

Supporting Information

Mechanistic Investigation of Rh(I)-Catalyzed Alkyne–Isatin Decarbonylative Coupling

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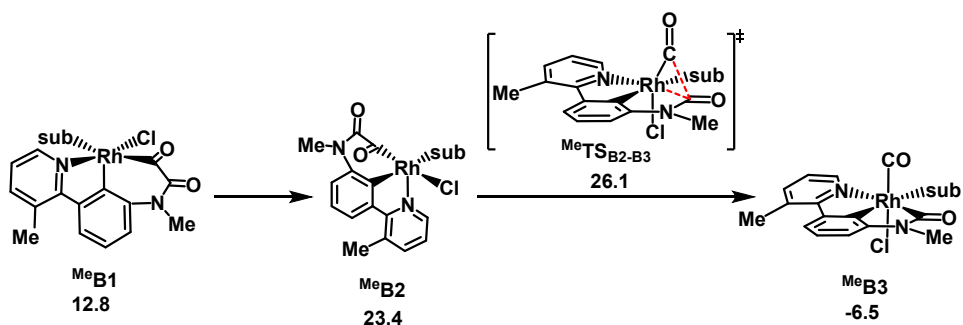
1. Table S1. Calculation results by different methods (M06, B3LYP and PBE0)^a

| | Me _{A1} | Me _{TS_{A1-B}} | Me _B | Me _{B1} | Me _{TS_{B1-C}} | Me _C | Me _{TS_{C2-D}} | Me _{A1'} | Me _{TS_{A1'-B'}} | Me _{B'} | Me _{C'} | Me _{C1'} | Me _{TS_{C1'-D'}} |
|-------|------------------|---------------------------------|-----------------|------------------|---------------------------------|-----------------|---------------------------------|-------------------|-----------------------------------|------------------|------------------|-------------------|-----------------------------------|
| M06 | 0.8 | 7.9 | 0.4 | 12.8 | 22.1 | -7.8 | 20.9 | 3.1 | 16.1 | 14.4 | 21.1 | 28.2 | 27.4 |
| B3LYP | 15.0 | 21.7 | 10.6 | 19.0 | 30.3 | 2.0 | 25.7 | 17.6 | 23.1 | 16.8 | 24.3 | 51.0 | 50.1 |
| PBE0 | 13.9 | 19.3 | 9.9 | 19.0 | 31.4 | 2.4 | 25.7 | 16.3 | 22.1 | 16.8 | 23.4 | 39.5 | 39.5 |

^aAll of the values are solvent-corrected free energies in kcal/mol.

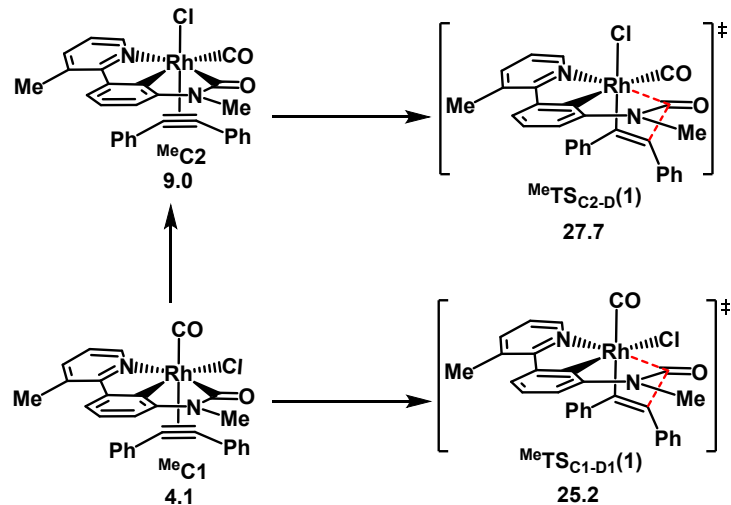
2. Schemes S1-S9 (Other possible pathways):

Scheme S1. Other possible decarbonylation step^a



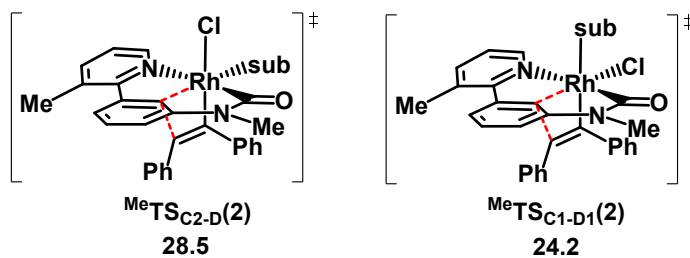
^aAll of the values are solvent-corrected free energies in kcal/mol.

Scheme S2. Possible pathways of acyl migratory insertion^a



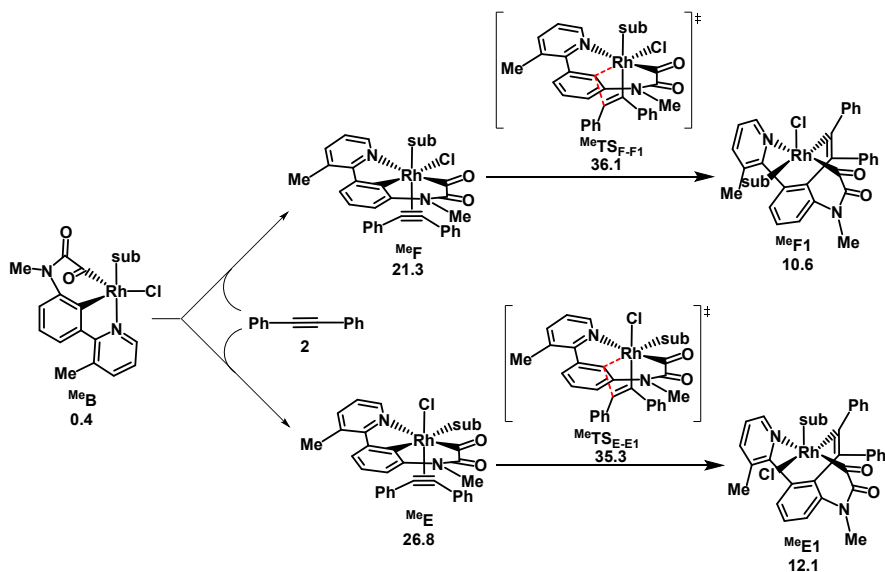
^aAll of the values are solvent-corrected free energies in kcal/mol.

Scheme S3. Other possible transition states for alkyne insertion^a



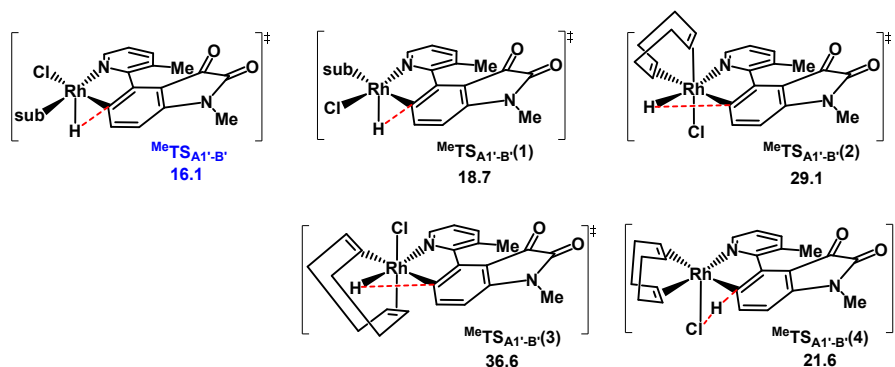
^aAll of the values are solvent-corrected free energies in kcal/mol.

