

Optimized Cartesian coordinates of all optimized structures.

A

| | | | |
|---|--------------|--------------|--------------|
| P | 1.805423000 | -0.455813000 | -0.194108000 |
| P | -1.784517000 | 0.293699000 | 0.134033000 |
| O | 0.753568000 | -2.134747000 | 4.140727000 |
| O | 0.166359000 | -0.579833000 | 5.735661000 |
| O | -1.336612000 | -3.775821000 | 2.535823000 |
| O | -0.691423000 | -5.666659000 | 1.385306000 |
| O | -5.361240000 | -4.515408000 | -0.235885000 |
| O | -5.161062000 | 5.223074000 | -0.452972000 |
| O | 4.417040000 | 1.053622000 | 5.028620000 |
| O | 6.039261000 | -0.883968000 | -4.436584000 |
| C | -1.166469000 | 0.086537000 | 1.873704000 |
| C | -0.346531000 | -1.040731000 | 2.208047000 |
| C | 0.000599000 | -1.142728000 | 3.548294000 |
| C | -0.358742000 | -0.208403000 | 4.517130000 |
| C | -1.112898000 | 0.899548000 | 4.203114000 |
| C | -1.515919000 | 1.017171000 | 2.860900000 |
| C | 0.575044000 | -1.937941000 | 5.542493000 |
| C | 1.086633000 | -2.100196000 | 0.278618000 |
| C | 1.467860000 | -3.262216000 | -0.400907000 |
| C | 0.924296000 | -4.526579000 | -0.115009000 |
| C | -0.010934000 | -4.576005000 | 0.893425000 |
| C | -0.403554000 | -3.429201000 | 1.580834000 |
| C | 0.090374000 | -2.161047000 | 1.308545000 |
| C | -1.281116000 | -5.201541000 | 2.600854000 |
| C | -2.962886000 | -1.120137000 | -0.001864000 |
| C | -3.749965000 | -1.516602000 | 1.090260000 |
| C | -4.619556000 | -2.606499000 | 1.016919000 |
| C | -4.658165000 | -3.318782000 | -0.214341000 |
| C | -4.027797000 | -2.841453000 | -1.383771000 |
| C | -3.132647000 | -1.766120000 | -1.224235000 |
| C | -4.261506000 | -3.349053000 | -2.834601000 |
| C | -2.975714000 | -4.017031000 | -3.378694000 |
| C | -5.457036000 | -4.311406000 | -3.023171000 |
| C | -4.587516000 | -2.111885000 | -3.717623000 |
| C | -5.549631000 | -2.952393000 | 2.208939000 |
| C | -7.023092000 | -2.935456000 | 1.731417000 |
| C | -5.422722000 | -1.915218000 | 3.346696000 |
| C | -5.227760000 | -4.331377000 | 2.830314000 |
| C | -4.520702000 | -5.669380000 | -0.205470000 |
| C | -2.881077000 | 1.782804000 | 0.171160000 |
| C | -2.296565000 | 3.057916000 | 0.236904000 |

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| C | -4.266813000 | 1.695860000 | 0.058423000 |
| C | -5.092127000 | 2.828358000 | -0.061869000 |
| C | -4.442790000 | 4.079308000 | -0.136263000 |
| C | -3.052658000 | 4.228556000 | 0.127749000 |
| C | -2.399450000 | 5.614772000 | 0.367500000 |
| C | -0.934180000 | 5.474342000 | 0.832592000 |
| C | -2.387323000 | 6.497822000 | -0.902767000 |
| C | -5.409344000 | 5.379100000 | -1.850648000 |
| C | -3.166958000 | 6.347730000 | 1.496818000 |
| C | -6.627894000 | 2.580891000 | -0.060155000 |
| C | -7.054735000 | 1.903622000 | -1.384704000 |
| C | -7.503284000 | 3.834404000 | 0.172877000 |
| C | -6.969089000 | 1.619664000 | 1.112309000 |
| C | 2.660218000 | 0.023317000 | 1.374721000 |
| C | 2.532388000 | 1.310831000 | 1.900209000 |
| C | 3.119463000 | 1.674228000 | 3.121464000 |
| C | 3.859688000 | 0.678546000 | 3.815733000 |
| C | 4.098571000 | -0.610649000 | 3.266279000 |
| C | 3.444998000 | -0.906191000 | 2.061549000 |
| C | 5.026566000 | -1.700962000 | 3.878725000 |
| C | 6.295232000 | -1.102722000 | 4.532635000 |
| C | 4.247163000 | -2.581633000 | 4.887248000 |
| C | 5.543390000 | -2.669643000 | 2.782791000 |
| C | 4.404479000 | 3.777867000 | 3.686871000 |
| C | 3.811389000 | 0.580425000 | 6.232138000 |
| C | 2.996957000 | 3.133961000 | 3.635825000 |
| C | 2.122407000 | 3.995708000 | 2.700702000 |
| C | 5.079109000 | -0.927477000 | -3.436153000 |
| C | 5.499927000 | -0.582504000 | -2.123975000 |
| C | 7.810875000 | -1.613992000 | -2.112740000 |
| C | 4.518611000 | -0.521391000 | -1.125787000 |
| C | 3.170727000 | -0.780873000 | -1.397813000 |
| C | 2.814398000 | -1.187726000 | -2.687574000 |
| C | 3.754003000 | -1.341073000 | -3.719217000 |
| C | 5.975505000 | 0.249716000 | -5.302680000 |
| C | 7.593225000 | 0.876437000 | -2.499660000 |
| C | 2.535203000 | -0.880790000 | -5.910044000 |
| C | 3.248859000 | -1.957462000 | -5.055790000 |
| C | 2.207644000 | -3.069933000 | -4.748546000 |
| C | 7.179879000 | -0.081470000 | -0.255336000 |
| C | 2.336238000 | 3.219185000 | 5.033765000 |
| C | 6.991471000 | -0.346215000 | -1.764814000 |
| C | 4.356472000 | -2.646244000 | -5.888202000 |
| H | -1.402829000 | 1.628216000 | 4.952360000 |

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|---|--------------|--------------|--------------|
| H | -2.147230000 | 1.855706000 | 2.591207000 |
| H | 1.519707000 | -2.111375000 | 6.057922000 |
| H | -0.214598000 | -2.610723000 | 5.910038000 |
| H | 2.221946000 | -3.194299000 | -1.175787000 |
| H | 1.236605000 | -5.416005000 | -0.651205000 |
| H | -2.291685000 | -5.602329000 | 2.691673000 |
| H | -0.652909000 | -5.504755000 | 3.452605000 |
| H | -3.662265000 | -0.965463000 | 2.017266000 |
| H | -2.527983000 | -1.447078000 | -2.064719000 |
| H | -2.129715000 | -3.323410000 | -3.379371000 |
| H | -3.136202000 | -4.351476000 | -4.411561000 |
| H | -2.697374000 | -4.894904000 | -2.783496000 |
| H | -5.288261000 | -5.306818000 | -2.610932000 |
| H | -5.627461000 | -4.436117000 | -4.099526000 |
| H | -6.375566000 | -3.914152000 | -2.581495000 |
| H | -5.483819000 | -1.596895000 | -3.351347000 |
| H | -4.782895000 | -2.439057000 | -4.746047000 |
| H | -3.765799000 | -1.394830000 | -3.755804000 |
| H | -7.691860000 | -3.166251000 | 2.570387000 |
| H | -7.195385000 | -3.669837000 | 0.942170000 |
| H | -7.296449000 | -1.944751000 | 1.349172000 |
| H | -6.137271000 | -2.165720000 | 4.138903000 |
| H | -5.650843000 | -0.898575000 | 3.008524000 |
| H | -4.422615000 | -1.912374000 | 3.794999000 |
| H | -4.171587000 | -4.385718000 | 3.117491000 |
| H | -5.454845000 | -5.150708000 | 2.147883000 |
| H | -5.827993000 | -4.479072000 | 3.736859000 |
| H | -3.856462000 | -5.655904000 | 0.666988000 |
| H | -3.902551000 | -5.748652000 | -1.105555000 |
| H | -5.186205000 | -6.534670000 | -0.146030000 |
| H | -1.222938000 | 3.128708000 | 0.365484000 |
| H | -4.723747000 | 0.715210000 | 0.050602000 |
| H | -0.538100000 | 6.469007000 | 1.065592000 |
| H | -0.287137000 | 5.041324000 | 0.062993000 |
| H | -0.850375000 | 4.867704000 | 1.740959000 |
| H | -3.388281000 | 6.831202000 | -1.178690000 |
| H | -1.943007000 | 5.963446000 | -1.750296000 |
| H | -1.780489000 | 7.393409000 | -0.721190000 |
| H | -6.062522000 | 4.589615000 | -2.238410000 |
| H | -4.475690000 | 5.374400000 | -2.424685000 |
| H | -5.905272000 | 6.346143000 | -1.969021000 |
| H | -4.213467000 | 6.510402000 | 1.232372000 |
| H | -2.703298000 | 7.323533000 | 1.688759000 |
| H | -3.129361000 | 5.771223000 | 2.429012000 |

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| H | -6.517013000 | 0.962906000 | -1.546096000 |
| H | -6.860575000 | 2.547993000 | -2.249393000 |
| H | -8.128737000 | 1.679864000 | -1.368386000 |
| H | -8.536488000 | 3.506563000 | 0.340633000 |
| H | -7.517753000 | 4.520021000 | -0.674452000 |
| H | -7.180844000 | 4.395906000 | 1.054394000 |
| H | -6.662169000 | 2.050339000 | 2.072413000 |
| H | -6.494300000 | 0.639920000 | 1.014427000 |
| H | -8.052130000 | 1.453633000 | 1.147229000 |
| H | 1.945992000 | 2.033640000 | 1.347809000 |
| H | 3.553176000 | -1.893865000 | 1.632952000 |
| H | 6.084235000 | -0.440647000 | 5.369963000 |
| H | 6.868005000 | -0.525569000 | 3.797413000 |
| H | 6.936495000 | -1.917335000 | 4.889990000 |
| H | 4.889665000 | -3.393096000 | 5.251637000 |
| H | 3.371880000 | -3.028643000 | 4.403788000 |
| H | 3.900565000 | -2.021974000 | 5.758417000 |
| H | 6.290588000 | -3.338424000 | 3.224194000 |
| H | 6.021723000 | -2.132306000 | 1.958043000 |
| H | 4.755376000 | -3.305497000 | 2.367649000 |
| H | 4.331803000 | 4.810841000 | 4.050301000 |
| H | 4.855325000 | 3.805981000 | 2.687640000 |
| H | 5.071973000 | 3.224632000 | 4.351007000 |
| H | 4.338657000 | -0.299183000 | 6.615984000 |
| H | 2.752013000 | 0.344539000 | 6.085996000 |
| H | 3.899725000 | 1.378334000 | 6.975124000 |
| H | 1.092886000 | 3.623313000 | 2.649793000 |
| H | 2.514934000 | 4.056952000 | 1.682416000 |
| H | 2.082619000 | 5.017548000 | 3.094062000 |
| H | 7.450437000 | -2.477283000 | -1.540659000 |
| H | 8.867275000 | -1.460098000 | -1.857908000 |
| H | 7.743825000 | -1.852043000 | -3.175927000 |
| H | 4.800440000 | -0.244149000 | -0.120243000 |
| H | 1.767421000 | -1.379879000 | -2.894012000 |
| H | 6.950284000 | 0.320290000 | -5.793499000 |
| H | 5.782625000 | 1.171160000 | -4.742342000 |
| H | 5.203545000 | 0.132086000 | -6.069432000 |
| H | 8.582123000 | 1.105232000 | -2.083325000 |
| H | 6.964700000 | 1.765625000 | -2.370723000 |
| H | 7.724021000 | 0.692360000 | -3.565372000 |
| H | 3.209367000 | -0.072002000 | -6.208475000 |
| H | 1.702614000 | -0.430357000 | -5.359389000 |
| H | 2.133112000 | -1.334461000 | -6.825066000 |
| H | 1.928537000 | -3.567552000 | -5.684584000 |

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| H | 1.285938000 | -2.687444000 | -4.303295000 |
| H | 2.628296000 | -3.829634000 | -4.078953000 |
| H | 6.813935000 | -0.911258000 | 0.357604000 |
| H | 6.678631000 | 0.836095000 | 0.073593000 |
| H | 8.248743000 | 0.034447000 | -0.044328000 |
| H | 1.410948000 | 2.632762000 | 5.070894000 |
| H | 2.077974000 | 4.262639000 | 5.251471000 |
| H | 2.998032000 | 2.878944000 | 5.827906000 |
| H | 3.885021000 | -3.195705000 | -6.711879000 |
| H | 4.916199000 | -3.367189000 | -5.282463000 |
| H | 5.075761000 | -1.954787000 | -6.324613000 |
| Cu | 0.002572000 | 0.475499000 | -1.329041000 |
| N | 0.025512000 | 1.795647000 | -3.054461000 |
| C | 0.284513000 | 3.064572000 | -3.219990000 |
| C | -0.653808000 | 1.117761000 | -4.038105000 |
| C | 1.203650000 | 3.872673000 | -2.432536000 |
| C | 1.196250000 | 5.273509000 | -2.606616000 |
| C | 2.190857000 | 3.320064000 | -1.590212000 |
| C | 2.119812000 | 6.088340000 | -1.956069000 |
| H | 0.457697000 | 5.718299000 | -3.270425000 |
| C | 3.121905000 | 4.136581000 | -0.953295000 |
| H | 2.245939000 | 2.242449000 | -1.482808000 |
| C | 3.091528000 | 5.525210000 | -1.124747000 |
| H | 2.088032000 | 7.164612000 | -2.106447000 |
| H | 3.891778000 | 3.682684000 | -0.333974000 |
| H | 3.823650000 | 6.156226000 | -0.628380000 |
| C | -0.821234000 | -0.262073000 | -3.903468000 |
| O | -0.472146000 | -0.941234000 | -2.891541000 |
| O | -1.392586000 | -1.011789000 | -4.903161000 |
| C | -1.787614000 | -0.384522000 | -6.116008000 |
| H | -0.933763000 | 0.081349000 | -6.623299000 |
| H | -2.193353000 | -1.178992000 | -6.745992000 |
| H | -2.563442000 | 0.372634000 | -5.945657000 |
| H | -0.947525000 | 1.658133000 | -4.933345000 |
| H | -0.147856000 | 3.571416000 | -4.092165000 |

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|---|--------------|--------------|--------------|
| C | -1.362430000 | 1.329915000 | -0.000011000 |
| C | 0.008971000 | 1.092829000 | 0.000012000 |
| C | 0.515336000 | -0.220503000 | 0.000033000 |
| C | -0.406495000 | -1.281617000 | 0.000013000 |
| C | -1.781277000 | -1.046456000 | 0.000020000 |
| C | -2.265782000 | 0.261843000 | -0.000017000 |
| H | -1.730752000 | 2.352570000 | -0.000051000 |

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| H | 0.694090000 | 1.935650000 | 0.000039000 |
| H | -0.035038000 | -2.304033000 | 0.000025000 |
| H | -2.472438000 | -1.885226000 | 0.000036000 |
| H | -3.335871000 | 0.450627000 | -0.000079000 |
| C | 1.955042000 | -0.529522000 | -0.000049000 |
| H | 2.186652000 | -1.594877000 | -0.000099000 |
| C | 2.977889000 | 0.335058000 | 0.000008000 |
| H | 2.840909000 | 1.413097000 | 0.000125000 |
| H | 4.004931000 | -0.017091000 | -0.000044000 |

TS1^H

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| P | 1.679556000 | -0.868544000 | -0.459466000 |
| P | -1.832888000 | -0.311782000 | 0.366990000 |
| O | 0.528203000 | -4.825380000 | 1.934064000 |
| O | -0.023854000 | -4.590396000 | 4.158557000 |
| O | -1.597053000 | -5.068764000 | -0.274841000 |
| O | -1.039333000 | -5.854137000 | -2.366683000 |
| O | -5.279869000 | -3.645024000 | -3.242418000 |
| O | -5.155209000 | 3.956319000 | 2.971177000 |
| O | 4.354280000 | -3.026290000 | 4.479725000 |
| O | 5.524465000 | 1.577535000 | -4.321334000 |
| C | -1.303117000 | -1.618656000 | 1.575106000 |
| C | -0.523470000 | -2.733755000 | 1.122223000 |
| C | -0.188911000 | -3.659753000 | 2.100878000 |
| C | -0.528217000 | -3.525342000 | 3.445294000 |
| C | -1.250366000 | -2.445333000 | 3.900012000 |
| C | -1.636328000 | -1.502235000 | 2.930905000 |
| C | 0.350974000 | -5.540702000 | 3.156458000 |
| C | 0.852589000 | -2.403783000 | -1.093007000 |
| C | 1.175514000 | -2.901245000 | -2.361693000 |
| C | 0.586868000 | -4.057286000 | -2.902529000 |
| C | -0.329215000 | -4.704564000 | -2.105182000 |
| C | -0.667535000 | -4.221925000 | -0.842001000 |
| C | -0.130686000 | -3.067397000 | -0.287923000 |
| C | -1.565522000 | -6.238353000 | -1.093889000 |
| C | -2.987874000 | -1.251049000 | -0.724983000 |
| C | -3.846406000 | -2.228474000 | -0.197973000 |
| C | -4.691032000 | -2.986144000 | -1.011479000 |
| C | -4.613002000 | -2.754664000 | -2.413417000 |
| C | -3.907271000 | -1.661087000 | -2.960424000 |
| C | -3.058909000 | -0.954633000 | -2.085327000 |
| C | -4.012871000 | -1.130435000 | -4.418361000 |
| C | -2.666073000 | -1.332505000 | -5.153219000 |
| C | -5.150485000 | -1.734732000 | -5.273801000 |

