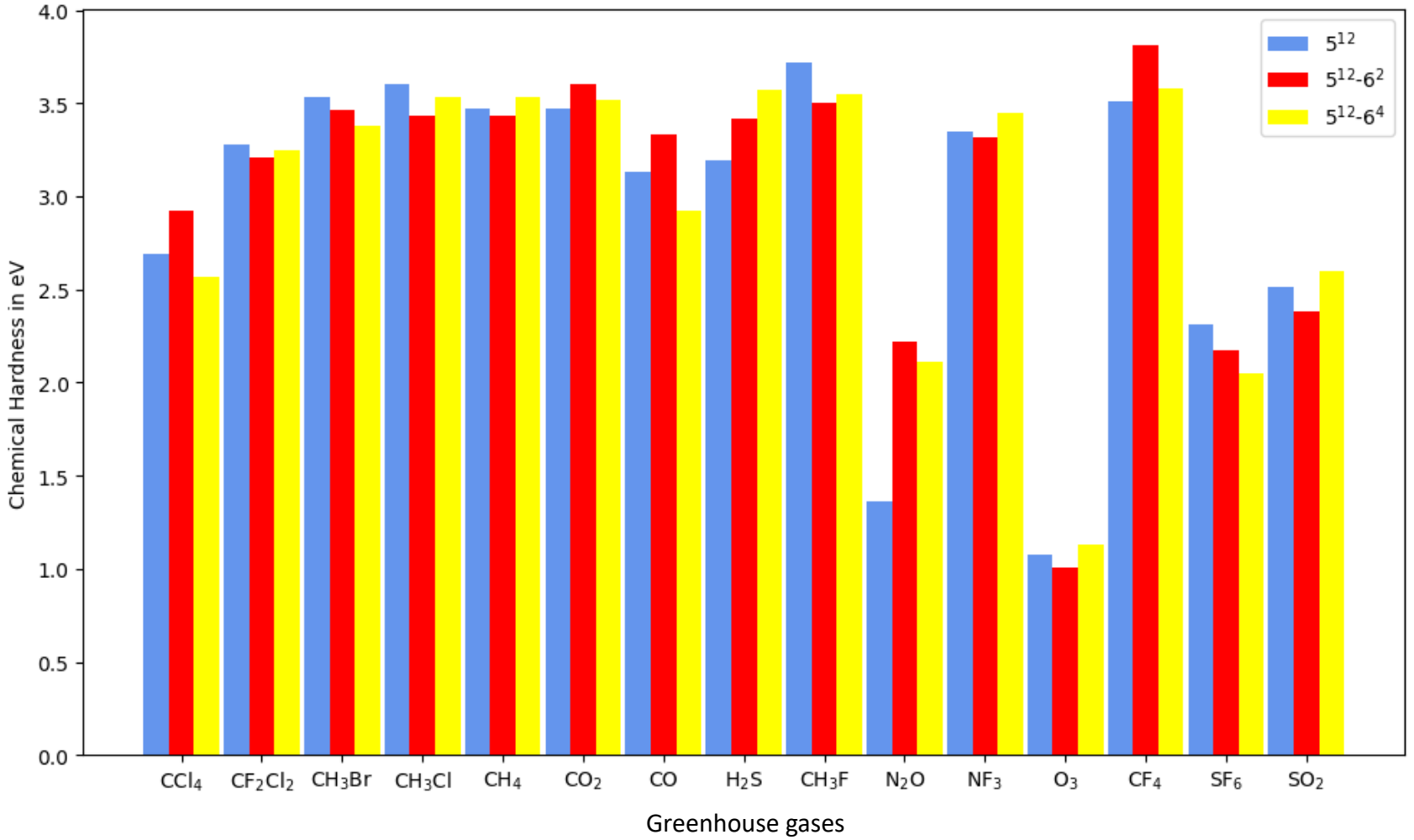


Figure S41. Bar plot for the electronegativity among the Greenhouse gases encapsulation in 5^{12}, $5^{12}6^2$ and $5^{12}6^4$ clathrate hydrates.

