

1a.xyz

44	-1.366070000	-3.835426000	0.239893000
15	-2.939919000	-2.363196000	-0.636201000
6	-0.478478000	-2.347731000	0.879571000
16	0.458978000	-5.257692000	0.788171000
16	-2.518155000	-5.885719000	-0.633492000
16	-2.404279000	-4.497833000	2.353755000
6	-3.944514000	-5.350644000	1.800085000
6	-3.783581000	-6.355450000	0.657590000
6	-1.380387000	-5.970647000	2.894565000
6	0.088301000	-5.823008000	2.521845000
6	-1.249714000	-7.245628000	-0.384747000
6	0.176397000	-6.731427000	-0.288606000
1	-4.595007000	-4.516027000	1.508002000
1	-4.407582000	-5.836250000	2.671559000
1	-4.737178000	-6.466373000	0.124466000
1	-3.503962000	-7.350453000	1.022847000
1	-1.822243000	-6.868797000	2.449931000
1	-1.482245000	-6.042796000	3.986357000
1	0.635220000	-6.760131000	2.698265000
1	0.570623000	-5.043485000	3.128737000
1	-1.345688000	-7.915950000	-1.249599000
1	-1.543437000	-7.802575000	0.512129000
1	0.537159000	-6.364240000	-1.260100000
1	0.854159000	-7.530078000	0.046661000
6	-0.529159000	-3.661267000	-1.692904000
6	0.665330000	-3.139282000	-2.049584000
1	1.315952000	-2.719007000	-1.274788000
16	0.271452000	-1.082788000	1.424175000
1	-4.032208000	-1.844376000	0.125787000
1	-3.674783000	-2.783569000	-1.782200000
1	-2.427646000	-1.137825000	-1.138408000
6	1.240275000	-3.076855000	-3.405664000
6	0.491562000	-3.308782000	-4.577380000
6	1.090782000	-3.243480000	-5.833514000
6	2.453408000	-2.942497000	-5.953397000
6	3.208302000	-2.699382000	-4.803295000
6	2.605777000	-2.760604000	-3.545818000
1	-0.577090000	-3.521066000	-4.506823000
1	0.491067000	-3.415760000	-6.728323000
1	2.918096000	-2.887360000	-6.938337000
1	4.268172000	-2.455957000	-4.885348000
1	3.199848000	-2.563989000	-2.650475000
1	-1.151327000	-4.083128000	-2.497719000

1b.xyz

44	-1.384027000	-3.809862000	0.152705000
15	-3.051846000	-2.238718000	-0.282867000
6	-0.437403000	-2.339408000	0.749571000
16	0.435879000	-5.291259000	0.524791000
16	-2.682248000	-5.817494000	-0.652653000
16	-2.252346000	-4.489217000	2.345153000
6	-3.859605000	-5.291399000	1.920585000
6	-3.815466000	-6.284561000	0.761123000
6	-1.224670000	-5.990793000	2.772868000
6	0.208620000	-5.853725000	2.284048000
6	-1.431498000	-7.213972000	-0.539000000
6	0.019720000	-6.761883000	-0.510671000
1	-4.508792000	-4.436132000	1.690343000
1	-4.262525000	-5.770719000	2.824865000
1	-4.817460000	-6.382950000	0.321938000
1	-3.515020000	-7.284928000	1.094025000
1	-1.716176000	-6.870210000	2.343003000
1	-1.241016000	-6.086593000	3.867611000
1	0.759432000	-6.796804000	2.409469000
1	0.746402000	-5.081224000	2.852123000
1	-1.601113000	-7.834622000	-1.429158000
1	-1.690198000	-7.807001000	0.345398000
1	0.344384000	-6.424907000	-1.503349000
1	0.678617000	-7.586662000	-0.201582000
6	-0.582988000	-3.582646000	-1.860556000
6	0.664484000	-3.083978000	-2.064107000
1	1.247680000	-2.792692000	-1.185984000
16	0.341411000	-1.072997000	1.249742000
1	-3.522246000	-1.476368000	0.827690000
1	-4.321573000	-2.600849000	-0.823857000
1	-2.748062000	-1.154887000	-1.152964000
6	1.406235000	-2.872826000	-3.328134000
6	0.798339000	-2.604481000	-4.571798000
6	1.567901000	-2.422416000	-5.720646000
6	2.963146000	-2.500527000	-5.660537000
6	3.585116000	-2.735356000	-4.430854000
6	2.815500000	-2.906043000	-3.279305000
1	-0.286395000	-2.522677000	-4.639986000
1	1.073228000	-2.212885000	-6.670021000
1	3.560317000	-2.364775000	-6.563121000
1	4.672986000	-2.778069000	-4.367387000
1	3.310968000	-3.075972000	-2.320331000
6	-1.395441000	-4.137836000	-2.981084000
6	-2.621726000	-3.581213000	-3.391861000
6	-3.361947000	-4.130626000	-4.440095000
6	-2.898684000	-5.265913000	-5.112119000
6	-1.677383000	-5.829197000	-4.733415000
6	-0.939141000	-5.271667000	-3.687233000
1	-2.985739000	-2.667945000	-2.919703000
1	-4.298618000	-3.661260000	-4.743770000
1	-3.474031000	-5.694057000	-5.933556000
1	-1.284072000	-6.693776000	-5.269807000
1	0.042398000	-5.684546000	-3.446218000

1c.xyz

44	-1.249478000	-3.916857000	0.261413000
15	-2.817568000	-2.444893000	-0.622975000
6	-0.422301000	-2.428035000	0.974595000
16	0.572468000	-5.344718000	0.819387000
16	-2.398501000	-5.974216000	-0.614459000
16	-2.301319000	-4.589142000	2.367203000
6	-3.837915000	-5.444825000	1.810784000
6	-3.658453000	-6.456101000	0.679321000
6	-1.281690000	-6.064410000	2.909361000
6	0.189096000	-5.919354000	2.546532000
6	-1.123665000	-7.329298000	-0.382855000
6	0.299577000	-6.809080000	-0.272531000
1	-4.487274000	-4.613824000	1.506005000
1	-4.307179000	-5.924731000	2.682015000
1	-4.608053000	-6.586769000	0.143492000
1	-3.364403000	-7.443387000	1.054071000
1	-1.721380000	-6.960269000	2.458149000
1	-1.391031000	-6.140271000	4.000113000
1	0.731484000	-6.859804000	2.719034000
1	0.671349000	-5.146033000	3.161278000
1	-1.210989000	-7.984371000	-1.260131000
1	-1.419302000	-7.903546000	0.502540000
1	0.660793000	-6.431675000	-1.240142000
1	0.979639000	-7.607893000	0.057621000
6	-0.297151000	-3.678068000	-1.642350000
6	-0.912386000	-4.096018000	-2.841722000
6	-0.257459000	-3.997653000	-4.078374000
6	1.033225000	-3.472210000	-4.152296000
6	1.659544000	-3.043621000	-2.978051000
6	1.004358000	-3.142613000	-1.745174000
1	-1.925353000	-4.505366000	-2.839428000
1	-0.768866000	-4.328809000	-4.983824000
1	1.542024000	-3.388344000	-5.113356000
1	2.664921000	-2.620795000	-3.017516000
1	1.524471000	-2.785775000	-0.855274000
16	0.249821000	-1.165199000	1.619044000
1	-3.871722000	-1.892752000	0.167706000
1	-3.598847000	-2.876983000	-1.732231000
1	-2.303806000	-1.238527000	-1.167329000

1d.xyz

6	-0.094658000	-0.073851000	0.027921000
6	-1.463839000	-0.003132000	0.026365000
6	2.302891000	-3.333905000	-0.110920000
6	1.789815000	-4.647981000	-0.196488000
44	1.154387000	1.686620000	0.023404000
15	2.167239000	0.762128000	1.921373000
6	0.014970000	2.558724000	1.186788000
16	-0.067130000	2.341379000	-1.902614000
16	2.726141000	0.502291000	-1.562089000
16	2.645595000	3.581965000	-0.388011000
6	4.269413000	2.766391000	-0.721448000
6	4.224253000	1.607502000	-1.714318000
6	2.195137000	4.112167000	-2.129045000
6	0.712808000	3.948998000	-2.423945000
6	1.929417000	0.760752000	-3.240603000
6	0.449409000	1.092402000	-3.162997000
1	4.587260000	2.430259000	0.274297000
1	4.986528000	3.531358000	-1.053459000
1	5.096226000	0.957079000	-1.562460000
1	4.266166000	1.956007000	-2.752844000
1	2.808780000	3.528651000	-2.823343000
1	2.482340000	5.168801000	-2.221097000
1	0.505761000	4.093865000	-3.493824000
1	0.116090000	4.688228000	-1.871029000
1	2.066166000	-0.181102000	-3.788881000
1	2.498972000	1.542411000	-3.756230000
1	-0.139589000	0.217457000	-2.852036000
1	0.072099000	1.425608000	-4.140863000
6	0.660194000	-1.256676000	0.019442000
1	-1.901250000	0.997692000	0.056520000
16	-0.951956000	3.294920000	2.177812000
1	2.691489000	1.612429000	2.939970000
1	3.290502000	-0.101906000	1.773912000
1	1.344470000	-0.075854000	2.720192000
6	-2.477706000	-1.059116000	0.006681000
6	-2.200708000	-2.444065000	-0.012670000
6	-3.233694000	-3.378403000	-0.017242000
6	-4.569977000	-2.963468000	-0.003932000
6	-4.865805000	-1.597019000	0.014089000
6	-3.834346000	-0.660470000	0.019016000
1	-1.166735000	-2.782062000	-0.017247000
1	-2.996079000	-4.443111000	-0.027837000
1	-5.373701000	-3.700555000	-0.005013000
1	-5.903511000	-1.262134000	0.027523000
1	-4.073621000	0.405205000	0.038100000
6	1.432543000	-2.214400000	-0.027323000
6	2.652094000	-5.738329000	-0.277583000
6	4.038300000	-5.547981000	-0.271970000
6	4.560713000	-4.253260000	-0.186239000
6	3.705851000	-3.157236000	-0.106782000
1	0.710552000	-4.798527000	-0.198505000
1	2.240717000	-6.745794000	-0.343255000
1	4.708957000	-6.405443000	-0.332377000
1	5.640278000	-4.099035000	-0.179632000
1	4.112383000	-2.147261000	-0.044142000

1e.xyz

44	-1.283454000	-3.754779000	0.200409000
15	-2.926164000	-2.140816000	-0.329063000
6	-0.333357000	-2.340745000	0.922003000
16	0.459586000	-5.293508000	0.681191000
16	-2.532727000	-5.701702000	-0.793372000
16	-2.361711000	-4.463930000	2.264972000
6	-3.938920000	-5.212363000	1.664660000
6	-3.812796000	-6.173726000	0.483788000
6	-1.416230000	-6.007026000	2.745455000
6	0.058738000	-5.908086000	2.388642000
6	-1.331080000	-7.131684000	-0.613934000
6	0.118558000	-6.701965000	-0.464122000
1	-4.544812000	-4.334996000	1.402708000
1	-4.433210000	-5.707962000	2.512860000
1	-4.769264000	-6.226646000	-0.053037000
1	-3.572243000	-7.192581000	0.809118000
1	-1.894480000	-6.861442000	2.254716000
1	-1.532788000	-6.123517000	3.831805000
1	0.565528000	-6.873125000	2.529769000
1	0.569865000	-5.172883000	3.026476000
1	-1.442395000	-7.735699000	-1.524379000
1	-1.667832000	-7.733605000	0.237660000
1	0.517711000	-6.313791000	-1.411922000
1	0.745948000	-7.549956000	-0.153060000
6	-0.372977000	-3.434206000	-1.687559000
6	0.949617000	-3.240333000	-1.892723000
1	1.658348000	-3.241668000	-1.062205000
16	0.470327000	-1.140031000	1.524063000
1	-3.676434000	-1.687620000	0.801448000
1	-4.009870000	-2.440853000	-1.195303000
1	-2.511396000	-0.886232000	-0.834736000
6	1.546544000	-2.971044000	-3.227019000
8	0.940073000	-2.700572000	-4.252191000
6	3.595678000	-2.817476000	-4.407147000
8	2.909155000	-3.059719000	-3.149992000
1	4.661283000	-2.875082000	-4.170497000
6	-1.329563000	-3.371021000	-2.835686000
8	-2.164249000	-2.477441000	-2.956283000
8	-1.267540000	-4.452894000	-3.645031000
6	-2.109647000	-4.360929000	-4.832555000
1	-2.034973000	-5.337015000	-5.317820000
1	-1.719292000	-3.571070000	-5.484046000
1	-3.144601000	-4.133794000	-4.554544000
1	3.333616000	-1.828400000	-4.799608000
1	3.319030000	-3.581695000	-5.143444000

1f.xyz

44	-1.292963000	-5.305459000	-0.931803000
15	-3.326571000	-4.173495000	-1.153623000
6	-1.226257000	-4.651523000	0.799767000
16	0.837421000	-6.349621000	-0.754642000
16	-1.367054000	-6.161882000	-3.266515000
16	-2.274108000	-7.512934000	-0.387272000
6	-3.238787000	-7.900227000	-1.907602000
6	-2.547005000	-7.622235000	-3.243857000

6	-0.832726000	-8.683747000	-0.552479000
6	0.457917000	-8.040706000	-0.070327000
6	0.255342000	-7.090076000	-3.481453000
6	1.348615000	-6.701048000	-2.497417000
1	-4.135186000	-7.277556000	-1.787286000
1	-3.565140000	-8.949250000	-1.858992000
1	-3.300741000	-7.408971000	-4.013435000
1	-1.971758000	-8.488092000	-3.591789000
1	-0.762595000	-9.000767000	-1.598729000
1	-1.064400000	-9.565159000	0.061304000
1	1.323507000	-8.684720000	-0.280741000
1	0.430831000	-7.865843000	1.014444000
1	0.588466000	-6.878031000	-4.506379000
1	0.018074000	-8.157509000	-3.420826000
1	1.828775000	-5.761553000	-2.794813000
1	2.127670000	-7.476655000	-2.459986000
14	-0.325042000	-3.158524000	-1.737904000
16	-1.229491000	-4.163005000	2.293415000
1	-4.451000000	-4.734025000	-0.468357000
1	-3.918536000	-4.009765000	-2.433792000
1	-3.441670000	-2.848759000	-0.663568000
6	0.021381000	-1.852447000	-0.409719000
8	-1.568007000	-2.596029000	-2.752516000
6	1.271471000	-3.234685000	-2.780393000
6	-1.456292000	-1.365990000	-3.510732000
6	-2.802676000	-0.664662000	-3.575326000
1	-3.138213000	-0.361544000	-2.573265000
1	-3.564548000	-1.322329000	-4.018461000
1	-2.728845000	0.237877000	-4.199113000
1	-1.102993000	-1.617180000	-4.523818000
1	-0.706553000	-0.700926000	-3.052232000
1	0.377898000	-0.917743000	-0.870446000
1	0.806223000	-2.196064000	0.281503000
1	-0.869081000	-1.616080000	0.190495000
1	1.528746000	-2.210592000	-3.096538000
1	1.170566000	-3.836153000	-3.696609000
1	2.130112000	-3.603402000	-2.196703000