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| C | -4.314180000 | 0.392233000 | -4.349122000 |
| C | -5.722286000 | -3.961219000 | -0.385524000 |
| C | -7.143995000 | -3.568503000 | -0.859072000 |
| C | -5.711753000 | -3.883135000 | 1.157174000 |
| C | -5.450133000 | -5.437525000 | -0.754800000 |
| C | -4.413941000 | -4.592802000 | -3.869612000 |
| C | -2.935616000 | 0.832893000 | 1.311722000 |
| C | -2.351215000 | 1.736560000 | 2.214023000 |
| C | -4.311439000 | 0.903551000 | 1.104139000 |
| C | -5.121533000 | 1.881498000 | 1.710321000 |
| C | -4.462906000 | 2.852345000 | 2.496829000 |
| C | -3.090931000 | 2.733728000 | 2.855357000 |
| C | -2.440577000 | 3.606522000 | 3.960730000 |
| C | -1.005063000 | 3.134975000 | 4.279575000 |
| C | -2.347278000 | 5.100593000 | 3.568868000 |
| C | -5.316386000 | 4.998170000 | 2.008546000 |
| C | -3.265197000 | 3.467178000 | 5.265479000 |
| C | -6.655879000 | 1.762271000 | 1.481608000 |
| C | -7.001785000 | 2.131451000 | 0.018928000 |
| C | -7.537475000 | 2.599708000 | 2.437369000 |
| C | -7.076506000 | 0.286115000 | 1.724590000 |
| C | 2.599315000 | -1.505719000 | 1.005154000 |
| C | 2.542065000 | -0.802622000 | 2.210747000 |
| C | 3.138235000 | -1.287758000 | 3.381731000 |
| C | 3.807356000 | -2.539413000 | 3.302962000 |
| C | 3.985583000 | -3.230078000 | 2.073245000 |
| C | 3.328106000 | -2.696202000 | 0.954295000 |
| C | 4.848594000 | -4.510496000 | 1.871742000 |
| C | 6.116832000 | -4.525904000 | 2.758670000 |
| C | 3.999849000 | -5.784660000 | 2.106477000 |
| C | 5.367067000 | -4.600179000 | 0.412691000 |
| C | 4.541657000 | -0.062427000 | 5.092060000 |
| C | 3.675771000 | -4.090199000 | 5.148121000 |
| C | 3.096529000 | -0.434956000 | 4.677971000 |
| C | 2.322501000 | 0.884384000 | 4.465106000 |
| C | 4.680351000 | 0.812716000 | -3.527542000 |
| C | 5.227538000 | 0.102526000 | -2.430348000 |
| C | 7.277774000 | -0.820305000 | -3.569899000 |
| C | 4.317389000 | -0.481702000 | -1.532659000 |
| C | 2.936040000 | -0.399698000 | -1.726116000 |
| C | 2.454181000 | 0.174336000 | -2.911198000 |
| C | 3.305366000 | 0.734256000 | -3.870797000 |
| C | 5.605104000 | 2.950156000 | -3.905643000 |
| C | 7.576820000 | 1.129664000 | -2.000704000 |

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| C | 2.819627000 | 2.618086000 | -5.604888000 |
| C | 2.753175000 | 1.108475000 | -5.274605000 |
| C | 1.274283000 | 0.682884000 | -5.422139000 |
| C | 7.044249000 | -1.122029000 | -1.110590000 |
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| H | -4.622259000 | -1.277371000 | 0.650553000 |
| H | -1.319265000 | 0.108834000 | 2.969250000 |
| H | -6.381478000 | 2.736448000 | 4.988414000 |
| H | -6.250101000 | 2.450393000 | 3.230192000 |
| H | -4.810869000 | 2.917210000 | 4.156581000 |
| H | -8.645985000 | 0.034359000 | 2.085396000 |
| H | -7.353091000 | 1.096066000 | 1.511908000 |
| H | -7.719806000 | 0.977538000 | 3.248757000 |
| H | -3.771079000 | 2.540114000 | 5.888897000 |
| H | -2.377451000 | 2.876229000 | 4.833010000 |
| H | -2.135898000 | 2.451784000 | 6.533901000 |
| H | -0.793517000 | 0.526144000 | 6.389245000 |
| H | -0.518777000 | 0.975316000 | 4.702688000 |
| H | -0.978023000 | -0.687101000 | 5.118137000 |
| H | -6.293327000 | -2.591221000 | 1.258992000 |
| H | -6.755487000 | -1.185322000 | 0.275572000 |
| H | -7.966114000 | -2.024608000 | 1.251345000 |
| H | -1.519514000 | -0.782684000 | -5.630568000 |
| H | -2.456674000 | 0.329207000 | -6.641519000 |
| H | -3.034691000 | -1.314410000 | -6.388364000 |
| H | -2.940782000 | 0.129106000 | 7.359970000 |
| H | -3.246488000 | -1.164279000 | 6.188738000 |
| H | -4.438611000 | 0.132937000 | 6.407360000 |
| Cu | -0.210706000 | 0.895227000 | 0.257079000 |
| N | -0.235804000 | 2.801122000 | 0.597141000 |
| C | -0.927767000 | 3.909237000 | -0.015266000 |
| C | 0.905045000 | 3.403671000 | 1.233109000 |
| C | -2.331015000 | 3.637683000 | -0.517206000 |
| C | -2.815342000 | 4.311093000 | -1.647194000 |
| C | -3.207996000 | 2.797806000 | 0.183422000 |
| C | -4.138943000 | 4.157576000 | -2.066565000 |
| H | -2.149795000 | 4.973833000 | -2.195398000 |
| C | -4.527563000 | 2.630101000 | -0.241319000 |
| H | -2.842811000 | 2.277983000 | 1.062880000 |
| C | -5.001008000 | 3.311729000 | -1.365746000 |
| H | -4.493792000 | 4.696165000 | -2.942012000 |
| H | -5.184615000 | 1.962075000 | 0.309490000 |
| H | -6.030705000 | 3.185547000 | -1.691602000 |
| C | 1.506269000 | 2.521157000 | 2.317632000 |
| O | 0.958387000 | 1.546033000 | 2.798311000 |
| O | 2.730444000 | 2.834502000 | 2.818287000 |
| C | 3.555909000 | 3.865508000 | 2.267005000 |

| | | | |
|---|--------------|--------------|--------------|
| H | 3.069963000 | 4.843788000 | 2.308007000 |
| H | 4.447869000 | 3.882430000 | 2.896702000 |
| H | 3.844224000 | 3.633648000 | 1.237027000 |
| H | 1.722833000 | 3.644351000 | 0.517464000 |
| H | -0.357666000 | 4.351913000 | -0.865921000 |
| C | -0.938415000 | 5.021684000 | 1.115159000 |
| C | 0.410524000 | 4.778187000 | 1.831685000 |
| H | -1.750610000 | 4.745720000 | 1.795343000 |
| H | 1.124440000 | 5.584189000 | 1.635493000 |
| C | -1.181035000 | 6.434139000 | 0.633935000 |
| C | -2.381586000 | 7.091749000 | 0.939507000 |
| C | -0.245587000 | 7.119043000 | -0.160214000 |
| C | -2.640172000 | 8.383822000 | 0.478473000 |
| H | -3.124382000 | 6.578863000 | 1.546054000 |
| C | -0.499241000 | 8.409104000 | -0.626943000 |
| H | 0.695229000 | 6.638165000 | -0.417335000 |
| C | -1.698762000 | 9.049714000 | -0.307715000 |
| H | -3.578646000 | 8.869475000 | 0.734484000 |
| H | 0.242125000 | 8.915546000 | -1.240481000 |
| H | 0.272119000 | 4.723828000 | 2.916799000 |
| H | -1.896102000 | 10.056147000 | -0.667635000 |

PhCH=CHF

| | | | |
|---|--------------|--------------|--------------|
| C | 1.904745000 | 1.322031000 | 0.017714000 |
| C | 0.532153000 | 1.096164000 | 0.073684000 |
| C | 0.014157000 | -0.213172000 | 0.054726000 |
| C | 0.926048000 | -1.281967000 | -0.000934000 |
| C | 2.300906000 | -1.055858000 | -0.053305000 |
| C | 2.797637000 | 0.248133000 | -0.047723000 |
| H | 2.280897000 | 2.341605000 | 0.034507000 |
| H | -0.141435000 | 1.945349000 | 0.148466000 |
| H | 0.546793000 | -2.301112000 | -0.009010000 |
| H | 2.983660000 | -1.900249000 | -0.097782000 |
| H | 3.868410000 | 0.427968000 | -0.086197000 |
| C | -1.423328000 | -0.511374000 | 0.096398000 |
| H | -1.707090000 | -1.545853000 | 0.278884000 |
| C | -2.414244000 | 0.361600000 | -0.091866000 |
| H | -2.314946000 | 1.419063000 | -0.314961000 |
| F | -3.704970000 | -0.020013000 | -0.027341000 |

TS1^{F1}

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|---|--------------|--------------|--------------|
| P | -1.780839000 | -0.751484000 | 0.467565000 |
| P | 1.761212000 | -0.525249000 | -0.403278000 |
| O | -1.073127000 | -4.740962000 | -2.014890000 |

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|---|--------------|--------------|--------------|
| O | -0.523714000 | -4.524812000 | -4.242601000 |
| O | 1.054952000 | -5.252463000 | 0.149164000 |
| O | 0.439585000 | -6.030149000 | 2.227559000 |
| O | 4.833729000 | -4.245168000 | 3.161161000 |
| O | 5.484057000 | 3.416294000 | -2.982233000 |
| O | -4.737050000 | -2.563120000 | -4.450222000 |
| O | -5.386194000 | 1.862816000 | 4.467509000 |
| C | 1.093585000 | -1.754921000 | -1.623809000 |
| C | 0.206880000 | -2.791150000 | -1.180543000 |
| C | -0.236099000 | -3.656993000 | -2.171115000 |
| C | 0.100341000 | -3.534311000 | -3.517190000 |
| C | 0.929449000 | -2.529489000 | -3.961757000 |
| C | 1.422916000 | -1.650101000 | -2.981573000 |
| C | -0.995965000 | -5.445482000 | -3.253878000 |
| C | -1.103360000 | -2.374424000 | 1.060389000 |
| C | -1.463551000 | -2.868961000 | 2.320080000 |
| C | -0.990327000 | -4.091886000 | 2.825949000 |
| C | -0.151355000 | -4.807858000 | 2.003030000 |
| C | 0.222632000 | -4.329904000 | 0.748148000 |
| C | -0.200385000 | -3.113878000 | 0.227964000 |
| C | 0.910472000 | -6.433650000 | 0.939049000 |
| C | 2.815662000 | -1.587657000 | 0.675810000 |
| C | 3.573790000 | -2.637905000 | 0.134985000 |
| C | 4.333543000 | -3.490064000 | 0.938450000 |
| C | 4.269127000 | -3.276748000 | 2.344062000 |
| C | 3.675993000 | -2.126122000 | 2.907356000 |
| C | 2.910462000 | -1.320814000 | 2.040966000 |
| C | 3.827830000 | -1.631652000 | 4.374018000 |
| C | 2.454781000 | -1.667635000 | 5.086960000 |
| C | 4.862087000 | -2.386110000 | 5.241006000 |
| C | 4.324702000 | -0.160436000 | 4.326978000 |
| C | 5.268772000 | -4.550203000 | 0.300248000 |
| C | 6.718801000 | -4.302803000 | 0.786109000 |
| C | 5.273631000 | -4.446548000 | -1.240933000 |
| C | 4.855260000 | -5.999446000 | 0.644079000 |
| C | 3.868315000 | -5.111256000 | 3.760974000 |
| C | 2.969488000 | 0.514674000 | -1.340093000 |
| C | 2.476908000 | 1.475832000 | -2.237953000 |
| C | 4.345162000 | 0.452060000 | -1.128607000 |
| C | 5.247324000 | 1.350559000 | -1.728282000 |
| C | 4.687288000 | 2.384365000 | -2.511359000 |
| C | 3.310713000 | 2.400561000 | -2.872439000 |
| C | 2.751279000 | 3.336047000 | -3.976269000 |
| C | 1.275758000 | 3.011480000 | -4.296235000 |

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|---|--------------|--------------|--------------|
| C | 2.809031000 | 4.832010000 | -3.584382000 |
| C | 5.745792000 | 4.436791000 | -2.018044000 |
| C | 3.558092000 | 3.114830000 | -5.280971000 |
| C | 6.762626000 | 1.083401000 | -1.497039000 |
| C | 7.139750000 | 1.416146000 | -0.033329000 |
| C | 7.722320000 | 1.832601000 | -2.450849000 |
| C | 7.039892000 | -0.426188000 | -1.740403000 |
| C | -2.776047000 | -1.269845000 | -0.994371000 |
| C | -2.655673000 | -0.570372000 | -2.197200000 |
| C | -3.318692000 | -0.978285000 | -3.361871000 |
| C | -4.123094000 | -2.147511000 | -3.279327000 |
| C | -4.360802000 | -2.821604000 | -2.050645000 |
| C | -3.632489000 | -2.371641000 | -0.939134000 |
| C | -5.357290000 | -3.999426000 | -1.839337000 |
| C | -6.623306000 | -3.886153000 | -2.722011000 |
| C | -4.649926000 | -5.358123000 | -2.069173000 |
| C | -5.876420000 | -4.022514000 | -0.377420000 |
| C | -4.603467000 | 0.411414000 | -5.038552000 |
| C | -4.181203000 | -3.686460000 | -5.134499000 |
| C | -3.202571000 | -0.125342000 | -4.653673000 |
| C | -2.280444000 | 1.096147000 | -4.446139000 |
| C | -4.597403000 | 1.087833000 | 3.633889000 |
| C | -5.198276000 | 0.557643000 | 2.461341000 |
| C | -7.456789000 | -0.068052000 | 3.409518000 |
| C | -4.358218000 | -0.085157000 | 1.541745000 |
| C | -2.978811000 | -0.193365000 | 1.754530000 |
| C | -2.451541000 | 0.257805000 | 2.968329000 |
| C | -3.247505000 | 0.829624000 | 3.972475000 |
| C | -5.135658000 | 3.267467000 | 4.361742000 |
| C | -7.253488000 | 2.059781000 | 2.059790000 |
| C | -1.517211000 | 2.198777000 | 5.246421000 |
| C | -2.572498000 | 1.072250000 | 5.353046000 |
| C | -1.846775000 | -0.239342000 | 5.764962000 |
| C | -7.132945000 | -0.152187000 | 0.943356000 |
| C | -2.605531000 | -0.921584000 | -5.839404000 |
| C | -6.729947000 | 0.612226000 | 2.222334000 |
| C | -3.538915000 | 1.387679000 | 6.518227000 |
| H | 1.205198000 | -2.432519000 | -5.006197000 |
| H | 2.106340000 | -0.870677000 | -3.297117000 |
| H | -1.988060000 | -5.801970000 | -3.531899000 |
| H | -0.281055000 | -6.276715000 | -3.159869000 |
| H | -2.154983000 | -2.300399000 | 2.929992000 |
| H | -1.289999000 | -4.460250000 | 3.800964000 |
| H | 1.877749000 | -6.925063000 | 1.043734000 |

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|---|-------------|--------------|--------------|
| H | 0.168467000 | -7.098224000 | 0.470794000 |
| H | 3.552606000 | -2.792060000 | -0.936090000 |
| H | 2.370140000 | -0.469248000 | 2.440443000 |
| H | 1.719926000 | -1.038035000 | 4.574771000 |
| H | 2.554272000 | -1.297595000 | 6.114933000 |
| H | 2.051694000 | -2.686299000 | 5.133755000 |
| H | 4.550263000 | -3.393394000 | 5.520213000 |
| H | 4.997529000 | -1.823819000 | 6.172871000 |
| H | 5.835113000 | -2.457232000 | 4.747493000 |
| H | 5.304667000 | -0.101852000 | 3.837436000 |
| H | 4.438783000 | 0.218420000 | 5.350004000 |
| H | 3.641216000 | 0.509563000 | 3.802771000 |
| H | 7.397206000 | -5.034435000 | 0.329352000 |
| H | 6.796560000 | -4.393130000 | 1.871507000 |
| H | 7.061319000 | -3.302518000 | 0.495719000 |
| H | 5.991102000 | -5.169609000 | -1.644896000 |
| H | 5.577415000 | -3.453511000 | -1.589343000 |
| H | 4.294038000 | -4.678800000 | -1.674261000 |
| H | 3.813328000 | -6.177423000 | 0.356492000 |
| H | 4.976480000 | -6.219739000 | 1.704751000 |
| H | 5.480901000 | -6.705682000 | 0.084191000 |
| H | 3.242663000 | -5.598963000 | 3.004528000 |
| H | 3.211462000 | -4.571921000 | 4.451666000 |
| H | 4.432905000 | -5.866075000 | 4.314482000 |
| H | 1.411419000 | 1.504163000 | -2.429902000 |
| H | 4.731685000 | -0.313555000 | -0.468604000 |
| H | 0.946143000 | 3.641704000 | -5.129558000 |
| H | 0.607135000 | 3.213231000 | -3.452511000 |
| H | 1.139891000 | 1.967888000 | -4.601908000 |
| H | 3.831933000 | 5.208833000 | -3.559466000 |
| H | 2.342668000 | 5.011138000 | -2.608425000 |
| H | 2.260505000 | 5.426457000 | -4.325106000 |
| H | 6.348314000 | 4.061773000 | -1.183109000 |
| H | 4.815452000 | 4.858934000 | -1.621126000 |
| H | 6.304280000 | 5.217895000 | -2.540150000 |
| H | 4.615391000 | 3.349148000 | -5.143856000 |
| H | 3.162374000 | 3.758496000 | -6.076445000 |
| H | 3.473248000 | 2.074970000 | -5.619064000 |
| H | 6.537114000 | 0.840064000 | 0.677569000 |
| H | 6.992587000 | 2.478763000 | 0.190706000 |
| H | 8.195178000 | 1.179973000 | 0.150637000 |
| H | 8.730661000 | 1.422582000 | -2.316627000 |
| H | 7.782922000 | 2.903366000 | -2.256592000 |
| H | 7.440123000 | 1.696282000 | -3.498720000 |