Scheme S4. Alkyne migratory insertion precedes decarbonylation step^a



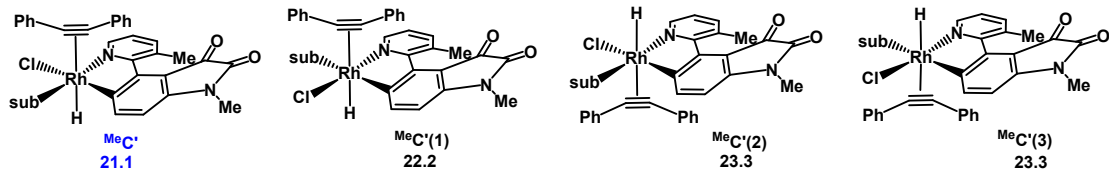
^aAll of the values are solvent-corrected free energies in kcal/mol.

Scheme S5. Other possible transition states about C–H activation^a



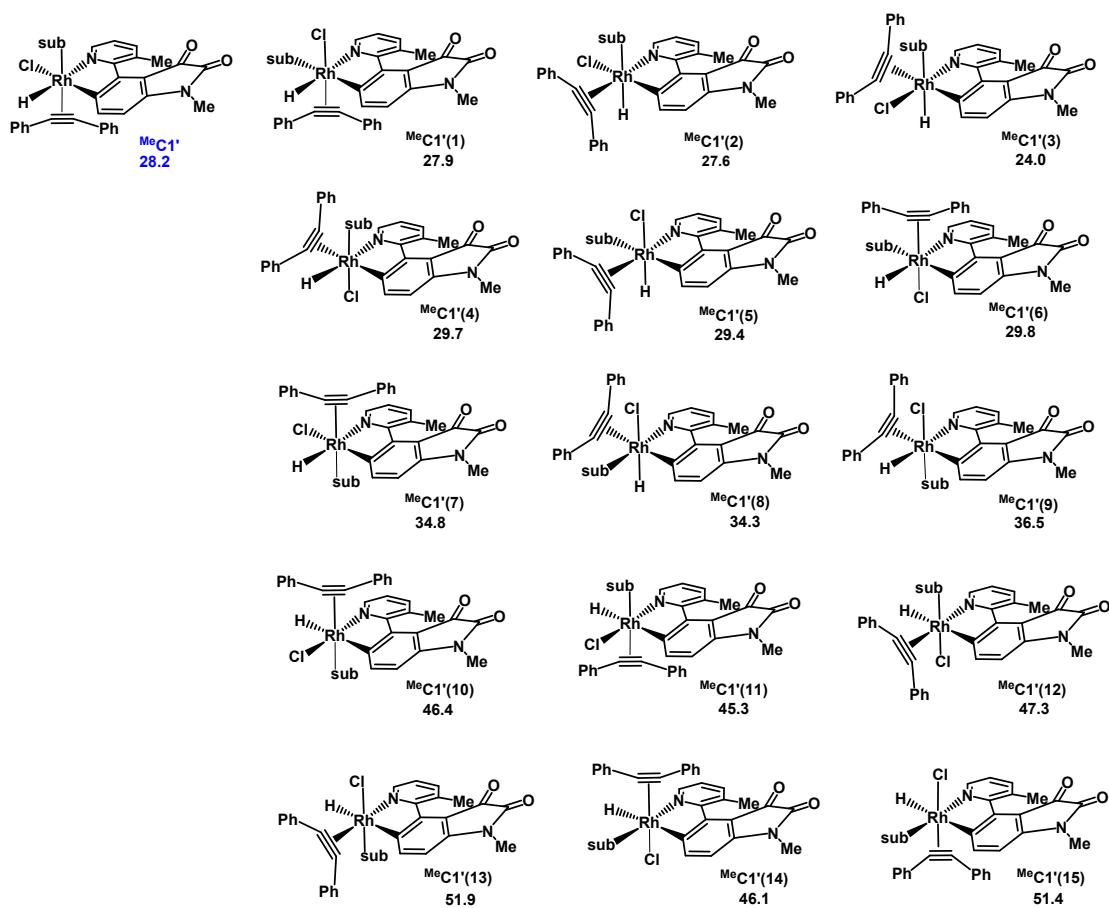
^aAll of the values are solvent-corrected free energies in kcal/mol.

Scheme S6. Isomers of $\text{MeC}^{\beta\text{a}}$



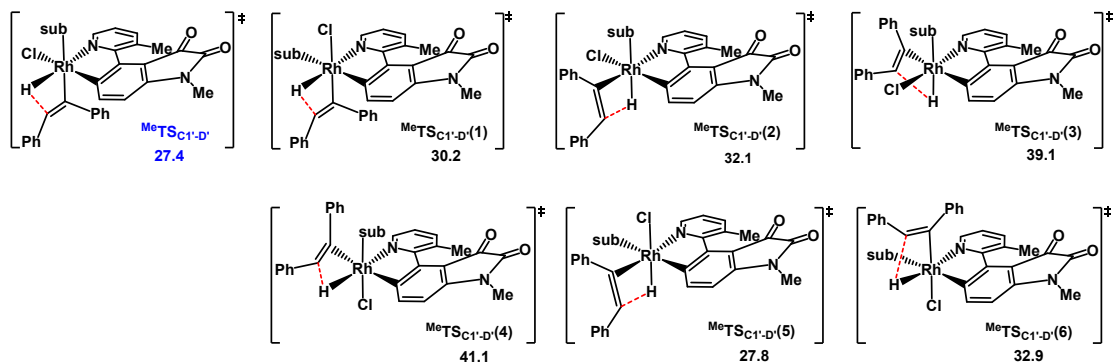
^aAll of the values are solvent-corrected free energies in kcal/mol.

Scheme S7. Isomers of $\text{MeC1}^{\beta\text{a}}$



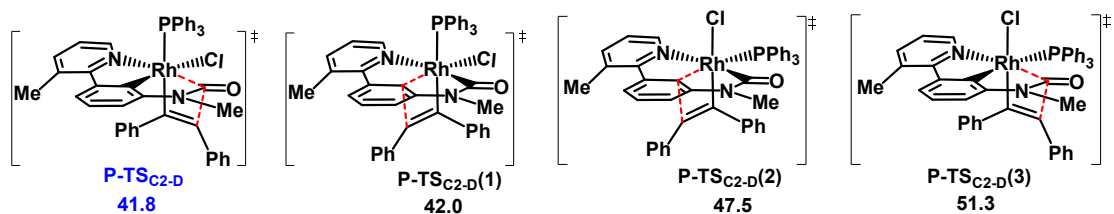
^aAll of the values are solvent-corrected free energies in kcal/mol.

Scheme S8. Isomers of $\text{Me}^{\text{TS}}_{\text{C1-D}}$,^a



^aAll of the values are solvent-corrected free energies in kcal/mol.

Scheme S9. Other possible transition states about alkynes migratory insertion using Wilkinson's catalyst^a



^aAll of the values are solvent-corrected free energies in kcal/mol.

