3FPHA dimers

3D1

C -0.748061000 1.768602000 2.990240000

C 0.068714000 1.323962000 2.195452000

C 1.008406000 0.799764000 1.252296000

C 1.253014000 -0.594246000 1.200171000

C 1.684627000 1.662724000 0.354742000

C 2.158557000 -1.075116000 0.256449000

C 2.590320000 1.138515000 -0.576311000

C 2.840527000 -0.243671000 -0.637717000

H -1.454047000 2.158580000 3.698252000

H 0.733496000 -1.283467000 1.867722000

H 1.475652000 2.734005000 0.384784000

F 2.378916000 -2.425347000 0.193783000

H 3.104395000 1.810091000 -1.270808000

H 3.538319000 -0.674881000 -1.359990000

C -1.089398000 3.171118000 -1.827372000

C -1.179338000 1.983593000 -1.546991000

C -1.273998000 0.595760000 -1.210860000

C -2.096692000 0.184660000 -0.133620000

C -0.539970000 -0.372931000 -1.939112000

C -2.152943000 -1.172436000 0.179367000

C -0.627112000 -1.727580000 -1.593880000

C -1.437635000 -2.146932000 -0.524838000

H -1.025237000 4.211615000 -2.082187000

H -2.654357000 0.910870000 0.459162000

H 0.103416000 -0.048890000 -2.760081000

F -2.936332000 -1.566455000 1.230464000

H -0.046714000 -2.469143000 -2.150564000

H -1.512293000 -3.197284000 -0.232604000

3D2

C 0.715034000 1.876461000 2.940802000

C -0.092217000 1.401585000 2.153805000

C -1.020527000 0.841871000 1.219914000

C -1.252208000 -0.555274000 1.206483000

C -1.697845000 1.672345000 0.292996000

C -2.146369000 -1.071521000 0.270654000

C -2.592057000 1.113120000 -0.628750000

C -2.829291000 -0.272497000 -0.651926000

H 1.412241000 2.293612000 3.641997000

H -0.731688000 -1.219953000 1.897747000

H -1.498668000 2.745921000 0.293680000

F -2.354584000 -2.424872000 0.245816000

H -3.107453000 1.759615000 -1.345736000

H -3.517955000 -0.730759000 -1.366258000

C 1.138382000 3.143566000 -1.838820000

C 1.214644000 1.957227000 -1.549565000

C 1.292087000 0.571046000 -1.202629000

C 2.092572000 0.160458000 -0.108572000

C 0.562222000 -0.396423000 -1.936667000

C 2.131301000 -1.194808000 0.214736000

C 0.631435000 -1.749289000 -1.580549000

C 1.419666000 -2.168089000 -0.494799000

H 1.086780000 4.182855000 -2.101293000

H 2.645631000 0.886211000 0.489068000

H -0.063819000 -0.072631000 -2.771057000

F 2.892373000 -1.588116000 1.282511000

H 0.054495000 -2.489807000 -2.142227000

H 1.479370000 -3.216836000 -0.193551000

3D3

C -3.973563000 -0.399817000 -0.718795000

C -2.862746000 -0.820030000 -0.424859000

C -1.558472000 -1.294876000 -0.076572000

C -0.555972000 -1.397589000 -1.071157000

C -1.253388000 -1.650474000 1.261115000

C 0.710409000 -1.845446000 -0.698745000

C 0.033046000 -2.096113000 1.593405000

C 1.036627000 -2.198247000 0.614483000

H -4.954745000 -0.046360000 -0.972288000

H -0.758232000 -1.118139000 -2.106259000

H -2.027028000 -1.560112000 2.027348000

F 1.677143000 -1.930970000 -1.661774000

H 0.264211000 -2.361468000 2.629732000

H 2.051564000 -2.521875000 0.854722000

C 3.970476000 0.390899000 0.719024000

C 2.860766000 0.814083000 0.425172000

C 1.558002000 1.293062000 0.076894000

C 0.553507000 1.391371000 1.069894000

C 1.256586000 1.657779000 -1.259166000

C -0.711058000 1.844496000 0.697690000

C -0.028168000 2.108342000 -1.591395000

C -1.033649000 2.206400000 -0.613951000

H 4.950664000 0.034707000 0.972535000

H 0.752609000 1.103661000 2.103309000