lg.xyz

44	-1.094167000	-3.805977000	0.612115000
15	-2.651017000	-2.333518000	-0.283616000
6	-0.266365000	-2.320607000	1.327817000
16	0.723676000	-5.235181000	1.178774000
16	-2.245820000	-5.864587000	-0.261218000
16	-2.152624000	-4.469482000	2.715326000
6	-3.690419000	-5.322263000	2.157959000
6	-3.511966000	-6.338123000	1.030380000
6	-1.138503000	-5.944865000	3.268406000
6	0.333775000	-5.803559000	2.907780000
6	-0.975029000	-7.220635000	-0.014472000
6	0.448834000	-6.701884000	0.091194000
1	-4.335492000	-4.489805000	1.847980000
1	-4.163919000	-5.797051000	3.029664000
1	-4.460573000	-6.466779000	0.492267000
1	-3.222812000	-7.325206000	1.409483000
1	-1.578783000	-6.842926000	2.822110000
1	-1.249755000	-6.013877000	4.359446000
1	0.874892000	-6.743406000	3.087249000
1	0.814394000	-5.027269000	3.520117000
1	-1.063102000	-7.885411000	-0.884373000
1	-1.272187000	-7.784316000	0.877164000
1	0.806670000	-6.324865000	-0.877841000
1	1.128546000	-7.500975000	0.421572000
6	-0.145995000	-3.569342000	-1.297662000
6	-0.748366000	-3.992870000	-2.501532000
6	-0.108269000	-3.883937000	-3.740930000
6	1.181254000	-3.328946000	-3.837902000
6	1.796179000	-2.893489000	-2.645742000
6	1.144987000	-3.009900000	-1.417732000
1	-1.753460000	-4.421093000	-2.505572000
1	-0.622332000	-4.223029000	-4.643159000
1	2.792798000	-2.447490000	-2.684688000
1	1.668979000	-2.641204000	-0.535081000
16	0.406358000	-1.059407000	1.977162000
1	-3.740335000	-1.817384000	0.485365000
1	-3.388515000	-2.748475000	-1.428363000
1	-2.138657000	-1.105674000	-0.778409000
7	1.818785000	-3.205553000	-5.053256000
1	1.371822000	-3.500324000	-5.909163000
1	2.737189000	-2.791299000	-5.119571000

lh.xyz

44	-1.091127000	-3.804197000	0.594340000
15	-2.646150000	-2.329853000	-0.304943000
6	-0.259014000	-2.315417000	1.300909000
16	0.731587000	-5.230728000	1.153282000
16	-2.240720000	-5.863021000	-0.273743000
16	-2.137964000	-4.465452000	2.700648000
6	-3.676942000	-5.320930000	2.149911000
6	-3.501728000	-6.337245000	1.022270000
6	-1.119706000	-5.939997000	3.249326000
6	0.350925000	-5.798508000	2.883563000
6	-0.968013000	-7.218983000	-0.034593000
6	0.455961000	-6.699771000	0.068743000
1	-4.324528000	-4.489587000	1.842363000
1	-4.145911000	-5.795996000	3.023940000
1	-4.452099000	-6.467020000	0.487632000
1	-3.210080000	-7.323957000	1.400395000
1	-1.561257000	-6.837729000	2.803701000
1	-1.227720000	-6.009616000	4.340605000
1	0.892475000	-6.738842000	3.059160000
1	0.835082000	-5.023210000	3.494302000
1	-1.058464000	-7.881285000	-0.906091000
1	-1.262410000	-7.785392000	0.856232000
1	0.814619000	-6.326805000	-0.901452000
1	1.136224000	-7.497499000	0.401106000
6	-0.146396000	-3.572883000	-1.315859000
6	-0.758485000	-3.986971000	-2.516516000
6	-0.114656000	-3.880224000	-3.757633000
6	1.173833000	-3.341452000	-3.831772000
6	1.807554000	-2.916733000	-2.656987000
6	1.152940000	-3.030007000	-1.429949000
1	-1.767405000	-4.405196000	-2.518808000
1	-0.625924000	-4.209771000	-4.666085000
1	2.808360000	-2.488453000	-2.720381000
1	1.678753000	-2.672864000	-0.543983000
16	0.421843000	-1.052821000	1.936924000
1	-3.714725000	-1.779033000	0.467990000
1	-3.407874000	-2.758859000	-1.428779000
1	-2.121730000	-1.122805000	-0.837119000
8	1.863593000	-3.197321000	-5.012622000
1	1.295514000	-3.497588000	-5.745635000

li.xyz

44	-1.246065000	-3.921290000	0.262339000
15	-2.804307000	-2.448674000	-0.631490000
6	-0.417891000	-2.434820000	0.976962000
16	0.572465000	-5.349888000	0.827024000
16	-2.397493000	-5.980121000	-0.611952000
16	-2.306704000	-4.583854000	2.365651000
6	-3.843749000	-5.435642000	1.804650000
6	-3.664116000	-6.452272000	0.678136000
6	-1.289621000	-6.057608000	2.917289000
6	0.182343000	-5.915537000	2.556024000
6	-1.126412000	-7.336068000	-0.366495000
6	0.297352000	-6.816899000	-0.260734000
1	-4.486008000	-4.601970000	1.491974000
1	-4.321418000	-5.908720000	2.674995000
1	-4.612127000	-6.580185000	0.138753000
1	-3.376459000	-7.439606000	1.057750000
1	-1.729525000	-6.955977000	2.471262000
1	-1.399716000	-6.127007000	4.008393000
1	0.723943000	-6.854912000	2.736700000
1	0.663046000	-5.138251000	3.167083000
1	-1.214560000	-7.999764000	-1.237190000
1	-1.423096000	-7.900822000	0.524641000
1	0.655984000	-6.440831000	-1.229871000
1	0.977569000	-7.615591000	0.069418000
6	-0.297993000	-3.682191000	-1.643694000
6	-0.905171000	-4.109471000	-2.841488000
6	-0.257079000	-3.992639000	-4.080029000
6	1.024854000	-3.440090000	-4.183760000
6	1.635325000	-3.009709000	-2.994051000
6	0.993088000	-3.124780000	-1.757934000
1	-1.910350000	-4.536998000	-2.840960000
1	-0.772547000	-4.330899000	-4.982242000
1	2.632155000	-2.562777000	-3.032123000
1	1.514800000	-2.757694000	-0.873362000
16	0.255711000	-1.173565000	1.623485000
1	-3.894418000	-1.931709000	0.134867000
1	-3.538488000	-2.863481000	-1.778374000
1	-2.290879000	-1.220478000	-1.124799000
6	1.724604000	-3.308006000	-5.516268000
1	2.161941000	-2.306903000	-5.639164000
1	2.547610000	-4.033970000	-5.606981000
1	1.032912000	-3.482146000	-6.350643000

1j.xyz

44	-1.250856000	-3.921398000	0.269606000
15	-2.812401000	-2.447426000	-0.620020000
6	-0.423545000	-2.434674000	0.986331000
16	0.569010000	-5.350940000	0.830829000
16	-2.400704000	-5.980426000	-0.605029000
16	-2.306568000	-4.586842000	2.371853000
6	-3.844722000	-5.437703000	1.812103000
6	-3.666640000	-6.453743000	0.685018000
6	-1.289164000	-6.061497000	2.920794000
6	0.182436000	-5.918512000	2.559693000
6	-1.129345000	-7.337106000	-0.363198000
6	0.294424000	-6.818183000	-0.256915000
1	-4.487763000	-4.603931000	1.501394000
1	-4.320380000	-5.911259000	2.683264000
1	-4.615036000	-6.581826000	0.146466000
1	-3.377731000	-7.441136000	1.063399000
1	-1.729091000	-6.959180000	2.473486000
1	-1.399772000	-6.131977000	4.011740000
1	0.724456000	-6.858165000	2.737515000
1	0.663834000	-5.142366000	3.171562000
1	-1.218218000	-7.999380000	-1.234918000
1	-1.425700000	-7.903305000	0.527064000
1	0.654919000	-6.444378000	-1.226136000
1	0.974521000	-7.616559000	0.074205000
6	-0.305252000	-3.677473000	-1.636557000
6	-0.915145000	-4.105866000	-2.835425000
6	-0.275081000	-4.000018000	-4.078662000
6	0.997776000	-3.448405000	-4.122183000
6	1.644090000	-3.002177000	-2.974811000
6	0.986856000	-3.118023000	-1.745266000
1	-1.919588000	-4.534421000	-2.832712000
1	-0.756501000	-4.330817000	-4.998701000
9	1.630490000	-3.336010000	-5.324815000
1	2.639987000	-2.565682000	-3.050240000
1	1.505866000	-2.752458000	-0.858847000
16	0.249992000	-1.174036000	1.632919000
1	-3.900731000	-1.929277000	0.147226000
1	-3.547729000	-2.862179000	-1.766331000
1	-2.296747000	-1.220890000	-1.115237000

1k.xyz

44	-1.087857000	-3.807597000	0.594755000
15	-2.664235000	-2.334046000	-0.280632000
6	-0.259916000	-2.317195000	1.310784000
16	0.729463000	-5.233910000	1.177743000
16	-2.228517000	-5.868480000	-0.279310000
16	-2.156871000	-4.466344000	2.696846000
6	-3.689616000	-5.321532000	2.129585000
6	-3.503401000	-6.338254000	1.004115000
6	-1.141748000	-5.937231000	3.256727000
6	0.331836000	-5.792367000	2.906399000
6	-0.958652000	-7.224837000	-0.025425000
6	0.464836000	-6.708074000	0.097040000
1	-4.334705000	-4.490403000	1.816092000
1	-4.167493000	-5.796212000	2.998925000
1	-4.448052000	-6.466769000	0.459155000
1	-3.217244000	-7.325345000	1.385329000
1	-1.576835000	-6.836242000	2.807367000
1	-1.260845000	-6.005865000	4.346889000
1	0.874554000	-6.730260000	3.091238000
1	0.807804000	-5.012993000	3.518386000
1	-1.038787000	-7.885632000	-0.899043000
1	-1.265327000	-7.792339000	0.860447000
1	0.841744000	-6.344669000	-0.869805000
1	1.137955000	-7.505452000	0.444402000
6	-0.132878000	-3.559650000	-1.297517000
6	-0.753125000	-3.960274000	-2.501787000
6	-0.101957000	-3.839794000	-3.733283000
6	1.193517000	-3.311712000	-3.804189000
6	1.827049000	-2.902992000	-2.618456000
6	1.174419000	-3.022968000	-1.394112000
1	-1.764219000	-4.372204000	-2.501034000
1	-0.606869000	-4.154032000	-4.650333000
1	2.833138000	-2.485266000	-2.683180000
1	1.693268000	-2.683256000	-0.496923000
16	0.414201000	-1.056756000	1.953469000
1	-3.720965000	-1.795743000	0.514956000
1	-3.441447000	-2.759100000	-1.395475000
1	-2.154977000	-1.120219000	-0.812810000
6	1.868980000	-3.182422000	-5.116781000
1	1.258328000	-3.524532000	-5.989876000
8	2.998191000	-2.744218000	-5.277072000

1m.xyz

44	-1.082178000	-3.808155000	0.587214000
15	-2.657119000	-2.335240000	-0.289552000
6	-0.251825000	-2.319939000	1.302868000
16	0.731296000	-5.241037000	1.167175000
16	-2.237668000	-5.870571000	-0.273619000
16	-2.146323000	-4.455458000	2.692776000
6	-3.684709000	-5.309914000	2.140345000
6	-3.508228000	-6.330564000	1.016940000
6	-1.135185000	-5.927994000	3.256150000
6	0.337618000	-5.794019000	2.899026000
6	-0.970678000	-7.229351000	-0.019186000
6	0.454586000	-6.715012000	0.088982000
1	-4.332864000	-4.479809000	1.830642000
1	-4.154075000	-5.781639000	3.015951000
1	-4.455841000	-6.457430000	0.476886000
1	-3.223429000	-7.317615000	1.399223000
1	-1.577591000	-6.827088000	2.814261000
1	-1.250426000	-5.989329000	4.347169000
1	0.874322000	-6.735638000	3.082395000
1	0.822214000	-5.017345000	3.507560000
1	-1.059185000	-7.896444000	-0.887209000
1	-1.271814000	-7.789229000	0.873384000
1	0.822408000	-6.352411000	-0.881677000
1	1.130399000	-7.513233000	0.429005000
6	-0.133022000	-3.562243000	-1.311870000
6	-0.745580000	-3.990030000	-2.512079000
6	-0.108020000	-3.878122000	-3.750546000
6	1.168698000	-3.324595000	-3.801370000
6	1.812405000	-2.881166000	-2.646212000
6	1.160259000	-3.001486000	-1.418570000
1	-1.748393000	-4.421155000	-2.505986000
1	-0.584879000	-4.206328000	-4.672541000
1	2.807151000	-2.445541000	-2.725062000
1	1.678190000	-2.640214000	-0.530279000
16	0.420936000	-1.060895000	1.949507000
1	-3.738854000	-1.825433000	0.490881000
1	-3.400459000	-2.747805000	-1.431592000
1	-2.150319000	-1.104318000	-0.783759000
7	1.850475000	-3.198545000	-5.108498000
8	1.240567000	-3.600015000	-6.111288000
8	2.984120000	-2.696769000	-5.115066000

2a.xyz

44	0.135731000	-0.041663000	0.052761000
6	2.101318000	-0.201625000	0.374800000
6	2.180837000	1.241364000	0.099579000
6	2.238806000	1.780483000	-1.164044000
1	2.317732000	1.901565000	0.962294000
15	-0.026124000	0.483980000	2.338086000
16	0.269691000	-0.643000000	-2.244303000
16	-2.316142000	0.466003000	-0.391682000
16	-0.599188000	-2.197336000	0.491796000
6	-2.345174000	-2.021982000	1.105135000
6	-3.217211000	-1.004677000	0.362916000
6	-0.986473000	-2.970645000	-1.180487000
6	-0.046972000	-2.473149000	-2.258893000
6	-2.524952000	0.070812000	-2.209077000
6	-1.230652000	0.131058000	-3.005786000
1	-2.214298000	-1.747392000	2.160289000
1	-2.803198000	-3.021398000	1.085179000
1	-3.950953000	-0.572640000	1.055017000
1	-3.782062000	-1.472437000	-0.451608000
1	-2.032253000	-2.745402000	-1.416729000
1	-0.883359000	-4.056046000	-1.044124000
1	-0.404450000	-2.741677000	-3.262809000
1	0.962072000	-2.891005000	-2.136893000
1	-3.234276000	0.807993000	-2.609570000
1	-2.994117000	-0.917176000	-2.278053000
1	-0.904324000	1.170969000	-3.146492000
1	-1.365470000	-0.311888000	-4.004140000
1	2.263343000	1.078414000	-2.001390000
16	3.232590000	-1.259392000	0.870127000
1	0.254867000	-0.539022000	3.291993000
1	-1.246331000	0.950062000	2.912842000
1	0.826026000	1.485381000	2.890678000
6	2.474200000	3.169852000	-1.525361000
6	2.371386000	4.246840000	-0.617557000
6	2.711292000	5.537103000	-1.012420000
6	3.165240000	5.782124000	-2.316508000
6	3.260612000	4.729714000	-3.231862000
6	2.906899000	3.439235000	-2.843658000
1	2.019857000	4.072386000	0.400501000
1	2.629376000	6.361154000	-0.303042000
1	3.443782000	6.793360000	-2.615671000
1	3.618722000	4.914024000	-4.245111000
1	2.997937000	2.613812000	-3.552821000

2b.xyz

44	-0.091404000	0.056281000	0.179876000
6	1.846074000	-0.265170000	-0.050429000
6	2.099422000	1.230972000	0.049059000
6	2.555281000	1.680236000	1.273724000
6	2.023247000	2.102097000	-1.167071000
15	0.034645000	-0.008113000	2.527621000
16	-0.132910000	-0.079847000	-2.209931000
16	-2.400841000	1.100621000	-0.011650000
16	-1.227724000	-1.956057000	0.221092000
6	-2.902118000	-1.574606000	0.956567000
6	-3.570057000	-0.279423000	0.487585000
6	-1.792442000	-2.296357000	-1.538341000
6	-0.769360000	-1.793094000	-2.531650000
6	-2.723524000	1.131695000	-1.863332000
6	-1.475421000	1.070897000	-2.729950000
1	-2.705002000	-1.552001000	2.035483000
1	-3.542670000	-2.445986000	0.759644000
1	-4.180752000	0.137623000	1.298275000
1	-4.237849000	-0.448419000	-0.364657000
1	-2.767578000	-1.815972000	-1.676913000
1	-1.921669000	-3.385181000	-1.614608000
1	-1.153851000	-1.818447000	-3.560842000
1	0.149405000	-2.396549000	-2.499069000
1	-3.260456000	2.068469000	-2.064796000
1	-3.405056000	0.301809000	-2.081201000
1	-0.942042000	2.033101000	-2.734470000
1	-1.735897000	0.833723000	-3.772605000
1	2.508999000	0.939801000	2.078790000
16	2.916810000	-1.423616000	-0.455130000
1	-0.955488000	-0.716475000	3.274254000
1	0.010191000	1.182173000	3.314368000
1	1.161194000	-0.623445000	3.148591000
6	3.249183000	2.892582000	1.684911000
6	3.795059000	3.856084000	0.801637000
6	4.535431000	4.926959000	1.292897000
6	4.741325000	5.079340000	2.669936000
6	4.214099000	4.137775000	3.560595000
6	3.489557000	3.054267000	3.072849000
1	3.664192000	3.748472000	-0.273246000
1	4.964900000	5.646452000	0.595125000
1	5.323386000	5.922043000	3.045331000
1	4.385336000	4.241594000	4.632180000
1	3.107702000	2.304804000	3.769675000
6	1.205549000	3.250232000	-1.134732000
6	1.099499000	4.083308000	-2.247997000
6	1.804047000	3.780052000	-3.420227000
6	2.616580000	2.643419000	-3.462164000
6	2.728041000	1.807428000	-2.345409000
1	0.659394000	3.488089000	-0.219968000
1	0.471401000	4.973708000	-2.197992000
1	1.722948000	4.430712000	-4.291823000
1	3.173145000	2.405342000	-4.369051000
1	3.369876000	0.925995000	-2.380167000