3. Table of energy values

Table S2. Energies (in Hartree) for the related TSs and intermediates.

| Species | E_0 | E | H_{433} | G_{433} | $E_{(sol, M06)}$ |
|------------------------|--------------|--------------|--------------|--------------|------------------|
| 1 | -837.958241 | -837.942525 | -837.941581 | -838.001292 | -838.4307408 |
| 2 | -538.821452 | -538.810224 | -538.809280 | -538.861282 | -539.1598141 |
| 3 | -1263.594803 | -1263.570119 | -1263.569175 | -1263.649039 | -1264.3589266 |
| 4 | -1376.835682 | -1376.808152 | -1376.807208 | -1376.894891 | -1377.6430081 |
| CO | -113.243564 | -113.241204 | -113.240259 | -113.262702 | -113.2862799 |
| cod | -311.581462 | -311.573993 | -311.573048 | -311.613211 | -311.8548235 |
| A | -881.330817 | -881.320959 | -881.320015 | -881.366553 | -882.697262 |
| MeA1 | -2245.687256 | -2245.650435 | -2245.649491 | -2245.756527 | -2247.723607 |
| MeTS _{A1-B} | -2245.687765 | -2245.653009 | -2245.652065 | -2245.750890 | -2247.719427 |
| MeB | -2245.695467 | -2245.659861 | -2245.658917 | -2245.761160 | -2247.729157 |
| MeB1 | -2245.673538 | -2245.638283 | -2245.637339 | -2245.737985 | -2247.711353 |
| MeTS _{B1-C} | -2245.659336 | -2245.624054 | -2245.623110 | -2245.724071 | -2247.693702 |
| MeC | -2245.708385 | -2245.672576 | -2245.671632 | -2245.773552 | -2247.742116 |
| MeC1 | -1946.552129 | -1946.520842 | -1946.519897 | -1946.612900 | -1948.4529979 |
| MeTS _{C1-D1} | -1946.521781 | -1946.490460 | -1946.489516 | -1946.584649 | -1948.4181408 |
| MeD1 | -1946.544227 | -1946.512462 | -1946.511518 | -1946.607499 | -1948.4433735 |
| MeC2 | -1946.541675 | -1946.509909 | -1946.508965 | -1946.603592 | -1948.4428519 |
| MeTS _{C2-D} | -1946.524146 | -1946.492925 | -1946.491981 | -1946.586630 | -1948.4222062 |
| MeD | -1946.556604 | -1946.525019 | -1946.524075 | -1946.620701 | -1948.4564571 |
| MeD2 | -1946.563446 | -1946.531969 | -1946.531025 | -1946.626846 | -1948.4607274 |
| MeTS _{D2-A} | -1946.561039 | -1946.530316 | -1946.529372 | -1946.622829 | -1948.4560419 |
| MeA1' | -2245.698743 | -2245.663477 | -2245.662533 | -2245.762969 | -2247.7274358 |
| MeTS _{A1'} | -2245.653174 | -2245.618225 | -2245.617281 | -2245.718330 | -2247.6779399 |
| MeTS _{A1'-B'} | -2245.672638 | -2245.637787 | -2245.636843 | -2245.736735 | -2247.7022636 |
| MeB' | -2245.676458 | -2245.641780 | -2245.640835 | -2245.739508 | -2247.7086129 |
| MeC' | -2784.503590 | -2784.455052 | -2784.454108 | -2784.587762 | -2786.8768131 |
| MeC1' | -2784.506312 | -2784.459625 | -2784.458681 | -2784.583274 | -2786.8746138 |
| MeTS _{C1'-D'} | -2784.506254 | -2784.459878 | -2784.458934 | -2784.583436 | -2786.8737955 |
| MeD' | -2784.514499 | -2784.466468 | -2784.465524 | -2784.597095 | -2786.8897595 |
| MeD1' | -2784.548316 | -2784.500782 | -2784.499838 | -2784.629870 | -2786.9147296 |
| MeTS _{D1'-A} | -2784.534661 | -2784.488303 | -2784.487359 | -2784.612378 | -2786.9002232 |
| PPh3 | -1035.418891 | -1035.402991 | -1035.402047 | -1035.465680 | -1035.9070264 |
| P-C1 | -3365.379226 | -3365.328541 | -3365.327597 | -3365.463112 | -3367.8728499 |
| P-C2 | -2868.748684 | -2868.702665 | -2868.701721 | -2868.826716 | -2871.0919575 |
| P-TS _{C2-D} | -2868.714806 | -2868.669407 | -2868.668463 | -2868.793405 | -2871.0555015 |

| | | | | | |
|---|--------------|--------------|--------------|--------------|---------------|
| P-D | -2868.749400 | -2868.704128 | -2868.703184 | -2868.827862 | -2871.0986165 |
| 2a | -391.250582 | -391.237819 | -391.236875 | -391.290006 | -391.6284426 |
| 2b | -422.455975 | -422.446765 | -422.445821 | -422.491414 | -422.7319175 |
| 2c | -460.544052 | -460.533937 | -460.532993 | -460.580959 | -460.8269598 |
| 2A | -1798.977003 | -1798.942958 | -1798.942014 | -1799.045924 | -1800.9147167 |
| TS_{2A} | -1798.950927 | -1798.917571 | -1798.916627 | -1799.018499 | -1800.8878239 |
| 2A' | -1798.967773 | -1798.934210 | -1798.933266 | -1799.034651 | -1800.9050372 |
| TS_{2A'} | -1798.950735 | -1798.917791 | -1798.916847 | -1799.017086 | -1800.8875584 |
| 2B | -1830.195207 | -1830.165937 | -1830.164992 | -1830.254368 | -1832.0295279 |
| TS_{2B} | -1830.168080 | -1830.139062 | -1830.138118 | -1830.227892 | -1832.0007694 |
| 2B' | -1830.175327 | -1830.145173 | -1830.144229 | -1830.237122 | -1832.00939 |
| TS_{2B'} | -1830.161287 | -1830.132191 | -1830.131246 | -1830.221644 | -1831.9945273 |
| 2C | -1868.277213 | -1868.246681 | -1868.245737 | -1868.337519 | -1870.1184452 |
| TS_{2C} | -1868.248310 | -1868.218025 | -1868.217081 | -1868.311630 | -1870.0928226 |
| 2C' | -1868.272126 | -1868.241263 | -1868.240319 | -1868.334211 | -1870.1126222 |
| TS_{2C'} | -1868.250293 | -1868.220044 | -1868.219100 | -1868.312237 | -1870.0888106 |
| NoDG_I | -551.862705 | -551.853133 | -551.852189 | -551.897584 | -552.1653272 |
| NoDG_A | -1433.231162 | -1433.210143 | -1433.209199 | -1433.282056 | -1434.8921256 |
| NoDG_AI | -1433.234085 | -1433.213001 | -1433.212057 | -1433.284819 | -1434.8895752 |
| NoDG_{TS_AI-B} | -1433.182276 | -1433.161562 | -1433.160618 | -1433.230758 | -1434.8377073 |
| NoDG_B | -1433.213966 | -1433.192851 | -1433.191907 | -1433.263891 | -1434.8725403 |
| NoDG_{TS_A-C} | -1433.175448 | -1433.155010 | -1433.154065 | -1433.222880 | -1434.8366226 |
| NoDG_C | -1433.187008 | -1433.165933 | -1433.164989 | -1433.235545 | -1434.8493491 |
| Me_{TS_AI-B}(1) | -2245.666295 | -2245.630987 | -2245.630043 | -2245.731842 | -2247.7056392 |
| Me_{TS_AI-B}(2) | -1946.530410 | -1946.500026 | -1946.499082 | -1946.591421 | -1948.4318066 |
| Me_{TS_AI-B}(3) | -1719.284335 | -1719.257677 | -1719.256733 | -1719.339453 | -1721.117552 |
| Me_{TS_AI-B}(4) | -1719.277261 | -1719.250928 | -1719.249984 | -1719.331165 | -1721.1146072 |
| Me_{TS_AI-B}(5) | -1719.275163 | -1719.248758 | -1719.247814 | -1719.329072 | -1721.1118109 |
| Me_{TS_AI-B}(6) | -1719.273567 | -1719.247625 | -1719.246681 | -1719.326574 | -1721.1115411 |
| Me_{TS_AI-B}(7) | -1719.266340 | -1719.239803 | -1719.238859 | -1719.320882 | -1721.1004465 |
| Me_{TS_AI-B}(8) | -1719.284145 | -1719.257253 | -1719.256309 | -1719.339985 | -1721.108642 |
| Me_{TS_AI-B}(9) | -1719.264628 | -1719.237452 | -1719.236507 | -1719.321764 | -1721.0952468 |
| Me_{TS_AI-B}(10) | -3083.623373 | -3083.571211 | -3083.570267 | -3083.706843 | -3086.1275386 |
| Me_{TS_AI-B}(11) | -2557.249017 | -2557.204967 | -2557.204023 | -2557.323957 | -2559.5480785 |
| Me_{TS_AI-B}(12) | -2557.240000 | -2557.195426 | -2557.194481 | -2557.317083 | -2559.5388326 |
| Me_{TS_AI-B}(13) | -3083.619107 | -3083.566942 | -3083.565998 | -3083.702439 | -3086.1169261 |
| Me_{TS_AI-B}(14) | -2245.636190 | -2245.599996 | -2245.599052 | -2245.702854 | -2247.6590165 |
| Me_{TS_AI-B}(15) | -2258.103719 | -2258.064211 | -2258.063267 | -2258.174195 | -2260.2643568 |
| Me_{TS_AI-B}(16) | -2485.342640 | -2485.299167 | -2485.298223 | -2485.417950 | -2487.5691072 |
| Me_{TS_AI-B}(17) | -1719.235542 | -1719.207860 | -1719.206916 | -1719.292972 | -1721.0726107 |