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|---|--------------|--------------|--------------|
| H | 6.760642000 | -0.715555000 | -2.760017000 |
| H | 6.503934000 | -1.077649000 | -1.045236000 |
| H | 8.109891000 | -0.627109000 | -1.613140000 |
| H | -2.019947000 | 0.304273000 | -2.218017000 |
| H | -3.733167000 | -2.893875000 | 0.003729000 |
| H | -6.420247000 | -3.948356000 | -3.788990000 |
| H | -7.133955000 | -2.933196000 | -2.542034000 |
| H | -7.318292000 | -4.692363000 | -2.458528000 |
| H | -5.333298000 | -6.183443000 | -1.832885000 |
| H | -3.769048000 | -5.446478000 | -1.424068000 |
| H | -4.322013000 | -5.489982000 | -3.103090000 |
| H | -6.664659000 | -4.778514000 | -0.291182000 |
| H | -6.304667000 | -3.057817000 | -0.087334000 |
| H | -5.102895000 | -4.289002000 | 0.349197000 |
| H | -4.534939000 | 1.009373000 | -5.956146000 |
| H | -4.998334000 | 1.058654000 | -4.247116000 |
| H | -5.310821000 | -0.402795000 | -5.210027000 |
| H | -4.680631000 | -4.615488000 | -4.839367000 |
| H | -3.103754000 | -3.774326000 | -4.958843000 |
| H | -4.357913000 | -3.530334000 | -6.202433000 |
| H | -1.249058000 | 0.796430000 | -4.225549000 |
| H | -2.629692000 | 1.758379000 | -3.649978000 |
| H | -2.259114000 | 1.683177000 | -5.370981000 |
| H | -7.154284000 | -1.118178000 | 3.500004000 |
| H | -8.541826000 | -0.044359000 | 3.247522000 |
| H | -7.239316000 | 0.437427000 | 4.352346000 |
| H | -4.773739000 | -0.484715000 | 0.627016000 |
| H | -1.383128000 | 0.169242000 | 3.137148000 |
| H | -5.844632000 | 3.756325000 | 5.034622000 |
| H | -5.296868000 | 3.623375000 | 3.337922000 |
| H | -4.115064000 | 3.522464000 | 4.664222000 |
| H | -8.298249000 | 2.037720000 | 1.726100000 |
| H | -6.675591000 | 2.610262000 | 1.307784000 |
| H | -7.221973000 | 2.612098000 | 2.998806000 |
| H | -1.974199000 | 3.155922000 | 4.970331000 |
| H | -0.750451000 | 1.965022000 | 4.500583000 |
| H | -1.015759000 | 2.337073000 | 6.212359000 |
| H | -1.369917000 | -0.102957000 | 6.742472000 |
| H | -1.064081000 | -0.533384000 | 5.060640000 |
| H | -2.558710000 | -1.069031000 | 5.850205000 |
| H | -6.825205000 | -1.202372000 | 0.979398000 |
| H | -6.714203000 | 0.298417000 | 0.035899000 |
| H | -8.223835000 | -0.132901000 | 0.844456000 |
| H | -1.682458000 | -1.435928000 | -5.547187000 |

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|----|--------------|--------------|--------------|
| H | -2.357205000 | -0.229829000 | -6.653471000 |
| H | -3.302422000 | -1.655289000 | -6.241502000 |
| H | -2.971643000 | 1.340829000 | 7.455668000 |
| H | -4.353309000 | 0.660108000 | 6.580832000 |
| H | -3.980324000 | 2.382898000 | 6.461506000 |
| Cu | -0.083865000 | 0.771763000 | 0.371063000 |
| N | 0.045506000 | 2.834403000 | 0.282236000 |
| C | -0.458165000 | 3.749987000 | -0.524750000 |
| C | 1.047657000 | 3.343294000 | 1.125823000 |
| C | -1.751442000 | 3.683696000 | -1.198332000 |
| C | -2.018396000 | 4.586245000 | -2.249398000 |
| C | -2.800889000 | 2.853804000 | -0.753132000 |
| C | -3.277829000 | 4.644225000 | -2.843472000 |
| H | -1.231471000 | 5.258179000 | -2.581388000 |
| C | -4.057439000 | 2.913392000 | -1.349865000 |
| H | -2.629713000 | 2.194262000 | 0.090359000 |
| C | -4.304489000 | 3.806849000 | -2.399101000 |
| H | -3.460500000 | 5.349909000 | -3.649788000 |
| H | -4.853115000 | 2.268756000 | -0.984916000 |
| H | -5.289532000 | 3.857493000 | -2.855398000 |
| C | 1.617337000 | 2.330165000 | 2.027164000 |
| O | 0.976549000 | 1.332395000 | 2.390380000 |
| O | 2.835335000 | 2.489654000 | 2.585279000 |
| C | 3.757054000 | 3.487662000 | 2.123304000 |
| H | 3.374494000 | 4.488016000 | 2.323879000 |
| H | 4.670821000 | 3.314252000 | 2.694361000 |
| H | 3.967597000 | 3.358887000 | 1.056214000 |
| H | 1.762661000 | 4.026026000 | 0.659415000 |
| H | 0.149384000 | 4.618420000 | -0.783857000 |
| C | -0.626105000 | 5.486429000 | 1.471584000 |
| C | 0.184286000 | 4.606712000 | 2.223348000 |
| H | -1.686616000 | 5.255523000 | 1.466682000 |
| C | -0.219045000 | 6.669949000 | 0.753884000 |
| C | -1.191045000 | 7.415605000 | 0.035235000 |
| C | 1.119239000 | 7.138828000 | 0.679282000 |
| C | -0.852648000 | 8.545345000 | -0.700690000 |
| H | -2.227177000 | 7.086052000 | 0.066181000 |
| C | 1.450508000 | 8.268185000 | -0.066922000 |
| H | 1.891331000 | 6.627097000 | 1.240667000 |
| C | 0.474675000 | 8.984893000 | -0.764104000 |
| H | -1.631139000 | 9.089173000 | -1.231910000 |
| H | 2.487034000 | 8.599141000 | -0.093912000 |
| H | -0.344117000 | 3.954072000 | 2.917152000 |
| H | 0.739275000 | 9.868786000 | -1.338196000 |

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|---|-------------|-------------|-------------|
| F | 1.304823000 | 5.145524000 | 2.872230000 |
|---|-------------|-------------|-------------|

INT1^{F1}

| | | | |
|---|--------------|--------------|--------------|
| P | -1.375720000 | -1.066584000 | 0.355274000 |
| P | 2.076744000 | 0.016613000 | -0.448445000 |
| O | 0.261568000 | -4.655203000 | -2.303359000 |
| O | 0.886130000 | -4.238273000 | -4.487279000 |
| O | 2.396369000 | -4.824600000 | -0.088020000 |
| O | 1.950550000 | -5.793160000 | 1.953115000 |
| O | 5.568728000 | -2.014508000 | 4.006349000 |
| O | 6.098221000 | 3.976719000 | -2.502907000 |
| O | -5.050437000 | -3.325276000 | -3.837070000 |
| O | -5.241142000 | 0.886203000 | 4.467005000 |
| C | 1.806175000 | -1.341925000 | -1.677561000 |
| C | 1.103043000 | -2.542068000 | -1.326054000 |
| C | 0.879897000 | -3.427136000 | -2.373016000 |
| C | 1.258678000 | -3.184712000 | -3.691673000 |
| C | 1.903473000 | -2.022771000 | -4.050213000 |
| C | 2.168733000 | -1.112277000 | -3.012991000 |
| C | 0.468310000 | -5.262684000 | -3.581198000 |
| C | -0.329168000 | -2.505169000 | 0.888957000 |
| C | -0.585257000 | -3.116110000 | 2.124581000 |
| C | 0.132367000 | -4.228586000 | 2.596489000 |
| C | 1.109071000 | -4.722240000 | 1.761255000 |
| C | 1.378611000 | -4.128249000 | 0.530586000 |
| C | 0.718427000 | -3.005894000 | 0.048883000 |
| C | 2.519345000 | -6.034247000 | 0.663029000 |
| C | 3.119426000 | -0.690553000 | 0.899133000 |
| C | 4.010044000 | -1.753203000 | 0.708528000 |
| C | 4.870783000 | -2.182393000 | 1.724401000 |
| C | 4.793809000 | -1.507261000 | 2.974051000 |
| C | 4.011304000 | -0.342595000 | 3.158994000 |
| C | 3.138473000 | -0.000380000 | 2.111404000 |
| C | 4.065362000 | 0.610056000 | 4.387850000 |
| C | 2.885029000 | 0.324365000 | 5.345652000 |
| C | 5.402100000 | 0.557543000 | 5.165190000 |
| C | 3.920630000 | 2.080549000 | 3.903731000 |
| C | 5.918659000 | -3.292578000 | 1.446586000 |
| C | 7.342654000 | -2.736412000 | 1.697840000 |
| C | 5.869917000 | -3.763423000 | -0.024332000 |
| C | 5.696041000 | -4.544395000 | 2.331314000 |
| C | 4.860942000 | -2.772385000 | 4.988182000 |
| C | 3.282947000 | 1.167099000 | -1.254774000 |
| C | 2.908227000 | 2.495224000 | -1.489615000 |

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| C | 4.571990000 | 0.764619000 | -1.608846000 |
| C | 5.522361000 | 1.647522000 | -2.140515000 |
| C | 5.151434000 | 3.013470000 | -2.193900000 |
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| C | 3.350437000 | 4.887421000 | -2.307221000 |
| C | 1.830143000 | 5.049597000 | -2.099807000 |
| C | 4.038726000 | 5.961154000 | -1.430312000 |
| C | 6.948816000 | 4.328150000 | -1.410099000 |
| C | 3.641852000 | 5.178949000 | -3.800928000 |
| C | 6.857028000 | 1.028961000 | -2.647992000 |
| C | 7.712047000 | 0.554400000 | -1.448766000 |
| C | 7.714131000 | 1.947961000 | -3.549763000 |
| C | 6.519444000 | -0.206381000 | -3.528611000 |
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| C | -4.268740000 | -2.833732000 | -2.803234000 |
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| C | -2.758585000 | -3.165687000 | -0.972132000 |
| C | -4.058859000 | -5.222490000 | -1.675016000 |
| C | -5.382014000 | -5.660827000 | -2.345666000 |
| C | -2.910804000 | -6.126441000 | -2.181039000 |
| C | -4.254263000 | -5.502541000 | -0.158824000 |
| C | -6.496441000 | -0.773236000 | -3.272831000 |
| C | -4.306232000 | -3.853039000 | -4.933864000 |
| C | -5.003455000 | -0.442092000 | -3.524090000 |
| C | -4.784418000 | 1.018097000 | -3.073805000 |
| C | -4.355057000 | 0.211056000 | 3.643775000 |
| C | -4.859052000 | -0.570750000 | 2.576411000 |
| C | -6.700110000 | -1.755188000 | 3.818172000 |
| C | -3.928662000 | -1.021340000 | 1.628032000 |
| C | -2.559763000 | -0.760889000 | 1.746275000 |
| C | -2.094073000 | -0.160707000 | 2.924958000 |
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| C | -5.482819000 | 2.243980000 | 4.041116000 |
| C | -7.340408000 | 0.127363000 | 2.270972000 |
| C | -2.669466000 | 2.235948000 | 5.627592000 |
| C | -2.414179000 | 0.744738000 | 5.303144000 |
| C | -0.888092000 | 0.528302000 | 5.385227000 |
| C | -6.555286000 | -2.038795000 | 1.346879000 |
| C | -4.709819000 | -0.496276000 | -5.042098000 |
| C | -6.339957000 | -1.030338000 | 2.496781000 |
| C | -3.068409000 | -0.132520000 | 6.399941000 |
| H | 2.206311000 | -1.826611000 | -5.072960000 |

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| H | 2.687435000 | -0.195443000 | -3.264841000 |
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| H | -1.386668000 | -2.728053000 | 2.741924000 |
| H | -0.087810000 | -4.684493000 | 3.555555000 |
| H | 3.573547000 | -6.289816000 | 0.771922000 |
| H | 1.957091000 | -6.835296000 | 0.160140000 |
| H | 4.020669000 | -2.255886000 | -0.249706000 |
| H | 2.460847000 | 0.835844000 | 2.236196000 |
| H | 1.928435000 | 0.434882000 | 4.826504000 |
| H | 2.897987000 | 1.033747000 | 6.182649000 |
| H | 2.921663000 | -0.685719000 | 5.765382000 |
| H | 5.556763000 | -0.371563000 | 5.711891000 |
| H | 5.414492000 | 1.375734000 | 5.895059000 |
| H | 6.257333000 | 0.693929000 | 4.494538000 |
| H | 4.665568000 | 2.320927000 | 3.136405000 |
| H | 4.081683000 | 2.754301000 | 4.753155000 |
| H | 2.928027000 | 2.305596000 | 3.505022000 |
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| H | 7.555022000 | -1.894864000 | 1.027763000 |
| H | 6.648769000 | -4.517938000 | -0.182507000 |
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| H | 4.906728000 | -4.213456000 | -0.286434000 |
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| H | 5.990787000 | -4.368471000 | 3.365846000 |
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| H | 4.150874000 | -3.465288000 | 4.523049000 |
| H | 4.321613000 | -2.126860000 | 5.688411000 |
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| H | 1.888162000 | 2.784304000 | -1.268984000 |
| H | 4.847960000 | -0.273633000 | -1.468182000 |
| H | 1.535570000 | 6.061120000 | -2.400594000 |
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| H | 1.251321000 | 4.345356000 | -2.704952000 |
| H | 5.092605000 | 6.082317000 | -1.681297000 |
| H | 3.954867000 | 5.717883000 | -0.364124000 |
| H | 3.550581000 | 6.930586000 | -1.588371000 |
| H | 7.576571000 | 3.487498000 | -1.095859000 |
| H | 6.367330000 | 4.673290000 | -0.547810000 |
| H | 7.587671000 | 5.139893000 | -1.767256000 |
| H | 4.708749000 | 5.108282000 | -4.022371000 |
| H | 3.302990000 | 6.190750000 | -4.056342000 |
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| H | 7.166117000 | -0.162156000 | -0.825166000 |
| H | 8.008781000 | 1.390035000 | -0.805516000 |
| H | 8.627250000 | 0.064875000 | -1.804171000 |
| H | 8.514663000 | 1.344379000 | -3.994514000 |
| H | 8.191058000 | 2.766443000 | -3.010799000 |
| H | 7.125562000 | 2.379419000 | -4.364473000 |
| H | 5.902686000 | 0.083697000 | -4.386988000 |
| H | 5.988676000 | -0.992277000 | -2.984384000 |
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| H | -2.254867000 | -3.816085000 | -0.268062000 |
| H | -5.325988000 | -5.703288000 | -3.433274000 |
| H | -6.209319000 | -4.996759000 | -2.078541000 |
| H | -5.631485000 | -6.668795000 | -1.992426000 |
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| H | -2.769028000 | -6.025204000 | -3.263499000 |
| H | -4.555926000 | -6.546800000 | -0.017365000 |
| H | -5.041294000 | -4.864966000 | 0.258651000 |
| H | -3.346017000 | -5.347268000 | 0.429453000 |
| H | -7.129414000 | -0.068877000 | -3.826698000 |
| H | -6.741731000 | -0.673428000 | -2.208521000 |
| H | -6.747535000 | -1.785864000 | -3.592969000 |
| H | -3.775901000 | -4.772567000 | -4.660971000 |
| H | -3.578591000 | -3.124682000 | -5.310240000 |
| H | -5.032999000 | -4.079691000 | -5.718310000 |
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| H | -5.483068000 | 1.664821000 | -3.616245000 |
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| H | -7.739385000 | -2.105806000 | 3.782805000 |
| H | -6.592347000 | -1.087898000 | 4.676170000 |
| H | -4.279974000 | -1.570467000 | 0.767201000 |
| H | -1.028917000 | -0.020846000 | 3.050373000 |
| H | -6.009182000 | 2.729856000 | 4.866503000 |
| H | -6.106988000 | 2.270122000 | 3.144088000 |
| H | -4.552063000 | 2.772590000 | 3.825738000 |
| H | -8.328975000 | -0.283803000 | 2.032086000 |
| H | -7.034738000 | 0.766589000 | 1.434678000 |
| H | -7.452142000 | 0.744358000 | 3.162912000 |
| H | -3.717135000 | 2.427426000 | 5.863450000 |
| H | -2.371467000 | 2.881205000 | 4.796148000 |
| H | -2.080646000 | 2.519627000 | 6.508820000 |
| H | -0.548350000 | 0.772124000 | 6.398081000 |

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| H | -0.343503000 | 1.174537000 | 4.689034000 |
| H | -0.606284000 | -0.512089000 | 5.185874000 |
| H | -5.898359000 | -2.911118000 | 1.435141000 |
| H | -6.396787000 | -1.588082000 | 0.360246000 |
| H | -7.589256000 | -2.399702000 | 1.379037000 |
| H | -3.643140000 | -0.344046000 | -5.243036000 |
| H | -5.259331000 | 0.305860000 | -5.549876000 |
| H | -5.024865000 | -1.440649000 | -5.487683000 |
| H | -2.678725000 | 0.151127000 | 7.385786000 |
| H | -2.841292000 | -1.193818000 | 6.241831000 |
| H | -4.153650000 | -0.008207000 | 6.412223000 |
| Cu | -0.035407000 | 0.813006000 | 0.039229000 |
| N | -0.754490000 | 2.720989000 | -0.355819000 |
| C | -1.284031000 | 3.278175000 | -1.412725000 |
| C | -1.032254000 | 3.456501000 | 0.851826000 |
| C | -1.266504000 | 2.758599000 | -2.778460000 |
| C | -1.833709000 | 3.568586000 | -3.785359000 |
| C | -0.705687000 | 1.522475000 | -3.153140000 |
| C | -1.837172000 | 3.158747000 | -5.115948000 |
| H | -2.281908000 | 4.519188000 | -3.506355000 |
| C | -0.702539000 | 1.118695000 | -4.485994000 |
| H | -0.274375000 | 0.877761000 | -2.393145000 |
| C | -1.266665000 | 1.933393000 | -5.473678000 |
| H | -2.282168000 | 3.796152000 | -5.875290000 |
| H | -0.259342000 | 0.162964000 | -4.752188000 |
| H | -1.261750000 | 1.615331000 | -6.512893000 |
| C | -0.111083000 | 2.997767000 | 1.943337000 |
| O | 0.257338000 | 1.821676000 | 2.026200000 |
| O | 0.336042000 | 3.825145000 | 2.900745000 |
| C | 0.025042000 | 5.227100000 | 2.916850000 |
| H | -1.049770000 | 5.375830000 | 3.013391000 |
| H | 0.542537000 | 5.620524000 | 3.793068000 |
| H | 0.404790000 | 5.726136000 | 2.019220000 |
| H | -0.980849000 | 4.539168000 | 0.697650000 |
| H | -1.702854000 | 4.278854000 | -1.323213000 |
| C | -3.599162000 | 3.667406000 | 0.325875000 |
| C | -2.630338000 | 3.198621000 | 1.270582000 |
| C | -3.837678000 | 5.023046000 | -0.069141000 |
| C | -4.660559000 | 5.305626000 | -1.198972000 |
| C | -3.280490000 | 6.155873000 | 0.589924000 |
| C | -4.886661000 | 6.602047000 | -1.640735000 |
| H | -5.117166000 | 4.470796000 | -1.727968000 |
| C | -3.503552000 | 7.452799000 | 0.131004000 |
| H | -2.715470000 | 6.006927000 | 1.502922000 |