2c.xyz

6	-1.626370000	0.308495000	0.021689000
6	-3.106663000	0.239221000	-0.118810000
44	-1.627164000	-1.698898000	0.042932000
15	-1.112271000	-1.486686000	2.315908000
16	-1.834815000	-1.727633000	-2.322421000
16	-2.211608000	-4.102377000	-0.011451000
16	0.543191000	-2.377436000	-0.210907000
6	0.616100000	-4.080446000	0.568085000
6	-0.578747000	-4.991989000	0.290914000
6	0.731415000	-2.915833000	-2.003028000
6	-0.102069000	-2.045508000	-2.915801000
6	-2.446392000	-4.495254000	-1.838959000
6	-2.770808000	-3.281534000	-2.693800000
1	0.714492000	-3.861982000	1.639159000
1	1.558340000	-4.540668000	0.239349000
1	-0.763244000	-5.642483000	1.154901000
1	-0.408730000	-5.642503000	-0.574377000
1	0.444127000	-3.971055000	-2.067634000
1	1.802318000	-2.825864000	-2.233546000
1	-0.166542000	-2.463953000	-3.930008000
1	0.316520000	-1.032236000	-2.994268000
1	-3.271141000	-5.218180000	-1.894925000
1	-1.534305000	-4.995903000	-2.182433000
1	-3.811206000	-2.957244000	-2.552450000
1	-2.636035000	-3.505244000	-3.762653000
6	-3.917435000	-0.302330000	0.914284000
6	-5.301971000	-0.475077000	0.730508000
6	-5.897217000	-0.109827000	-0.468180000
6	-5.112197000	0.448177000	-1.497489000
6	-3.746801000	0.616797000	-1.334100000
1	-3.507873000	-0.448929000	1.909231000
1	-5.906899000	-0.856128000	1.553738000
1	-5.587716000	0.766865000	-2.425582000
1	-3.147036000	1.065203000	-2.126180000
16	-0.630948000	1.597568000	0.028507000
1	0.129329000	-0.839674000	2.582469000
1	-0.939843000	-2.612952000	3.179381000
1	-1.916532000	-0.710703000	3.202978000
1	-6.973758000	-0.221165000	-0.602252000

2d.xyz

6	-1.249398000	0.769603000	4.162488000
6	-1.505937000	2.112664000	4.518694000
6	-0.083348000	-0.101597000	0.367033000
6	-0.747077000	0.376931000	-0.759835000
6	-1.435900000	-0.242978000	5.128724000
6	1.011174000	-1.147141000	0.139951000
44	2.277658000	0.348119000	-0.072745000
6	-0.490775000	0.188542000	1.694852000
6	-0.825094000	0.442392000	2.844030000
6	-1.867296000	0.084858000	6.412032000
6	-2.114077000	1.418201000	6.756852000
6	-1.931627000	2.429079000	5.807160000
1	-1.251705000	-1.280898000	4.852542000
1	-2.017666000	-0.706084000	7.147041000
1	-2.453047000	1.668546000	7.762528000
1	-2.127190000	3.468767000	6.070881000
1	-1.372800000	2.898939000	3.774488000
6	-1.948039000	1.172599000	-0.914241000
6	-2.713911000	1.704716000	0.151723000
6	-3.905650000	2.376610000	-0.102554000
6	-4.362675000	2.544695000	-1.415188000
6	-3.615460000	2.036615000	-2.484343000
6	-2.426089000	1.360601000	-2.236718000
1	-2.381330000	1.561381000	1.176409000
1	-4.493627000	2.761719000	0.731129000
1	-5.304045000	3.062479000	-1.603677000
1	-3.970988000	2.158068000	-3.507567000
1	-1.857079000	0.946539000	-3.071950000
1	-0.382870000	-0.030452000	-1.704767000
15	2.068530000	0.239166000	-2.396926000
16	2.554955000	0.276952000	2.284513000
16	3.398256000	2.575307000	-0.007424000
16	4.389187000	-0.521291000	-0.278380000
6	5.409357000	0.813790000	-1.107018000
6	5.144333000	2.243625000	-0.638612000
6	5.185059000	-0.412763000	1.424480000
6	4.157447000	-0.634393000	2.510695000
6	3.779585000	2.839312000	1.816929000
6	2.904008000	2.029941000	2.757826000
1	5.171141000	0.690011000	-2.170299000
1	6.463859000	0.535428000	-0.972847000
1	5.284332000	2.943429000	-1.471734000
1	5.829426000	2.548391000	0.160229000
1	5.662542000	0.570025000	1.507267000
1	5.964473000	-1.187345000	1.447078000
1	4.550133000	-0.373866000	3.503542000
1	3.828817000	-1.682999000	2.543121000
1	3.636661000	3.911526000	2.007788000
1	4.841435000	2.609981000	1.960374000
1	1.889215000	2.446371000	2.823174000
1	3.321635000	2.023071000	3.775758000
16	0.863167000	-2.764282000	0.213776000
1	1.321727000	-0.832978000	-2.970143000
1	3.238040000	0.061346000	-3.198133000
1	1.500388000	1.303436000	-3.162257000

2e.xyz

6	-0.170601000	0.792445000	-0.135892000
44	2.128879000	-0.218216000	0.138796000
6	1.150524000	1.498838000	-0.130969000
15	2.112620000	0.057375000	2.486093000
16	2.204795000	-0.417890000	-2.246558000
16	2.992054000	-2.596865000	0.211057000
16	4.345388000	0.395559000	0.071092000
6	5.258671000	-0.966966000	0.956785000
6	4.811729000	-2.392761000	0.625689000
6	4.968674000	0.002474000	-1.660539000
6	3.886745000	0.224649000	-2.692161000
6	3.113424000	-3.072157000	-1.600610000
6	2.237566000	-2.239502000	-2.523634000
1	5.109703000	-0.734208000	2.018190000
1	6.327037000	-0.825384000	0.738609000
1	4.991695000	-3.045342000	1.489479000
1	5.374095000	-2.811551000	-0.216567000
1	5.322961000	-1.034136000	-1.656983000
1	5.826755000	0.667978000	-1.829747000
1	4.161167000	-0.203735000	-3.666467000
1	3.692601000	1.296380000	-2.841922000
1	2.809256000	-4.125952000	-1.660977000
1	4.171458000	-3.011110000	-1.880545000
1	1.172842000	-2.484851000	-2.406314000
1	2.507644000	-2.414755000	-3.575964000
6	-0.797806000	0.463525000	1.028993000
1	-0.372496000	0.761578000	1.987589000
16	1.397260000	3.083000000	-0.407388000
1	3.322474000	-0.044280000	3.235453000
1	1.333237000	-0.814811000	3.301883000
1	1.677233000	1.295246000	3.042074000
6	-2.165987000	-0.115104000	1.081924000
8	-2.826241000	-0.460024000	0.115573000
6	-3.955463000	-0.650730000	2.536087000
8	-2.586514000	-0.180277000	2.373376000
1	-4.136287000	-0.644030000	3.613556000
6	-0.833917000	0.431373000	-1.459493000
8	-0.631272000	-0.633805000	-2.023908000
8	-1.580174000	1.438226000	-1.916122000
6	-2.306354000	1.152703000	-3.150834000
1	-2.803727000	2.089973000	-3.409395000
1	-3.035149000	0.356534000	-2.963096000
1	-1.607176000	0.845075000	-3.935939000
1	-4.059690000	-1.660508000	2.123619000
1	-4.645537000	0.026585000	2.019522000

3a.xyz

44	-1.312678000	-3.800104000	0.247761000
15	-2.948776000	-2.323693000	-0.495452000
6	0.003327000	-2.698288000	-0.813233000
16	0.466323000	-5.189828000	0.933805000
16	-2.201826000	-5.589788000	-0.932868000
16	-2.572107000	-4.607052000	2.136662000
6	-4.010826000	-5.476322000	1.332132000

6	-3.690302000	-6.259215000	0.065143000
6	-1.590037000	-6.095271000	2.718912000
6	-0.093892000	-5.885663000	2.566283000
6	-1.021950000	-7.052065000	-0.645641000
6	0.373242000	-6.620521000	-0.247038000
1	-4.704996000	-4.650110000	1.131345000
1	-4.476860000	-6.121271000	2.089693000
1	-4.534992000	-6.223094000	-0.634056000
1	-3.476647000	-7.313990000	0.272020000
1	-1.937562000	-6.963957000	2.147864000
1	-1.844083000	-6.251765000	3.776883000
1	0.459929000	-6.819577000	2.740597000
1	0.278938000	-5.140822000	3.284023000
1	-1.001461000	-7.610311000	-1.591580000
1	-1.477970000	-7.690954000	0.118518000
1	0.942591000	-6.244236000	-1.108173000
1	0.940976000	-7.455014000	0.190253000
6	0.627142000	-2.517119000	-2.079263000
6	1.718151000	-1.705104000	-2.261551000
1	2.110143000	-1.211504000	-1.365841000
16	0.179179000	-1.862147000	0.637024000
1	-4.121748000	-2.054122000	0.277410000
1	-3.611010000	-2.534117000	-1.742901000
1	-2.535706000	-0.973026000	-0.696344000
6	2.443565000	-1.439504000	-3.483025000
6	1.970599000	-1.811778000	-4.764100000
6	2.707326000	-1.506166000	-5.902128000
6	3.935712000	-0.837519000	-5.789874000
6	4.420944000	-0.464628000	-4.531827000
6	3.677289000	-0.752456000	-3.391416000
1	1.009850000	-2.318104000	-4.864597000
1	2.326668000	-1.779707000	-6.886573000
1	4.509214000	-0.601086000	-6.687058000
1	5.374324000	0.056501000	-4.444302000
1	4.046465000	-0.455642000	-2.408024000
1	0.227332000	-3.097321000	-2.914485000

3b.xyz

44	-1.293425000	-3.749706000	-0.083233000
15	-2.990636000	-2.299625000	-0.732175000
6	-0.120698000	-2.790118000	-1.441608000
16	0.547547000	-5.084605000	0.523213000
16	-2.356889000	-5.642404000	-0.890537000
16	-2.279239000	-4.276817000	2.039885000
6	-3.824905000	-5.213369000	1.578647000
6	-3.716289000	-6.127356000	0.362504000
6	-1.237489000	-5.700367000	2.678965000
6	0.223785000	-5.546417000	2.296935000
6	-1.171738000	-7.093967000	-0.567082000
6	0.272759000	-6.662293000	-0.421016000
1	-4.551463000	-4.408094000	1.412072000
1	-4.149053000	-5.770034000	2.468147000
1	-4.646088000	-6.105963000	-0.218886000
1	-3.523302000	-7.169770000	0.639580000
1	-1.664533000	-6.627625000	2.280378000
1	-1.345968000	-5.710338000	3.772505000
1	0.792365000	-6.462096000	2.513933000
1	0.695547000	-4.723099000	2.851734000
1	-1.289306000	-7.772807000	-1.422338000
1	-1.530377000	-7.608789000	0.330528000
1	0.726611000	-6.432619000	-1.394448000
1	0.878269000	-7.447415000	0.054645000
6	0.331619000	-2.698834000	-2.799494000
6	-0.247987000	-3.572272000	-3.698058000
1	-1.032176000	-4.204028000	-3.267663000
16	0.251806000	-1.822409000	-0.126920000
1	-4.020772000	-1.905730000	0.177884000
1	-3.848977000	-2.606012000	-1.833020000
1	-2.584474000	-0.994274000	-1.138973000
6	-0.019833000	-3.773901000	-5.115081000
6	1.131830000	-3.329046000	-5.809900000
6	1.270125000	-3.571458000	-7.172310000
6	0.263904000	-4.241789000	-7.879964000
6	-0.876437000	-4.699880000	-7.209931000
6	-1.007466000	-4.484691000	-5.841602000
1	1.921434000	-2.806461000	-5.272499000
1	2.167412000	-3.231888000	-7.690266000
1	0.373081000	-4.412532000	-8.951724000
1	-1.657691000	-5.227480000	-7.757193000
1	-1.892778000	-4.848365000	-5.316031000
6	1.312485000	-1.628640000	-3.168691000
6	2.639800000	-1.672046000	-2.713881000
6	3.541581000	-0.664153000	-3.067226000
6	3.124104000	0.405312000	-3.864402000
6	1.798667000	0.465485000	-4.305269000
6	0.898739000	-0.544878000	-3.961317000
1	2.972000000	-2.503970000	-2.090291000
1	4.572639000	-0.714337000	-2.716456000
1	3.827792000	1.192548000	-4.137427000
1	1.462747000	1.301058000	-4.920044000
1	-0.133131000	-0.498291000	-4.314452000

3c.xyz

44	2.558636000	-2.471659000	1.295995000
15	1.629149000	-4.431858000	2.143992000
6	0.695558000	-1.749735000	1.145419000
16	3.351416000	-0.401617000	0.489446000
16	3.245125000	-3.463241000	-0.674962000
16	4.791883000	-2.909420000	2.120714000
6	5.295656000	-4.408479000	1.136680000
6	4.851180000	-4.429796000	-0.321665000
6	5.831843000	-1.614223000	1.252468000
6	5.097400000	-0.292032000	1.115238000
6	3.986962000	-2.076538000	-1.742374000
6	3.512042000	-0.696178000	-1.337546000
1	4.848682000	-5.233213000	1.706161000
1	6.386662000	-4.506599000	1.217136000
1	4.636722000	-5.456688000	-0.642592000
1	5.614620000	-4.025335000	-0.995614000
1	6.114217000	-2.020625000	0.274689000
1	6.744886000	-1.481366000	1.849456000
1	5.645388000	0.402971000	0.462829000
1	4.973927000	0.198397000	2.091312000
1	3.685894000	-2.302335000	-2.774033000
1	5.076599000	-2.164613000	-1.676399000
1	2.489458000	-0.500963000	-1.688804000
1	4.163390000	0.088620000	-1.748326000
6	-0.423400000	-1.594357000	0.247268000
6	-0.458400000	-2.348199000	-0.949298000
6	-1.519279000	-2.213670000	-1.838940000
6	-2.550714000	-1.307953000	-1.560500000
6	-2.527394000	-0.547180000	-0.383008000
6	-1.481215000	-0.694449000	0.520639000
1	0.353581000	-3.048127000	-1.152173000
1	-1.547218000	-2.809930000	-2.751171000
1	-3.376764000	-1.193688000	-2.263439000
1	-3.330999000	0.159689000	-0.175208000
1	-1.453885000	-0.108184000	1.440448000
16	0.940698000	-1.194292000	2.702687000
1	0.444834000	-4.277763000	2.922868000
1	2.353973000	-5.261538000	3.053971000
1	1.182747000	-5.474971000	1.276860000