| | | | | | |
|---------------------------|--------------|--------------|--------------|--------------|---------------|
| MeB2 | -2245.654973 | -2245.618979 | -2245.618035 | -2245.721757 | -2247.6907099 |
| MeTS _{B2-B3} | -2245.648394 | -2245.612248 | -2245.611303 | -2245.716127 | -2247.683451 |
| MeB3 | -2245.701493 | -2245.664741 | -2245.663797 | -2245.771032 | -2247.734603 |
| MeTS _{C2-D} (1) | -1946.510173 | -1946.478859 | -1946.477915 | -1946.573542 | -1948.4105795 |
| MeTS _{C2-D} (2) | -2671.237897 | -2671.192088 | -2671.191144 | -2671.316031 | -2673.5612517 |
| MeTS _{C1-D1} (1) | -1946.519208 | -1946.488384 | -1946.487440 | -1946.580449 | -1948.4174873 |
| MeTS _{C1-D1} (2) | -2671.247277 | -2671.201988 | -2671.201044 | -2671.323926 | -2673.5698816 |
| MeE | -2784.504749 | -2784.457255 | -2784.456310 | -2784.584740 | -2786.8755206 |
| MeTS _{E-E1} | -2784.487531 | -2784.439836 | -2784.438892 | -2784.569348 | -2786.8576386 |
| MeE1 | -2784.527363 | -2784.479196 | -2784.478251 | -2784.609449 | -2786.8962911 |
| MeF | -2784.519815 | -2784.473763 | -2784.472819 | -2784.594064 | -2786.8927077 |
| MeTS _{F-F1} | -2784.496796 | -2784.450769 | -2784.449824 | -2784.572091 | -2786.8654366 |
| MeF1 | -2784.533530 | -2784.485750 | -2784.484806 | -2784.614430 | -2786.9002032 |
| MeTS _{A1'-B} (1) | -2245.669246 | -2245.634315 | -2245.633371 | -2245.733489 | -2247.6985191 |
| MeTS _{A1'-B} (2) | -1719.270806 | -1719.243990 | -1719.243046 | -1719.326683 | -1721.1013339 |
| MeTS _{A1'-B} (3) | -1719.257618 | -1719.231023 | -1719.230079 | -1719.312997 | -1721.0903807 |
| MeTS _{A1'-B} (4) | -1719.284972 | -1719.258510 | -1719.257566 | -1719.340899 | -1721.1119314 |
| MeC'(1) | -2784.502610 | -2784.453894 | -2784.452950 | -2784.586326 | -2786.8744083 |
| MeC'(2) | -2784.499127 | -2784.450953 | -2784.450009 | -2784.581246 | -2786.875344 |
| MeC'(3) | -2784.503793 | -2784.455077 | -2784.454133 | -2784.587037 | -2786.8731107 |
| MeC1'(1) | -2784.490902 | -2784.442527 | -2784.441582 | -2784.574455 | -2786.8655939 |
| MeC1'(2) | -2784.502195 | -2784.454574 | -2784.453630 | -2784.581996 | -2786.871125 |
| MeC1'(3) | -2784.508922 | -2784.460630 | -2784.459686 | -2784.590960 | -2786.8741872 |
| MeC1'(4) | -2784.500015 | -2784.452084 | -2784.451139 | -2784.579227 | -2786.8690418 |
| MeC1'(5) | -2784.493864 | -2784.446095 | -2784.445150 | -2784.574216 | -2786.8672657 |
| MeC1'(6) | -2784.490579 | -2784.441783 | -2784.440839 | -2784.575490 | -2786.8606993 |
| MeC1'(7) | -2784.494269 | -2784.448158 | -2784.447214 | -2784.569117 | -2786.86756 |
| MeC1'(8) | -2784.488095 | -2784.440450 | -2784.439506 | -2784.567771 | -2786.8614851 |
| MeC1'(9) | -2784.482785 | -2784.435390 | -2784.434445 | -2784.563767 | -2786.8551907 |
| MeC1'(10) | -2784.467379 | -2784.419992 | -2784.419048 | -2784.547673 | -2786.8396951 |
| MeC1'(11) | -2784.471524 | -2784.424284 | -2784.423340 | -2784.551745 | -2786.8419032 |
| MeC1'(12) | -2784.463946 | -2784.416170 | -2784.415226 | -2784.544575 | -2786.8376755 |
| MeC1'(13) | -2784.456589 | -2784.409108 | -2784.408164 | -2784.535049 | -2786.8335565 |
| MeC1'(14) | -2784.460657 | -2784.412835 | -2784.411891 | -2784.542204 | -2786.8387207 |
| MeC1'(15) | -2784.449057 | -2784.400961 | -2784.400017 | -2784.532159 | -2786.828311 |
| MeTS _{C1'-D} (1) | -2784.489617 | -2784.441892 | -2784.440948 | -2784.570991 | -2786.8634354 |
| MeTS _{C1'-D} (2) | -2784.494212 | -2784.447406 | -2784.446462 | -2784.572779 | -2786.8647542 |
| MeTS _{C1'-D} (3) | -2784.483318 | -2784.435953 | -2784.435009 | -2784.564354 | -2786.8494162 |
| MeTS _{C1'-D} (4) | -2784.480289 | -2784.433561 | -2784.432617 | -2784.558549 | -2786.8499608 |
| MeTS _{C1'-D} (5) | -2784.492988 | -2784.445010 | -2784.444066 | -2784.576767 | -2786.8636764 |

| | | | | | |
|-------------------------------|--------------|--------------|--------------|--------------|---------------|
| MeTS_{C1-D}(6) | -2784.488385 | -2784.440336 | -2784.439391 | -2784.570303 | -2786.8580386 |
| P-TS_{C2-D}(1) | -2868.718475 | -2868.673645 | -2868.672701 | -2868.793960 | -2871.0593722 |
| P-TS_{C2-D}(2) | -2868.704468 | -2868.658836 | -2868.657892 | -2868.782604 | -2871.0468854 |
| P-TS_{C2-D}(3) | -2868.699851 | -2868.654614 | -2868.653670 | -2868.777695 | -2871.0425306 |