H 2.031849000 1.571189000 -2.024213000

F -1.679564000 1.926463000 1.659269000

H -0.256314000 2.381524000 -2.626362000

H -2.047215000 2.534398000 -0.854204000

3D4

C 1.102564000 3.146764000 -1.850253000

C 1.191581000 1.962022000 -1.558114000

C 1.283277000 0.577702000 -1.207292000

C 2.089579000 0.178364000 -0.113333000

C 0.561956000 -0.399164000 -1.937264000

C 2.142328000 -1.175432000 0.214004000

C 0.645304000 -1.750231000 -1.577297000

C 1.439302000 -2.157876000 -0.491523000

H 1.040178000 4.184725000 -2.115612000

H 2.636292000 0.911412000 0.481241000

H -0.068645000 -0.084117000 -2.771575000

F 2.909009000 -1.557929000 1.281641000

H 0.074985000 -2.498188000 -2.135860000

H 1.509960000 -3.205087000 -0.187294000

C 0.705812000 1.881641000 2.941217000

C -0.098749000 1.401268000 2.154797000

C -1.024346000 0.835100000 1.222100000

C -1.244617000 -0.563867000 1.207568000

C -1.710455000 1.661056000 0.297621000

C -2.136502000 -1.086419000 0.273076000

C -2.601944000 1.095510000 -0.622911000

C -2.827864000 -0.291971000 -0.647166000

H 1.400854000 2.303484000 3.641750000

H -0.716750000 -1.225032000 1.896615000

H -1.520011000 2.736212000 0.298995000

F -2.333662000 -2.441374000 0.247149000

H -3.124099000 1.738529000 -1.338129000

H -3.514246000 -0.755011000 -1.360615000

2D5

C 4.072647000 0.785979000 -0.281322000

C 3.125152000 0.033936000 -0.096169000

C 2.001869000 -0.830246000 0.103302000

C 1.111408000 -0.594926000 1.178536000

C 1.758958000 -1.910758000 -0.781147000

C 0.010447000 -1.437095000 1.327396000

C 0.639606000 -2.733352000 -0.596053000

C -0.254846000 -2.504066000 0.463333000

H 4.919364000 1.429335000 -0.427238000

H 1.264980000 0.237090000 1.867567000

H 2.448814000 -2.088436000 -1.610120000

F -0.855154000 -1.198141000 2.358324000

H 0.452719000 -3.560434000 -1.287990000

H -1.146486000 -3.116473000 0.612690000

C -3.684510000 -1.327159000 -0.905689000

C -2.796495000 -0.487368000 -0.848113000

C -1.747026000 0.482966000 -0.774251000

C -1.709394000 1.404777000 0.300991000

C -0.732167000 0.520475000 -1.762376000

C -0.660903000 2.322482000 0.352554000

C 0.302771000 1.459592000 -1.672838000

C 0.352728000 2.376635000 -0.609505000

H -4.475833000 -2.050074000 -0.961868000

H -2.468555000 1.389070000 1.085043000

H -0.757575000 -0.202043000 -2.581092000

F -0.615774000 3.200335000 1.402464000

H 1.096552000 1.468240000 -2.425036000

H 1.162905000 3.102743000 -0.510946000

2D6

C -1.576453000 3.819312000 0.104061000

C -1.632734000 2.623968000 -0.151930000

C -1.668293000 1.220921000 -0.431858000

C -2.516712000 0.370073000 0.318668000

C -0.839224000 0.668543000 -1.439123000

C -2.498133000 -0.997471000 0.045258000

C -0.851223000 -0.710705000 -1.680519000

C -1.682915000 -1.566219000 -0.938069000

H -1.548445000 4.872862000 0.307678000

H -3.165384000 0.766970000 1.102300000

H -0.175686000 1.326065000 -2.005062000

F -3.307224000 -1.818904000 0.784190000

H -0.190117000 -1.134888000 -2.441418000

H -1.688408000 -2.646841000 -1.096947000

C 1.576766000 -3.819302000 -0.104263000

C 1.632920000 -2.623980000 0.151858000

C 1.668363000 -1.220943000 0.431840000

C 2.516699000 -0.369998000 -0.318675000

C 0.839258000 -0.668672000 1.439136000

C 2.498015000 0.997535000 -0.045208000