3d.xyz

6	0.792026000	-4.523979000	-4.562948000
6	1.790851000	-4.232190000	-3.639542000
6	5.019790000	-1.862278000	-4.313352000
6	6.011777000	-1.637597000	-3.334626000
44	0.410240000	-5.797374000	-1.043630000
15	-0.708339000	-3.784708000	-0.725844000
6	1.608344000	-4.761888000	-2.308925000
16	1.633679000	-7.766857000	-1.473013000
16	-1.433662000	-6.777363000	-2.045201000
16	-0.349099000	-6.801336000	1.000093000
6	-2.191936000	-6.924774000	0.748289000
6	-2.646571000	-7.291071000	-0.659594000
6	0.106056000	-8.610760000	0.804187000
6	1.423635000	-8.787224000	0.069566000
6	-0.892758000	-8.517137000	-2.585044000
6	0.607639000	-8.645720000	-2.748244000
1	-2.541501000	-5.925584000	1.037393000
1	-2.581008000	-7.636647000	1.488680000
1	-3.585088000	-6.780046000	-0.906620000
1	-2.814591000	-8.367466000	-0.776343000
1	-0.719461000	-9.103543000	0.278159000
1	0.174507000	-9.035138000	1.815561000
1	1.591566000	-9.839988000	-0.199415000
1	2.271162000	-8.464706000	0.690625000
1	-1.405918000	-8.709706000	-3.536710000
1	-1.278679000	-9.221415000	-1.840447000
1	0.955829000	-8.186097000	-3.682938000
1	0.919154000	-9.700294000	-2.758087000
6	2.933571000	-3.430405000	-3.893918000
1	-0.016676000	-5.135603000	-4.154741000
16	2.551031000	-4.556672000	-0.945881000
1	-1.366080000	-3.478093000	0.506292000
1	-1.781906000	-3.413278000	-1.591033000
1	0.071741000	-2.595326000	-0.830245000
6	0.632919000	-4.137890000	-5.941377000
6	1.577603000	-3.371770000	-6.668890000
6	1.337547000	-3.025584000	-7.993560000
6	0.157990000	-3.430024000	-8.630434000
6	-0.786541000	-4.194064000	-7.933142000
6	-0.552061000	-4.544589000	-6.609010000
1	2.494431000	-3.058523000	-6.176459000
1	2.073273000	-2.434223000	-8.539365000
1	-0.024275000	-3.150713000	-9.668849000
1	-1.704386000	-4.510905000	-8.428308000
1	-1.290802000	-5.135411000	-6.063773000
6	3.913978000	-2.716858000	-4.053741000
6	7.081346000	-0.786647000	-3.604412000
6	7.182003000	-0.148784000	-4.845449000
6	6.204991000	-0.366111000	-5.823109000
6	5.132115000	-1.213621000	-5.563597000
1	5.929933000	-2.136210000	-2.369047000
1	7.841533000	-0.617738000	-2.841508000
1	8.020027000	0.518111000	-5.051191000
1	6.279325000	0.130206000	-6.791057000
1	4.367739000	-1.378448000	-6.322446000

3e.xyz

44	-0.026853000	-0.051460000	-0.135216000
15	-2.292648000	-0.199248000	-0.709554000
6	-0.034743000	-2.029591000	-0.065003000
16	2.278411000	-0.031321000	0.380804000
16	-0.473772000	0.839214000	1.951214000
16	0.219726000	2.247231000	-0.894030000
6	-0.892788000	3.168084000	0.280082000
6	-0.889332000	2.683305000	1.726661000
6	1.886132000	2.747603000	-0.201335000
6	2.888565000	1.606887000	-0.247283000
6	1.210615000	1.037821000	2.806846000
6	2.278755000	0.131566000	2.231285000
1	-1.881201000	3.047693000	-0.181367000
1	-0.630762000	4.233014000	0.220260000
1	-1.886409000	2.799230000	2.169841000
1	-0.183599000	3.242268000	2.351517000
1	1.723246000	3.100445000	0.823214000
1	2.246041000	3.592370000	-0.805196000
1	3.802962000	1.858189000	0.309366000
1	3.183653000	1.376739000	-1.280814000
1	1.032933000	0.798806000	3.863856000
1	1.492565000	2.093807000	2.737056000
1	2.133209000	-0.909545000	2.550702000
1	3.284685000	0.447889000	2.542653000
6	-0.313250000	-3.125840000	0.841207000
6	-0.015589000	-4.417990000	0.558968000
1	0.434104000	-4.676767000	-0.401675000
16	0.436306000	-1.996102000	-1.667713000
1	-2.918804000	0.837121000	-1.467286000
1	-3.286199000	-0.340338000	0.302106000
1	-2.652337000	-1.301312000	-1.538485000
6	-0.291339000	-5.518128000	1.517743000
8	-0.843701000	-5.376600000	2.598325000
6	-0.087204000	-7.841351000	1.892231000
8	0.149028000	-6.699274000	1.019060000
1	0.293697000	-8.705901000	1.344286000
6	-1.026621000	-2.712710000	2.111811000
8	-2.220176000	-2.482770000	2.133699000
8	-0.170636000	-2.532858000	3.143310000
6	-0.826812000	-2.227076000	4.410531000
1	-0.014557000	-2.103204000	5.131277000
1	-1.473008000	-3.064077000	4.695254000
1	-1.422980000	-1.312132000	4.317928000
1	-1.159409000	-7.941494000	2.095239000
1	0.450539000	-7.705270000	2.837698000

3f.xyz

44	-1.204211000	-5.168796000	-0.922304000
15	-3.245061000	-4.029968000	-0.928135000
6	-0.310377000	-3.383329000	-0.690405000
16	0.909798000	-6.225149000	-0.912288000
16	-1.426523000	-5.747438000	-3.158563000
16	-2.181882000	-7.336922000	-0.423085000
6	-3.232178000	-7.655485000	-1.925989000

6	-2.634870000	-7.221760000	-3.261094000
6	-0.781605000	-8.532239000	-0.770463000
6	0.569028000	-7.966716000	-0.364629000
6	0.159728000	-6.670596000	-3.639820000
6	1.324173000	-6.372184000	-2.718031000
1	-4.153820000	-7.104570000	-1.698498000
1	-3.483405000	-8.724803000	-1.936271000
1	-3.426637000	-6.888952000	-3.943698000
1	-2.093903000	-8.036034000	-3.756191000
1	-0.812228000	-8.772362000	-1.839261000
1	-0.993107000	-9.449289000	-0.203059000
1	1.391226000	-8.599798000	-0.728375000
1	0.661335000	-7.899885000	0.728577000
1	0.388210000	-6.354973000	-4.666526000
1	-0.076707000	-7.739729000	-3.655052000
1	1.764484000	-5.389463000	-2.933793000
1	2.120157000	-7.123807000	-2.819452000
14	0.493887000	-1.878384000	-1.548599000
16	-0.457933000	-3.697376000	0.928674000
1	-4.437834000	-4.653364000	-0.447523000
1	-3.788730000	-3.527511000	-2.149133000
1	-3.316475000	-2.836443000	-0.151202000
6	2.250253000	-1.704230000	-0.900479000
8	-0.501197000	-0.628342000	-1.089929000
6	0.476387000	-2.152858000	-3.408919000
6	-0.263996000	0.734518000	-1.543702000
6	-0.594002000	1.713449000	-0.431479000
1	0.050206000	1.545931000	0.442441000
1	-1.641917000	1.607405000	-0.119066000
1	-0.440925000	2.744015000	-0.783883000
1	-0.896200000	0.916251000	-2.426908000
1	0.787464000	0.856230000	-1.855629000
1	2.767181000	-0.858759000	-1.380923000
1	2.844216000	-2.608509000	-1.103464000
1	2.249574000	-1.534964000	0.185884000
1	0.879078000	-1.276770000	-3.940028000
1	-0.542674000	-2.334491000	-3.779747000
1	1.102341000	-3.014026000	-3.690667000

3g.xyz

44	2.556694000	-2.473299000	1.289799000
15	1.619287000	-4.424118000	2.141073000
6	0.685567000	-1.746642000	1.132178000
16	3.348169000	-0.405193000	0.486286000
16	3.251274000	-3.466644000	-0.676577000
16	4.782431000	-2.906824000	2.124287000
6	5.298331000	-4.405868000	1.144029000
6	4.858179000	-4.434178000	-0.315207000
6	5.828389000	-1.610840000	1.262504000
6	5.092593000	-0.290241000	1.118896000
6	4.002573000	-2.080269000	-1.740857000
6	3.524426000	-0.699968000	-1.339873000
1	4.853436000	-5.230946000	1.714467000
1	6.389687000	-4.497365000	1.228686000
1	4.642368000	-5.462133000	-0.631535000
1	5.623780000	-4.033829000	-0.989157000

1	6.118265000	-2.017532000	0.286956000
1	6.736926000	-1.476523000	1.866032000
1	5.641940000	0.404299000	0.467159000
1	4.963800000	0.201610000	2.093577000
1	3.710321000	-2.306374000	-2.775056000
1	5.091743000	-2.167867000	-1.666122000
1	2.504329000	-0.505684000	-1.698753000
1	4.178596000	0.085028000	-1.746117000
6	-0.420402000	-1.594641000	0.246995000
6	-0.463965000	-2.329627000	-0.967743000
6	-1.516065000	-2.204744000	-1.850860000
6	-2.578317000	-1.305830000	-1.572369000
6	-2.544216000	-0.558180000	-0.364582000
6	-1.501304000	-0.712090000	0.522408000
1	0.350046000	-3.022308000	-1.186202000
1	-1.539643000	-2.796016000	-2.768113000
1	-3.353830000	0.140446000	-0.144787000
1	-1.485369000	-0.134466000	1.447718000
16	0.951309000	-1.188738000	2.694891000
1	0.432093000	-4.265480000	2.915143000
1	2.337671000	-5.256896000	3.054931000
1	1.172280000	-5.470801000	1.276900000
7	-3.610862000	-1.159682000	-2.446863000
1	-4.373830000	-0.524093000	-2.253504000
1	-3.653182000	-1.698153000	-3.302157000

3h.xyz

44	2.775680000	-2.655212000	1.242680000
15	1.843992000	-4.613998000	2.091017000
6	0.908650000	-1.930690000	1.084703000
16	3.576794000	-0.587749000	0.438910000
16	3.482558000	-3.652896000	-0.719414000
16	4.999708000	-3.089433000	2.089858000
6	5.518624000	-4.590125000	1.116135000
6	5.085475000	-4.620569000	-0.345374000
6	6.050268000	-1.795795000	1.232017000
6	5.316429000	-0.474697000	1.083963000
6	4.242498000	-2.269218000	-1.779539000
6	3.762690000	-0.887699000	-1.385151000
1	5.072086000	-5.414725000	1.686028000
1	6.609562000	-4.681210000	1.205851000
1	4.871951000	-5.649119000	-0.661260000
1	5.854832000	-4.221410000	-1.015692000
1	6.345010000	-2.203736000	0.258541000
1	6.955693000	-1.661722000	1.840234000
1	5.870766000	0.219656000	0.436254000
1	5.181317000	0.017165000	2.057781000
1	3.958150000	-2.497276000	-2.815469000
1	5.330887000	-2.357716000	-1.695967000
1	2.745324000	-0.693122000	-1.751454000
1	4.420075000	-0.104562000	-1.789655000
6	-0.208431000	-1.774632000	0.199483000
6	-0.255526000	-2.510702000	-1.011873000
6	-1.313667000	-2.380126000	-1.892746000
6	-2.353491000	-1.480338000	-1.593708000
6	-2.329297000	-0.732534000	-0.399089000
6	-1.277814000	-0.888902000	0.486924000
1	0.556364000	-3.204397000	-1.233470000
1	-1.365718000	-2.955788000	-2.816170000
1	-3.139028000	-0.033409000	-0.177765000
1	-1.254288000	-0.312719000	1.412669000
16	1.162230000	-1.373442000	2.645518000
1	0.657289000	-4.460375000	2.866699000
1	2.568208000	-5.443176000	3.002729000
1	1.400834000	-5.658797000	1.223428000
8	-3.357660000	-1.375270000	-2.503115000
1	-4.014478000	-0.726116000	-2.187704000

3i.xyz

44	2.559322000	-2.471924000	1.294375000
15	1.626118000	-4.429714000	2.143416000
6	0.696443000	-1.746939000	1.142503000
16	3.353289000	-0.402583000	0.488992000
16	3.247614000	-3.464344000	-0.675652000
16	4.790565000	-2.909677000	2.122389000
6	5.296536000	-4.408822000	1.139334000
6	4.853241000	-4.432240000	-0.319197000
6	5.832961000	-1.613753000	1.257625000
6	5.098136000	-0.292032000	1.118649000
6	3.994899000	-2.078163000	-1.741105000
6	3.519614000	-0.697644000	-1.337772000
1	4.849195000	-5.232953000	1.709349000
1	6.387515000	-4.506400000	1.221076000
1	4.637838000	-5.459505000	-0.638230000
1	5.617839000	-4.029987000	-0.993151000
1	6.118766000	-2.019764000	0.280678000
1	6.743861000	-1.480692000	1.857834000
1	5.647153000	0.403413000	0.467601000
1	4.971782000	0.198133000	2.094518000
1	3.697401000	-2.303676000	-2.773886000
1	5.084263000	-2.167042000	-1.671281000
1	2.498048000	-0.502284000	-1.691855000
1	4.172518000	0.086779000	-1.746949000
6	-0.418612000	-1.589755000	0.246422000
6	-0.458696000	-2.335264000	-0.955673000
6	-1.524115000	-2.205361000	-1.835400000
6	-2.578611000	-1.310571000	-1.568343000
6	-2.532890000	-0.559717000	-0.376982000
6	-1.484156000	-0.699721000	0.520861000
1	0.353006000	-3.032585000	-1.167596000
1	-1.549022000	-2.805942000	-2.746673000
1	-3.341024000	0.139993000	-0.156010000
1	-1.463662000	-0.116137000	1.442304000
16	0.945118000	-1.192921000	2.701914000
1	0.440398000	-4.272548000	2.919771000
1	2.348241000	-5.260859000	3.055017000
1	1.179506000	-5.473057000	1.276028000
6	-3.715464000	-1.150580000	-2.541744000
1	-3.424172000	-0.479358000	-3.366280000
1	-3.994148000	-2.113219000	-2.992161000
1	-4.601412000	-0.717657000	-2.060657000

3j.xyz

44	2.570301000	-2.472130000	1.291089000
15	1.627732000	-4.432497000	2.144024000
6	0.699624000	-1.746449000	1.148465000
16	3.359734000	-0.405448000	0.489238000
16	3.252640000	-3.465116000	-0.666183000
16	4.797463000	-2.909993000	2.128564000
6	5.301817000	-4.411627000	1.147968000
6	4.857597000	-4.437730000	-0.310131000
6	5.839073000	-1.613703000	1.263453000
6	5.103317000	-0.293363000	1.122984000
6	4.007232000	-2.083493000	-1.736246000
6	3.532637000	-0.701153000	-1.337814000
1	4.854241000	-5.233980000	1.720316000
1	6.392697000	-4.509645000	1.229273000
1	4.639094000	-5.464988000	-0.626943000
1	5.621906000	-4.038112000	-0.985823000
1	6.127537000	-2.020506000	0.287628000
1	6.748882000	-1.478767000	1.864977000
1	5.653353000	0.403127000	0.473769000
1	4.973638000	0.197004000	2.098374000
1	3.713158000	-2.312747000	-2.769147000
1	5.095970000	-2.173894000	-1.661402000
1	2.513560000	-0.503346000	-1.697388000
1	4.189396000	0.081254000	-1.744245000
6	-0.417633000	-1.592022000	0.257674000
6	-0.449115000	-2.330973000	-0.949311000
6	-1.507870000	-2.204295000	-1.838481000
6	-2.531371000	-1.311859000	-1.518353000
6	-2.542249000	-0.557555000	-0.343219000
6	-1.488488000	-0.709036000	0.546437000
1	0.369622000	-3.018740000	-1.164485000
1	-1.560278000	-2.773949000	-2.765367000
9	-3.557917000	-1.169971000	-2.387441000
1	-3.368529000	0.125981000	-0.150948000
1	-1.467342000	-0.134617000	1.473278000
16	0.952917000	-1.191110000	2.707709000
1	0.443954000	-4.270465000	2.918638000
1	2.350638000	-5.260281000	3.054728000
1	1.180837000	-5.473780000	1.275727000