E_0 = Sum of electronic and zero-point Energies in gas phase

E = Sum of electronic and thermal Energies in gas phase

H_{433} = Sum of electronic and thermal Enthalpies in gas phase

G_{433} = Sum of electronic and thermal Free Energies in gas phase

$E_{(sol,M06)}$ = Single point energies calculated by M06 in solvent

4. Calculated imaginary frequencies of all transition states species.

| Species | IF |
|--------------------------------------|---------|
| MeTS _{A1-B} | -201.85 |
| MeTS _{B1-C} | -98.96 |
| MeTS _{C1-D1} | -341.72 |
| MeTS _{C2-D} | -301.41 |
| MeTS _{D2-A} | -170.41 |
| MeTS _{A1'} | -288.19 |
| MeTS _{A1'-B'} | -715.42 |
| MeTS _{C1'-D'} | -365.38 |
| MeTS _{D1'-A} | -202.39 |
| P-TS _{C2-D} | -243.69 |
| TS _{2A} | -404.90 |
| TS _{2A'} | -322.02 |
| TS _{2B} | -399.13 |
| TS _{2B'} | -250.66 |
| TS _{2C} | -412.85 |
| TS _{2C'} | -256.63 |
| NoDG ⁺ TS _{A1-B} | -238.29 |
| NoDG ⁺ TS _{A-C} | -218.78 |
| MeTS _{A1-B} (1) | -185.82 |
| MeTS _{A1-B} (2) | -77.78 |
| MeTS _{A1-B} (3) | -135.93 |
| MeTS _{A1-B} (4) | -230.21 |
| MeTS _{A1-B} (5) | -240.24 |
| MeTS _{A1-B} (6) | -220.99 |
| MeTS _{A1-B} (7) | -229.86 |
| MeTS _{A1-B} (8) | -200.14 |
| MeTS _{A1-B} (9) | -241.22 |
| MeTS _{A1-B} (10) | -283.26 |
| MeTS _{A1-B} (11) | -284.20 |
| MeTS _{A1-B} (12) | -329.40 |
| MeTS _{A1-B} (13) | -383.94 |
| MeTS _{A1-B} (14) | -422.29 |
| MeTS _{A1-B} (15) | -328.77 |
| MeTS _{A1-B} (16) | -321.74 |
| MeTS _{A1-B} (17) | -402.43 |
| MeTS _{B2-B3} | -164.86 |
| MeTS _{C2-D} (1) | -231.47 |

| | |
|---------------------------------|---------|
| MeTS_{C2-D}(2) | -247.73 |
| MeTS_{C1-D1}(1) | -242.40 |
| MeTS_{C1-D1}(2) | -202.09 |
| MeTS_{E-E1} | -252.57 |
| MeTS_{F-F1} | -238.50 |
| MeTS_{A1'-B'}(1) | -602.19 |
| MeTS_{A1'-B'}(2) | -843.42 |
| MeTS_{A1'-B'}(3) | -816.79 |
| MeTS_{A1'-B'}(4) | -231.30 |
| MeTS_{C1'-D'}(1) | -406.08 |
| MeTS_{C1'-D'}(2) | -416.93 |
| MeTS_{C1'-D'}(3) | -376.99 |
| MeTS_{C1'-D'}(4) | -427.27 |
| MeTS_{C1'-D'}(5) | -538.32 |
| MeTS_{C1'-D'}(6) | -457.43 |
| P-TS_{C2-D}(1) | -211.97 |
| P-TS_{C2-D}(2) | -256.53 |
| P-TS_{C2-D}(3) | -262.70 |

5. Cartesian coordinates

31

1

| | | | |
|---|----------|----------|----------|
| C | -0.71021 | 0.17426 | -0.01448 |
| C | -1.97645 | 0.78618 | 0.08348 |
| C | -2.11372 | 2.14544 | 0.29309 |
| C | -0.93937 | 2.89971 | 0.37016 |
| C | 0.31626 | 2.31786 | 0.24701 |
| C | 0.45876 | 0.93569 | 0.0689 |
| H | -3.09102 | 2.61598 | 0.37888 |
| H | -1.01353 | 3.97532 | 0.52265 |
| H | 1.2139 | 2.93106 | 0.28255 |
| C | -0.94445 | -1.24215 | -0.31001 |
| C | -2.49059 | -1.40403 | -0.34768 |
| O | -0.18003 | -2.15883 | -0.50245 |
| O | -3.11571 | -2.41475 | -0.55611 |
| N | -3.00417 | -0.14918 | -0.08349 |
| C | -4.41241 | 0.15149 | -0.06213 |
| H | -4.71504 | 0.55694 | 0.91226 |
| H | -4.67305 | 0.87409 | -0.8471 |
| H | -4.94737 | -0.78547 | -0.24412 |
| C | 1.83026 | 0.37972 | -0.07439 |
| C | 2.34142 | -0.62811 | 0.76092 |
| C | 3.65834 | -1.02412 | 0.52544 |
| C | 3.80468 | 0.57651 | -1.22745 |
| C | 4.40206 | -0.43624 | -0.48535 |
| H | 4.09678 | -1.79902 | 1.15531 |
| H | 4.35686 | 1.08859 | -2.01768 |
| H | 5.42804 | -0.73954 | -0.6826 |
| C | 1.56629 | -1.25184 | 1.87905 |
| H | 0.83312 | -0.55948 | 2.30996 |
| H | 1.01953 | -2.13513 | 1.52454 |
| H | 2.23936 | -1.57478 | 2.68278 |
| N | 2.55746 | 0.98602 | -1.0234 |

24

2

| | | | |
|---|----------|----------|----------|
| C | -4.13248 | 0.87955 | 0.82453 |
| C | -2.74421 | 0.88151 | 0.82676 |
| C | -2.03383 | -0.0007 | -0.0003 |
| C | -2.74578 | -0.88203 | -0.82689 |
| C | -4.13406 | -0.87832 | -0.82377 |
| C | -4.83114 | 0.00105 | 0.00059 |
| H | -4.67399 | 1.56872 | 1.47044 |
| H | -2.18979 | 1.5649 | 1.46759 |
| H | -2.19266 | -1.56611 | -1.46811 |
| H | -4.67685 | -1.5668 | -1.46935 |
| H | -5.91973 | 0.00172 | 0.00089 |
| C | -0.60709 | -0.00121 | -0.00061 |
| C | 0.60709 | -0.00109 | -0.00044 |
| C | 2.03383 | -0.00065 | -0.00025 |
| C | 2.74527 | -0.82712 | 0.88162 |
| C | 2.74471 | 0.82654 | -0.88191 |
| C | 4.13356 | -0.82369 | 0.87901 |
| H | 2.19175 | -1.46843 | 1.56528 |
| C | 4.13299 | 0.82461 | -0.87885 |
| H | 2.1907 | 1.46728 | -1.56571 |
| C | 4.83114 | 0.00084 | 0.00021 |
| H | 4.67594 | -1.46914 | 1.56793 |
| H | 4.6749 | 1.47067 | -1.56758 |
| H | 5.91973 | 0.00145 | 0.00043 |