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| C | -4.302781000 | 7.697333000 | -0.988064000 |
| H | -5.524215000 | 6.765555000 | -2.507833000 |
| H | -3.059488000 | 8.287758000 | 0.670605000 |
| H | -4.479683000 | 8.711222000 | -1.336246000 |
| F | -2.652682000 | 3.844003000 | 2.575791000 |
| H | -4.164712000 | 2.895681000 | -0.188397000 |
| H | -2.717809000 | 2.129687000 | 1.461968000 |

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| P | 1.339917000 | -1.038359000 | -0.325436000 |
| P | -2.125158000 | 0.063692000 | 0.457582000 |
| O | -0.140421000 | -4.403932000 | 2.601315000 |
| O | -0.717287000 | -3.837775000 | 4.764735000 |
| O | -2.382472000 | -4.771837000 | 0.452043000 |
| O | -1.999094000 | -5.862607000 | -1.539666000 |
| O | -5.658761000 | -2.330895000 | -3.781723000 |
| O | -6.093485000 | 4.139001000 | 2.393700000 |
| O | 5.128270000 | -3.296070000 | 3.776416000 |
| O | 5.137795000 | 0.750670000 | -4.578025000 |
| C | -1.815964000 | -1.200635000 | 1.773209000 |
| C | -1.075147000 | -2.396970000 | 1.493048000 |
| C | -0.773060000 | -3.181432000 | 2.597840000 |
| C | -1.124832000 | -2.849554000 | 3.905315000 |
| C | -1.824694000 | -1.699547000 | 4.191119000 |
| C | -2.157991000 | -0.884616000 | 3.095730000 |
| C | 0.102471000 | -4.705458000 | 3.977935000 |
| C | 0.274917000 | -2.492272000 | -0.768509000 |
| C | 0.489374000 | -3.169755000 | -1.976419000 |
| C | -0.232998000 | -4.316122000 | -2.352000000 |
| C | -1.167159000 | -4.771181000 | -1.448574000 |
| C | -1.397981000 | -4.105661000 | -0.246378000 |
| C | -0.733790000 | -2.950207000 | 0.139759000 |
| C | -2.513745000 | -6.028772000 | -0.214167000 |
| C | -3.186876000 | -0.746717000 | -0.815481000 |
| C | -4.061065000 | -1.803001000 | -0.534190000 |
| C | -4.930468000 | -2.316956000 | -1.502564000 |
| C | -4.876882000 | -1.738520000 | -2.800849000 |
| C | -4.109108000 | -0.583906000 | -3.084601000 |
| C | -3.230690000 | -0.151122000 | -2.076168000 |
| C | -4.181016000 | 0.265756000 | -4.385910000 |
| C | -3.004787000 | -0.087931000 | -5.326431000 |
| C | -5.522466000 | 0.139467000 | -5.146419000 |
| C | -4.045370000 | 1.771918000 | -4.024701000 |
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| C | -7.396063000 | -2.882211000 | -1.390873000 |
| C | -5.885365000 | -3.772418000 | 0.375048000 |
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| C | -4.954086000 | -3.160781000 | -4.705644000 |
| C | -3.321034000 | 1.259271000 | 1.212220000 |
| C | -2.922781000 | 2.584978000 | 1.424664000 |
| C | -4.618423000 | 0.885112000 | 1.566839000 |
| C | -5.557292000 | 1.793971000 | 2.074807000 |
| C | -5.161639000 | 3.153270000 | 2.108269000 |
| C | -3.819764000 | 3.559420000 | 1.886994000 |
| C | -3.327696000 | 4.994776000 | 2.209722000 |
| C | -1.801846000 | 5.122708000 | 2.021928000 |
| C | -3.982596000 | 6.068024000 | 1.307071000 |
| C | -6.926347000 | 4.489135000 | 1.287563000 |
| C | -3.633813000 | 5.315408000 | 3.694534000 |
| C | -6.907222000 | 1.208693000 | 2.581292000 |
| C | -7.761927000 | 0.731727000 | 1.382799000 |
| C | -7.753425000 | 2.158038000 | 3.461646000 |
| C | -6.600629000 | -0.018977000 | 3.483646000 |
| C | 2.467802000 | -1.761233000 | 0.954120000 |
| C | 3.213711000 | -0.905098000 | 1.774660000 |
| C | 4.168557000 | -1.391442000 | 2.676886000 |
| C | 4.314466000 | -2.802653000 | 2.767908000 |
| C | 3.703419000 | -3.688524000 | 1.848631000 |
| C | 2.744903000 | -3.129015000 | 0.987353000 |
| C | 4.055853000 | -5.193490000 | 1.647549000 |
| C | 5.400033000 | -5.635745000 | 2.272149000 |
| C | 2.924649000 | -6.099031000 | 2.188009000 |
| C | 4.199386000 | -5.471575000 | 0.125106000 |
| C | 6.568677000 | -0.761053000 | 3.184943000 |
| C | 4.423198000 | -3.823292000 | 4.897432000 |
| C | 5.083770000 | -0.413282000 | 3.460459000 |
| C | 4.872862000 | 1.045060000 | 2.999796000 |
| C | 4.264342000 | 0.105766000 | -3.716133000 |
| C | 4.784471000 | -0.639181000 | -2.630849000 |
| C | 6.595986000 | -1.877779000 | -3.862019000 |
| C | 3.868740000 | -1.052052000 | -1.651327000 |
| C | 2.497050000 | -0.797818000 | -1.756156000 |
| C | 2.013858000 | -0.244400000 | -2.950776000 |
| C | 2.871164000 | 0.177399000 | -3.976475000 |
| C | 5.399721000 | 2.117799000 | -4.204414000 |
| C | 7.276780000 | 0.054743000 | -2.396446000 |
| C | 2.521720000 | 2.094022000 | -5.691769000 |
| C | 2.297919000 | 0.599445000 | -5.356741000 |

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| C | 0.775853000 | 0.349001000 | -5.425025000 |
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| C | 4.816545000 | -0.450774000 | 4.983756000 |
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| H | 6.257245000 | 2.594027000 | -3.313871000 |
| H | 4.744865000 | 3.025594000 | -4.135029000 |
| H | 8.656878000 | 0.189553000 | -2.174651000 |
| H | 7.359863000 | 1.229523000 | -1.571415000 |
| H | 7.699083000 | 1.128144000 | -3.315540000 |
| H | 3.667406000 | 2.673793000 | -5.862087000 |
| H | 2.286791000 | 2.972158000 | -4.778601000 |
| H | 2.022971000 | 2.558618000 | -6.478477000 |
| H | 0.720809000 | 0.603309000 | -6.327668000 |
| H | 0.466763000 | 1.038228000 | -4.634792000 |
| H | 0.951694000 | -0.613177000 | -5.067623000 |
| H | 6.352329000 | -2.472616000 | -1.329126000 |
| H | 6.817090000 | -1.069138000 | -0.342954000 |
| H | 8.018316000 | -1.886775000 | -1.348383000 |
| H | 1.579336000 | -0.709142000 | 5.633518000 |
| H | 2.483696000 | 0.426531000 | 6.648076000 |
| H | 3.104250000 | -1.202182000 | 6.397315000 |
| H | 2.851146000 | 0.259351000 | -7.341144000 |
| H | 3.202997000 | -1.039237000 | -6.189098000 |
| H | 4.368327000 | 0.279705000 | -6.419914000 |
| Cu | 0.196650000 | 0.848185000 | -0.161216000 |
| N | 0.035471000 | 2.763496000 | -0.357320000 |
| C | 0.729261000 | 3.890143000 | 0.231298000 |
| C | -1.179906000 | 3.280476000 | -0.932550000 |
| C | 2.203993000 | 3.688594000 | 0.519292000 |
| C | 2.787485000 | 4.291093000 | 1.641897000 |
| C | 3.032004000 | 2.983264000 | -0.363911000 |
| C | 4.161038000 | 4.198669000 | 1.878315000 |
| H | 2.158648000 | 4.848573000 | 2.332111000 |
| C | 4.403885000 | 2.879395000 | -0.125605000 |
| H | 2.587990000 | 2.512401000 | -1.234767000 |
| C | 4.975274000 | 3.487523000 | 0.995004000 |
| H | 4.592219000 | 4.680073000 | 2.752752000 |
| H | 5.024695000 | 2.315241000 | -0.816121000 |
| H | 6.044290000 | 3.408646000 | 1.177535000 |
| C | -1.612173000 | 2.517854000 | -2.189588000 |
| O | -0.948362000 | 1.658679000 | -2.736743000 |
| O | -2.813075000 | 2.816379000 | -2.749151000 |
| C | -3.813078000 | 3.597068000 | -2.075371000 |
| H | -3.444808000 | 4.574486000 | -1.760642000 |
| H | -4.612057000 | 3.724331000 | -2.808514000 |

| | | | |
|---|--------------|--------------|--------------|
| H | -4.199351000 | 3.054437000 | -1.206784000 |
| H | -2.050907000 | 3.261899000 | -0.246484000 |
| H | 0.264993000 | 4.247317000 | 1.176218000 |
| C | 0.506955000 | 5.032824000 | -0.827741000 |
| C | -0.951628000 | 4.802594000 | -1.224507000 |
| H | 1.098200000 | 4.727495000 | -1.700217000 |
| C | 0.895378000 | 6.444657000 | -0.457857000 |
| C | 1.844643000 | 7.126730000 | -1.233983000 |
| C | 0.363806000 | 7.106453000 | 0.662023000 |
| C | 2.248523000 | 8.423588000 | -0.914646000 |
| H | 2.276146000 | 6.629429000 | -2.099908000 |
| C | 0.769057000 | 8.401536000 | 0.986972000 |
| H | -0.372108000 | 6.608828000 | 1.282946000 |
| C | 1.710697000 | 9.067942000 | 0.200208000 |
| H | 2.985776000 | 8.927219000 | -1.534953000 |
| H | 0.343873000 | 8.892984000 | 1.858801000 |
| H | 2.023245000 | 10.077333000 | 0.455105000 |
| F | -1.833227000 | 5.553167000 | -0.413976000 |
| H | -1.166188000 | 5.109752000 | -2.252861000 |

PhCH=CF₂

| | | | |
|---|--------------|--------------|--------------|
| C | -2.068157000 | 1.342140000 | -0.000057000 |
| C | -0.717334000 | 1.001646000 | -0.000033000 |
| C | -0.319114000 | -0.349709000 | 0.000127000 |
| C | -1.323887000 | -1.335476000 | 0.000034000 |
| C | -2.673723000 | -0.990986000 | 0.000017000 |
| C | -3.053911000 | 0.352084000 | 0.000009000 |
| H | -2.352053000 | 2.391321000 | -0.000143000 |
| H | 0.029657000 | 1.786186000 | -0.000178000 |
| H | -1.036676000 | -2.384395000 | -0.000021000 |
| H | -3.428205000 | -1.773220000 | -0.000045000 |
| H | -4.105550000 | 0.624994000 | -0.000007000 |
| C | 1.077326000 | -0.797193000 | -0.000044000 |
| H | 1.254044000 | -1.868025000 | -0.000065000 |
| C | 2.187324000 | -0.059979000 | -0.000075000 |
| F | 3.411604000 | -0.572866000 | -0.000042000 |
| F | 2.253689000 | 1.267086000 | 0.000109000 |

TS1^{F2}

| | | | |
|---|--------------|--------------|--------------|
| P | 1.368564000 | -1.126685000 | -0.275137000 |
| P | -2.090531000 | -0.045722000 | 0.488743000 |
| O | -0.168740000 | -4.358261000 | 3.010001000 |
| O | -0.846723000 | -3.654610000 | 5.100212000 |
| O | -2.244332000 | -4.919167000 | 0.888784000 |

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|---|--------------|--------------|--------------|
| O | -1.797708000 | -6.176045000 | -0.988363000 |
| O | -5.430934000 | -2.797134000 | -3.684363000 |
| O | -6.236741000 | 4.042473000 | 1.956548000 |
| O | 5.450982000 | -2.329316000 | 3.976969000 |
| O | 5.198873000 | -0.013716000 | -4.718876000 |
| C | -1.787232000 | -1.212013000 | 1.894688000 |
| C | -1.043767000 | -2.427899000 | 1.725558000 |
| C | -0.816511000 | -3.147502000 | 2.892533000 |
| C | -1.227769000 | -2.732553000 | 4.157610000 |
| C | -1.910691000 | -1.551379000 | 4.338411000 |
| C | -2.181706000 | -0.807067000 | 3.178452000 |
| C | -0.414998000 | -4.792093000 | 4.350203000 |
| C | 0.361918000 | -2.674196000 | -0.504534000 |
| C | 0.609371000 | -3.458142000 | -1.641547000 |
| C | -0.067138000 | -4.657894000 | -1.916454000 |
| C | -0.998005000 | -5.057349000 | -0.984813000 |
| C | -1.264543000 | -4.290885000 | 0.146588000 |
| C | -0.643527000 | -3.081296000 | 0.433827000 |
| C | -2.339072000 | -6.232390000 | 0.334375000 |
| C | -3.097777000 | -0.964426000 | -0.753784000 |
| C | -3.933544000 | -2.041468000 | -0.433829000 |
| C | -4.762698000 | -2.638337000 | -1.390058000 |
| C | -4.710099000 | -2.118723000 | -2.712833000 |
| C | -3.998459000 | -0.939767000 | -3.036150000 |
| C | -3.149721000 | -0.426360000 | -2.040122000 |
| C | -4.107873000 | -0.136994000 | -4.364197000 |
| C | -2.868104000 | -0.393322000 | -5.251709000 |
| C | -5.397215000 | -0.412541000 | -5.173438000 |
| C | -4.138613000 | 1.382211000 | -4.032741000 |
| C | -5.759432000 | -3.755045000 | -0.980317000 |
| C | -7.203864000 | -3.308139000 | -1.319179000 |
| C | -5.715115000 | -4.024947000 | 0.540424000 |
| C | -5.463439000 | -5.099429000 | -1.690031000 |
| C | -4.643245000 | -3.617210000 | -4.548258000 |
| C | -3.344556000 | 1.157194000 | 1.135178000 |
| C | -2.966080000 | 2.477057000 | 1.374421000 |
| C | -4.678101000 | 0.790946000 | 1.373224000 |
| C | -5.652339000 | 1.723304000 | 1.733078000 |
| C | -5.245464000 | 3.084532000 | 1.810329000 |
| C | -3.888683000 | 3.468855000 | 1.764180000 |
| C | -3.310045000 | 4.859183000 | 2.151572000 |
| C | -2.203283000 | 4.627521000 | 3.215486000 |
| C | -2.680248000 | 5.533834000 | 0.909332000 |
| C | -6.554510000 | 4.724618000 | 0.741907000 |

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|---|--------------|--------------|--------------|
| C | -4.300190000 | 5.852474000 | 2.802507000 |
| C | -7.085395000 | 1.263665000 | 2.106312000 |
| C | -8.158757000 | 1.794752000 | 1.126388000 |
| C | -7.415232000 | 1.746837000 | 3.540988000 |
| C | -7.201311000 | -0.276215000 | 2.105665000 |
| C | 2.564824000 | -1.562874000 | 1.066157000 |
| C | 3.368518000 | -0.531580000 | 1.570667000 |
| C | 4.393313000 | -0.772600000 | 2.490248000 |
| C | 4.553234000 | -2.110805000 | 2.943052000 |
| C | 3.871207000 | -3.198505000 | 2.349532000 |
| C | 2.844311000 | -2.876260000 | 1.442836000 |
| C | 4.207017000 | -4.706103000 | 2.552293000 |
| C | 5.594007000 | -4.989789000 | 3.176022000 |
| C | 3.116373000 | -5.390027000 | 3.408428000 |
| C | 4.231239000 | -5.405861000 | 1.165274000 |
| C | 6.815925000 | -0.066497000 | 2.531484000 |
| C | 4.838226000 | -2.505586000 | 5.253557000 |
| C | 5.371519000 | 0.361104000 | 2.896086000 |
| C | 5.075612000 | 1.664359000 | 2.122276000 |
| C | 4.265367000 | -0.502370000 | -3.814575000 |
| C | 4.705417000 | -1.336087000 | -2.757086000 |
| C | 6.199019000 | -2.861222000 | -4.093087000 |
| C | 3.791578000 | -1.572282000 | -1.721951000 |
| C | 2.489841000 | -1.057459000 | -1.748552000 |
| C | 2.043788000 | -0.424713000 | -2.914168000 |
| C | 2.900303000 | -0.170465000 | -3.995109000 |
| C | 5.693644000 | 1.288659000 | -4.364888000 |
| C | 7.287035000 | -1.098413000 | -2.659146000 |
| C | 2.711565000 | 1.853188000 | -5.607989000 |
| C | 2.331472000 | 0.377871000 | -5.332647000 |
| C | 0.788767000 | 0.305751000 | -5.338925000 |
| C | 6.196993000 | -3.066678000 | -1.610500000 |
| C | 5.301134000 | 0.705178000 | 4.402828000 |
| C | 6.079386000 | -2.057685000 | -2.773662000 |
| C | 2.828047000 | -0.507899000 | -6.502536000 |
| H | -2.238258000 | -1.221394000 | 5.318147000 |
| H | -2.732656000 | 0.118990000 | 3.288701000 |
| H | 0.507879000 | -5.184291000 | 4.780646000 |
| H | -1.209808000 | -5.552492000 | 4.346988000 |
| H | 1.372009000 | -3.134976000 | -2.339588000 |
| H | 0.147803000 | -5.244096000 | -2.803164000 |
| H | -3.386204000 | -6.532735000 | 0.286398000 |
| H | -1.744020000 | -6.930117000 | 0.942445000 |
| H | -3.928306000 | -2.419233000 | 0.580425000 |