3k.xyz

44	2.783413000	-2.653896000	1.251200000
15	1.854994000	-4.617209000	2.101857000
6	0.922242000	-1.933661000	1.098466000
16	3.585061000	-0.585483000	0.442867000
16	3.484927000	-3.652243000	-0.713462000
16	5.012475000	-3.089930000	2.091350000
6	5.523253000	-4.591787000	1.116713000
6	5.085415000	-4.621415000	-0.343541000
6	6.059113000	-1.795624000	1.230583000
6	5.325005000	-0.474265000	1.085234000
6	4.240704000	-2.269672000	-1.776363000
6	3.763173000	-0.887545000	-1.381631000
1	5.076402000	-5.415017000	1.688415000
1	6.614127000	-4.686685000	1.202832000
1	4.869523000	-5.649790000	-0.658681000
1	5.853210000	-4.223890000	-1.016587000
1	6.351999000	-2.203424000	0.256544000
1	6.965682000	-1.661450000	1.837046000
1	5.878131000	0.220275000	0.436735000
1	5.192073000	0.017582000	2.059340000
1	3.951074000	-2.498795000	-2.810600000
1	5.329329000	-2.359296000	-1.697526000
1	2.745099000	-0.691657000	-1.745245000
1	4.420063000	-0.105343000	-1.788500000
6	-0.203623000	-1.781688000	0.201899000
6	-0.230214000	-2.534437000	-0.998034000
6	-1.285249000	-2.406858000	-1.887662000
6	-2.329498000	-1.508568000	-1.607872000
6	-2.313335000	-0.753536000	-0.421673000
6	-1.267213000	-0.892157000	0.481536000
1	0.589703000	-3.225015000	-1.200178000
1	-1.332276000	-2.984195000	-2.811349000
1	-3.128562000	-0.057208000	-0.214484000
1	-1.246535000	-0.309929000	1.403506000
16	1.160758000	-1.374800000	2.654548000
1	0.668616000	-4.462843000	2.877523000
1	2.581768000	-5.441656000	3.014887000
1	1.413440000	-5.661174000	1.233460000
6	-3.453257000	-1.356661000	-2.575463000
1	-4.241247000	-0.623792000	-2.278182000
8	-3.529299000	-1.974559000	-3.624607000

3m.xyz

44	2.779939000	-2.654425000	1.250403000
15	1.851912000	-4.618526000	2.098308000
6	0.918463000	-1.934461000	1.094572000
16	3.580765000	-0.585076000	0.443347000
16	3.478422000	-3.649534000	-0.716265000
16	5.010248000	-3.092216000	2.086396000
6	5.518618000	-4.592594000	1.108320000
6	5.079754000	-4.618299000	-0.351671000
6	6.055171000	-1.798075000	1.223496000
6	5.322601000	-0.475676000	1.081449000
6	4.228537000	-2.265132000	-1.780784000
6	3.752470000	-0.883764000	-1.381799000
1	5.072763000	-5.417341000	1.678541000
1	6.609616000	-4.687116000	1.193222000
1	4.864492000	-5.645798000	-0.669948000
1	5.846378000	-4.217706000	-1.024184000
1	6.344188000	-2.205716000	0.248261000
1	6.963853000	-1.665899000	1.827222000
1	5.874576000	0.218526000	0.431673000
1	5.192651000	0.015850000	2.056101000
1	3.934282000	-2.493044000	-2.813978000
1	5.317527000	-2.354381000	-1.707351000
1	2.733329000	-0.686373000	-1.741690000
1	4.407685000	-0.100736000	-1.789728000
6	-0.209317000	-1.778351000	0.196929000
6	-0.242478000	-2.532041000	-0.998121000
6	-1.298797000	-2.402526000	-1.890709000
6	-2.317307000	-1.496727000	-1.589841000
6	-2.318244000	-0.732582000	-0.419819000
6	-1.267174000	-0.882176000	0.475601000
1	0.570053000	-3.229080000	-1.205287000
1	-1.354806000	-2.978156000	-2.812036000
1	-3.138512000	-0.041366000	-0.237039000
1	-1.243836000	-0.297193000	1.395676000
16	1.152342000	-1.376559000	2.649694000
1	0.667140000	-4.464042000	2.876572000
1	2.580411000	-5.443362000	3.009356000
1	1.407699000	-5.661176000	1.229890000
7	-3.439138000	-1.339644000	-2.551839000
8	-4.324631000	-0.527339000	-2.259776000
8	-3.404014000	-2.032610000	-3.577086000

1TSa.xyz

44	0.146591000	-0.255665000	0.127119000
6	2.020292000	-0.155280000	0.387738000
6	1.390067000	1.515245000	-0.141624000
6	1.906024000	1.961409000	-1.327231000
1	1.432138000	2.200023000	0.712831000
15	0.027011000	0.214351000	2.402073000
16	0.272189000	-0.711164000	-2.187052000
16	-2.196703000	0.452065000	-0.268825000
16	-0.797249000	-2.410450000	0.410094000
6	-2.524453000	-2.099379000	1.031045000
6	-3.281076000	-0.965652000	0.339000000
6	-1.235119000	-2.981125000	-1.326077000
6	-0.230172000	-2.492311000	-2.349772000
6	-2.432612000	0.262213000	-2.121888000
6	-1.127916000	0.272435000	-2.897959000
1	-2.371176000	-1.888886000	2.097652000
1	-3.082828000	-3.043341000	0.961103000
1	-3.997348000	-0.511784000	1.035180000
1	-3.851322000	-1.322371000	-0.526196000
1	-2.245010000	-2.619873000	-1.548725000
1	-1.256176000	-4.079326000	-1.299735000
1	-0.593120000	-2.643983000	-3.376099000
1	0.728871000	-3.020034000	-2.253297000
1	-3.060815000	1.104760000	-2.440884000
1	-2.995960000	-0.662656000	-2.288726000
1	-0.694927000	1.282357000	-2.931601000
1	-1.283710000	-0.061696000	-3.934348000
1	1.975308000	1.251634000	-2.159042000
16	3.518356000	-0.377518000	0.878023000
1	0.383359000	-0.791630000	3.347362000
1	-1.191022000	0.638309000	3.015452000
1	0.868287000	1.255573000	2.893040000
6	2.465180000	3.269538000	-1.631079000
6	2.453404000	4.357935000	-0.729006000
6	3.028257000	5.574777000	-1.080858000
6	3.623962000	5.740015000	-2.339158000
6	3.636258000	4.678317000	-3.248823000
6	3.061398000	3.459382000	-2.898851000
1	1.988244000	4.249417000	0.251947000
1	3.015050000	6.405087000	-0.374144000
1	4.076046000	6.695349000	-2.607650000
1	4.098690000	4.800783000	-4.228495000
1	3.078491000	2.627123000	-3.605899000

1TSb.xyz

44	0.028877000	-0.117370000	0.158395000
6	1.893874000	-0.445790000	0.060752000
6	1.661743000	1.365917000	0.211112000
6	2.285938000	1.761012000	1.372035000

6	1.666548000	2.200071000	-1.019812000
15	0.011464000	-0.130612000	2.484233000
16	0.017175000	-0.325511000	-2.225200000
16	-2.063365000	1.228321000	-0.107695000
16	-1.477393000	-1.960537000	0.203031000
6	-3.065177000	-1.275568000	0.901006000
6	-3.484326000	0.104055000	0.390792000
6	-2.037095000	-2.202217000	-1.565727000
6	-0.909111000	-1.906626000	-2.532052000
6	-2.354507000	1.287484000	-1.971054000
6	-1.122980000	1.004340000	-2.814213000
1	-2.879498000	-1.258565000	1.981931000
1	-3.850346000	-2.022254000	0.718945000
1	-4.023679000	0.645405000	1.178450000
1	-4.155772000	0.037328000	-0.472519000
1	-2.897678000	-1.546041000	-1.736045000
1	-2.368866000	-3.246086000	-1.654117000
1	-1.269765000	-1.876703000	-3.570028000
1	-0.121024000	-2.670380000	-2.474364000
1	-2.715855000	2.302705000	-2.183400000
1	-3.168920000	0.586990000	-2.187529000
1	-0.454990000	1.877343000	-2.848539000
1	-1.405490000	0.759612000	-3.849255000
1	2.197368000	1.085293000	2.229147000
16	3.328505000	-1.070924000	-0.261556000
1	-0.982772000	-0.900861000	3.162380000
1	-0.148909000	1.071155000	3.237291000
1	1.134635000	-0.655338000	3.184292000
6	3.172409000	2.878361000	1.673835000
6	3.749252000	3.743423000	0.713007000
6	4.617313000	4.757848000	1.103445000
6	4.926375000	4.950618000	2.455041000
6	4.374063000	4.102321000	3.422042000
6	3.519670000	3.073927000	3.034304000
1	3.533745000	3.607453000	-0.345328000
1	5.061297000	5.403394000	0.344115000
1	5.603599000	5.751882000	2.752000000
1	4.620182000	4.237874000	4.475278000
1	3.106530000	2.403431000	3.791634000
6	0.887751000	3.373622000	-1.001356000
6	0.811361000	4.200716000	-2.119812000
6	1.503160000	3.863589000	-3.290956000
6	2.280519000	2.701952000	-3.320152000
6	2.369012000	1.876410000	-2.194058000
1	0.353108000	3.630598000	-0.085209000
1	0.214555000	5.111575000	-2.074227000
1	1.442060000	4.506615000	-4.168563000
1	2.831813000	2.436869000	-4.222854000
1	2.999132000	0.986934000	-2.222753000

1TSc.xyz

6	-1.528405000	0.319483000	0.004234000
6	-3.277351000	-0.329095000	-0.076945000
44	-1.400804000	-1.571856000	-0.058923000
15	-0.913869000	-1.300094000	2.210981000
16	-1.465088000	-1.650097000	-2.426080000
16	-2.415227000	-3.815180000	-0.065125000

16	0.641405000	-2.738640000	-0.184702000
6	0.324695000	-4.397711000	0.624540000
6	-1.056542000	-5.022546000	0.397947000
6	0.786012000	-3.322247000	-1.959711000
6	0.200526000	-2.304119000	-2.913050000
6	-2.601080000	-4.239815000	-1.892692000
6	-2.647019000	-3.028149000	-2.807396000
1	0.492496000	-4.186612000	1.688000000
1	1.129405000	-5.068500000	0.294984000
1	-1.409717000	-5.495680000	1.322694000
1	-1.041285000	-5.797382000	-0.376439000
1	0.278205000	-4.289942000	-2.034933000
1	1.857777000	-3.472322000	-2.150700000
1	0.114859000	-2.706467000	-3.932357000
1	0.817988000	-1.396316000	-2.960494000
1	-3.541903000	-4.799686000	-1.977767000
1	-1.778635000	-4.914197000	-2.154339000
1	-3.616932000	-2.515697000	-2.740040000
1	-2.491196000	-3.320348000	-3.856180000
6	-4.073936000	-0.414632000	1.085683000
6	-5.458484000	-0.249403000	1.022309000
6	-6.079091000	0.033659000	-0.197987000
6	-5.300895000	0.171228000	-1.353306000
6	-3.918053000	-0.003711000	-1.293178000
1	-3.624515000	-0.621166000	2.055000000
1	-6.054059000	-0.342289000	1.931303000
1	-5.773463000	0.424309000	-2.303391000
1	-3.326172000	0.153288000	-2.196517000
16	-1.243170000	1.878197000	0.173535000
1	0.214930000	-0.473920000	2.472838000
1	-0.550305000	-2.395370000	3.052543000
1	-1.816899000	-0.669009000	3.114918000
1	-7.161072000	0.162787000	-0.245545000

1TSd.xyz

6	-1.136002000	0.973940000	4.089448000
6	-1.431253000	2.278143000	4.544902000
6	0.125375000	0.331332000	0.281474000
6	-0.693942000	0.629211000	-0.795602000
6	-1.394067000	-0.122202000	4.941769000
6	1.087296000	-1.229753000	0.042506000
44	2.343226000	0.190269000	-0.042166000
6	-0.278523000	0.565876000	1.616837000
6	-0.632484000	0.764464000	2.773424000
6	-1.937235000	0.086319000	6.207575000
6	-2.228326000	1.381802000	6.648614000
6	-1.972003000	2.474594000	5.814285000
1	-1.180774000	-1.131233000	4.589452000
1	-2.143718000	-0.769047000	6.851265000
1	-2.659853000	1.538943000	7.637489000
1	-2.202095000	3.485559000	6.151442000
1	-1.245499000	3.128412000	3.887645000
6	-2.020481000	1.207544000	-0.886694000
6	-2.816450000	1.618095000	0.211892000
6	-4.083469000	2.155079000	0.005320000
6	-4.593253000	2.303851000	-1.289773000
6	-3.825129000	1.904591000	-2.389857000
6	-2.560561000	1.363440000	-2.190217000
1	-2.440082000	1.500475000	1.224685000
1	-4.684058000	2.457049000	0.863970000
1	-5.587663000	2.725609000	-1.440848000
1	-4.218359000	2.012596000	-3.400784000
1	-1.967281000	1.048038000	-3.051478000
1	-0.312217000	0.337963000	-1.777439000
15	2.134009000	0.200599000	-2.365816000
16	2.643789000	0.095237000	2.313367000
16	3.278369000	2.493872000	0.053458000
16	4.588271000	-0.470973000	-0.266928000
6	5.448290000	0.969008000	-1.085124000
6	5.043574000	2.357859000	-0.589811000
6	5.342970000	-0.297101000	1.443316000
6	4.337185000	-0.638145000	2.523103000
6	3.633028000	2.764323000	1.880098000
6	2.816489000	1.873607000	2.798362000
1	5.201816000	0.836552000	-2.146009000
1	6.530227000	0.809165000	-0.980605000
1	5.108395000	3.082382000	-1.411342000
1	5.699957000	2.716502000	0.210856000
1	5.711237000	0.730093000	1.541004000
1	6.202728000	-0.980853000	1.477747000
1	4.701826000	-0.348957000	3.519107000
1	4.126814000	-1.716659000	2.546364000
1	3.399583000	3.818487000	2.082714000
1	4.709654000	2.622638000	2.026272000
1	1.763692000	2.187218000	2.835940000
1	3.209909000	1.901798000	3.825219000
16	0.394254000	-2.662313000	0.101364000
1	1.294154000	-0.776189000	-2.974804000
1	3.284520000	-0.035876000	-3.178948000
1	1.649521000	1.342778000	-3.073736000

1TSe.xyz

6	-0.058932000	0.391933000	-0.037972000
44	2.222766000	-0.037614000	0.084923000
6	1.255422000	1.589625000	-0.025124000
15	2.213909000	0.128706000	2.421156000
16	2.255166000	-0.276588000	-2.278937000
16	2.797781000	-2.467877000	0.186779000
16	4.520278000	0.292436000	0.006013000
6	5.254657000	-1.156123000	0.921258000
6	4.638598000	-2.512854000	0.589786000
6	5.054831000	-0.203835000	-1.728672000
6	3.998941000	0.149459000	-2.754560000
6	2.845175000	-3.015298000	-1.610981000
6	2.083521000	-2.096965000	-2.548052000
1	5.101930000	-0.890805000	1.974861000
1	6.337937000	-1.153050000	0.737037000
1	4.735591000	-3.187298000	1.449633000
1	5.139442000	-2.993031000	-0.258213000
1	5.260449000	-1.279872000	-1.715281000
1	5.994485000	0.330653000	-1.926529000
1	4.201611000	-0.335039000	-3.720571000
1	3.951220000	1.233559000	-2.928228000
1	2.389738000	-4.014787000	-1.632220000
1	3.899831000	-3.116854000	-1.891396000
1	0.997298000	-2.205418000	-2.426491000
1	2.337980000	-2.301209000	-3.598794000
6	-0.790580000	0.228014000	1.094560000
1	-0.372057000	0.415704000	2.084119000
16	0.885848000	3.138770000	-0.133552000
1	3.439011000	0.211431000	3.149497000
1	1.605934000	-0.901136000	3.199900000
1	1.574274000	1.246525000	3.029334000
6	-2.236737000	-0.115368000	1.078317000
8	-2.900881000	-0.329951000	0.076824000
6	-4.157450000	-0.394999000	2.424570000
8	-2.724926000	-0.144595000	2.348098000
1	-4.389975000	-0.421151000	3.491566000
6	-0.718134000	0.118638000	-1.369743000
8	-0.659976000	-0.978219000	-1.912765000
8	-1.294237000	1.207769000	-1.895772000
6	-2.040935000	0.956085000	-3.124168000
1	-2.412128000	1.933993000	-3.437244000
1	-2.867033000	0.271435000	-2.904276000
1	-1.385840000	0.519110000	-3.885017000
1	-4.402929000	-1.347239000	1.941140000
1	-4.701244000	0.415555000	1.924586000