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3

| | | | |
|---|----------|---------|----------|
| C | 0.51381 | 1.49618 | -0.18004 |
| C | -0.05569 | 2.79818 | -0.24055 |
| C | 0.75367 | 3.9239 | -0.45672 |
| C | 2.1204 | 3.78405 | -0.58481 |
| C | 2.70559 | 2.53142 | -0.44336 |
| C | 1.93293 | 1.39945 | -0.21161 |
| H | 0.30899 | 4.91113 | -0.53041 |
| H | 2.73821 | 4.66091 | -0.76926 |
| H | 3.78588 | 2.41523 | -0.49832 |
| C | -2.31182 | 1.91681 | 0.15613 |

| | | | | | | | |
|---|----------|----------|----------|-----------|----------|----------|----------|
| O | -3.4894 | 2.13179 | 0.40848 | C | -4.63017 | -2.60134 | -0.08326 |
| N | -1.42144 | 2.9701 | -0.06942 | H | -5.20908 | -1.91457 | 1.87507 |
| C | -1.99048 | 4.30874 | -0.06025 | H | -3.85183 | -3.03526 | -2.04639 |
| H | -1.53368 | 4.92007 | 0.72769 | H | -5.35568 | -3.41324 | -0.10207 |
| H | -1.84301 | 4.79955 | -1.03011 | | | | |
| H | -3.0578 | 4.20093 | 0.13675 | | | | |
| C | 2.73489 | 0.17013 | 0.06094 | 55 | | | |
| C | 2.7236 | -0.43938 | 1.32889 | 4 | | | |
| C | 3.55018 | -1.5466 | 1.50041 | C | 2.66663 | -0.01365 | -0.13492 |
| C | 4.34255 | -1.26466 | -0.72311 | C | 3.2253 | 1.15449 | -0.68467 |
| C | 4.36246 | -1.98524 | 0.4636 | C | 2.42637 | 2.18584 | -1.1441 |
| H | 3.561 | -2.0565 | 2.46463 | C | 1.04722 | 2.01369 | -1.04456 |
| H | 4.99172 | -1.54536 | -1.55513 | C | 0.45801 | 0.85642 | -0.52198 |
| H | 5.0126 | -2.84956 | 0.58052 | C | 1.28381 | -0.17431 | -0.0276 |
| C | 1.89584 | 0.08135 | 2.46316 | H | 2.84811 | 3.09926 | -1.55885 |
| H | 2.00109 | 1.1687 | 2.57342 | H | 0.38685 | 2.80965 | -1.3901 |
| H | 0.82515 | -0.12159 | 2.32088 | C | 3.78454 | -0.85709 | 0.30046 |
| H | 2.19522 | -0.38692 | 3.40871 | C | 5.06745 | -0.05602 | -0.0652 |
| N | 3.55697 | -0.20929 | -0.92399 | O | 3.81004 | -1.94938 | 0.8174 |
| C | -1.75036 | 0.5707 | 0.01207 | O | 6.21386 | -0.38456 | 0.11718 |
| C | -0.40404 | 0.3635 | -0.1283 | N | 4.62293 | 1.11225 | -0.65453 |
| C | 0.08069 | -1.03325 | -0.2882 | C | 5.4976 | 2.15609 | -1.12272 |
| C | -0.2092 | -2.00186 | 0.67818 | H | 5.3561 | 2.33648 | -2.19651 |
| C | 0.77106 | -1.41777 | -1.43972 | H | 5.32247 | 3.09279 | -0.57682 |
| C | 0.20009 | -3.3173 | 0.50873 | H | 6.52445 | 1.82248 | -0.94524 |
| H | -0.77689 | -1.71909 | 1.5648 | C | 0.67262 | -1.32663 | 0.69549 |
| C | 1.17525 | -2.73639 | -1.61353 | C | 0.71552 | -2.64055 | 0.20976 |
| H | 1.00211 | -0.6729 | -2.20115 | C | 0.02467 | -3.601 | 0.94735 |
| C | 0.89651 | -3.68809 | -0.63809 | C | -0.60647 | -1.91574 | 2.5042 |
| H | -0.0299 | -4.05765 | 1.27309 | C | -0.64562 | -3.24748 | 2.10843 |
| H | 1.71923 | -3.01675 | -2.51437 | H | 0.01307 | -4.63311 | 0.59528 |
| H | 1.21825 | -4.71953 | -0.77349 | H | -1.11738 | -1.58854 | 3.41149 |
| C | -2.75483 | -0.52141 | -0.02876 | H | -1.19326 | -3.98467 | 2.69132 |
| C | -3.62283 | -0.72515 | 1.04789 | C | 1.43759 | -3.01937 | -1.0451 |
| C | -2.85856 | -1.35879 | -1.14302 | H | 2.49039 | -3.24434 | -0.82864 |
| C | -4.54599 | -1.76327 | 1.02463 | H | 0.99208 | -3.91272 | -1.49966 |
| H | -3.57045 | -0.05913 | 1.90708 | H | 1.42262 | -2.21446 | -1.79121 |
| C | -3.78745 | -2.3917 | -1.17039 | N | 0.02899 | -0.97312 | 1.81486 |
| H | -2.19326 | -1.20169 | -1.9915 | C | -1.62718 | -0.29324 | -1.09313 |

| | | | |
|---|----------|----------|----------|
| H | -0.98684 | -0.96318 | -1.67517 |
| C | -1.02295 | 0.75061 | -0.49026 |
| C | -3.03689 | -0.68954 | -1.0532 |
| C | -3.58168 | -1.36971 | -2.1503 |
| C | -3.85169 | -0.47928 | 0.06887 |
| C | -4.90515 | -1.79191 | -2.14807 |
| H | -2.95005 | -1.56173 | -3.0187 |
| C | -5.17162 | -0.90892 | 0.0743 |
| H | -3.43512 | 0.01037 | 0.94839 |
| C | -5.7075 | -1.55881 | -1.0355 |
| H | -5.31006 | -2.31005 | -3.01616 |
| H | -5.78688 | -0.74076 | 0.95694 |
| H | -6.74384 | -1.89259 | -1.02743 |
| C | -1.73721 | 1.84829 | 0.2015 |
| C | -1.37826 | 2.20268 | 1.50726 |
| C | -2.75342 | 2.56266 | -0.44212 |
| C | -2.0451 | 3.23082 | 2.16363 |
| H | -0.59283 | 1.63369 | 2.00605 |
| C | -3.41116 | 3.59664 | 0.21321 |
| H | -3.02683 | 2.2937 | -1.46237 |
| C | -3.06175 | 3.93052 | 1.51883 |
| H | -1.76963 | 3.48779 | 3.18552 |
| H | -4.20051 | 4.14531 | -0.29859 |
| H | -3.57956 | 4.73938 | 2.03229 |

2
CO

| | | | |
|---|------|------|----------|
| C | 0.00 | 0.00 | -0.64994 |
| O | 0.00 | 0.00 | 0.48746 |

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Cod

| | | | |
|---|----------|----------|----------|
| C | -0.05524 | 1.68991 | -0.19969 |
| C | 1.17274 | 1.25347 | -0.49316 |
| C | -1.17279 | -1.25348 | -0.49308 |
| C | 1.90982 | 0.02809 | -0.045 |
| C | 0.05521 | -1.68994 | -0.19972 |
| C | 1.10905 | -1.0616 | 0.67172 |
| H | 2.3856 | -0.41973 | -0.93403 |

| | | | |
|---|----------|----------|----------|
| H | 2.75244 | 0.33752 | 0.59739 |
| H | 1.81567 | -1.84453 | 0.98212 |
| H | 0.68776 | -0.66718 | 1.60367 |
| C | -1.10901 | 1.06156 | 0.67181 |
| H | -0.68767 | 0.66702 | 1.60368 |
| C | -1.9098 | -0.02802 | -0.04504 |
| H | -2.75259 | -0.33736 | 0.59718 |
| H | -2.38536 | 0.41987 | -0.93416 |
| H | -0.36191 | 2.62095 | -0.68353 |
| H | 1.75769 | 1.88364 | -1.1692 |
| H | -1.75781 | -1.88367 | -1.16904 |
| H | 0.36181 | -2.621 | -0.68355 |
| H | -1.81558 | 1.84448 | 0.98233 |