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|---|--------------|--------------|--------------|
| H | -2.517965000 | 0.424972000 | -2.266667000 |
| H | -1.948854000 | -0.121723000 | -4.724932000 |
| H | -2.924689000 | 0.213072000 | -6.164441000 |
| H | -2.783492000 | -1.442392000 | -5.554301000 |
| H | -5.423788000 | -1.399400000 | -5.634319000 |
| H | -5.465644000 | 0.327132000 | -5.980119000 |
| H | -6.291396000 | -0.312092000 | -4.549489000 |
| H | -4.944473000 | 1.616604000 | -3.327561000 |
| H | -4.321115000 | 1.947170000 | -4.954269000 |
| H | -3.196875000 | 1.748901000 | -3.616395000 |
| H | -7.915255000 | -4.090697000 | -1.025871000 |
| H | -7.323513000 | -3.116563000 | -2.386922000 |
| H | -7.467408000 | -2.395825000 | -0.770965000 |
| H | -6.459547000 | -4.790477000 | 0.787344000 |
| H | -5.962588000 | -3.131681000 | 1.124523000 |
| H | -4.736567000 | -4.387403000 | 0.871500000 |
| H | -4.404283000 | -5.370803000 | -1.612410000 |
| H | -5.732524000 | -5.068804000 | -2.746033000 |
| H | -6.054061000 | -5.900009000 | -1.226581000 |
| H | -3.967965000 | -4.264754000 | -3.977474000 |
| H | -4.051667000 | -3.019476000 | -5.248958000 |
| H | -5.347468000 | -4.233862000 | -5.113306000 |
| H | -1.923273000 | 2.744868000 | 1.243174000 |
| H | -4.957967000 | -0.246226000 | 1.251187000 |
| H | -1.753847000 | 5.587241000 | 3.496806000 |
| H | -1.398399000 | 3.979903000 | 2.863914000 |
| H | -2.626451000 | 4.175657000 | 4.120118000 |
| H | -3.433900000 | 5.733361000 | 0.138095000 |
| H | -1.900890000 | 4.908278000 | 0.461552000 |
| H | -2.223800000 | 6.491413000 | 1.188358000 |
| H | -5.689216000 | 5.264039000 | 0.341248000 |
| H | -7.343925000 | 5.439447000 | 0.987717000 |
| H | -6.916833000 | 4.027856000 | -0.022835000 |
| H | -5.037140000 | 6.254395000 | 2.105984000 |
| H | -3.723951000 | 6.703447000 | 3.185669000 |
| H | -4.836606000 | 5.403807000 | 3.642575000 |
| H | -7.895210000 | 1.566784000 | 0.086745000 |
| H | -8.302601000 | 2.870933000 | 1.225166000 |
| H | -9.121507000 | 1.313424000 | 1.338101000 |
| H | -8.422365000 | 1.416406000 | 3.824702000 |
| H | -7.378242000 | 2.835554000 | 3.614079000 |
| H | -6.707945000 | 1.325497000 | 4.265260000 |
| H | -6.480422000 | -0.745052000 | 2.784940000 |
| H | -7.060871000 | -0.701737000 | 1.105441000 |

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|---|--------------|--------------|--------------|
| H | -8.204408000 | -0.559066000 | 2.443372000 |
| H | 3.193497000 | 0.476139000 | 1.215208000 |
| H | 2.264221000 | -3.676031000 | 0.999364000 |
| H | 5.656825000 | -4.734180000 | 4.233595000 |
| H | 6.390270000 | -4.452005000 | 2.653162000 |
| H | 5.798585000 | -6.063832000 | 3.087980000 |
| H | 3.333074000 | -6.460889000 | 3.512264000 |
| H | 2.131208000 | -5.280478000 | 2.945824000 |
| H | 3.066926000 | -4.961203000 | 4.416230000 |
| H | 4.494315000 | -6.462081000 | 1.295295000 |
| H | 4.981125000 | -4.950204000 | 0.509935000 |
| H | 3.267857000 | -5.375304000 | 0.649481000 |
| H | 7.518292000 | 0.734490000 | 2.794049000 |
| H | 6.906139000 | -0.249225000 | 1.453843000 |
| H | 7.114080000 | -0.972157000 | 3.063297000 |
| H | 4.265856000 | -3.438718000 | 5.304673000 |
| H | 4.171897000 | -1.669450000 | 5.495044000 |
| H | 5.651574000 | -2.544781000 | 5.982930000 |
| H | 4.095076000 | 2.083020000 | 2.372005000 |
| H | 5.127382000 | 1.520346000 | 1.037301000 |
| H | 5.829699000 | 2.413408000 | 2.389175000 |
| H | 5.397096000 | -3.604865000 | -4.171304000 |
| H | 7.157291000 | -3.395311000 | -4.122666000 |
| H | 6.146313000 | -2.202827000 | -4.962988000 |
| H | 4.104927000 | -2.149275000 | -0.863723000 |
| H | 1.019085000 | -0.080391000 | -2.958754000 |
| H | 6.178346000 | 1.688657000 | -5.259302000 |
| H | 6.423852000 | 1.228257000 | -3.552302000 |
| H | 4.882635000 | 1.951367000 | -4.053429000 |
| H | 8.202252000 | -1.677749000 | -2.485278000 |
| H | 7.169189000 | -0.403197000 | -1.819525000 |
| H | 7.435028000 | -0.524357000 | -3.574382000 |
| H | 3.758919000 | 1.961573000 | -5.895550000 |
| H | 2.516265000 | 2.487880000 | -4.737638000 |
| H | 2.108726000 | 2.233051000 | -6.442363000 |
| H | 0.425270000 | 0.578726000 | -6.336253000 |
| H | 0.331509000 | 0.994788000 | -4.622504000 |
| H | 0.429926000 | -0.706895000 | -5.122082000 |
| H | 5.384829000 | -3.801681000 | -1.621900000 |
| H | 6.203023000 | -2.575026000 | -0.630746000 |
| H | 7.140731000 | -3.614968000 | -1.707826000 |
| H | 4.271841000 | 0.917499000 | 4.712997000 |
| H | 5.898379000 | 1.603932000 | 4.600332000 |
| H | 5.702995000 | -0.096015000 | 5.023945000 |

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|----|--------------|--------------|--------------|
| H | 2.409105000 | -0.140904000 | -7.447941000 |
| H | 2.498679000 | -1.546006000 | -6.372186000 |
| H | 3.916499000 | -0.498545000 | -6.581937000 |
| Cu | 0.005526000 | 0.744863000 | -0.149450000 |
| N | 0.552717000 | 2.765082000 | 0.155924000 |
| C | 1.006684000 | 3.432022000 | 1.182345000 |
| C | 0.536900000 | 3.486719000 | -1.056970000 |
| C | 1.191120000 | 2.932413000 | 2.543668000 |
| C | 1.730042000 | 3.825006000 | 3.494870000 |
| C | 0.835677000 | 1.638925000 | 2.971078000 |
| C | 1.906026000 | 3.438833000 | 4.820930000 |
| H | 2.014607000 | 4.825446000 | 3.177325000 |
| C | 1.002878000 | 1.258420000 | 4.300183000 |
| H | 0.420348000 | 0.934703000 | 2.256619000 |
| C | 1.537571000 | 2.154266000 | 5.231944000 |
| H | 2.324868000 | 4.141848000 | 5.536089000 |
| H | 0.710007000 | 0.258701000 | 4.608702000 |
| H | 1.661968000 | 1.855315000 | 6.269459000 |
| C | -0.223883000 | 2.821882000 | -2.113323000 |
| O | -0.422911000 | 1.595870000 | -2.133403000 |
| O | -0.708505000 | 3.504138000 | -3.173961000 |
| C | -0.748871000 | 4.935423000 | -3.198942000 |
| H | 0.256481000 | 5.357539000 | -3.213115000 |
| H | -1.269819000 | 5.190511000 | -4.123380000 |
| H | -1.314060000 | 5.328467000 | -2.346472000 |
| H | 0.363078000 | 4.559156000 | -0.955329000 |
| H | 1.220620000 | 4.494555000 | 1.060444000 |
| C | 3.224626000 | 4.188171000 | -0.613249000 |
| C | 2.412323000 | 3.619777000 | -1.591332000 |
| H | 3.710287000 | 3.474497000 | 0.042407000 |
| C | 3.335116000 | 5.587470000 | -0.274437000 |
| C | 4.060643000 | 5.955758000 | 0.889351000 |
| C | 2.753691000 | 6.646139000 | -1.018061000 |
| C | 4.193387000 | 7.282484000 | 1.282505000 |
| H | 4.525484000 | 5.170928000 | 1.482588000 |
| C | 2.884611000 | 7.972962000 | -0.612560000 |
| H | 2.222677000 | 6.424659000 | -1.936122000 |
| C | 3.601465000 | 8.309096000 | 0.538000000 |
| H | 4.763109000 | 7.519438000 | 2.178568000 |
| H | 2.426158000 | 8.756411000 | -1.212565000 |
| H | 3.703608000 | 9.346297000 | 0.844962000 |
| F | 2.222397000 | 4.289895000 | -2.781852000 |
| F | 2.676138000 | 2.316965000 | -1.887827000 |

INT1^{F2}

| | | | |
|---|--------------|--------------|--------------|
| P | -1.403988000 | -1.114783000 | 0.260923000 |
| P | 2.080981000 | -0.092993000 | -0.497591000 |
| O | 0.008387000 | -4.234841000 | -3.181004000 |
| O | 0.701855000 | -3.469156000 | -5.244442000 |
| O | 2.091136000 | -4.947882000 | -1.109990000 |
| O | 1.625389000 | -6.275789000 | 0.712784000 |
| O | 5.377905000 | -3.105298000 | 3.525015000 |
| O | 6.219460000 | 4.029176000 | -1.900533000 |
| O | -5.614510000 | -2.000784000 | -3.940777000 |
| O | -5.126695000 | -0.052242000 | 4.803589000 |
| C | 1.738379000 | -1.194321000 | -1.946869000 |
| C | 0.955240000 | -2.391030000 | -1.823143000 |
| C | 0.697913000 | -3.053007000 | -3.017666000 |
| C | 1.118639000 | -2.600919000 | -4.266921000 |
| C | 1.844013000 | -1.439179000 | -4.402541000 |
| C | 2.144559000 | -0.752615000 | -3.214589000 |
| C | 0.229608000 | -4.620009000 | -4.540494000 |
| C | -0.439597000 | -2.697840000 | 0.408294000 |
| C | -0.698790000 | -3.525302000 | 1.511493000 |
| C | -0.053988000 | -4.754481000 | 1.725289000 |
| C | 0.857175000 | -5.136709000 | 0.767295000 |
| C | 1.135476000 | -4.327255000 | -0.330866000 |
| C | 0.545897000 | -3.089220000 | -0.557496000 |
| C | 2.154284000 | -6.287073000 | -0.616201000 |
| C | 3.077385000 | -1.083595000 | 0.696242000 |
| C | 3.875011000 | -2.172775000 | 0.323622000 |
| C | 4.696146000 | -2.832550000 | 1.245066000 |
| C | 4.675108000 | -2.363857000 | 2.587409000 |
| C | 4.009943000 | -1.173575000 | 2.964098000 |
| C | 3.164871000 | -0.595972000 | 2.000758000 |
| C | 4.170399000 | -0.421564000 | 4.316408000 |
| C | 2.926394000 | -0.643609000 | 5.206855000 |
| C | 5.448828000 | -0.787374000 | 5.106753000 |
| C | 4.277941000 | 1.103318000 | 4.030348000 |
| C | 5.650575000 | -3.964535000 | 0.780367000 |
| C | 7.112289000 | -3.587353000 | 1.129656000 |
| C | 5.589478000 | -4.163306000 | -0.750640000 |
| C | 5.308159000 | -5.326866000 | 1.432376000 |
| C | 4.564457000 | -3.925768000 | 4.364565000 |
| C | 3.347986000 | 1.114353000 | -1.109562000 |
| C | 2.956638000 | 2.417014000 | -1.416969000 |
| C | 4.698198000 | 0.768132000 | -1.267990000 |
| C | 5.671266000 | 1.708244000 | -1.612771000 |

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| C | 5.242143000 | 3.055618000 | -1.765706000 |
| C | 3.876795000 | 3.411416000 | -1.803619000 |
| C | 3.289504000 | 4.769030000 | -2.283352000 |
| C | 2.251057000 | 4.462535000 | -3.396654000 |
| C | 2.574901000 | 5.480957000 | -1.109816000 |
| C | 6.456501000 | 4.770163000 | -0.702046000 |
| C | 4.291814000 | 5.758324000 | -2.921464000 |
| C | 7.131437000 | 1.266444000 | -1.890139000 |
| C | 8.137768000 | 1.857990000 | -0.874365000 |
| C | 7.530642000 | 1.702030000 | -3.322414000 |
| C | 7.277575000 | -0.269360000 | -1.823098000 |
| C | -2.642290000 | -1.455584000 | -1.068675000 |
| C | -3.439803000 | -0.382378000 | -1.489603000 |
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| C | -4.688370000 | -1.857988000 | -2.918910000 |
| C | -4.012358000 | -2.990059000 | -2.407757000 |
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| C | -3.321065000 | -5.133789000 | -3.597497000 |
| C | -4.398657000 | -5.248800000 | -1.337537000 |
| C | -6.902620000 | 0.194141000 | -2.327970000 |
| C | -5.034336000 | -2.110300000 | -5.239880000 |
| C | -5.460662000 | 0.620168000 | -2.704137000 |
| C | -5.122636000 | 1.869069000 | -1.861157000 |
| C | -4.218957000 | -0.534385000 | 3.870838000 |
| C | -4.693604000 | -1.332387000 | 2.800460000 |
| C | -6.190782000 | -2.864870000 | 4.123494000 |
| C | -3.803725000 | -1.556745000 | 1.742409000 |
| C | -2.491865000 | -1.068102000 | 1.758832000 |
| C | -2.012591000 | -0.477312000 | 2.932803000 |
| C | -2.844362000 | -0.234228000 | 4.035242000 |
| C | -5.605688000 | 1.267041000 | 4.490950000 |
| C | -7.271831000 | -1.046651000 | 2.754909000 |
| C | -2.580432000 | 1.747530000 | 5.687643000 |
| C | -2.241369000 | 0.269657000 | 5.375216000 |
| C | -0.701039000 | 0.159025000 | 5.354644000 |
| C | -6.236058000 | -3.005809000 | 1.636381000 |
| C | -5.422939000 | 1.052686000 | -4.189129000 |
| C | -6.079913000 | -2.029745000 | 2.823097000 |
| C | -2.739571000 | -0.629512000 | 6.534113000 |
| H | 2.181208000 | -1.082100000 | -5.369410000 |
| H | 2.728274000 | 0.156786000 | -3.289496000 |
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| H | 0.993531000 | -5.410529000 | -4.575735000 |
| H | -1.445612000 | -3.212867000 | 2.231231000 |
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| H | 3.193140000 | -6.617442000 | -0.591454000 |
| H | 1.535431000 | -6.940244000 | -1.249406000 |
| H | 3.846776000 | -2.508382000 | -0.705021000 |
| H | 2.566643000 | 0.267887000 | 2.267819000 |
| H | 2.016962000 | -0.310903000 | 4.698382000 |
| H | 3.020366000 | -0.070498000 | 6.137776000 |
| H | 2.792735000 | -1.696585000 | 5.476853000 |
| H | 5.426273000 | -1.787527000 | 5.538433000 |
| H | 5.559622000 | -0.076814000 | 5.934602000 |
| H | 6.343535000 | -0.714518000 | 4.480013000 |
| H | 5.094630000 | 1.316909000 | 3.331082000 |
| H | 4.488797000 | 1.631283000 | 4.967616000 |
| H | 3.356736000 | 1.529697000 | 3.625020000 |
| H | 7.791692000 | -4.382849000 | 0.797938000 |
| H | 7.244557000 | -3.447617000 | 2.203860000 |
| H | 7.408115000 | -2.663057000 | 0.619613000 |
| H | 6.306710000 | -4.940906000 | -1.037092000 |
| H | 5.863547000 | -3.252394000 | -1.294451000 |
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| H | 5.580354000 | -5.350958000 | 2.487863000 |
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| H | 3.984699000 | -3.330299000 | 5.077086000 |
| H | 5.249625000 | -4.574572000 | 4.916721000 |
| H | 1.904293000 | 2.669020000 | -1.344324000 |
| H | 4.991948000 | -0.257309000 | -1.092471000 |
| H | 1.793200000 | 5.396473000 | -3.743103000 |
| H | 1.444250000 | 3.807147000 | -3.063618000 |
| H | 2.738021000 | 3.986898000 | -4.255997000 |
| H | 3.278584000 | 5.729420000 | -0.306099000 |
| H | 1.782585000 | 4.857730000 | -0.682384000 |
| H | 2.115953000 | 6.415374000 | -1.454639000 |
| H | 5.558293000 | 5.302200000 | -0.369743000 |
| H | 7.239460000 | 5.495233000 | -0.938142000 |
| H | 6.796012000 | 4.116079000 | 0.109502000 |
| H | 4.978409000 | 6.208266000 | -2.203100000 |
| H | 3.718700000 | 6.577223000 | -3.372943000 |
| H | 4.885329000 | 5.288197000 | -3.709750000 |
| H | 7.821942000 | 1.663030000 | 0.157411000 |
| H | 8.264603000 | 2.932753000 | -1.006494000 |