1TSg.xyz

6	-1.500004000	0.306001000	0.019119000
6	-3.287084000	-0.411033000	-0.041282000
44	-1.410343000	-1.584177000	-0.051800000
15	-0.977205000	-1.341299000	2.227929000
16	-1.538309000	-1.705004000	-2.407588000
16	-2.330538000	-3.871934000	0.002158000
16	0.690828000	-2.673892000	-0.214549000
6	0.444640000	-4.315495000	0.642164000

6	-0.890758000	-5.018611000	0.386837000
6	0.781612000	-3.303185000	-1.977684000
6	0.122578000	-2.337835000	-2.939779000
6	-2.608087000	-4.308854000	-1.808354000
6	-2.718313000	-3.100281000	-2.721815000
1	0.563779000	-4.061265000	1.703358000
1	1.290275000	-4.959632000	0.364569000
1	-1.196989000	-5.576078000	1.280958000
1	-0.827655000	-5.738213000	-0.437060000
1	0.303931000	-4.288755000	-2.003237000
1	1.847758000	-3.424700000	-2.214255000
1	0.006621000	-2.779483000	-3.939676000
1	0.710387000	-1.415510000	-3.046930000
1	-3.544131000	-4.882057000	-1.841972000
1	-1.791518000	-4.973296000	-2.111749000
1	-3.688708000	-2.598267000	-2.600243000
1	-2.618254000	-3.393800000	-3.777074000
6	-4.099678000	-0.462786000	1.117476000
6	-5.466585000	-0.228596000	1.069145000
6	-6.100061000	0.102654000	-0.149114000
6	-5.294598000	0.222916000	-1.303866000
6	-3.930514000	-0.023955000	-1.241759000
1	-3.672017000	-0.710396000	2.087919000
1	-6.061911000	-0.306908000	1.981416000
1	-5.750202000	0.520937000	-2.250804000
1	-3.343716000	0.124648000	-2.149828000
16	-1.216003000	1.861021000	0.196274000
1	0.305932000	-0.809911000	2.547326000
1	-0.961833000	-2.439197000	3.144183000
1	-1.748789000	-0.444839000	3.021744000
7	-7.468851000	0.262292000	-0.216640000
1	-7.843072000	0.767058000	-1.014215000
1	-7.962488000	0.444165000	0.651403000

1TSh.xyz

6	-1.520581000	0.314849000	-0.000591000
6	-3.312644000	-0.326127000	-0.041994000
44	-1.465688000	-1.579312000	-0.041710000
15	-1.035524000	-1.361567000	2.241520000
16	-1.613155000	-1.667854000	-2.398326000
16	-2.395424000	-3.857530000	-0.002167000
16	0.618551000	-2.653108000	-0.219400000
6	0.387098000	-4.313865000	0.611083000
6	-0.953861000	-5.009510000	0.368111000
6	0.721109000	-3.251990000	-1.995074000
6	0.051553000	-2.279750000	-2.942163000
6	-2.675743000	-4.275762000	-1.816510000
6	-2.798567000	-3.057005000	-2.713630000
1	0.526728000	-4.079225000	1.674237000
1	1.227218000	-4.951762000	0.304727000
1	-1.257163000	-5.564586000	1.264544000
1	-0.903810000	-5.728500000	-0.457025000
1	0.259015000	-4.244337000	-2.038053000
1	1.790134000	-3.352117000	-2.228991000
1	-0.058698000	-2.705097000	-3.949618000
1	0.628211000	-1.348419000	-3.033480000
1	-3.607239000	-4.856228000	-1.853764000
1	-1.854598000	-4.929296000	-2.130992000
1	-3.765598000	-2.553849000	-2.569601000
1	-2.718914000	-3.337353000	-3.774144000
6	-4.111836000	-0.367209000	1.124737000
6	-5.473782000	-0.087735000	1.093244000
6	-6.087144000	0.274596000	-0.115829000
6	-5.314557000	0.369509000	-1.284677000
6	-3.957311000	0.075384000	-1.238160000
1	-3.682679000	-0.638932000	2.087305000
1	-6.066664000	-0.149458000	2.009662000
1	-5.791624000	0.688512000	-2.210945000
1	-3.377959000	0.200421000	-2.153619000
16	-1.175123000	1.862890000	0.128521000
1	0.222089000	-0.782908000	2.578343000
1	-0.972613000	-2.483200000	3.125273000
1	-1.844526000	-0.526245000	3.065233000
8	-7.418703000	0.557295000	-0.219110000
1	-7.833893000	0.468996000	0.659524000

1TSi.xyz

6	-1.544608000	0.339941000	0.004501000
6	-3.242929000	-0.317545000	-0.059972000
44	-1.379129000	-1.551567000	-0.067709000
15	-0.869393000	-1.279676000	2.201511000
16	-1.419978000	-1.633735000	-2.431143000
16	-2.449838000	-3.777082000	-0.083934000
16	0.632233000	-2.794603000	-0.165750000
6	0.257071000	-4.447653000	0.632891000
6	-1.146487000	-5.025130000	0.415612000
6	0.790691000	-3.358538000	-1.945219000
6	0.240779000	-2.316587000	-2.895235000
6	-2.603704000	-4.208219000	-1.912550000
6	-2.612861000	-2.999574000	-2.832726000
1	0.439644000	-4.247903000	1.696056000
1	1.038558000	-5.140856000	0.294130000
1	-1.522787000	-5.459056000	1.350475000
1	-1.158493000	-5.820213000	-0.337938000
1	0.266877000	-4.315768000	-2.040996000
1	1.862220000	-3.526089000	-2.122689000
1	0.166082000	-2.705774000	-3.920613000
1	0.876982000	-1.421151000	-2.920079000
1	-3.550467000	-4.755049000	-2.015539000
1	-1.785798000	-4.895387000	-2.154094000
1	-3.577925000	-2.475759000	-2.789820000
1	-2.436547000	-3.298706000	-3.876301000
6	-4.029582000	-0.419581000	1.105871000
6	-5.421447000	-0.318808000	1.047893000
6	-6.084879000	-0.079467000	-0.163396000
6	-5.299721000	0.090291000	-1.319218000
6	-3.911183000	-0.021579000	-1.270712000
1	-3.569967000	-0.593726000	2.075267000
1	-6.000624000	-0.433450000	1.965799000
1	-5.783665000	0.318735000	-2.270948000
1	-3.335862000	0.158192000	-2.179838000
16	-1.252324000	1.901279000	0.153326000
1	0.221242000	-0.401956000	2.459878000
1	-0.434715000	-2.370404000	3.015086000
1	-1.784397000	-0.714278000	3.138058000
6	-7.588609000	0.017765000	-0.224530000
1	-7.995466000	-0.626818000	-1.016477000
1	-7.906974000	1.045795000	-0.452095000
1	-8.048504000	-0.273851000	0.726878000

1TSj.xyz

6	-1.551326000	0.337750000	-0.000970000
6	-3.256143000	-0.307936000	-0.074387000
44	-1.396144000	-1.556144000	-0.060984000
15	-0.881536000	-1.275104000	2.204299000
16	-1.432103000	-1.633630000	-2.427046000
16	-2.455965000	-3.783089000	-0.085727000
16	0.621485000	-2.779658000	-0.170363000
6	0.258072000	-4.434511000	0.629265000
6	-1.142643000	-5.020412000	0.413494000
6	0.784763000	-3.345206000	-1.947256000
6	0.232458000	-2.304412000	-2.895929000
6	-2.604040000	-4.212494000	-1.916592000
6	-2.615135000	-3.004184000	-2.836747000
1	0.440182000	-4.233905000	1.692314000
1	1.042968000	-5.123445000	0.289776000
1	-1.515014000	-5.455220000	1.349453000
1	-1.150642000	-5.816900000	-0.338699000
1	0.264591000	-4.304381000	-2.042985000
1	1.857557000	-3.508797000	-2.120725000
1	0.157806000	-2.691675000	-3.921923000
1	0.864906000	-1.406240000	-2.919464000
1	-3.548333000	-4.762934000	-2.022486000
1	-1.782843000	-4.896240000	-2.156704000
1	-3.583638000	-2.486342000	-2.801602000
1	-2.430095000	-3.301207000	-3.879411000
6	-4.038326000	-0.409824000	1.099389000
6	-5.427852000	-0.319586000	1.061735000
6	-6.042436000	-0.086248000	-0.165106000
6	-5.314604000	0.089644000	-1.341724000
6	-3.926608000	-0.018649000	-1.286625000
1	-3.568485000	-0.575979000	2.066035000
1	-6.033567000	-0.428427000	1.960804000
1	-5.839616000	0.312849000	-2.270284000
1	-3.353516000	0.158416000	-2.198217000
16	-1.254155000	1.898589000	0.154117000
1	0.199046000	-0.382469000	2.450561000
1	-0.428294000	-2.357443000	3.018656000
1	-1.796024000	-0.716833000	3.145600000
9	-7.396506000	-0.011572000	-0.215432000

1Tsk.xyz

6	-1.551102000	0.316869000	0.012520000
6	-3.263354000	-0.248135000	-0.063437000
44	-1.427619000	-1.577924000	-0.056011000
15	-0.931596000	-1.330669000	2.220249000
16	-1.511789000	-1.658888000	-2.421801000
16	-2.406793000	-3.843146000	-0.059561000
16	0.627255000	-2.702212000	-0.192364000
6	0.349194000	-4.368459000	0.616958000
6	-1.016404000	-5.023303000	0.386005000
6	0.774995000	-3.284677000	-1.968510000
6	0.162678000	-2.280667000	-2.919337000
6	-2.605834000	-4.265735000	-1.885397000
6	-2.676487000	-3.052792000	-2.796934000
1	0.511166000	-4.154686000	1.680818000
1	1.169891000	-5.019496000	0.287212000
1	-1.355091000	-5.517597000	1.305081000
1	-0.984293000	-5.786804000	-0.398980000
1	0.287974000	-4.263350000	-2.039260000
1	1.849060000	-3.410982000	-2.163728000
1	0.077442000	-2.686377000	-3.937311000
1	0.760507000	-1.360128000	-2.972947000
1	-3.539855000	-4.838031000	-1.962917000
1	-1.777084000	-4.928603000	-2.156616000
1	-3.654027000	-2.555606000	-2.724601000
1	-2.523571000	-3.340110000	-3.847563000
6	-4.053020000	-0.340432000	1.103771000
6	-5.439734000	-0.237038000	1.034647000
6	-6.075720000	-0.009998000	-0.194616000
6	-5.297137000	0.159178000	-1.354290000
6	-3.915193000	0.049851000	-1.287084000
1	-3.593522000	-0.507400000	2.074911000
1	-6.040010000	-0.344906000	1.940975000
1	-5.805948000	0.372078000	-2.295728000
1	-3.323480000	0.219128000	-2.187918000
16	-1.221584000	1.870669000	0.181347000
1	0.223386000	-0.541109000	2.482791000
1	-0.604856000	-2.441809000	3.056248000
1	-1.812366000	-0.675067000	3.129242000
6	-7.558807000	0.043939000	-0.261102000
8	-8.191985000	0.189643000	-1.294511000
1	-8.076983000	-0.073630000	0.721762000

1Tsm.xyz

6	-1.546833000	0.316777000	0.005413000
6	-3.273848000	-0.261122000	-0.064007000
44	-1.428544000	-1.577363000	-0.058154000
15	-0.929291000	-1.325403000	2.218473000
16	-1.504680000	-1.659046000	-2.424359000
16	-2.410628000	-3.841775000	-0.064863000
16	0.624884000	-2.706271000	-0.186072000
6	0.341619000	-4.373620000	0.619753000
6	-1.026971000	-5.023746000	0.391509000
6	0.781893000	-3.282107000	-1.963316000
6	0.174874000	-2.274012000	-2.913391000
6	-2.594505000	-4.267851000	-1.891690000
6	-2.661305000	-3.057418000	-2.806547000
1	0.506990000	-4.163220000	1.683699000
1	1.159408000	-5.026624000	0.286613000
1	-1.369754000	-5.509949000	1.313439000
1	-0.997844000	-5.793038000	-0.387963000
1	0.295884000	-4.260762000	-2.040923000
1	1.857117000	-3.407029000	-2.152896000
1	0.097717000	-2.674494000	-3.934002000
1	0.771177000	-1.351990000	-2.957642000
1	-3.526074000	-4.843268000	-1.975300000
1	-1.761720000	-4.928631000	-2.155262000
1	-3.641441000	-2.564130000	-2.744891000
1	-2.497795000	-3.346366000	-3.855102000
6	-4.059999000	-0.351826000	1.106204000
6	-5.447766000	-0.250419000	1.053343000
6	-6.056921000	-0.021564000	-0.178755000
6	-5.313224000	0.153438000	-1.347320000
6	-3.928159000	0.038176000	-1.281976000
1	-3.598281000	-0.518955000	2.076318000
1	-6.065176000	-0.357774000	1.943198000
1	-5.830214000	0.368477000	-2.280860000
1	-3.344090000	0.205500000	-2.187618000
16	-1.237792000	1.873882000	0.167881000
1	0.204958000	-0.504961000	2.474814000
1	-0.564747000	-2.430369000	3.045797000
1	-1.821094000	-0.699262000	3.137034000
7	-7.538341000	0.032629000	-0.249271000
8	-8.045952000	0.222335000	-1.364050000
8	-8.162563000	-0.127441000	0.808992000

Fragment analysis

1a Catalyst

0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
1.99	2.00	2.00	2.00	2.00	2.00	2.00	2.00
2.00	2.00	2.00	2.00	2.00	2.00	2.00	2.00
2.00	2.00	2.00	2.00	2.00	2.00	2.00	2.00
2.00	2.00	2.00	2.00	2.00	2.00	2.00	2.00
2.00	2.00	2.00	1.99	2.00	2.00	2.00	1.99
2.00	2.00	1.99	2.00	2.00	2.00	2.00	1.99
1.98	1.95	0.80	0.01	0.01	0.01	0.00	0.00
0.00	0.00	0.00	0.01	-0.01			

1a Ligand

0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
0.00	0.00	2.02	2.03	2.00			
2.05	2.01	2.01	1.99	2.00	2.01	2.00	
2.00	2.00	2.03	2.00	2.00			
2.00	1.99	2.00	1.96*	1.19	0.03	0.00	
0.01	0.00	0.00	0.00	0.00			

1TSa Catalyst

0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
1.99	2.00	2.00	2.00	2.00	2.00	2.00	2.00
2.00	2.00	2.00	2.00	2.00	2.00	2.00	2.00
2.00	2.00	2.00	2.00	2.00	2.00	2.00	2.00
2.00	2.00	2.00	2.00	2.00	2.00	2.00	2.00
1.99	2.00	2.00	2.00	2.00	1.95	1.99	1.90
1.98	1.96	1.99	1.98	1.99			
2.00	1.99	0.95	0.09	0.07	0.03	0.01	
0.04	0.01	0.01	0.00	0.00			

1TSa Ligand

0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
0.00	0.00	2.02	2.03	2.00			
2.05	2.01	2.01	1.99	2.00	2.00	2.00	2.00
2.00	2.00	2.02	2.00	2.00			
2.00	1.96	2.00	1.76*	1.21	0.07	0.00	
0.02	0.00	0.01	-0.01	0.00			