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A

| | | | |
|----|----------|----------|----------|
| C | -1.24504 | -1.1594 | -0.88331 |
| C | -1.32762 | 0.16552 | -1.33559 |
| C | -0.23609 | -0.07476 | 1.4759 |
| C | -2.09708 | 1.25669 | -0.61998 |
| C | -0.08608 | 1.22902 | 0.92156 |
| C | -1.18697 | 2.06023 | 0.31632 |
| H | -2.54817 | 1.9325 | -1.3579 |
| H | -2.9386 | 0.81556 | -0.06825 |
| H | -0.70693 | 2.8687 | -0.25211 |
| H | -1.77077 | 2.5553 | 1.11181 |
| C | -1.84854 | -1.69164 | 0.39522 |
| H | -2.93273 | -1.85895 | 0.27747 |
| C | -1.56612 | -0.79326 | 1.60541 |
| H | -2.36746 | -0.05357 | 1.74345 |
| H | -1.56152 | -1.40214 | 2.51829 |
| Rh | 0.59828 | -0.19456 | -0.43441 |
| Cl | 2.80347 | 0.04764 | 0.25668 |
| H | -1.0081 | -1.92482 | -1.63107 |
| H | -1.1257 | 0.34162 | -2.39652 |
| H | 0.55396 | -0.39503 | 2.16031 |
| H | 0.7925 | 1.7924 | 1.24828 |
| H | -1.40654 | -2.68076 | 0.57769 |

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MeA1

| | | | |
|----|----------|----------|----------|
| C | 2.36856 | 0.67551 | 0.37104 |
| C | 2.39891 | 2.07377 | 0.06021 |
| C | 2.97214 | 2.56771 | -1.08066 |
| C | 3.55838 | 1.64463 | -1.98079 |
| C | 3.55104 | 0.29255 | -1.73701 |
| C | 2.94256 | -0.23482 | -0.56197 |
| H | 2.99315 | 3.63618 | -1.28747 |
| H | 4.02272 | 2.02145 | -2.89059 |
| H | 3.99686 | -0.40274 | -2.447 |
| C | 1.95064 | 0.55203 | 1.77573 |
| C | 1.47639 | 1.98232 | 2.15462 |
| O | 2.00704 | -0.35899 | 2.57185 |
| O | 0.94798 | 2.33575 | 3.18488 |
| N | 1.80891 | 2.79845 | 1.0912 |
| C | 1.55999 | 4.21746 | 1.06362 |
| H | 1.00491 | 4.47088 | 1.97202 |
| H | 2.50014 | 4.78467 | 1.04465 |
| H | 0.96091 | 4.47955 | 0.18114 |
| C | 3.03579 | -1.67783 | -0.22241 |
| C | 4.16225 | -2.47939 | -0.0816 |
| C | 3.91898 | -3.81959 | 0.23966 |
| C | 1.55374 | -3.42527 | 0.21097 |
| C | 2.6235 | -4.29624 | 0.38649 |
| H | 4.76582 | -4.49167 | 0.38038 |
| H | 0.50863 | -3.71899 | 0.27713 |
| H | 2.43672 | -5.33755 | 0.63649 |
| C | 5.55009 | -1.94435 | -0.25104 |
| H | 5.92837 | -2.11965 | -1.26799 |
| H | 5.59221 | -0.86407 | -0.06946 |
| H | 6.24512 | -2.43355 | 0.44213 |
| N | 1.78734 | -2.14908 | -0.0831 |
| Rh | 0.65322 | -0.51671 | -0.51145 |
| Cl | -1.06224 | -1.95703 | -1.27217 |
| C | -3.01458 | -0.09592 | 0.31863 |
| C | -3.5663 | -1.16346 | 1.03643 |
| C | -3.14538 | -1.44541 | 2.3252 |
| C | -2.15507 | -0.62446 | 2.86904 |

| | | | |
|---|----------|----------|----------|
| C | -1.57649 | 0.42454 | 2.15444 |
| C | -1.98743 | 0.67806 | 0.84422 |
| H | -3.55869 | -2.27515 | 2.89524 |
| H | -1.8068 | -0.81682 | 3.88224 |
| H | -0.80186 | 1.0252 | 2.62537 |
| C | -3.63519 | -0.07986 | -1.00863 |
| C | -4.59889 | -1.29998 | -1.00916 |
| O | -3.52397 | 0.70845 | -1.91799 |
| O | -5.31021 | -1.67986 | -1.90607 |
| N | -4.50576 | -1.84793 | 0.26125 |
| C | -5.1855 | -3.05248 | 0.65874 |
| H | -4.46528 | -3.84874 | 0.8911 |
| H | -5.82297 | -2.87608 | 1.53529 |
| H | -5.80946 | -3.36644 | -0.18347 |
| C | -1.39395 | 1.68022 | -0.08143 |
| C | -1.9376 | 2.96475 | -0.1898 |
| C | -1.5034 | 3.76537 | -1.24352 |
| C | -0.05446 | 2.00754 | -1.94657 |
| C | -0.57904 | 3.27264 | -2.15348 |
| H | -1.92661 | 4.76245 | -1.36725 |
| H | 0.69163 | 1.58015 | -2.61364 |
| H | -0.26108 | 3.85713 | -3.01334 |
| C | -3.00379 | 3.42446 | 0.75506 |
| H | -2.72731 | 3.24761 | 1.80215 |
| H | -3.20543 | 4.49445 | 0.62775 |
| H | -3.94306 | 2.8831 | 0.57408 |
| N | -0.42442 | 1.23856 | -0.91257 |

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MeTS_{A1-B}

| | | | |
|---|----------|---------|---------|
| C | 0.75026 | 0.23595 | 1.19425 |
| C | -0.40254 | 0.44175 | 1.97524 |
| C | -0.8464 | 1.72753 | 2.27325 |
| C | -0.08769 | 2.80468 | 1.81828 |
| C | 1.12737 | 2.6207 | 1.15811 |
| C | 1.58315 | 1.32932 | 0.87095 |
| H | -1.76701 | 1.89237 | 2.83168 |
| H | -0.44851 | 3.81578 | 2.00754 |
| H | 1.68642 | 3.49408 | 0.83532 |