C 0.851148000 0.710569000 1.680589000

C 1.682774000 1.566173000 0.938161000

H 1.548905000 -4.872823000 -0.308051000

H 3.165384000 -0.766814000 -1.102338000

H 0.175796000 -1.326281000 2.005062000

F 3.307020000 1.819070000 -0.784123000

H 0.190027000 1.134649000 2.441534000

H 1.688227000 2.646783000 1.097080000

2D7

C 0.338371000 2.668203000 -2.277354000

C -0.263204000 1.686153000 -1.864958000

C -0.948443000 0.531401000 -1.371058000

C -2.018559000 0.680819000 -0.455108000

C -0.552248000 -0.766292000 -1.778745000

C -2.651738000 -0.466596000 0.019310000

C -1.218104000 -1.893331000 -1.280469000

C -2.282028000 -1.757908000 -0.371838000

H 0.855921000 3.530996000 -2.650815000

H -2.326905000 1.667035000 -0.105526000

H 0.282704000 -0.875676000 -2.474544000

F -3.676847000 -0.322265000 0.915581000

H -0.903315000 -2.892832000 -1.595482000

H -2.813462000 -2.623361000 0.032128000

C -0.338459000 2.668064000 2.277490000

C 0.263175000 1.686085000 1.865009000

C 0.948438000 0.531363000 1.371072000

C 2.018540000 0.680832000 0.455113000

C 0.552285000 -0.766351000 1.778732000

C 2.651743000 -0.466554000 -0.019342000

C 1.218166000 -1.893360000 1.280421000

C 2.282074000 -1.757885000 0.371780000

H -0.856029000 3.530827000 2.650991000

H 2.326854000 1.667066000 0.105551000

H -0.282655000 -0.875775000 2.474540000

F 3.676836000 -0.322172000 -0.915623000

H 0.903408000 -2.892877000 1.595414000

H 2.813527000 -2.623314000 -0.032213000

2D8

C 0.862492000 3.330748000 -0.766832000

C -0.000205000 2.467498000 -0.684313000

C -0.995922000 1.445234000 -0.579013000

C -0.915655000 0.296549000 -1.403749000

C -2.055365000 1.563718000 0.354874000

C -1.891228000 -0.689064000 -1.266606000

C -3.017817000 0.550816000 0.458274000

C -2.947936000 -0.593906000 -0.355200000

H 1.615706000 4.090940000 -0.848125000

H -0.099067000 0.171035000 -2.116291000

H -2.105570000 2.446265000 0.996898000

F -1.803417000 -1.806726000 -2.052346000

H -3.832463000 0.647784000 1.182756000

H -3.685056000 -1.398097000 -0.288292000

C 4.057317000 0.090784000 -1.571664000

C 3.162916000 -0.261083000 -0.814377000

C 2.102156000 -0.670235000 0.055235000

C 1.673793000 0.184065000 1.100236000

C 1.458441000 -1.918845000 -0.135181000

C 0.615364000 -0.231076000 1.906775000

C 0.399145000 -2.298389000 0.699361000

C -0.040014000 -1.454178000 1.733252000

H 4.849821000 0.394051000 -2.228872000

H 2.133621000 1.161025000 1.254368000

H 1.788015000 -2.572654000 -0.946394000

F 0.193169000 0.602586000 2.906399000

H -0.103515000 -3.256169000 0.535640000

H -0.874144000 -1.722756000 2.385409000

2D9

C -1.040209000 3.812663000 -0.253966000

C -1.329735000 2.650560000 -0.003205000

C -1.654792000 1.284278000 0.272565000

C -0.887922000 0.551193000 1.209994000

C -2.729553000 0.650525000 -0.400086000

C -1.214406000 -0.785345000 1.435639000

C -3.024466000 -0.695236000 -0.143551000

C -2.265243000 -1.434932000 0.779834000

H -0.799578000 4.839018000 -0.455794000

H -0.042722000 1.006199000 1.728538000

H -3.319106000 1.221102000 -1.122260000

F -0.463505000 -1.494986000 2.331353000

H -3.852884000 -1.180030000 -0.669565000

H -2.468048000 -2.488644000 0.985399000

C 3.898252000 1.121321000 1.599936000

C 3.121910000 0.675000000 0.766009000