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| H | 9.120488000 | 1.391165000 | -1.014619000 |
| H | 8.557849000 | 1.382069000 | -3.537842000 |
| H | 7.477424000 | 2.786158000 | -3.439775000 |
| H | 6.872432000 | 1.238906000 | -4.067136000 |
| H | 6.606688000 | -0.778593000 | -2.524228000 |
| H | 7.087195000 | -0.660460000 | -0.817200000 |
| H | 8.303922000 | -0.542554000 | -2.091850000 |
| H | -3.238639000 | 0.599251000 | -1.078949000 |
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| H | -6.008560000 | -5.774015000 | -3.267104000 |
| H | -3.559905000 | -6.193423000 | -3.754421000 |
| H | -2.325951000 | -5.067151000 | -3.148234000 |
| H | -3.281516000 | -4.651933000 | -4.581585000 |
| H | -4.686148000 | -6.291203000 | -1.517823000 |
| H | -5.127542000 | -4.813056000 | -0.645747000 |
| H | -3.426281000 | -5.264416000 | -0.838133000 |
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| H | -6.969056000 | -0.050673000 | -1.260932000 |
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| H | -4.472052000 | -3.043785000 | -5.356716000 |
| H | -4.366008000 | -1.267400000 | -5.450369000 |
| H | -5.865252000 | -2.101844000 | -5.950171000 |
| H | -4.141673000 | 2.287637000 | -2.108648000 |
| H | -5.149333000 | 1.660653000 | -0.785874000 |
| H | -5.869652000 | 2.645062000 | -2.062652000 |
| H | -5.400883000 | -3.623994000 | 4.168589000 |
| H | -7.157674000 | -3.382921000 | 4.156436000 |
| H | -6.111479000 | -2.230049000 | 5.008769000 |
| H | -4.143884000 | -2.102718000 | 0.874091000 |
| H | -0.979400000 | -0.158760000 | 2.969203000 |
| H | -6.085041000 | 1.643303000 | 5.398381000 |
| H | -6.336764000 | 1.241044000 | 3.677447000 |
| H | -4.787302000 | 1.930136000 | 4.200488000 |
| H | -8.200428000 | -1.605400000 | 2.584714000 |
| H | -7.157184000 | -0.333456000 | 1.930042000 |
| H | -7.392297000 | -0.492426000 | 3.686256000 |
| H | -3.620097000 | 1.874353000 | 5.994781000 |
| H | -2.384218000 | 2.396792000 | 4.828203000 |
| H | -1.955951000 | 2.094265000 | 6.520660000 |
| H | -0.314552000 | 0.400610000 | 6.351337000 |
| H | -0.238013000 | 0.853011000 | 4.646572000 |
| H | -0.370664000 | -0.856634000 | 5.108720000 |

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| H | -5.436862000 | -3.754764000 | 1.612944000 |
| H | -6.251619000 | -2.488225000 | 0.670175000 |
| H | -7.187320000 | -3.540269000 | 1.737047000 |
| H | -4.398159000 | 1.263161000 | -4.515005000 |
| H | -6.006210000 | 1.973039000 | -4.316008000 |
| H | -5.857905000 | 0.298161000 | -4.845579000 |
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| H | -2.438138000 | -1.672248000 | 6.375851000 |
| H | -3.825866000 | -0.595545000 | 6.632447000 |
| Cu | -0.003288000 | 0.726210000 | 0.153864000 |
| N | -0.502454000 | 2.743729000 | -0.078533000 |
| C | -0.990906000 | 3.450042000 | -1.065757000 |
| C | -0.526167000 | 3.468239000 | 1.167302000 |
| C | -1.208629000 | 3.000460000 | -2.439781000 |
| C | -1.754747000 | 3.934453000 | -3.345879000 |
| C | -0.876918000 | 1.718532000 | -2.917705000 |
| C | -1.958826000 | 3.598345000 | -4.681230000 |
| H | -2.023933000 | 4.924369000 | -2.984905000 |
| C | -1.068924000 | 1.389734000 | -4.257300000 |
| H | -0.461397000 | 0.982791000 | -2.235852000 |
| C | -1.609554000 | 2.325906000 | -5.144850000 |
| H | -2.383531000 | 4.330303000 | -5.362921000 |
| H | -0.792908000 | 0.399308000 | -4.608275000 |
| H | -1.754745000 | 2.066896000 | -6.190391000 |
| C | 0.348151000 | 2.776767000 | 2.179957000 |
| O | 0.508763000 | 1.555637000 | 2.176695000 |
| O | 0.982379000 | 3.454847000 | 3.148987000 |
| C | 0.983017000 | 4.888432000 | 3.231607000 |
| H | -0.024979000 | 5.264106000 | 3.403362000 |
| H | 1.620999000 | 5.119990000 | 4.085725000 |
| H | 1.413018000 | 5.335154000 | 2.329271000 |
| H | -0.238017000 | 4.519229000 | 1.041797000 |
| H | -1.179266000 | 4.510639000 | -0.911359000 |
| C | -3.013466000 | 4.254403000 | 0.800685000 |
| C | -2.102821000 | 3.584057000 | 1.678963000 |
| H | -3.692645000 | 3.602846000 | 0.263671000 |
| C | -3.020221000 | 5.650490000 | 0.492699000 |
| C | -3.854256000 | 6.135066000 | -0.558251000 |
| C | -2.211744000 | 6.626078000 | 1.142462000 |
| C | -3.868918000 | 7.471999000 | -0.930286000 |
| H | -4.496457000 | 5.425841000 | -1.077115000 |
| C | -2.226971000 | 7.964316000 | 0.753182000 |
| H | -1.606274000 | 6.333726000 | 1.992871000 |
| C | -3.048274000 | 8.408129000 | -0.285106000 |

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|---|--------------|-------------|--------------|
| H | -4.527239000 | 7.792694000 | -1.735554000 |
| H | -1.595248000 | 8.674614000 | 1.283791000 |
| H | -3.060498000 | 9.454139000 | -0.578244000 |
| F | -1.935832000 | 4.168949000 | 2.954990000 |
| F | -2.496675000 | 2.285687000 | 1.911437000 |

TS2^{F2}

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| P | -1.324849000 | -1.153143000 | 0.348231000 |
| P | 2.075265000 | 0.074031000 | -0.431111000 |
| O | 0.308776000 | -4.420369000 | -2.729151000 |
| O | 0.845123000 | -3.748924000 | -4.871853000 |
| O | 2.485579000 | -4.783755000 | -0.603730000 |
| O | 2.120354000 | -5.964567000 | 1.339126000 |
| O | 5.662662000 | -2.363878000 | 3.740347000 |
| O | 6.091034000 | 4.186614000 | -2.184685000 |
| O | -5.063447000 | -3.081931000 | -3.957154000 |
| O | -5.123748000 | 0.276934000 | 4.717248000 |
| C | 1.787936000 | -1.150536000 | -1.790519000 |
| C | 1.126378000 | -2.400421000 | -1.551866000 |
| C | 0.892080000 | -3.173589000 | -2.681934000 |
| C | 1.217233000 | -2.776973000 | -3.977065000 |
| C | 1.813941000 | -1.561842000 | -4.226243000 |
| C | 2.093291000 | -0.763840000 | -3.104166000 |
| C | 0.499717000 | -4.880459000 | -4.069269000 |
| C | -0.229760000 | -2.614960000 | 0.697862000 |
| C | -0.432948000 | -3.352136000 | 1.873293000 |
| C | 0.312355000 | -4.496923000 | 2.203683000 |
| C | 1.261601000 | -4.890827000 | 1.287764000 |
| C | 1.481039000 | -4.169964000 | 0.116687000 |
| C | 0.792744000 | -3.013300000 | -0.223892000 |
| C | 2.644856000 | -6.063155000 | 0.011948000 |
| C | 3.148034000 | -0.761232000 | 0.818480000 |
| C | 4.049773000 | -1.785835000 | 0.509247000 |
| C | 4.930764000 | -2.305127000 | 1.464106000 |
| C | 4.860820000 | -1.766656000 | 2.778817000 |
| C | 4.060914000 | -0.642490000 | 3.095007000 |
| C | 3.173405000 | -0.203690000 | 2.097025000 |
| C | 4.109385000 | 0.166889000 | 4.422702000 |
| C | 2.968576000 | -0.276929000 | 5.368429000 |
| C | 5.469996000 | 0.082293000 | 5.154700000 |
| C | 3.891901000 | 1.675846000 | 4.118915000 |
| C | 5.991810000 | -3.362163000 | 1.057487000 |
| C | 7.410584000 | -2.812291000 | 1.349158000 |
| C | 5.930656000 | -3.675347000 | -0.454516000 |

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| C | 5.800919000 | -4.704723000 | 1.806228000 |
| C | 4.993742000 | -3.240743000 | 4.647328000 |
| C | 3.273010000 | 1.295618000 | -1.145420000 |
| C | 2.906833000 | 2.643816000 | -1.239902000 |
| C | 4.547172000 | 0.917907000 | -1.573533000 |
| C | 5.494595000 | 1.838913000 | -2.041396000 |
| C | 5.139600000 | 3.206551000 | -1.948729000 |
| C | 3.818465000 | 3.629057000 | -1.649068000 |
| C | 3.362822000 | 5.100138000 | -1.835336000 |
| C | 1.848748000 | 5.256437000 | -1.586277000 |
| C | 4.079348000 | 6.074099000 | -0.869133000 |
| C | 6.972895000 | 4.417117000 | -1.085082000 |
| C | 3.631064000 | 5.535859000 | -3.298014000 |
| C | 6.806165000 | 1.261170000 | -2.647560000 |
| C | 7.688687000 | 0.658813000 | -1.528544000 |
| C | 7.649617000 | 2.257939000 | -3.476507000 |
| C | 6.426924000 | 0.125317000 | -3.638261000 |
| C | -2.442859000 | -1.786891000 | -0.983115000 |
| C | -3.203954000 | -0.868167000 | -1.717924000 |
| C | -4.146250000 | -1.280035000 | -2.668272000 |
| C | -4.263123000 | -2.677703000 | -2.899659000 |
| C | -3.636502000 | -3.638462000 | -2.070490000 |
| C | -2.692940000 | -3.149603000 | -1.151083000 |
| C | -3.949027000 | -5.164413000 | -2.040317000 |
| C | -5.297633000 | -5.560816000 | -2.686464000 |
| C | -2.808245000 | -5.966661000 | -2.708586000 |
| C | -4.048650000 | -5.630765000 | -0.561399000 |
| C | -6.555688000 | -0.642303000 | -3.117974000 |
| C | -4.344825000 | -3.470410000 | -5.126612000 |
| C | -5.076595000 | -0.246405000 | -3.357675000 |
| C | -4.887310000 | 1.165767000 | -2.762043000 |
| C | -4.255857000 | -0.315590000 | 3.814298000 |
| C | -4.754613000 | -1.027092000 | 2.703305000 |
| C | -7.108871000 | -1.445097000 | 3.765744000 |
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| C | -2.472083000 | -1.043328000 | 1.798837000 |
| C | -1.998597000 | -0.521408000 | 3.012764000 |
| C | -2.863096000 | -0.170010000 | 4.052168000 |
| C | -5.645174000 | 1.529775000 | 4.255782000 |
| C | -6.892588000 | -0.689515000 | 1.371050000 |
| C | -2.644472000 | 1.831768000 | 5.651268000 |
| C | -2.309438000 | 0.339492000 | 5.406504000 |
| C | -0.773582000 | 0.203793000 | 5.469238000 |
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| C | -4.812661000 | -0.135188000 | -4.878035000 |
| C | -6.219785000 | -1.503222000 | 2.502097000 |
| C | -2.890634000 | -0.518141000 | 6.558007000 |
| H | 2.070485000 | -1.243333000 | -5.230650000 |
| H | 2.576684000 | 0.190862000 | -3.270462000 |
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| H | -7.316942000 | 1.452354000 | 1.627367000 |
| H | -7.549678000 | 1.562636000 | 3.386384000 |
| H | -2.555376000 | 3.692776000 | 4.333023000 |
| H | -1.103052000 | 2.879292000 | 3.720199000 |
| H | -1.188779000 | 3.384398000 | 5.415489000 |
| H | -0.659472000 | 1.038500000 | 6.225954000 |
| H | -0.422871000 | 0.599256000 | 4.540447000 |
| H | -1.522806000 | -0.358645000 | 5.560037000 |
| H | -6.426589000 | -2.263334000 | 1.686378000 |
| H | -6.891566000 | -0.928609000 | 0.608413000 |
| H | -8.073740000 | -1.626442000 | 1.720471000 |
| H | -1.689695000 | -0.850238000 | -5.640574000 |
| H | -2.502853000 | 0.323260000 | -6.688623000 |
| H | -3.257656000 | -1.237027000 | -6.378341000 |
| H | -2.487321000 | 1.993228000 | 7.097761000 |
| H | -3.675373000 | 0.798172000 | 6.553268000 |
| H | -3.934622000 | 2.517278000 | 6.246026000 |
| Cu | -0.145122000 | 0.814627000 | 0.093680000 |
| N | 0.138180000 | 2.722896000 | 0.259725000 |
| C | -0.462806000 | 3.875267000 | -0.384964000 |
| C | 1.403022000 | 3.157779000 | 0.796606000 |
| C | -1.949393000 | 3.774604000 | -0.664817000 |
| C | -2.490595000 | 4.359556000 | -1.817023000 |
| C | -2.822324000 | 3.178018000 | 0.253781000 |
| C | -3.868376000 | 4.353118000 | -2.047964000 |
| H | -1.826273000 | 4.834066000 | -2.535410000 |
| C | -4.198582000 | 3.157805000 | 0.020833000 |
| H | -2.410258000 | 2.724981000 | 1.148343000 |
| C | -4.728220000 | 3.746818000 | -1.130171000 |
| H | -4.267460000 | 4.818900000 | -2.945704000 |
| H | -4.855731000 | 2.674449000 | 0.739164000 |
| H | -5.800505000 | 3.734637000 | -1.309588000 |
| C | 1.792319000 | 2.388010000 | 2.071177000 |
| O | 1.043010000 | 1.625259000 | 2.651388000 |
| O | 3.045772000 | 2.507692000 | 2.558452000 |
| C | 4.063766000 | 3.304293000 | 1.934024000 |
| H | 3.768778000 | 4.350903000 | 1.860977000 |
| H | 4.929886000 | 3.214401000 | 2.592269000 |
| H | 4.318092000 | 2.909609000 | 0.945827000 |
| H | 2.256120000 | 3.045423000 | 0.097151000 |

| | | | |
|---|--------------|--------------|--------------|
| H | 0.026282000 | 4.146081000 | -1.345758000 |
| C | -0.153682000 | 5.048321000 | 0.615619000 |
| C | 1.271769000 | 4.696871000 | 1.028029000 |
| H | -0.764430000 | 4.843514000 | 1.501377000 |
| C | -0.397930000 | 6.468903000 | 0.167712000 |
| C | -1.234170000 | 7.296485000 | 0.931093000 |
| C | 0.159831000 | 6.998108000 | -1.007780000 |
| C | -1.505507000 | 8.608719000 | 0.542447000 |
| H | -1.679557000 | 6.903442000 | 1.841979000 |
| C | -0.112737000 | 8.308597000 | -1.401422000 |
| H | 0.811567000 | 6.385361000 | -1.620903000 |
| C | -0.944582000 | 9.120909000 | -0.628198000 |
| H | -2.156853000 | 9.228383000 | 1.153554000 |
| H | 0.329709000 | 8.696822000 | -2.315567000 |
| H | -1.154184000 | 10.141977000 | -0.936240000 |
| F | 2.211605000 | 5.361758000 | 0.258534000 |
| F | 1.540684000 | 5.072586000 | 2.326022000 |

PhCF=CF₂

| | | | |
|---|--------------|--------------|--------------|
| C | -2.300240000 | -1.388171000 | 0.000033000 |
| C | -0.928509000 | -1.148378000 | 0.000032000 |
| C | -0.439733000 | 0.172227000 | -0.000002000 |
| C | -1.361210000 | 1.235058000 | -0.000025000 |
| C | -2.731704000 | 0.983475000 | -0.000024000 |
| C | -3.209418000 | -0.327582000 | 0.000002000 |
| H | -2.659769000 | -2.413620000 | 0.000060000 |
| H | -0.242238000 | -1.985742000 | 0.000060000 |
| H | -0.996894000 | 2.255443000 | -0.000043000 |
| H | -3.427475000 | 1.818133000 | -0.000045000 |
| H | -4.278171000 | -0.522457000 | 0.000006000 |
| C | 0.988923000 | 0.496673000 | 0.000002000 |
| C | 2.051229000 | -0.317602000 | -0.000019000 |
| F | 3.301802000 | 0.113078000 | -0.000004000 |
| F | 1.986058000 | -1.643379000 | -0.000040000 |
| F | 1.288642000 | 1.820750000 | 0.000041000 |

TS1^{F3}

| | | | |
|---|--------------|--------------|--------------|
| P | 1.336315000 | -1.121578000 | -0.298211000 |
| P | -2.105331000 | 0.053182000 | 0.440822000 |
| O | -0.308009000 | -4.379765000 | 2.832841000 |
| O | -0.909716000 | -3.696060000 | 4.953578000 |
| O | -2.425206000 | -4.806613000 | 0.690680000 |
| O | -2.019630000 | -6.011931000 | -1.228554000 |
| O | -5.597320000 | -2.519119000 | -3.726780000 |