3a Catalyst

0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
2.00	2.00	2.00	2.00	2.00	2.00	2.00	2.00
2.00	2.00	2.00	1.98	2.00	2.00	2.00	2.00
2.00	2.00	2.00	2.00	2.00	2.00	2.00	2.00
2.00	2.00	2.00	2.00	2.00	2.00	2.00	2.00
2.00	2.00	2.00	2.00	2.00	2.00	2.00	2.00
2.00	1.99	2.00	2.00	2.00	2.00	1.93	1.95
1.98	1.99	1.93	1.89	1.98			
1.99	1.98	1.37	0.29	0.01	0.01	0.00	
0.02	0.02	0.00	0.00	0.00			

3a Ligand

0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
0.00	0.00	2.03	2.03	2.00			
2.04	2.00	2.01	1.97	2.00	2.00	2.00	1.99
1.99	2.00	2.00	2.00	2.00			
2.00	1.97	2.00	1.70*	0.94	0.05	0.00	
0.01	0.00	0.00	0.01	0.00			

1b Catalyst								
	0.00	1.98	2.00	2.00	2.00	1.99	2.00	
2.00	2.00	2.00	2.00	2.00	2.00			
	1.99	2.00	2.00	2.00	2.00	1.99	1.99	2.00
2.00	2.00	2.00	2.00	2.00	2.00			
	2.00	2.00	1.99	1.99	1.98	1.99	2.00	
2.00	1.99	2.00	2.00	1.99				
	2.00	2.00	2.00	1.99	2.00	2.00	1.98	
1.97	0.77	0.01	0.01	0.00				
1b Ligand								
	0.00	0.00	0.00	2.03	2.00	2.01	1.99	
2.00	2.00	2.01	1.99	2.00				
	2.00	2.00	2.00	1.99	2.00	2.00	2.00	
2.00	2.00	2.00	2.00	2.00				
	2.01	1.99	2.00	1.99	1.99	2.00	2.00	
1.99	1.96	1.99	2.00	1.94*				
	1.30	0.03	0.00	0.01	0.00	0.01	0.01	
0.00	0.00	0.01	0.00	0.00				
1TSb Catalyst								
	0.00	1.98	2.00	2.00	2.00	2.00	2.00	
2.00	1.99	2.00	2.00	2.00				
	1.99	2.00	2.00	2.00	2.00	2.00	1.96	2.00
2.00	2.00	2.00	2.00	2.00	2.00			
	2.00	1.99	2.00	1.99	2.00	1.98	2.00	
1.99	2.00	2.00	1.99	1.94				
	1.91	1.96	1.98	1.98	1.98	1.98	1.98	1.99
1.99	0.97	0.02	0.14	0.02				
1TSb Ligand								
	0.00	0.00	0.00	2.03	2.00	1.99	1.99	
2.00	2.00	2.00	1.99	2.00				
	2.00	2.01	2.00	1.99	2.00	2.00	2.00	
2.00	2.00	2.00	1.99	2.00				
	2.00	1.98	2.00	1.99	2.00	2.00	2.00	
1.97	1.94	1.98	2.00	1.73*				
	1.34	0.07	0.01	0.03	0.00	0.01	0.02	
0.00	0.01	0.00	0.00	0.00				
3b Catalyst								
	0.00	2.00	2.00	2.00	2.00	2.00	2.00	
2.00	1.96	2.00	2.00	2.00				
	2.00	2.00	2.00	2.00	2.00	2.00	1.89	1.99
2.00	2.00	2.00	2.00	2.00	2.00			
	2.00	2.00	2.00	2.00	1.99	1.99	2.00	
1.99	2.00	2.00	2.00	1.94				
	1.95	1.99	1.99	1.96	1.85	1.98	1.99	
1.97	1.36	0.29	0.02	0.01				
3b Ligand								
	0.00	0.00	0.00	2.05	2.01	2.01	1.99	
2.00	2.00	2.00	1.99	2.00				
	2.00	2.00	1.99	1.98	2.00	2.00	2.00	
2.00	2.00	2.00	1.99	2.00				
	2.00	1.99	2.00	1.97	1.99	1.99	2.00	
1.97	1.94	2.00	2.00	1.67*				
	1.05	0.06	0.00	0.04	0.00	0.00	0.02	
0.00	0.02	0.00	0.00	0.00				

1c Catalyst

	0.00	0.00	0.00	0.00	0.00	1.98	2.00
2.00	2.00	2.01	2.00	2.00			
	2.00	2.00	2.00	2.00	2.00	2.00	2.00
2.00	2.00	1.99	2.00	2.00			
	2.00	2.00	2.00	2.00	2.00	2.00	2.00
2.00	2.00	1.99	2.00	2.00			
	1.99	2.00	2.00	1.99	2.00	2.00	2.00
1.99	2.00	2.00	1.99	1.96			
	0.78	0.01	0.01	0.00	0.01	0.00	0.00
0.00	0.01	-0.01	0.00	0.00			
1c Ligand							
	0.00	0.00	0.00	0.00	0.00	0.00	0.00
2.07	2.00	2.02	1.99	1.99			
	2.06	1.99	1.99	1.99	2.00	2.01	1.99
1.99	1.97*	1.21	0.01	0.03			
1TSc Catalyst							
	0.00	0.00	0.00	0.00	0.00	1.99	2.00
2.00	2.00	2.00	2.00	2.00			
	2.01	2.00	2.00	2.00	2.00	2.00	2.00
2.00	2.00	1.96	2.00	2.00			
	2.00	2.00	2.00	2.00	2.00	2.00	2.00
1.99	2.00	1.99	1.98	2.00			
	2.00	1.97	1.99	1.98	1.92	1.96	1.98
1.99	1.99	1.99	1.99	1.99			
	1.05	0.04	0.06	0.04	0.03	0.01	0.00
0.02	0.00	0.01	0.00	0.00			
1TSc Ligand							
	0.00	0.00	0.00	0.00	0.00	0.00	0.00
2.06	2.00	2.01	1.99	1.98			
	2.05	1.99	1.99	1.99	2.00	2.00	1.99
1.99	1.84*	1.18	0.01	0.05			
3c Catalyst							
	0.00	0.00	0.00	0.00	0.00	2.00	2.00
2.00	2.00	2.00	2.00	2.00			
	1.97	2.00	2.00	2.00	2.00	2.00	2.00
2.00	2.00	1.92	1.99	2.00			
	2.00	2.00	2.00	2.00	2.00	2.00	2.00
2.00	2.00	1.99	2.00	1.99			
	2.00	2.00	2.00	1.93	1.95	1.98	1.99
1.89	1.96	1.98	2.00	1.98			
	1.37	0.21	0.02	0.01	0.00	0.01	0.02
0.00	0.01	0.00	0.00	0.00			
3c Ligand							
	0.00	0.00	0.00	0.00	0.00	0.00	0.00
2.08	2.00	1.99	1.99	1.96			
	2.06	1.98	1.98	1.99	1.97	1.99	1.99
2.00	1.78*	0.93	0.00	0.04			
1d Catalyst							
	0.00	0.00	0.00	0.00	0.00	1.98	2.00
2.00	2.00	2.00	2.00	2.00			
	2.00	2.00	2.00	2.00	2.00	2.00	2.00
2.00	2.00	1.99	2.00	2.00			
	2.00	2.00	2.00	2.00	2.00	2.00	2.00
2.00	1.99	1.99	2.00	2.00			
	1.99	2.00	2.00	2.00	2.00	2.00	2.00
1.99	2.00	2.00	1.99	1.96			

	0.74	0.01	0.01	0.01	0.00	0.00	0.01
0.01	0.00	0.02	0.00	-0.01			
1d Ligand							
	0.00	0.00	0.00	2.00	2.01	2.02	2.01
2.00	2.01	2.00	2.00	2.00			
	1.99	2.00	2.00	1.99	2.00	1.99	2.00
2.00	2.00	2.01	2.00	2.00			
	2.00	2.00	2.01	2.00	2.00	2.00	2.00
2.00	1.99	2.00	1.93	1.99			
	2.00	1.99	2.00	1.97*	1.31	0.02	0.00
0.01	0.00	0.01	0.00	0.02			
1TSd Catalyst							
	0.00	0.00	0.00	0.00	0.00	1.98	2.00
2.00	2.00	2.00	2.00	2.00			
	2.00	2.00	2.00	2.00	1.99	2.00	2.00
2.00	2.00	1.96	2.00	2.00			
	2.00	2.00	2.00	2.00	2.00	1.99	1.99
2.00	2.00	1.99	1.99	2.00			
	2.00	2.00	1.98	1.96	1.92	1.97	1.98
1.98	1.98	1.99	1.99	1.99			
	0.94	0.07	0.09	0.02	0.06	0.01	0.01
0.01	0.01	0.02	0.00	0.00			
1TSd Ligand							
	0.00	0.00	0.00	2.00	2.01	2.01	2.00
2.00	2.00	2.00	1.98	2.00			
	2.00	1.99	2.00	1.99	2.00	1.99	2.00
2.00	2.00	2.00	2.00	2.00			
	2.00	2.00	2.00	2.00	2.00	2.00	2.00
2.00	1.99	1.97	1.98	1.98			
	2.00	1.94	2.00	1.79*	1.30	0.05	0.04
0.00	0.00	0.01	0.00	0.00			
3d Catalyst							
	0.00	0.00	0.00	0.00	0.00	2.00	2.00
2.00	2.00	2.00	2.00	2.00			
	1.96	2.00	2.00	2.00	2.00	2.00	2.00
2.00	2.00	1.89	1.99	2.00			
	2.00	2.00	2.00	2.00	2.00	2.00	2.00
2.00	1.99	1.99	2.00	1.99			
	2.00	2.00	2.00	1.94	1.95	1.99	1.99
2.00	1.82	1.99	1.99	1.97			
	1.35	0.28	0.01	0.01	0.00	0.02	0.02
0.00	0.00	0.00	0.00	0.00			
3d Ligand							
	0.00	0.00	0.00	2.01	2.02	2.02	2.01
2.00	2.01	2.00	1.99	1.99			
	1.99	2.00	2.00	1.98	2.00	1.99	2.00
2.00	2.00	2.00	2.00	2.00			
	1.99	2.00	1.99	2.00	2.00	2.00	2.00
1.99	1.98	1.99	1.90	1.96			
	2.00	1.96	1.99	1.78*	1.05	0.03	0.00
0.02	0.00	0.01	0.00	0.05			
1e Catalyst							
	0.00	0.00	0.00	0.00	0.00	0.00	0.00
0.00	0.00	1.98	2.00	2.00			
	2.00	2.00	2.00	2.00	2.00	2.00	2.00
2.00	2.00	2.00	2.00	2.00			

	2.00	1.99	2.00	2.00	2.00	2.00	2.00
2.00	2.00	2.00	2.00	2.00	2.00		
	1.99	2.00	2.00	2.00	1.99	2.00	2.00
1.99	1.99	2.00	2.00	2.00	1.99		
	2.00	2.00	1.99	1.94	0.67	0.00	0.01
0.01	0.00	0.00	0.01	0.00			
1e Ligand							
	0.00	0.00	0.00	0.00	0.00	0.00	0.00
0.00	0.00	0.00	0.00	2.01			
	2.00	2.00	1.98	2.07	2.00	2.00	1.99
1.98	1.99	2.01	2.00	2.00			
	2.00	2.00	2.00	2.01	1.99	2.00	1.99
1.99	2.00	2.00	1.99	1.99			
	1.94	1.96*	1.41	0.05	0.01	0.00	0.01
0.00	0.00	0.00	0.00	0.00			
1TSe Catalyst							
	0.00	0.00	0.00	0.00	0.00	1.99	2.00
2.00	2.00	2.00	2.00	2.00			
	2.00	2.00	2.00	2.00	2.00	2.00	2.00
2.00	2.00	1.95	2.00	2.00			
	2.00	2.00	2.00	2.00	2.00	1.99	2.00
2.00	1.99	1.99	2.00	1.99			
	2.00	2.00	1.97	1.96	1.91	1.96	1.95
1.96	1.98	1.99	1.99	1.99			
	0.98	0.07	0.06	0.01	0.06	0.00	0.01
0.01	0.01	0.01	0.00	0.00			
1TSe Ligand							
	0.00	0.00	0.00	0.00	0.00	0.00	0.00
0.00	0.00	2.01	2.00	2.00			
	1.99	2.04	2.00	2.00	1.99	1.99	1.99
2.01	2.00	2.00	2.00	2.00			
	1.99	2.00	1.99	2.00	1.99	1.99	2.00
2.00	1.91	1.94	1.94	1.93*			
	1.33	0.09	0.03	0.00	0.01	0.00	0.00
0.00	0.01	0.00	0.00	0.00			
3e Catalyst							
	0.00	0.00	0.00	0.00	0.00	0.00	0.00
0.00	0.00	2.00	2.00	2.00			
	2.00	2.00	2.00	2.00	1.97	2.00	2.00
2.00	2.00	2.00	2.00	2.00			
	2.00	1.93	2.00	2.00	2.00	2.00	2.00
2.00	2.00	2.00	2.00	2.00			
	2.00	1.99	2.00	1.99	2.00	2.00	2.00
1.94	1.94	1.97	1.98	1.94			
	1.90	1.98	1.99	1.97	1.31	0.13	0.04
0.01	0.00	0.02	0.02	0.00			
3e Ligand							
	0.00	0.00	0.00	0.00	0.00	0.00	0.00
0.00	0.00	0.00	0.00	2.02			
	2.00	1.99	2.00	2.07	2.00	2.00	1.98
1.98	1.98	2.00	2.00	2.00			
	1.99	2.00	1.99	2.00	1.98	2.00	1.98
1.99	2.00	1.99	1.93	1.93			
	1.90	1.91*	1.12	0.06	0.03	0.00	0.01
0.01	0.00	0.01	0.01	0.00			
1g Catalyst							
	0.00	0.00	0.00	0.00	0.00	0.00	1.98
2.00	2.00	2.00	2.01	2.00			

	2.00	2.00	2.00	2.00	2.00	2.00	2.00
2.00	2.00	2.00	1.99	2.00			
	2.00	2.00	2.00	2.00	2.00	2.00	2.00
2.00	2.00	2.00	1.99	2.00	2.00		
	2.00	1.99	2.00	2.00	1.99	2.00	2.00
2.00	1.99	2.00	2.00	1.99			
	1.96	0.80	0.02	0.01	0.00	0.01	0.00
0.00	0.00	0.01	-0.01	0.00			
1g Ligand							
	0.00	0.00	0.00	0.00	0.00	0.00	0.00
0.00	2.01	2.06	2.00	2.04			
	1.99	1.98	2.03	1.99	2.00	1.99	2.03
1.99	2.00	1.99	1.99	1.99			
	1.20	1.94*	0.00	0.03	0.00	0.00	0.00
0.00	0.00	0.01	0.01	0.00			
1TSg Catalyst							
	0.00	0.00	0.00	0.00	0.00	0.00	1.99
2.00	2.00	2.00	2.00	2.00			
	2.00	2.00	2.00	2.00	2.00	2.00	2.00
2.00	2.00	2.00	1.96	2.00			
	2.00	2.00	2.00	2.00	2.00	2.00	2.00
2.00	1.99	2.00	1.98	1.99			
	2.00	2.00	1.97	2.00	1.98	1.92	1.98
1.98	1.99	1.99	1.99	1.99			
	1.99	0.98	0.05	0.07	0.04	0.02	0.02
0.00	0.02	0.00	0.01	0.00			
1TSg Ligand							
	0.00	0.00	0.00	0.00	0.00	0.00	0.00
0.00	2.01	2.05	2.00	2.03			
	2.00	1.98	2.02	1.99	1.99	1.99	2.02
1.99	2.00	1.99	1.97	1.99			
	1.78*	1.22	0.01	0.04	0.00	-0.01	0.00
0.01	-0.01	0.01	0.01	0.00			
3g Catalyst							
	0.00	0.00	0.00	0.00	0.00	0.00	2.00
2.00	2.00	2.00	2.00	2.00			
	2.00	1.97	2.00	2.00	2.00	2.00	2.00
2.00	2.00	2.00	1.91	2.00			
	2.00	2.00	2.00	2.00	2.00	2.00	2.00
2.00	2.00	2.00	1.99	2.00			
	1.99	2.00	2.00	2.00	1.93	1.94	1.98
1.99	1.86	1.98	1.98	2.00			
	1.98	1.38	0.31	0.02	0.01	0.00	0.01
0.02	0.00	0.01	0.00	0.00			
3g Ligand							
	0.00	0.00	0.00	0.00	0.00	0.00	0.00
0.00	2.01	2.05	2.00	2.02			
	1.99	1.95	2.03	1.99	1.97	1.98	1.99
2.02	2.00	1.99	1.97	2.00			
	1.68*	0.90	0.00	0.04	0.00	0.00	0.02
0.01	0.03	0.01	0.01	0.02			
1h Catalyst							
	0.00	0.00	0.00	0.00	0.00	0.00	1.98
2.00	2.00	2.00	2.01	2.00			
	2.00	2.00	2.00	2.00	2.00	2.00	2.00
2.00	2.00	2.00	1.99	2.00			