C 2.188636000 0.163614000 -0.191319000

C 1.810006000 -1.201167000 -0.151446000

C 1.614370000 1.020596000 -1.162530000

C 0.866339000 -1.655697000 -1.071386000

C 0.670241000 0.522105000 -2.069181000

C 0.281129000 -0.827193000 -2.034347000

H 4.591881000 1.507875000 2.322099000

H 2.221711000 -1.880500000 0.596977000

H 1.893488000 2.076377000 -1.178111000

F 0.485815000 -2.969343000 -1.018624000

H 0.213545000 1.196174000 -2.799468000

H -0.466424000 -1.232322000 -2.720136000

2D10

C -4.424940000 1.089672000 -1.098414000

C -3.518961000 0.522309000 -0.502765000

C -2.442177000 -0.129898000 0.178814000

C -2.059793000 -1.442537000 -0.194949000

C -1.735649000 0.535685000 1.210232000

C -0.984185000 -2.035204000 0.464578000

C -0.661621000 -0.098456000 1.848651000

C -0.269342000 -1.396497000 1.482931000

H -5.229076000 1.583179000 -1.610272000

H -2.583206000 -1.978822000 -0.989158000

H -2.016339000 1.555616000 1.481401000

F -0.602367000 -3.294038000 0.084862000

H -0.106727000 0.432141000 2.627525000

H 0.576944000 -1.900837000 1.954897000

C 0.354526000 3.870408000 0.552629000

C 0.790969000 2.805147000 0.137906000

C 1.277163000 1.542369000 -0.328056000

C 2.462902000 0.993855000 0.219817000

C 0.565089000 0.820784000 -1.317559000

C 2.888901000 -0.255079000 -0.232008000

C 1.027979000 -0.430525000 -1.742981000

C 2.200601000 -0.988176000 -1.204112000

H -0.014786000 4.817744000 0.896516000

H 3.031655000 1.526799000 0.984631000

H -0.359590000 1.237736000 -1.721802000

F 4.028644000 -0.788088000 0.308225000

H 0.463657000 -0.990015000 -2.494602000

H 2.572208000 -1.967560000 -1.515218000

2D11

C -0.335316000 3.523347000 0.479893000

C 0.285184000 2.563395000 0.043939000

C 0.991264000 1.425382000 -0.459935000

C 2.195246000 1.006675000 0.158012000

C 0.482132000 0.699583000 -1.565282000

C 2.846751000 -0.116679000 -0.349946000

C 1.168978000 -0.422626000 -2.044690000

C 2.366755000 -0.845990000 -1.442889000

H -0.869901000 4.375309000 0.854469000

H 2.602064000 1.538222000 1.020290000

H -0.458377000 1.013986000 -2.022819000

F 4.005362000 -0.526809000 0.253502000

H 0.765113000 -0.983489000 -2.892793000

H 2.917585000 -1.720211000 -1.799228000

C -4.398842000 0.710615000 -1.128705000

C -3.468873000 0.114879000 -0.601734000

C -2.364092000 -0.572726000 -0.005380000

C -1.685036000 0.001037000 1.096473000

C -1.925989000 -1.816364000 -0.525948000

C -0.588723000 -0.676766000 1.628621000

C -0.819087000 -2.463760000 0.038250000

C -0.130486000 -1.898001000 1.124854000

H -5.224288000 1.227020000 -1.580415000

H -1.982696000 0.968433000 1.503189000

H -2.454701000 -2.256427000 -1.375362000

F 0.074774000 -0.113031000 2.682488000

H -0.478991000 -3.418249000 -0.375101000

H 0.743780000 -2.378050000 1.570672000

2D12

C 3.180054000 1.275185000 -1.715919000

C 2.140094000 1.436419000 -1.093782000

C 0.924379000 1.600006000 -0.361460000

C -0.317935000 1.503082000 -1.028921000

C 0.951046000 1.841049000 1.032114000

C -1.486162000 1.644515000 -0.285653000

C -0.246013000 1.978578000 1.742412000

C -1.485660000 1.880312000 1.090971000

H 4.095990000 1.150794000 -2.259373000

H -0.363942000 1.302318000 -2.099219000

H 1.912942000 1.897127000 1.543620000

F -2.685658000 1.536339000 -0.933092000