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|---|--------------|--------------|--------------|
| O | -6.213952000 | 4.120780000 | 2.090299000 |
| O | 5.096951000 | -2.879938000 | 4.060030000 |
| O | 5.188133000 | 0.059583000 | -4.706624000 |
| C | -1.817780000 | -1.146057000 | 1.822732000 |
| C | -1.127833000 | -2.386009000 | 1.612958000 |
| C | -0.908063000 | -3.142581000 | 2.757312000 |
| C | -1.273092000 | -2.738963000 | 4.039900000 |
| C | -1.897446000 | -1.532591000 | 4.261445000 |
| C | -2.162600000 | -0.751558000 | 3.124113000 |
| C | -0.531160000 | -4.831051000 | 4.170977000 |
| C | 0.262988000 | -2.608644000 | -0.620017000 |
| C | 0.487466000 | -3.359963000 | -1.782718000 |
| C | -0.233054000 | -4.523469000 | -2.101617000 |
| C | -1.181600000 | -4.921546000 | -1.187090000 |
| C | -1.424500000 | -4.186142000 | -0.029905000 |
| C | -0.760798000 | -3.011381000 | 0.299157000 |
| C | -2.553850000 | -6.098930000 | 0.095343000 |
| C | -3.152771000 | -0.817491000 | -0.805763000 |
| C | -4.033063000 | -1.858744000 | -0.487453000 |
| C | -4.896006000 | -2.410186000 | -1.440579000 |
| C | -4.831607000 | -1.883884000 | -2.760323000 |
| C | -4.065861000 | -0.738994000 | -3.082554000 |
| C | -3.188435000 | -0.270587000 | -2.088755000 |
| C | -4.142753000 | 0.071132000 | -4.408546000 |
| C | -2.938198000 | -0.266504000 | -5.317573000 |
| C | -5.462583000 | -0.118550000 | -5.193137000 |
| C | -4.065909000 | 1.589256000 | -4.080223000 |
| C | -5.936345000 | -3.485853000 | -1.029888000 |
| C | -7.363748000 | -2.971242000 | -1.343271000 |
| C | -5.883105000 | -3.776520000 | 0.486758000 |
| C | -5.710519000 | -4.833443000 | -1.759555000 |
| C | -4.866898000 | -3.373542000 | -4.607640000 |
| C | -3.332964000 | 1.265255000 | 1.123135000 |
| C | -2.990642000 | 2.619414000 | 1.217511000 |
| C | -4.610156000 | 0.872037000 | 1.527558000 |
| C | -5.580356000 | 1.781194000 | 1.971569000 |
| C | -5.244463000 | 3.153448000 | 1.878157000 |
| C | -3.924057000 | 3.593923000 | 1.601781000 |
| C | -3.495015000 | 5.073024000 | 1.787635000 |
| C | -1.979720000 | 5.252844000 | 1.563028000 |
| C | -4.209835000 | 6.030823000 | 0.804149000 |
| C | -7.079524000 | 4.331732000 | 0.973551000 |
| C | -3.795063000 | 5.511706000 | 3.243207000 |
| C | -6.895087000 | 1.186903000 | 2.554394000 |

| | | | |
|---|--------------|--------------|--------------|
| C | -7.747555000 | 0.569128000 | 1.420589000 |
| C | -7.767373000 | 2.174542000 | 3.364261000 |
| C | -6.519329000 | 0.059041000 | 3.555529000 |
| C | 2.453747000 | -1.699610000 | 1.058363000 |
| C | 3.223201000 | -0.751820000 | 1.747089000 |
| C | 4.164714000 | -1.128508000 | 2.712785000 |
| C | 4.282640000 | -2.516197000 | 2.998198000 |
| C | 3.647559000 | -3.508855000 | 2.215257000 |
| C | 2.696719000 | -3.055359000 | 1.285126000 |
| C | 3.962414000 | -5.034795000 | 2.241618000 |
| C | 5.316789000 | -5.405144000 | 2.891479000 |
| C | 2.828934000 | -5.814050000 | 2.947876000 |
| C | 4.052573000 | -5.557274000 | 0.781099000 |
| C | 6.575353000 | -0.461353000 | 3.059248000 |
| C | 4.392423000 | -3.227319000 | 5.250541000 |
| C | 5.104240000 | -0.073267000 | 3.354494000 |
| C | 4.874144000 | 1.328124000 | 2.752124000 |
| C | 4.271658000 | -0.449494000 | -3.796098000 |
| C | 4.741235000 | -1.203315000 | -2.693599000 |
| C | 6.358231000 | -2.691229000 | -3.921109000 |
| C | 3.820513000 | -1.459703000 | -1.668033000 |
| C | 2.489068000 | -1.037440000 | -1.744088000 |
| C | 2.030748000 | -0.478092000 | -2.942708000 |
| C | 2.891622000 | -0.214587000 | -4.016161000 |
| C | 5.591959000 | 1.405502000 | -4.397834000 |
| C | 7.300567000 | -0.786787000 | -2.567972000 |
| C | 2.645861000 | 1.703636000 | -5.749838000 |
| C | 2.317626000 | 0.234737000 | -5.387918000 |
| C | 0.778533000 | 0.109000000 | -5.405083000 |
| C | 6.324076000 | -2.764502000 | -1.430855000 |
| C | 4.901928000 | 0.056177000 | 4.883177000 |
| C | 6.160972000 | -1.829302000 | -2.648617000 |
| C | 2.864378000 | -0.699877000 | -6.495612000 |
| H | -2.186178000 | -1.209339000 | 5.255556000 |
| H | -2.668243000 | 0.195096000 | 3.268390000 |
| H | 0.390803000 | -5.258031000 | 4.568998000 |
| H | -1.347295000 | -5.568481000 | 4.176445000 |
| H | 1.268157000 | -3.043485000 | -2.463749000 |
| H | -0.034927000 | -5.086763000 | -3.006942000 |
| H | -3.607702000 | -6.373763000 | 0.045268000 |
| H | -1.970685000 | -6.828874000 | 0.676710000 |
| H | -4.033462000 | -2.248109000 | 0.522270000 |
| H | -2.519138000 | 0.551279000 | -2.315075000 |
| H | -1.993930000 | -0.062652000 | -4.804528000 |

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|---|--------------|--------------|--------------|
| H | -2.967244000 | 0.347563000 | -6.226474000 |
| H | -2.930923000 | -1.316885000 | -5.626343000 |
| H | -5.566100000 | -1.103262000 | -5.647231000 |
| H | -5.496050000 | 0.620940000 | -6.002170000 |
| H | -6.335480000 | 0.045587000 | -4.552486000 |
| H | -4.835940000 | 1.876802000 | -3.354941000 |
| H | -4.235472000 | 2.163575000 | -4.998410000 |
| H | -3.091372000 | 1.894404000 | -3.690570000 |
| H | -8.105363000 | -3.725461000 | -1.050418000 |
| H | -7.488105000 | -2.760733000 | -2.406897000 |
| H | -7.579378000 | -2.055178000 | -0.780723000 |
| H | -6.657164000 | -4.511261000 | 0.735784000 |
| H | -6.083659000 | -2.880144000 | 1.084794000 |
| H | -4.916909000 | -4.185595000 | 0.799594000 |
| H | -4.660507000 | -5.144133000 | -1.714062000 |
| H | -6.006119000 | -4.781571000 | -2.807579000 |
| H | -6.318054000 | -5.616450000 | -1.288123000 |
| H | -4.194901000 | -4.038231000 | -4.053157000 |
| H | -4.280366000 | -2.802537000 | -5.334207000 |
| H | -5.609636000 | -3.971371000 | -5.142906000 |
| H | -1.978243000 | 2.908619000 | 0.965353000 |
| H | -4.860163000 | -0.181517000 | 1.499634000 |
| H | -1.711602000 | 6.297293000 | 1.757762000 |
| H | -1.684770000 | 5.024501000 | 0.532205000 |
| H | -1.384724000 | 4.629153000 | 2.236913000 |
| H | -5.267518000 | 6.147214000 | 1.040614000 |
| H | -4.116334000 | 5.680425000 | -0.231071000 |
| H | -3.749830000 | 7.025041000 | 0.860979000 |
| H | -7.688768000 | 3.447724000 | 0.757296000 |
| H | -6.511911000 | 4.594983000 | 0.073795000 |
| H | -7.735718000 | 5.162195000 | 1.246419000 |
| H | -4.859639000 | 5.436002000 | 3.473167000 |
| H | -3.483747000 | 6.553494000 | 3.390653000 |
| H | -3.238818000 | 4.892455000 | 3.956651000 |
| H | -7.188203000 | -0.194032000 | 0.868489000 |
| H | -8.071822000 | 1.325647000 | 0.697605000 |
| H | -8.646368000 | 0.096035000 | 1.835155000 |
| H | -8.548244000 | 1.601917000 | 3.879332000 |
| H | -8.269889000 | 2.919735000 | 2.747704000 |
| H | -7.182751000 | 2.703703000 | 4.122256000 |
| H | -5.904354000 | 0.452490000 | 4.373035000 |
| H | -5.971843000 | -0.765612000 | 3.091213000 |
| H | -7.432024000 | -0.362464000 | 3.992390000 |
| H | 3.092936000 | 0.295794000 | 1.504369000 |

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|---|-------------|--------------|--------------|
| H | 2.147773000 | -3.782706000 | 0.700813000 |
| H | 5.329546000 | -5.281385000 | 3.974061000 |
| H | 6.137553000 | -4.811824000 | 2.477435000 |
| H | 5.525030000 | -6.461257000 | 2.680828000 |
| H | 3.029940000 | -6.892176000 | 2.908383000 |
| H | 1.863534000 | -5.625358000 | 2.468856000 |
| H | 2.743263000 | -5.532735000 | 4.003841000 |
| H | 4.315142000 | -6.621474000 | 0.791946000 |
| H | 4.828765000 | -5.024752000 | 0.221544000 |
| H | 3.113087000 | -5.463980000 | 0.229856000 |
| H | 7.250619000 | 0.287188000 | 3.492413000 |
| H | 6.758461000 | -0.488316000 | 1.978325000 |
| H | 6.829075000 | -1.436532000 | 3.479554000 |
| H | 3.849853000 | -4.173087000 | 5.141525000 |
| H | 3.681998000 | -2.443551000 | 5.537718000 |
| H | 5.146835000 | -3.338165000 | 6.033972000 |
| H | 3.875744000 | 1.718771000 | 2.971572000 |
| H | 5.017171000 | 1.347202000 | 1.668171000 |
| H | 5.599431000 | 2.022262000 | 3.192469000 |
| H | 5.608766000 | -3.489975000 | -3.972151000 |
| H | 7.350176000 | -3.160669000 | -3.907712000 |
| H | 6.278643000 | -2.083744000 | -4.825490000 |
| H | 4.151636000 | -1.978053000 | -0.780117000 |
| H | 0.987464000 | -0.203355000 | -3.022393000 |
| H | 6.042911000 | 1.810021000 | -5.307799000 |
| H | 6.327941000 | 1.422243000 | -3.589015000 |
| H | 4.737468000 | 2.017220000 | -4.099483000 |
| H | 8.246871000 | -1.293679000 | -2.341893000 |
| H | 7.118230000 | -0.052724000 | -1.774589000 |
| H | 7.432793000 | -0.259872000 | -3.513448000 |
| H | 3.693489000 | 1.835531000 | -6.024755000 |
| H | 2.408950000 | 2.379234000 | -4.921928000 |
| H | 2.044179000 | 2.006889000 | -6.615744000 |
| H | 0.416188000 | 0.322035000 | -6.417305000 |
| H | 0.295417000 | 0.818120000 | -4.725634000 |
| H | 0.448285000 | -0.902612000 | -5.142267000 |
| H | 5.565967000 | -3.554851000 | -1.417414000 |
| H | 6.274164000 | -2.223292000 | -0.478937000 |
| H | 7.305678000 | -3.248795000 | -1.481724000 |
| H | 3.848821000 | 0.236545000 | 5.127635000 |
| H | 5.477411000 | 0.912815000 | 5.255013000 |
| H | 5.247066000 | -0.826994000 | 5.421415000 |
| H | 2.447199000 | -0.407798000 | -7.467664000 |
| H | 2.574254000 | -1.740562000 | -6.306345000 |

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|----|--------------|--------------|--------------|
| H | 3.953098000 | -0.651003000 | -6.559986000 |
| Cu | 0.018045000 | 0.788495000 | -0.185299000 |
| N | 0.594648000 | 2.797562000 | 0.074846000 |
| C | 1.031951000 | 3.476100000 | 1.098240000 |
| C | 0.620988000 | 3.497179000 | -1.154283000 |
| C | 1.155681000 | 3.011936000 | 2.476290000 |
| C | 1.700182000 | 3.911852000 | 3.416799000 |
| C | 0.745384000 | 1.742799000 | 2.926819000 |
| C | 1.825790000 | 3.556472000 | 4.757491000 |
| H | 2.036261000 | 4.889346000 | 3.080900000 |
| C | 0.863376000 | 1.393486000 | 4.269398000 |
| H | 0.328413000 | 1.032369000 | 2.219491000 |
| C | 1.402197000 | 2.297480000 | 5.191495000 |
| H | 2.251910000 | 4.263240000 | 5.464456000 |
| H | 0.531202000 | 0.411869000 | 4.595477000 |
| H | 1.490350000 | 2.022118000 | 6.239173000 |
| C | -0.141981000 | 2.828049000 | -2.210099000 |
| O | -0.375223000 | 1.609218000 | -2.203637000 |
| O | -0.579509000 | 3.499959000 | -3.299141000 |
| C | -0.617788000 | 4.931712000 | -3.340261000 |
| H | 0.385977000 | 5.355903000 | -3.307914000 |
| H | -1.094251000 | 5.177594000 | -4.290670000 |
| H | -1.225060000 | 5.331247000 | -2.519767000 |
| H | 0.450895000 | 4.571554000 | -1.065557000 |
| H | 1.285373000 | 4.528482000 | 0.957446000 |
| C | 3.388114000 | 3.839906000 | -0.651858000 |
| C | 2.477179000 | 3.603838000 | -1.689910000 |
| C | 3.759284000 | 5.071613000 | -0.014140000 |
| C | 4.626944000 | 5.043594000 | 1.108382000 |
| C | 3.296507000 | 6.343761000 | -0.443932000 |
| C | 5.002245000 | 6.215503000 | 1.756690000 |
| H | 5.003553000 | 4.089166000 | 1.457119000 |
| C | 3.675357000 | 7.505177000 | 0.222392000 |
| H | 2.651504000 | 6.418006000 | -1.310895000 |
| C | 4.529812000 | 7.460036000 | 1.327904000 |
| H | 5.673500000 | 6.154872000 | 2.610714000 |
| H | 3.301333000 | 8.462169000 | -0.135156000 |
| H | 4.825620000 | 8.372374000 | 1.838098000 |
| F | 2.367442000 | 4.595004000 | -2.635681000 |
| F | 2.626580000 | 2.411015000 | -2.326888000 |
| F | 3.870216000 | 2.679343000 | -0.078456000 |

INT1^{F3}

| | | | |
|---|--------------|--------------|-------------|
| P | -1.372399000 | -1.145824000 | 0.309137000 |
|---|--------------|--------------|-------------|

| | | | |
|---|--------------|--------------|--------------|
| P | 2.087675000 | -0.031165000 | -0.436454000 |
| O | 0.249784000 | -4.471868000 | -2.788644000 |
| O | 0.897278000 | -3.830308000 | -4.909029000 |
| O | 2.331014000 | -4.906521000 | -0.627020000 |
| O | 1.887071000 | -6.087466000 | 1.298954000 |
| O | 5.486634000 | -2.586505000 | 3.815253000 |
| O | 6.245685000 | 3.968504000 | -2.128562000 |
| O | -5.241546000 | -2.748438000 | -4.008426000 |
| O | -5.231728000 | 0.199418000 | 4.652269000 |
| C | 1.798801000 | -1.249480000 | -1.801827000 |
| C | 1.084875000 | -2.474916000 | -1.584412000 |
| C | 0.869081000 | -3.243711000 | -2.721584000 |
| C | 1.261623000 | -2.865942000 | -4.004029000 |
| C | 1.911390000 | -1.674496000 | -4.233048000 |
| C | 2.171549000 | -0.881161000 | -3.103218000 |
| C | 0.486944000 | -4.947218000 | -4.116314000 |
| C | -0.332043000 | -2.652648000 | 0.638462000 |
| C | -0.579355000 | -3.389716000 | 1.805965000 |
| C | 0.117787000 | -4.562360000 | 2.141569000 |
| C | 1.067582000 | -4.984335000 | 1.239149000 |
| C | 1.333398000 | -4.263526000 | 0.077816000 |
| C | 0.692708000 | -3.080565000 | -0.268259000 |
| C | 2.435437000 | -6.194653000 | -0.017671000 |
| C | 3.108842000 | -0.893729000 | 0.836441000 |
| C | 3.967712000 | -1.961335000 | 0.547678000 |
| C | 4.812218000 | -2.509808000 | 1.518961000 |
| C | 4.749539000 | -1.953092000 | 2.826123000 |
| C | 4.011701000 | -0.781634000 | 3.115833000 |
| C | 3.151358000 | -0.316436000 | 2.105913000 |
| C | 4.104184000 | 0.060948000 | 4.420353000 |
| C | 2.871712000 | -0.198428000 | 5.317281000 |
| C | 5.400009000 | -0.162705000 | 5.235252000 |
| C | 4.101856000 | 1.570321000 | 4.045921000 |
| C | 5.833257000 | -3.615259000 | 1.140294000 |
| C | 7.267861000 | -3.126307000 | 1.462061000 |
| C | 5.792186000 | -3.930968000 | -0.371656000 |
| C | 5.569131000 | -4.944073000 | 1.891020000 |
| C | 4.719407000 | -3.400610000 | 4.703283000 |
| C | 3.336696000 | 1.154427000 | -1.125167000 |
| C | 2.999802000 | 2.504577000 | -1.278249000 |
| C | 4.622702000 | 0.744786000 | -1.482349000 |
| C | 5.605575000 | 1.635760000 | -1.935456000 |
| C | 5.270008000 | 3.010928000 | -1.903061000 |
| C | 3.943894000 | 3.462950000 | -1.676203000 |