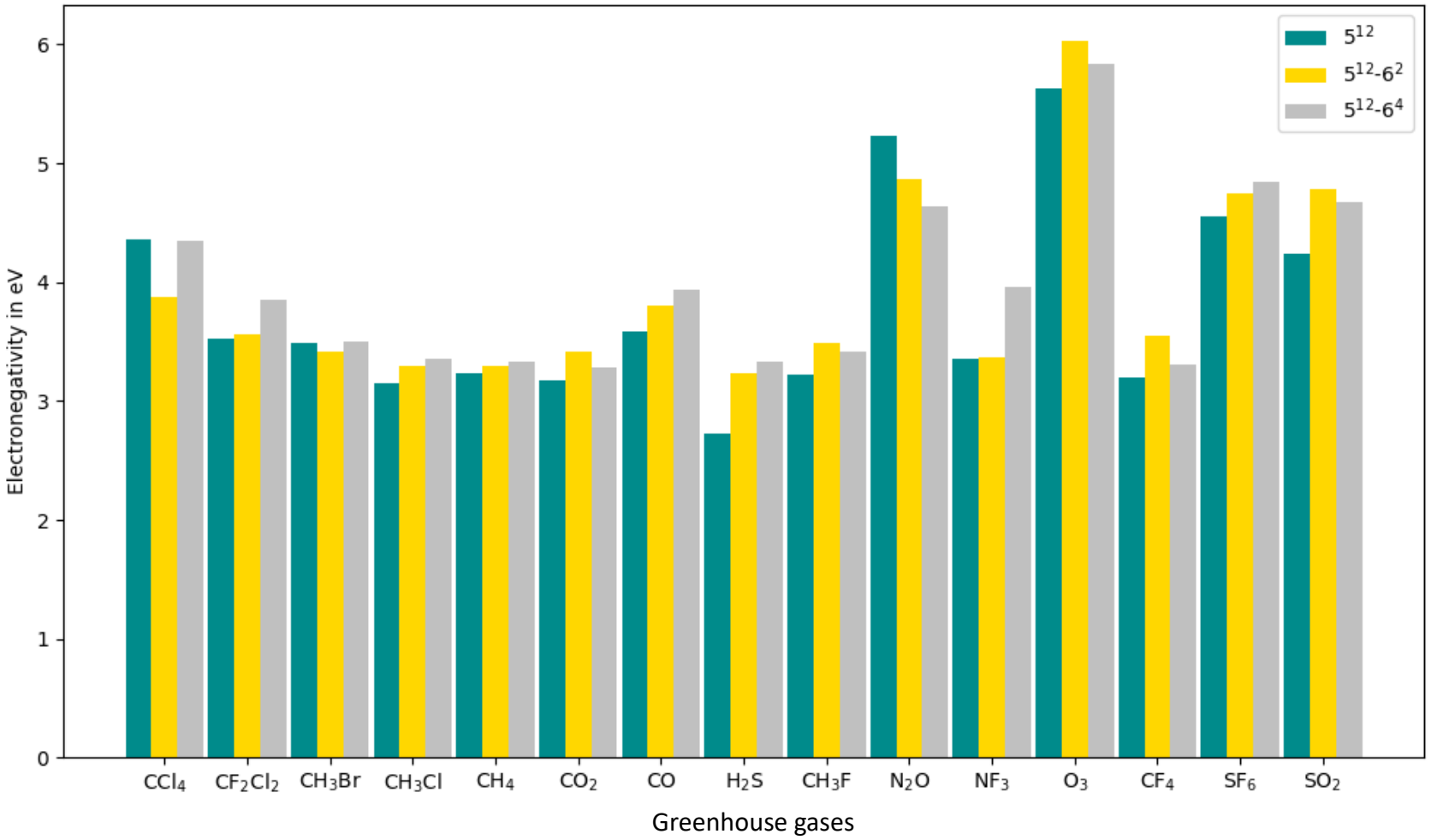
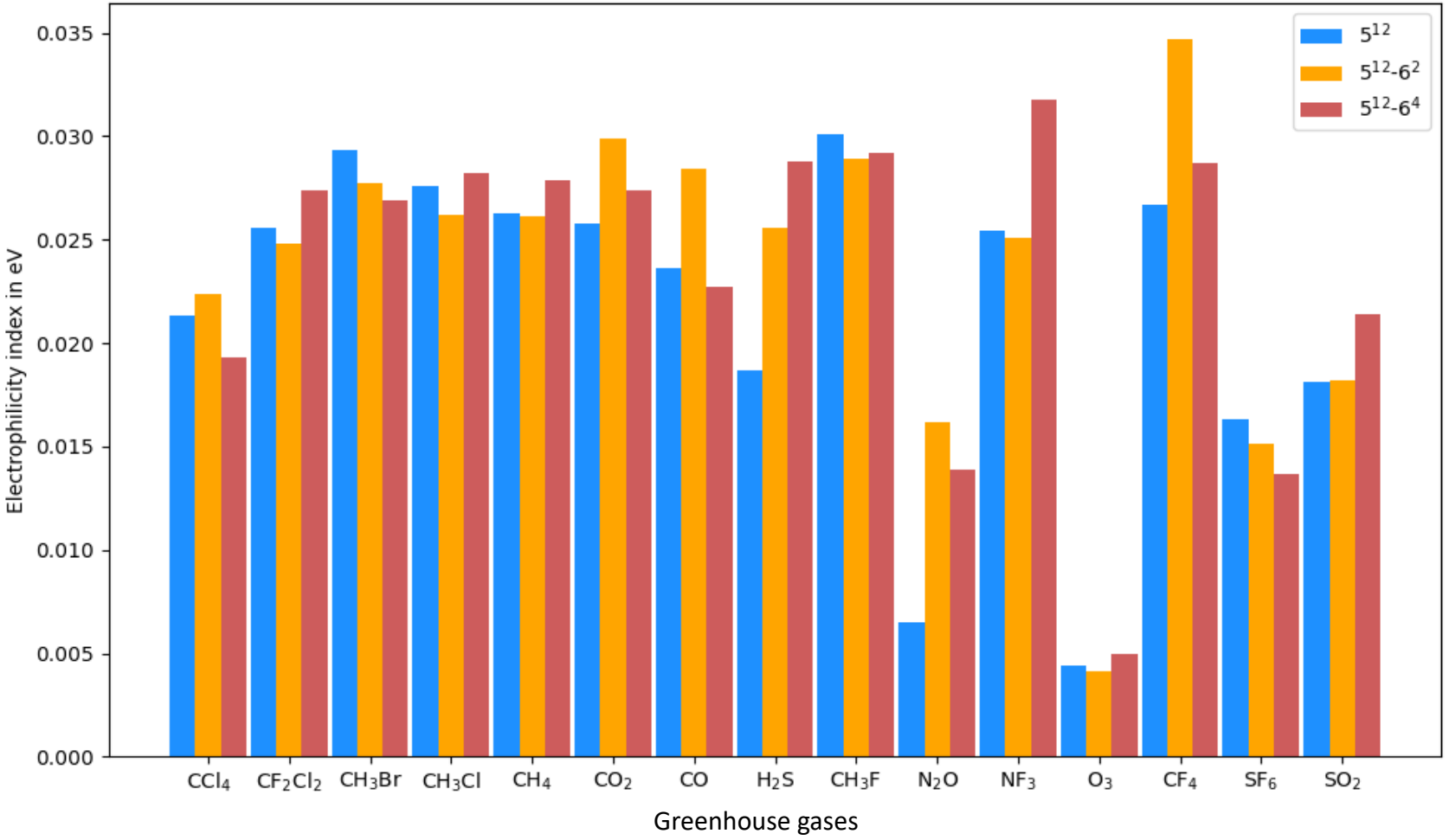


Figure S42. Bar plot for the electrophilicity index among the Greenhouse gases encapsulation in 5^{12}, $5^{12}6^2$ and $5^{12}6^4$ clathrate hydrates.



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