H -0.219051000 2.157421000 2.820745000

H -2.430669000 1.969570000 1.630067000

C 3.158040000 -1.314454000 1.717835000

C 2.116615000 -1.461880000 1.094738000

C 0.899382000 -1.610260000 0.361701000

C 0.923769000 -1.850601000 -1.032059000

C -0.341952000 -1.499378000 1.028761000

C -0.274534000 -1.974114000 -1.742815000

C -1.511480000 -1.627097000 0.285025000

C -1.513211000 -1.862179000 -1.091700000

H 4.075050000 -1.202055000 2.262084000

H 1.885168000 -1.917195000 -1.543242000

H -0.386077000 -1.298744000 2.099163000

H -0.249267000 -2.152530000 -2.821259000

F -2.709872000 -1.505384000 0.932106000

H -2.458969000 -1.940399000 -1.631190000

2D13

C -2.438047000 3.654570000 -0.159682000

C -2.523665000 2.436709000 -0.078496000

C -2.587856000 1.008948000 0.001948000

C -2.111261000 0.344396000 1.158331000

C -3.099641000 0.248758000 -1.080164000

C -2.154141000 -1.049354000 1.192538000

C -3.125203000 -1.151271000 -1.005550000

C -2.648387000 -1.820987000 0.135139000

H -2.386429000 4.724958000 -0.223313000

H -1.699611000 0.902687000 2.001155000

H -3.465103000 0.765217000 -1.971130000

F -1.682940000 -1.686459000 2.304365000

H -3.513944000 -1.732791000 -1.846952000

H -2.647413000 -2.911141000 0.208413000

C 5.680346000 0.829608000 0.843099000

C 4.544104000 0.595997000 0.453534000

C 3.214048000 0.325863000 -0.003112000

C 2.846576000 -0.991317000 -0.376002000

C 2.254888000 1.367444000 -0.086091000

C 1.542657000 -1.218480000 -0.817264000

C 0.954825000 1.094697000 -0.532847000

C 0.581236000 -0.207637000 -0.907525000

H 6.676744000 1.034380000 1.185943000

H 3.562218000 -1.814218000 -0.320519000

H 2.542141000 2.381463000 0.203848000

F 1.189807000 -2.493108000 -1.174478000

H 0.215689000 1.899492000 -0.585306000

H -0.428982000 -0.441611000 -1.248259000

2D14

C -5.818198000 0.804335000 0.734641000

C -4.662720000 0.562083000 0.412806000

C -3.309912000 0.281809000 0.035873000

C -2.939810000 -1.030301000 -0.352188000

C -2.331083000 1.308051000 0.047012000

C -1.613444000 -1.267700000 -0.713912000

C -1.008790000 1.025450000 -0.322170000

C -0.631895000 -0.272012000 -0.710309000

H -6.831616000 1.016414000 1.017934000

H -3.670684000 -1.841427000 -0.369195000

H -2.620803000 2.318312000 0.347413000

F -1.258686000 -2.537008000 -1.087709000

H -0.256713000 1.819608000 -0.307345000

H 0.393279000 -0.512932000 -0.996453000

C 2.299826000 3.698357000 -0.196757000

C 2.451023000 2.485653000 -0.137491000

C 2.590744000 1.062208000 -0.077482000

C 2.280166000 0.372023000 1.119939000

C 3.013746000 0.330927000 -1.216264000

C 2.396452000 -1.017972000 1.138554000

C 3.117258000 -1.066181000 -1.155922000

C 2.806768000 -1.761444000 0.026255000

H 2.190737000 4.765250000 -0.244683000

H 1.940891000 0.907357000 2.008735000

H 3.248984000 0.866816000 -2.139004000

F 2.087458000 -1.680236000 2.291743000

H 3.436554000 -1.625562000 -2.040339000

H 2.869635000 -2.850353000 0.091124000

2D15

C -1.490520000 3.625533000 -0.494822000

C -1.867335000 2.502304000 -0.190220000

C -2.264169000 1.173942000 0.165425000

C -2.874399000 0.333219000 -0.798823000

C -2.026499000 0.680178000 1.472536000

C -3.223192000 -0.965366000 -0.425517000

C -2.389763000 -0.631453000 1.806205000

C -2.995204000 -1.475045000 0.858126000