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| C | 3.521624000 | 4.933952000 | -1.929634000 |
| C | 2.002393000 | 5.124501000 | -1.744340000 |
| C | 4.217119000 | 5.930283000 | -0.970832000 |
| C | 7.083896000 | 4.222698000 | -0.999815000 |
| C | 3.853372000 | 5.313229000 | -3.395000000 |
| C | 6.933627000 | 1.018106000 | -2.460941000 |
| C | 7.754908000 | 0.443136000 | -1.282428000 |
| C | 7.828896000 | 1.972906000 | -3.285048000 |
| C | 6.581362000 | -0.146646000 | -3.427858000 |
| C | -2.517398000 | -1.688165000 | -1.036875000 |
| C | -3.299367000 | -0.712891000 | -1.671731000 |
| C | -4.271220000 | -1.049321000 | -2.620813000 |
| C | -4.402521000 | -2.425483000 | -2.952975000 |
| C | -3.753874000 | -3.448070000 | -2.221728000 |
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| C | -2.959695000 | -5.735771000 | -3.025780000 |
| C | -4.168841000 | -5.529048000 | -0.842839000 |
| C | -6.689524000 | -0.370698000 | -2.883337000 |
| C | -4.561684000 | -3.050859000 | -5.225339000 |
| C | -5.225204000 | 0.033224000 | -3.191788000 |
| C | -4.984490000 | 1.404056000 | -2.526766000 |
| C | -4.306731000 | -0.350625000 | 3.775942000 |
| C | -4.764665000 | -1.173094000 | 2.718045000 |
| C | -6.363887000 | -2.603870000 | 4.034777000 |
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| C | -2.516084000 | -1.021435000 | 1.758325000 |
| C | -2.064235000 | -0.400583000 | 2.928317000 |
| C | -2.930036000 | -0.087549000 | 3.984415000 |
| C | -5.657364000 | 1.516820000 | 4.259075000 |
| C | -7.329082000 | -0.807960000 | 2.554613000 |
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| C | -2.366021000 | 0.450920000 | 5.327320000 |
| C | -0.826496000 | 0.335030000 | 5.360185000 |
| C | -6.313937000 | -2.840864000 | 1.555298000 |
| C | -5.055581000 | 0.231929000 | -4.716820000 |
| C | -6.173594000 | -1.824218000 | 2.709342000 |
| C | -2.910942000 | -0.414121000 | 6.491041000 |
| H | 2.222779000 | -1.371798000 | -5.226774000 |
| H | 2.696662000 | 0.053896000 | -3.253270000 |
| H | -0.435631000 | -5.364431000 | -4.523091000 |
| H | 1.290663000 | -5.697789000 | -4.097160000 |
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| H | 3.484928000 | -6.482807000 | 0.047545000 |
| H | 1.849517000 | -6.922515000 | -0.598700000 |
| H | 3.966526000 | -2.372826000 | -0.453262000 |
| H | 2.503699000 | 0.528852000 | 2.308086000 |
| H | 1.944781000 | 0.032306000 | 4.784267000 |
| H | 2.913771000 | 0.437353000 | 6.210556000 |
| H | 2.814094000 | -1.239255000 | 5.652622000 |
| H | 5.448847000 | -1.135181000 | 5.723874000 |
| H | 5.452534000 | 0.600868000 | 6.020547000 |
| H | 6.291185000 | -0.060079000 | 4.607423000 |
| H | 4.903167000 | 1.801925000 | 3.334677000 |
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| H | 3.153238000 | 1.905147000 | 3.618562000 |
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| H | 7.384598000 | -2.899353000 | 2.523145000 |
| H | 7.510577000 | -2.225753000 | 0.885606000 |
| H | 6.554096000 | -4.685285000 | -0.598582000 |
| H | 6.018112000 | -3.049038000 | -0.982064000 |
| H | 4.821852000 | -4.325708000 | -0.689792000 |
| H | 4.514378000 | -5.236243000 | 1.833040000 |
| H | 5.848034000 | -4.877517000 | 2.942833000 |
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| H | 4.869944000 | -0.307187000 | -1.408306000 |
| H | 1.738953000 | 6.160227000 | -1.985114000 |
| H | 1.686520000 | 4.937952000 | -0.711171000 |
| H | 1.419428000 | 4.474743000 | -2.404097000 |
| H | 5.279357000 | 6.037429000 | -1.190469000 |
| H | 4.102941000 | 5.621325000 | 0.075524000 |
| H | 3.758828000 | 6.921210000 | -1.076382000 |
| H | 7.685651000 | 3.347244000 | -0.733685000 |
| H | 6.494612000 | 4.522103000 | -0.125706000 |
| H | 7.748315000 | 5.040911000 | -1.289096000 |
| H | 4.922657000 | 5.227805000 | -3.598408000 |
| H | 3.546636000 | 6.348219000 | -3.591197000 |
| H | 3.312063000 | 4.665732000 | -4.094725000 |
| H | 7.179928000 | -0.297795000 | -0.716210000 |
| H | 8.061974000 | 1.226491000 | -0.580832000 |
| H | 8.663204000 | -0.046371000 | -1.655099000 |
| H | 8.622093000 | 1.379982000 | -3.756397000 |

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| H | 8.316323000 | 2.741090000 | -2.684872000 |
| H | 7.265728000 | 2.472596000 | -4.078463000 |
| H | 5.986572000 | 0.215513000 | -4.274234000 |
| H | 6.022406000 | -0.953536000 | -2.946238000 |
| H | 7.504040000 | -0.584011000 | -3.826371000 |
| H | -3.155918000 | 0.325297000 | -1.397632000 |
| H | -2.216540000 | -3.784221000 | -0.755848000 |
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| H | -5.655760000 | -6.373730000 | -2.758242000 |
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| H | -1.991559000 | -5.573752000 | -2.542716000 |
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| H | -4.434007000 | -6.592093000 | -0.879071000 |
| H | -4.941577000 | -5.008484000 | -0.267259000 |
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| H | -7.373439000 | 0.398070000 | -3.264073000 |
| H | -6.848812000 | -0.450194000 | -1.801169000 |
| H | -6.953495000 | -1.324186000 | -3.344975000 |
| H | -3.999490000 | -3.989070000 | -5.155583000 |
| H | -3.872544000 | -2.246711000 | -5.508147000 |
| H | -5.333868000 | -3.153808000 | -5.992291000 |
| H | -3.992682000 | 1.810475000 | -2.747245000 |
| H | -5.103567000 | 1.370654000 | -1.440434000 |
| H | -5.720753000 | 2.117766000 | -2.913910000 |
| H | -5.601931000 | -3.385133000 | 4.141469000 |
| H | -7.347935000 | -3.089542000 | 4.047359000 |
| H | -6.299466000 | -1.937373000 | 4.897746000 |
| H | -4.165530000 | -2.033353000 | 0.844711000 |
| H | -1.023488000 | -0.112683000 | 2.994851000 |
| H | -6.146167000 | 1.955838000 | 5.132647000 |
| H | -6.366939000 | 1.472565000 | 3.428195000 |
| H | -4.809093000 | 2.134859000 | 3.955752000 |
| H | -8.266331000 | -1.344016000 | 2.360418000 |
| H | -7.154856000 | -0.126521000 | 1.713845000 |
| H | -7.473732000 | -0.219888000 | 3.461525000 |
| H | -3.755324000 | 2.076805000 | 5.860325000 |
| H | -2.480529000 | 2.563647000 | 4.721642000 |
| H | -2.107245000 | 2.303481000 | 6.434084000 |
| H | -0.470615000 | 0.610863000 | 6.359368000 |
| H | -0.341708000 | 1.003951000 | 4.642175000 |
| H | -0.490070000 | -0.688844000 | 5.160421000 |
| H | -5.539235000 | -3.614373000 | 1.594449000 |
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| H | -7.285414000 | -3.341115000 | 1.636927000 |
| H | -4.008414000 | 0.426367000 | -4.975741000 |
| H | -5.641427000 | 1.102049000 | -5.037647000 |
| H | -5.409969000 | -0.628049000 | -5.286324000 |
| H | -2.500775000 | -0.055949000 | 7.443733000 |
| H | -2.611715000 | -1.462539000 | 6.371166000 |
| H | -4.000178000 | -0.369932000 | 6.547385000 |
| Cu | -0.038902000 | 0.744836000 | 0.129520000 |
| N | -0.611866000 | 2.731287000 | -0.201171000 |
| C | -1.038172000 | 3.381473000 | -1.248470000 |
| C | -0.699257000 | 3.505081000 | 1.013314000 |
| C | -1.147393000 | 2.879400000 | -2.613649000 |
| C | -1.677893000 | 3.759032000 | -3.581364000 |
| C | -0.742354000 | 1.594879000 | -3.023373000 |
| C | -1.795199000 | 3.367685000 | -4.912324000 |
| H | -2.010523000 | 4.746814000 | -3.271902000 |
| C | -0.849587000 | 1.211158000 | -4.357124000 |
| H | -0.340573000 | 0.900139000 | -2.292215000 |
| C | -1.374575000 | 2.094398000 | -5.307131000 |
| H | -2.210990000 | 4.056565000 | -5.642517000 |
| H | -0.521911000 | 0.219176000 | -4.654740000 |
| H | -1.455016000 | 1.791395000 | -6.347790000 |
| C | 0.178137000 | 2.899143000 | 2.070642000 |
| O | 0.386607000 | 1.685405000 | 2.129511000 |
| O | 0.748648000 | 3.648268000 | 3.030195000 |
| C | 0.732069000 | 5.083328000 | 3.011932000 |
| H | -0.285924000 | 5.461477000 | 3.102101000 |
| H | 1.320939000 | 5.382817000 | 3.880012000 |
| H | 1.207555000 | 5.470917000 | 2.104489000 |
| H | -0.462669000 | 4.562153000 | 0.845090000 |
| H | -1.306001000 | 4.432386000 | -1.139843000 |
| C | -3.255686000 | 4.099902000 | 0.579531000 |
| C | -2.295433000 | 3.571742000 | 1.508883000 |
| C | -3.366637000 | 5.425540000 | 0.082895000 |
| C | -4.193768000 | 5.701333000 | -1.046116000 |
| C | -2.664784000 | 6.532166000 | 0.645575000 |
| C | -4.291729000 | 6.982712000 | -1.571885000 |
| H | -4.754903000 | 4.887069000 | -1.491052000 |
| C | -2.769600000 | 7.805959000 | 0.095357000 |
| H | -2.074133000 | 6.391584000 | 1.543592000 |
| C | -3.577395000 | 8.053716000 | -1.018269000 |
| H | -4.938124000 | 7.151269000 | -2.431262000 |
| H | -2.220272000 | 8.623868000 | 0.557993000 |
| H | -3.660538000 | 9.053414000 | -1.434861000 |

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|---|--------------|-------------|--------------|
| F | -2.182185000 | 4.331019000 | 2.686561000 |
| F | -2.607781000 | 2.296250000 | 1.885520000 |
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TS2^{F3}

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|---|--------------|--------------|--------------|
| P | -1.302377000 | -1.124827000 | 0.337504000 |
| P | 2.134641000 | 0.069467000 | -0.459998000 |
| O | 0.153176000 | -4.273262000 | -2.852684000 |
| O | 0.690216000 | -3.565327000 | -4.984218000 |
| O | 2.436649000 | -4.761445000 | -0.792406000 |
| O | 2.105028000 | -5.995474000 | 1.123456000 |
| O | 5.775137000 | -2.517048000 | 3.570408000 |
| O | 6.146077000 | 4.206776000 | -2.171885000 |
| O | -5.140898000 | -3.131602000 | -3.845271000 |
| O | -4.926138000 | 0.195821000 | 4.899864000 |
| C | 1.815710000 | -1.114534000 | -1.847110000 |
| C | 1.090553000 | -2.333784000 | -1.632908000 |
| C | 0.775381000 | -3.048007000 | -2.781004000 |
| C | 1.103895000 | -2.630990000 | -4.070089000 |
| C | 1.791318000 | -1.459580000 | -4.292174000 |
| C | 2.133385000 | -0.712036000 | -3.152287000 |
| C | -0.110592000 | -4.488737000 | -4.241431000 |
| C | -0.207746000 | -2.594824000 | 0.645917000 |
| C | -0.389166000 | -3.359660000 | 1.806619000 |
| C | 0.348050000 | -4.524312000 | 2.083289000 |
| C | 1.264024000 | -4.906907000 | 1.129292000 |
| C | 1.462911000 | -4.155199000 | -0.026420000 |
| C | 0.782219000 | -2.980552000 | -0.314242000 |
| C | 2.590525000 | -6.061994000 | -0.221342000 |
| C | 3.218523000 | -0.807330000 | 0.749659000 |
| C | 4.090271000 | -1.843321000 | 0.395537000 |
| C | 4.986144000 | -2.398728000 | 1.315640000 |
| C | 4.963238000 | -1.883866000 | 2.641322000 |
| C | 4.197890000 | -0.748274000 | 2.999757000 |
| C | 3.290658000 | -0.273558000 | 2.036584000 |
| C | 4.305671000 | 0.039228000 | 4.337126000 |
| C | 3.177092000 | -0.383383000 | 5.306564000 |
| C | 5.681087000 | -0.096558000 | 5.032978000 |
| C | 4.127236000 | 1.558272000 | 4.058316000 |
| C | 6.011821000 | -3.470736000 | 0.860427000 |
| C | 7.450351000 | -2.964156000 | 1.133084000 |
| C | 5.910498000 | -3.744597000 | -0.657036000 |
| C | 5.801982000 | -4.825733000 | 1.580942000 |
| C | 5.107259000 | -3.393817000 | 4.478437000 |

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| C | 3.332033000 | 1.302128000 | -1.156454000 |
| C | 2.964785000 | 2.650455000 | -1.242859000 |
| C | 4.608623000 | 0.930608000 | -1.582453000 |
| C | 5.555386000 | 1.856570000 | -2.042414000 |
| C | 5.197506000 | 3.222848000 | -1.942586000 |
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| C | 1.903404000 | 5.266307000 | -1.564341000 |
| C | 4.134729000 | 6.082609000 | -0.850475000 |
| C | 7.028285000 | 4.432850000 | -1.071269000 |
| C | 3.680164000 | 5.555401000 | -3.280570000 |
| C | 6.870042000 | 1.284807000 | -2.647630000 |
| C | 7.752069000 | 0.681982000 | -1.528409000 |
| C | 7.711183000 | 2.287112000 | -3.472283000 |
| C | 6.496800000 | 0.150320000 | -3.642217000 |
| C | -2.448208000 | -1.762144000 | -0.968861000 |
| C | -3.203652000 | -0.858014000 | -1.727228000 |
| C | -4.158353000 | -1.294742000 | -2.655740000 |
| C | -4.306078000 | -2.698663000 | -2.825858000 |
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| C | -4.020765000 | -5.155855000 | -1.863735000 |
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| C | -2.911588000 | -6.013057000 | -2.517669000 |
| C | -4.094355000 | -5.553598000 | -0.363010000 |
| C | -6.556690000 | -0.604727000 | -3.059346000 |
| C | -4.464106000 | -3.595647000 | -5.010270000 |
| C | -5.076942000 | -0.274745000 | -3.380179000 |
| C | -4.815549000 | 1.165448000 | -2.892685000 |
| C | -4.106659000 | -0.351647000 | 3.925949000 |
| C | -4.661778000 | -0.976515000 | 2.789076000 |
| C | -6.982037000 | -1.425892000 | 3.903792000 |
| C | -3.777673000 | -1.262798000 | 1.734483000 |
| C | -2.408505000 | -1.015701000 | 1.816428000 |
| C | -1.882644000 | -0.564024000 | 3.036110000 |
| C | -2.703126000 | -0.250275000 | 4.122105000 |
| C | -5.441401000 | 1.486944000 | 4.549845000 |
| C | -6.832719000 | -0.425871000 | 1.589034000 |
| C | -2.378258000 | 1.659254000 | 5.813686000 |
| C | -2.086929000 | 0.175792000 | 5.478562000 |
| C | -0.552319000 | 0.012895000 | 5.470339000 |
| C | -6.209619000 | -2.818946000 | 2.022595000 |
| C | -4.869449000 | -0.273168000 | -4.913785000 |
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| C | -2.638209000 | -0.731828000 | 6.605847000 |
| H | 2.063324000 | -1.134376000 | -5.290377000 |
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| H | -1.172479000 | -4.297627000 | -4.445889000 |
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| H | -7.627027000 | 1.227588000 | 3.271720000 |
| H | -2.792659000 | 3.640160000 | 4.244759000 |
| H | -1.303161000 | 2.917374000 | 3.628861000 |
| H | -1.406881000 | 3.422869000 | 5.323475000 |
| H | -0.745216000 | 1.134370000 | 6.175600000 |
| H | -0.466065000 | 0.692504000 | 4.497371000 |
| H | -1.507922000 | -0.324957000 | 5.520411000 |
| H | -6.303022000 | -2.585611000 | 1.691850000 |
| H | -6.820695000 | -1.306138000 | 0.571688000 |
| H | -7.979542000 | -2.029624000 | 1.691926000 |
| H | -1.561900000 | -1.168672000 | -5.624961000 |
| H | -2.422386000 | -0.080578000 | -6.726348000 |
| H | -3.095621000 | -1.667388000 | -6.367180000 |
| H | -2.634332000 | 1.983673000 | 7.022504000 |
| H | -3.736010000 | 0.703073000 | 6.490726000 |
| H | -4.108767000 | 2.395762000 | 6.155459000 |
| Cu | -0.187528000 | 0.772168000 | 0.042750000 |
| N | 0.045979000 | 2.691584000 | 0.092155000 |
| C | -0.652699000 | 3.807662000 | -0.511472000 |
| C | 1.259203000 | 3.201963000 | 0.677907000 |
| C | -2.121754000 | 3.597927000 | -0.821723000 |
| C | -2.669418000 | 4.131208000 | -1.995974000 |
| C | -2.974081000 | 2.946570000 | 0.078771000 |
| C | -4.034922000 | 4.020695000 | -2.268116000 |
| H | -2.020926000 | 4.645821000 | -2.701116000 |
| C | -4.337107000 | 2.822893000 | -0.196111000 |
| H | -2.560066000 | 2.540894000 | 0.992647000 |
| C | -4.874017000 | 3.360807000 | -1.368436000 |
| H | -4.439582000 | 4.446124000 | -3.183139000 |
| H | -4.978761000 | 2.302091000 | 0.509784000 |
| H | -5.936744000 | 3.267636000 | -1.578562000 |
| C | 1.643527000 | 2.472310000 | 1.979033000 |
| O | 0.920087000 | 1.675990000 | 2.544322000 |
| O | 2.871797000 | 2.672311000 | 2.504295000 |
| C | 3.876993000 | 3.484389000 | 1.879366000 |
| H | 3.540698000 | 4.512184000 | 1.741097000 |
| H | 4.718542000 | 3.469663000 | 2.574396000 |
| H | 4.189648000 | 3.051947000 | 0.924085000 |
| H | 2.145155000 | 3.129205000 | 0.016085000 |
| H | -0.180994000 | 4.163913000 | -1.453754000 |
| C | -0.434732000 | 4.979980000 | 0.506954000 |

| | | | |
|---|--------------|-------------|--------------|
| C | 1.038964000 | 4.731031000 | 0.888516000 |
| C | -0.790190000 | 6.381600000 | 0.066714000 |
| C | -1.652147000 | 7.156951000 | 0.853907000 |
| C | -0.294286000 | 6.929022000 | -1.127267000 |
| C | -2.011460000 | 8.445598000 | 0.458152000 |
| H | -2.042340000 | 6.743127000 | 1.775617000 |
| C | -0.656217000 | 8.217361000 | -1.520788000 |
| H | 0.378710000 | 6.355420000 | -1.754245000 |
| C | -1.515788000 | 8.982253000 | -0.730472000 |
| H | -2.681948000 | 9.029940000 | 1.083072000 |
| H | -0.262019000 | 8.623586000 | -2.448808000 |
| H | -1.795836000 | 9.986160000 | -1.038698000 |
| F | 1.878196000 | 5.437685000 | 0.050521000 |
| F | 1.315323000 | 5.168811000 | 2.153049000 |
| F | -1.149532000 | 4.675424000 | 1.669898000 |