	2.00	2.00	2.00	2.00	2.00	2.00	2.00
2.00	2.00	2.00	1.99	2.00			
	2.00	1.99	2.00	2.00	1.99	2.00	2.00
2.00	1.99	2.00	2.00	1.99			
	1.96	0.79	0.01	0.01	0.00	0.01	0.00
0.00	0.00	0.01	-0.01	0.00			
1h Ligand							
	0.00	0.00	0.00	0.00	0.00	0.00	0.00
0.00	2.00	2.07	2.00	2.03			
	1.99	1.99	2.02	2.01	2.00	2.02	2.00
2.00	2.00	1.99	2.00	1.99			
	1.96*	1.20	0.01	0.03	0.00	0.00	0.00
0.00	0.00	0.01	0.00	0.00			
1TSh Catalyst							
	0.00	0.00	0.00	0.00	0.00	0.00	1.99
2.00	2.00	2.00	2.00	2.00			
	2.00	2.00	2.00	2.00	2.00	2.00	2.00
2.00	2.00	2.00	1.96	2.00			
	2.00	2.00	2.00	2.00	2.00	2.00	2.00
2.00	1.99	2.00	1.98	1.99			
	2.00	2.00	1.97	2.00	1.97	1.92	1.97
1.98	1.99	1.99	1.99	1.99			
	2.00	0.99	0.05	0.07	0.03	0.02	0.02
0.00	0.02	0.00	0.01	0.00			
1TSh Ligand							
	0.00	0.00	0.00	0.00	0.00	0.00	0.00
0.00	2.00	2.06	2.00	2.02			
	1.99	1.99	2.01	2.00	1.99	2.02	1.99
2.00	1.99	1.99	1.98	1.99			
	1.82*	1.21	0.01	0.04	0.00	-0.01	0.00
-0.01	0.01	0.01	0.00	0.00			
3h Catalyst							
	0.00	0.00	0.00	0.00	0.00	0.00	2.00
2.00	2.00	2.00	2.00	2.00			
	2.00	1.97	2.00	2.00	2.00	2.00	2.00
2.00	2.00	2.00	1.91	1.99			
	2.00	2.00	2.00	2.00	2.00	2.00	2.00
2.00	2.00	2.00	1.99	2.00			
	1.99	2.00	2.00	2.00	1.93	1.95	1.98
1.99	1.89	1.95	1.98	1.99			
	1.98	1.37	0.26	0.02	0.01	0.00	0.01
0.02	0.00	0.01	0.00	0.00			
3h Ligand							
	0.00	0.00	0.00	0.00	0.00	0.00	0.00
0.00	2.00	2.07	2.00	2.00			
	1.99	1.97	2.02	2.00	1.97	2.01	1.99
2.00	1.99	1.99	1.97	2.00			
	1.74*	0.92	0.00	0.04	0.00	0.02	0.00
0.03	0.01	0.01	0.01	0.03			
1i Catalyst							
	0.00	0.00	0.00	0.00	0.00	0.00	1.98
2.00	2.00	2.00	2.01	2.00			
	2.00	2.00	2.00	2.00	2.00	2.00	2.00
2.00	2.00	2.00	1.99	2.00			

	2.00	2.00	2.00	2.00	2.00	2.00	2.00
2.00	2.00	2.00	1.99	2.00			
	2.00	1.99	2.00	2.00	1.99	2.00	2.00
2.00	1.99	2.00	2.00	1.99			
	1.96	0.79	0.01	0.01	0.00	0.01	0.00
0.00	0.00	0.01	-0.01	0.00			
1i Ligand							
	0.00	0.00	0.00	0.00	0.00	0.00	0.00
0.00	2.07	2.00	2.00	2.04			
	1.99	1.98	2.03	1.99	1.99	2.00	2.00
2.00	2.01	2.00	1.99	1.99			
	1.96*	1.20	0.01	0.03	0.00	0.00	0.00
0.00	0.00	0.00	0.00	0.01			
1TSi Catalyst							
	0.00	0.00	0.00	0.00	0.00	0.00	1.99
2.00	2.00	2.00	2.00	2.00			
	2.00	2.01	2.00	2.00	2.00	2.00	2.00
2.00	2.00	2.00	1.95	2.00			
	2.00	2.00	2.00	2.00	2.00	2.00	2.00
2.00	2.00	2.00	1.99	1.98			
	2.00	2.00	1.97	1.98	2.00	1.91	1.96
1.97	1.99	1.99	1.99	1.99			
	1.97	1.10	0.04	0.08	0.04	0.03	0.01
0.00	0.02	0.00	0.00	0.00			
1TSi Ligand							
	0.00	0.00	0.00	0.00	0.00	0.00	0.00
0.00	2.06	1.99	2.00	2.03			
	1.99	1.98	2.02	1.99	1.99	2.00	2.00
2.00	2.01	1.99	1.99	1.99			
	1.81*	1.16	0.02	0.04	0.00	-0.01	0.00
0.01	0.00	0.00	0.00	0.01			
3i Catalyst							
	0.00	0.00	0.00	0.00	0.00	0.00	2.00
2.00	2.00	2.00	2.00	2.00			
	2.00	1.97	2.00	2.00	2.00	2.00	2.00
2.00	2.00	2.00	1.91	1.99			
	2.00	2.00	2.00	2.00	2.00	2.00	2.00
2.00	2.00	2.00	1.99	2.00			
	1.99	2.00	2.00	2.00	1.93	1.94	1.98
1.99	1.88	1.97	1.98	2.00			
	1.98	1.38	0.23	0.02	0.01	0.00	0.01
0.02	0.00	0.01	0.00	0.00			
3i Ligand							
	0.00	0.00	0.00	0.00	0.00	0.00	0.00
0.00	2.08	1.97	2.00	2.02			
	1.99	1.96	2.02	1.98	1.99	2.00	2.00
1.99	1.99	1.98	1.99	2.00			
	1.76*	0.93	0.01	0.04	0.00	0.02	0.00
0.01	0.00	0.03	0.00	0.01			
1j Catalyst							
	0.00	0.00	0.00	0.00	0.00	0.00	1.98
2.00	2.00	2.00	2.01	2.00			
	2.00	2.00	2.00	2.00	2.00	2.00	2.00
2.00	2.00	2.00	1.99	2.00			

	2.00	2.00	2.00	2.00	2.00	2.00	2.00
2.00	2.00	2.00	1.99	2.00			
	2.00	1.99	2.00	2.00	1.99	2.00	2.00
2.00	1.99	2.00	2.00	1.99			
	1.96	0.77	0.01	0.01	0.00	0.01	0.00
0.00	0.00	0.01	-0.01	0.00			
1j Ligand							
	0.00	0.00	0.00	0.00	0.00	0.00	0.00
0.00	2.00	2.07	2.00	2.03			
	1.99	1.99	2.03	1.99	2.00	2.00	2.02
1.99	2.00	2.01	1.99	1.99			
	1.97*	1.22	0.01	0.03	0.00	0.00	0.00
0.00	0.00	0.01	0.00	0.00			
1TSj Catalyst							
	0.00	0.00	0.00	0.00	0.00	0.00	1.99
2.00	2.00	2.00	2.00	2.00			
	2.00	2.01	2.00	2.00	2.00	2.00	2.00
2.00	2.00	2.00	1.95	2.00			
	2.00	2.00	2.00	2.00	2.00	2.00	2.00
2.00	2.00	2.00	1.99	1.98			
	2.00	2.00	1.97	1.98	2.00	1.91	1.95
1.98	1.99	1.99	1.99	1.98			
	1.98	1.08	0.04	0.07	0.04	0.03	0.01
0.00	0.02	0.00	0.00	0.00			
1TSj Ligand							
	0.00	0.00	0.00	0.00	0.00	0.00	0.00
0.00	2.00	2.05	2.00	2.02			
	2.00	1.98	2.03	1.99	1.99	2.00	2.02
2.00	2.00	1.99	1.99	1.99			
	1.82*	1.17	0.01	0.05	-0.01	0.00	0.00
-0.01	0.01	0.01	0.00	0.00			
3j Catalyst							
	0.00	0.00	0.00	0.00	0.00	0.00	2.00
2.00	2.00	2.00	2.00	2.00			
	2.00	1.97	2.00	2.00	2.00	2.00	2.00
2.00	2.00	2.00	1.92	1.99			
	2.00	2.00	2.00	2.00	2.00	2.00	2.00
2.00	2.00	2.00	1.99	2.00			
	2.00	2.00	2.00	2.00	1.93	1.95	1.98
1.99	1.89	1.95	1.98	2.00			
	1.98	1.37	0.23	0.01	0.01	0.00	0.01
0.02	0.00	0.00	0.00	0.00			
3j Ligand							
	0.00	0.00	0.00	0.00	0.00	0.00	0.00
0.00	2.00	2.07	2.00	2.00			
	1.99	1.96	2.04	1.98	1.97	2.00	2.01
1.99	1.99	1.98	1.99	2.00			
	1.77*	0.92	0.00	0.04	0.02	0.00	0.00
0.03	0.01	0.01	0.02	0.00			
1k Catalyst							
	0.00	0.00	0.00	0.00	0.00	0.00	0.00
1.98	2.00	2.00	2.00	2.01			
	2.00	2.00	2.00	2.00	2.00	2.00	2.00
2.00	2.00	2.00	2.00	1.99			

	2.00	2.00	2.00	2.00	2.00	2.00	2.00
2.00	2.00	2.00	2.00	1.99			
	2.00	2.00	1.99	2.00	2.00	1.99	2.00
2.00	2.00	1.99	2.00	2.00			
	1.99	1.96	0.76	0.01	0.01	0.00	0.00
0.00	0.00	0.00	0.01	-0.01			
1k Ligand							
	0.00	0.00	0.00	0.00	0.00	0.00	0.00
0.00	0.00	2.00	2.07	2.02			
	2.00	2.01	1.99	2.00	2.01	1.99	1.99
2.00	2.01	2.02	2.00	2.00			
	1.99	1.99	1.97*	2.00	1.23	0.03	0.01
0.02	0.00	0.00	0.00	0.00			
1TSk Catalyst							
	0.00	0.00	0.00	0.00	0.00	0.00	0.00
1.99	2.00	2.00	2.00	2.00			
	2.00	2.00	2.01	2.00	2.00	2.00	2.00
2.00	2.00	2.00	2.00	1.95			
	2.00	2.00	2.00	2.00	2.00	2.00	2.00
2.00	2.00	2.00	2.00	1.99			
	1.98	2.00	2.00	1.97	2.00	1.97	1.91
1.95	1.97	1.98	1.99	1.99			
	1.99	1.99	1.07	0.05	0.06	0.04	0.03
0.01	0.00	0.02	0.00	0.00			
1TSk Ligand							
	0.00	0.00	0.00	0.00	0.00	0.00	0.00
0.00	0.00	2.00	2.05	2.00			
	2.00	2.00	1.99	2.00	2.00	1.99	1.99
2.00	2.01	2.01	2.01	1.99			
	1.99	1.98	1.85*	2.00	1.17	0.05	0.01
0.02	-0.01	0.00	0.00	0.00			
3k Catalyst							
	0.00	0.00	0.00	0.00	0.00	0.00	0.00
2.00	2.00	2.00	2.00	2.00			
	2.00	2.00	1.97	2.00	2.00	2.00	2.00
2.00	2.00	2.00	2.00	1.92			
	1.99	2.00	2.00	2.00	2.00	2.00	2.00
2.00	2.00	2.00	2.00	1.99			
	2.00	1.99	2.00	2.00	2.00	1.94	1.94
1.98	1.99	1.92	1.93	1.98			
	1.99	1.98	1.36	0.19	0.02	0.01	0.00
0.01	0.02	0.00	0.00	0.00			
3k Ligand							
	0.00	0.00	0.00	0.00	0.00	0.00	0.00
0.00	0.00	2.00	2.07	2.00			
	2.00	1.99	1.98	2.00	2.00	1.98	1.99
2.00	2.00	2.00	2.00	1.98			
	1.99	1.99	1.82*	2.00	0.93	0.03	0.00
0.02	0.01	0.02	0.00	0.02			
1m Catalyst							
	0.00	0.00	0.00	0.00	0.00	0.00	0.00
0.00	1.98	2.00	2.00	2.00			
	2.01	2.00	2.00	2.00	2.00	2.00	2.00
2.00	2.00	2.00	2.00	2.00			
	1.99	2.00	2.00	2.00	2.00	2.00	2.00
2.00	2.00	2.00	2.00	2.00			

	1.99	2.00	2.00	1.99	2.00	2.00	1.99
2.00	2.00	2.00	1.99	2.00			
	2.00	1.99	1.96	0.74	0.01	0.01	0.00
0.00	0.00	0.00	0.00	0.01			
1m Ligand							
	0.00	0.00	0.00	0.00	0.00	0.00	0.00
0.00	0.00	0.00	2.00	2.00			
	2.05	2.04	2.00	2.01	1.99	1.99	2.01
2.00	2.00	2.00	1.99	2.04			
	1.99	2.01	1.99	2.00	2.00	1.98	
1.99*	2.00	1.24	0.02	0.01	0.03		
1Tsm Catalyst							
	0.00	0.00	0.00	0.00	0.00	0.00	0.00
0.00	1.99	2.00	2.00	2.00			
	2.00	2.00	2.00	2.01	2.00	2.00	2.00
2.00	2.00	2.00	2.00	2.00			
	1.95	2.00	2.00	2.00	2.00	2.00	2.00
2.00	2.00	2.00	2.00	2.00			
	1.99	1.98	2.00	2.00	1.97	2.00	1.97
1.91	1.95	1.97	1.98	1.99			
	1.99	1.99	1.99	1.05	0.04	0.05	0.03
0.03	0.01	0.00	0.02	0.00			
1Tsm Ligand							
	0.00	0.00	0.00	0.00	0.00	0.00	0.00
0.00	0.00	0.00	2.00	2.00			
	2.04	2.02	2.00	2.00	1.99	1.99	2.01
2.00	2.00	1.99	2.00	2.03			
	2.00	2.00	1.99	2.00	2.00	1.99	
1.86*	2.00	1.18	0.04	0.01	0.04		
3m Catalyst							
	0.00	0.00	0.00	0.00	0.00	0.00	0.00
0.00	2.00	2.00	2.00	2.00			
	2.00	2.00	2.00	1.97	2.00	2.00	2.00
2.00	2.00	2.00	2.00	2.00			
	1.92	1.99	2.00	2.00	2.00	2.00	2.00
2.00	2.00	2.00	2.00	2.00			
	1.99	2.00	1.99	2.00	2.00	2.00	1.94
1.94	1.98	1.98	1.91	1.94			
	1.98	1.99	1.98	1.35	0.17	0.02	0.01
0.00	0.01	0.02	0.00	0.00			
3m Ligand							
	0.00	0.00	0.00	0.00	0.00	0.00	0.00
0.00	0.00	0.00	2.00	2.00			
	2.06	2.01	2.00	1.99	1.99	1.98	2.01
2.00	1.99	1.98	1.98	2.02			
	1.99	1.99	1.99	2.00	2.00	2.00	
1.82*	2.00	0.93	0.02	0.00	0.03		