H -1.172034000 4.616039000 -0.759045000

H -3.064485000 0.684269000 -1.814994000

H -1.544943000 1.327794000 2.208889000

F -3.808358000 -1.775492000 -1.358049000

H -2.195095000 -1.008565000 2.814678000

H -3.283876000 -2.501768000 1.096458000

C 3.746201000 3.053384000 0.040152000

C 3.248476000 1.936846000 -0.014362000

C 2.663771000 0.630933000 -0.077595000

C 3.491289000 -0.518694000 -0.015581000

C 1.259983000 0.476528000 -0.199921000

C 2.889847000 -1.775660000 -0.078908000

C 0.696546000 -0.805364000 -0.259605000

C 1.506951000 -1.952485000 -0.200562000

H 4.184018000 4.032209000 0.087601000

H 4.575636000 -0.430632000 0.079443000

H 0.624556000 1.363591000 -0.247513000

F 3.690989000 -2.884375000 -0.018629000

H -0.386782000 -0.916134000 -0.348638000

H 1.087427000 -2.960813000 -0.245947000

2D16

C -2.022427000 -1.085005000 0.132616000

C -3.081521000 -2.027252000 0.134158000

C -2.314576000 0.294131000 -0.018134000

C -4.407500000 -1.596055000 -0.012368000

C -3.646731000 0.679532000 -0.160746000

C -4.709629000 -0.230625000 -0.162359000

C -0.661241000 -1.502588000 0.280931000

C 0.512065000 -1.824796000 0.403725000

H -2.852571000 -3.089777000 0.250104000

H -1.516411000 1.039890000 -0.023397000

H -5.220521000 -2.329166000 -0.010551000

F -3.925751000 2.013628000 -0.306034000

H -5.736129000 0.126570000 -0.277979000

H 1.552623000 -2.065244000 0.511441000

C 2.136587000 1.177834000 0.192505000

C 2.568648000 0.783053000 1.483237000

C 2.693781000 0.555461000 -0.951520000

C 3.538709000 -0.218113000 1.624855000

C 3.657220000 -0.436194000 -0.768310000

C 4.097676000 -0.845064000 0.496161000

C 1.135573000 2.189265000 0.039572000

C 0.276523000 3.051152000 -0.088522000

H 2.130759000 1.260555000 2.363016000

H 2.374059000 0.833114000 -1.957771000

H 3.865668000 -0.519894000 2.624706000

F 4.191100000 -1.038229000 -1.873577000

H 4.857013000 -1.626235000 0.583218000

H -0.481580000 3.803191000 -0.201074000

2D17

C -6.080539000 0.389928000 -0.719424000

C -4.888712000 0.255190000 -0.477145000

C -3.493296000 0.100032000 -0.195300000

C -3.034157000 -1.046282000 0.500794000

C -2.560708000 1.085791000 -0.606777000

C -1.668260000 -1.165748000 0.758515000

C -1.196473000 0.925375000 -0.327132000

C -0.729903000 -0.207577000 0.361704000

H -7.125969000 0.508313000 -0.932085000

H -3.728252000 -1.822158000 0.830370000

H -2.918471000 1.968682000 -1.142627000

F -1.228751000 -2.273980000 1.432333000

H -0.483329000 1.690104000 -0.646796000

H 0.327648000 -0.352406000 0.587711000

C 3.370003000 -2.588956000 -2.118165000

C 3.164943000 -1.663126000 -1.345522000

C 2.919866000 -0.583406000 -0.438813000

C 2.545327000 0.689452000 -0.937572000

C 3.037554000 -0.776186000 0.961276000

C 2.301827000 1.716873000 -0.026537000

C 2.783010000 0.284207000 1.842423000

C 2.408912000 1.550297000 1.358155000

H 3.549401000 -3.402118000 -2.795678000

H 2.438751000 0.866183000 -2.009624000

H 3.319666000 -1.760230000 1.343128000

F 1.926249000 2.940138000 -0.513022000

H 2.869078000 0.125430000 2.921462000

H 2.197639000 2.387611000 2.027467000

2D18

C -5.133013000 2.472983000 0.480967000

C -4.230753000 1.662907000 0.316462000

C -3.172618000 0.717051000 0.125677000

C -3.468674000 -0.599619000 -0.307824000

C -1.824649000 1.084962000 0.366776000

C -2.413910000 -1.495861000 -0.483974000

C -0.794665000 0.153451000 0.178199000

C -1.076951000 -1.154831000 -0.251895000

H -5.924584000 3.183748000 0.623966000

H -4.496609000 -0.912761000 -0.502057000

H -1.599256000 2.101498000 0.699515000

F -2.704499000 -2.766052000 -0.902938000

H 0.240784000 0.445196000 0.367411000

H -0.289526000 -1.895548000 -0.406940000

C 3.398534000 3.015251000 -1.803734000

C 3.178476000 2.062007000 -1.069389000

C 2.914651000 0.950315000 -0.207461000

C 2.736810000 -0.344966000 -0.755192000

C 2.818339000 1.133039000 1.195735000

C 2.470017000 -1.404008000 0.112273000

C 2.546466000 0.040890000 2.031701000

C 2.366966000 -1.247605000 1.498517000

H 3.593139000 3.850618000 -2.449336000

H 2.797391000 -0.515853000 -1.831742000

H 2.953594000 2.133261000 1.614531000

F 2.284688000 -2.650189000 -0.421464000

H 2.467340000 0.191054000 3.112565000

H 2.145870000 -2.110834000 2.130682000

2D19

C -0.356547000 -1.533595000 0.480943000

C 0.756249000 -1.052035000 0.321859000

C 2.042362000 -0.454522000 0.127448000

C 3.215563000 -1.248477000 0.170107000

C 2.149799000 0.939625000 -0.110279000

C 4.449000000 -0.626560000 -0.025126000

C 3.409387000 1.523821000 -0.301510000

C 4.580824000 0.746308000 -0.261388000

H -1.349970000 -1.916051000 0.618604000

H 3.163715000 -2.324243000 0.350774000

H 1.241000000 1.546500000 -0.142184000

F 5.580317000 -1.396204000 0.016705000

H 3.486481000 2.600425000 -0.485094000

H 5.572468000 1.182090000 -0.408048000

C -0.948568000 3.265670000 -0.224168000

C -1.646001000 2.274417000 -0.056643000

C -2.461081000 1.114960000 0.142507000

C -2.898475000 0.358099000 -0.972047000

C -2.829435000 0.711295000 1.450092000

C -3.683795000 -0.771684000 -0.743764000

C -3.619419000 -0.430813000 1.637314000

C -4.058002000 -1.191922000 0.538247000

H -0.348768000 4.143577000 -0.371279000

H -2.622974000 0.640178000 -1.990046000

H -2.483494000 1.293935000 2.307173000

F -4.102067000 -1.502754000 -1.820297000

H -3.897839000 -0.738486000 2.649942000

H -4.676038000 -2.084830000 0.660934000

2D20

C -0.712732000 2.009693000 -0.034412000

C -1.745133000 1.364971000 0.093049000

C -2.953898000 0.612619000 0.244964000

C -3.596906000 0.066529000 -0.894234000

C -3.516222000 0.403615000 1.529866000

C -4.771268000 -0.664099000 -0.711592000

C -4.698292000 -0.336696000 1.669621000

C -5.344308000 -0.882715000 0.546267000

H 0.217648000 2.539182000 -0.143469000

H -3.188710000 0.211412000 -1.896777000

H -3.018500000 0.826625000 2.406291000

F -5.388793000 -1.189235000 -1.813402000

H -5.126671000 -0.492935000 2.664820000

H -6.266735000 -1.462664000 0.632692000

C 2.773917000 3.303725000 -0.368138000

C 2.973814000 2.102531000 -0.243118000

C 3.231778000 0.700368000 -0.098454000

C 4.569794000 0.232088000 -0.113216000

C 2.168034000 -0.223143000 0.058855000

C 4.798063000 -1.136574000 0.029064000

C 2.442577000 -1.590755000 0.198506000

C 3.765133000 -2.067715000 0.185517000

H 2.604694000 4.358149000 -0.478878000

H 5.408986000 0.920597000 -0.232923000

H 1.136218000 0.136373000 0.070602000

F 6.089964000 -1.585757000 0.014556000

H 1.616519000 -2.298598000 0.319253000

H 3.999907000 -3.129885000 0.292738000