| | | | | | | | |
|----|----------|----------|----------|------------|----------|----------|----------|
| C | 1.25093 | -1.33326 | 1.77322 | H | -0.45263 | 4.91537 | -0.85229 |
| C | -0.05144 | -1.78281 | 2.46505 | H | -1.79743 | 5.21483 | -1.99356 |
| O | 2.34829 | -1.56052 | 2.24292 | H | -2.05362 | 5.43132 | -0.2392 |
| O | -0.25767 | -2.89283 | 2.90023 | C | -1.90539 | -1.37096 | -0.94468 |
| N | -0.9527 | -0.73579 | 2.4756 | C | -3.20284 | -1.88042 | -1.06887 |
| C | -2.24626 | -0.85197 | 3.11366 | C | -3.44181 | -3.15562 | -0.55764 |
| H | -2.37409 | -1.90618 | 3.37688 | C | -1.15521 | -3.31378 | 0.09336 |
| H | -2.29167 | -0.24911 | 4.0311 | C | -2.41597 | -3.88357 | 0.02176 |
| H | -3.04235 | -0.53848 | 2.42871 | H | -4.4425 | -3.58007 | -0.63895 |
| C | 2.84937 | 0.98662 | 0.20282 | H | -0.30991 | -3.8419 | 0.52616 |
| C | 4.02637 | 1.75646 | 0.21122 | H | -2.57616 | -4.88655 | 0.40788 |
| C | 5.14905 | 1.21562 | -0.41589 | C | -4.29992 | -1.10368 | -1.72728 |
| C | 3.9168 | -0.74265 | -0.97473 | H | -3.94706 | -0.57314 | -2.62016 |
| C | 5.10415 | -0.03059 | -1.01928 | H | -5.11893 | -1.76707 | -2.02813 |
| H | 6.07719 | 1.78726 | -0.41096 | H | -4.70841 | -0.35597 | -1.03382 |
| H | 3.79432 | -1.72798 | -1.4213 | N | -0.91214 | -2.07458 | -0.35481 |
| H | 5.97837 | -0.46003 | -1.50146 | | | | |
| C | 4.15635 | 3.08671 | 0.89207 | 64 | | | |
| H | 3.72056 | 3.90444 | 0.30119 | MeB | | | |
| H | 3.67108 | 3.09572 | 1.87534 | C | 0.56323 | 0.12458 | 1.08969 |
| H | 5.21503 | 3.33021 | 1.03925 | C | -0.44774 | 0.43966 | 2.00111 |
| N | 2.83119 | -0.24292 | -0.38002 | C | -0.50132 | 1.71161 | 2.57489 |
| Rh | 1.03381 | -1.25944 | -0.27006 | C | 0.52049 | 2.62082 | 2.3067 |
| Cl | 1.52763 | -2.73617 | -2.0851 | C | 1.62736 | 2.25216 | 1.55073 |
| C | -1.96195 | 1.16288 | -1.03346 | C | 1.67465 | 0.98156 | 0.95386 |
| C | -1.45754 | 2.3757 | -1.54155 | H | -1.32098 | 1.99799 | 3.23243 |
| C | -0.56264 | 2.40631 | -2.5937 | H | 0.46942 | 3.61885 | 2.73991 |
| C | -0.16782 | 1.17687 | -3.13006 | H | 2.44522 | 2.95929 | 1.45588 |
| C | -0.62146 | -0.03388 | -2.61462 | C | 0.42839 | -2.17226 | 1.76911 |
| C | -1.5115 | -0.06039 | -1.53225 | C | -0.97426 | -1.8887 | 2.34491 |
| H | -0.1783 | 3.34392 | -2.99047 | O | 1.25954 | -2.80731 | 2.34621 |
| H | 0.529 | 1.16184 | -3.96613 | O | -1.66848 | -2.81885 | 2.70708 |
| H | -0.25286 | -0.97333 | -3.02398 | N | -1.36835 | -0.57547 | 2.34566 |
| C | -2.8706 | 1.50239 | 0.05676 | C | -2.67069 | -0.25785 | 2.9062 |
| C | -2.79047 | 3.04744 | 0.19308 | H | -3.2851 | -1.15986 | 2.84753 |
| O | -3.59387 | 0.81253 | 0.74259 | H | -2.5935 | 0.04206 | 3.96067 |
| O | -3.3223 | 3.73478 | 1.03239 | H | -3.13388 | 0.54692 | 2.32657 |
| N | -1.97284 | 3.46968 | -0.83431 | C | 2.83048 | 0.35598 | 0.28994 |
| C | -1.53969 | 4.83269 | -0.9977 | C | 4.07275 | 0.937 | -0.0238 |

| | | | | | | | |
|----|----------|----------|----------|-------------|----------|----------|----------|
| C | 5.08352 | 0.09334 | -0.48533 | C | -3.99075 | 0.26671 | -2.47331 |
| C | 3.60689 | -1.76417 | -0.40287 | H | -3.29983 | 0.71075 | -3.20027 |
| C | 4.87673 | -1.26757 | -0.64698 | H | -4.8622 | -0.11262 | -3.01925 |
| H | 6.05564 | 0.52753 | -0.72079 | H | -4.33462 | 1.06857 | -1.80715 |
| H | 3.32804 | -2.80001 | -0.58582 | N | -1.42447 | -1.72268 | -0.53993 |
| H | 5.66693 | -1.92876 | -0.99141 | | | | |
| C | 4.35642 | 2.40501 | 0.08412 | 64 | | | |
| H | 3.55584 | 3.00691 | -0.36703 | MeB1 | | | |
| H | 4.47305 | 2.73535 | 1.12548 | C | 0.85779 | 0.72257 | -0.84907 |
| H | 5.2891 | 2.64879 | -0.43812 | C | 1.21176 | 2.07257 | -0.79322 |
| N | 2.62676 | -0.96971 | 0.03011 | C | 0.36635 | 3.01369 | -1.39297 |
| Rh | 0.63102 | -1.51685 | -0.05754 | C | -0.74241 | 2.59259 | -2.12071 |
| Cl | 0.98221 | -3.1993 | -1.80221 | C | -0.99067 | 1.24094 | -2.32895 |
| C | -1.30358 | 1.68621 | -1.08908 | C | -0.16148 | 0.28596 | -1.72202 |
| C | -0.36867 | 2.70278 | -1.35938 | H | 0.60046 | 4.07552 | -1.3255 |
| C | 0.70218 | 2.49156 | -2.21128 | H | -1.39707 | 3.33059 | -2.58358 |
| C | 0.82744 | 1.22173 | -2.78037 | H | -1.82232 | 0.95262 | -2.96277 |
| C | -0.06211 | 0.18834 | -2.48854 | C | 3.54275 | 1.6346 | -0.28225 |
| C | -1.13926 | 0.40673 | -1.61755 | O | 4.65684 | 1.99517 | 0.0217 |
| H | 1.4218 | 3.27874 | -2.42952 | N | 2.42705 | 2.44837 | -0.19964 |
| H | 1.65695 | 1.02296 | -3.45702 | C | 2.60552 | 3.77817 | 0.3459 |
| H | 0.08989 | -0.80405 | -2.91399 | H | 2.7739 | 4.53362 | -0.43532 |
| C | -2.26465 | 2.22901 | -0.13124 | H | 1.71691 | 4.05028 | 0.9292 |
| C | -1.76001 | 3.6649 | 0.18314 | H | 3.48378 | 3.75486 | 0.996 |
| O | -3.26779 | 1.749 | 0.34923 | C | -0.11507 | -1.15134 | -1.99619 |
| O | -2.22103 | 4.44438 | 0.9801 | C | -0.93064 | -1.9185 | -2.85212 |
| N | -0.6655 | 3.86363 | -0.63919 | C | -0.55085 | -3.24132 | -3.07469 |
| C | 0.19139 | 5.017 | -0.55246 | C | 1.32064 | -2.98302 | -1.6376 |
| H | 1.18976 | 4.73088 | -0.18811 | C | 0.58953 | -3.78328 | -2.49609 |
| H | 0.2911 | 5.51259 | -1.52638 | H | -1.16487 | -3.85312 | -3.73538 |
| H | -0.26554 | 5.71051 | 0.16023 | H | 2.22446 | -3.32898 | -1.13658 |
| C | -2.01692 | -0.73612 | -1.24774 | H | 0.9026 | -4.8033 | -2.70109 |
| C | -3.34268 | -0.82592 | -1.68249 | C | -2.15637 | -1.39025 | -3.53349 |
| C | -4.04479 | -1.9859 | -1.35835 | H | -2.86717 | -0.94648 | -2.82293 |
| C | -2.10433 | -2.84628 | -0.27522 | H | -1.90576 | -0.63221 | -4.2882 |
| C | -3.42577 | -3.00767 | -0.65756 | H | -2.67569 | -2.20388 | -4.05288 |
| H | -5.08062 | -2.08624 | -1.68206 | N | 0.95409 | -1.72758 | -1.37921 |
| H | -1.56611 | -3.62515 | 0.25757 | Rh | 1.7668 | -0.66915 | 0.19413 |
| H | -3.94716 | -3.9296 | -0.41537 | Cl | 2.70573 | 0.09985 | 2.22722 |

| | | | | | | | |
|---|----------|----------|----------|----|----------|----------|----------|
| C | 3.28857 | 0.17326 | -0.72382 | C | -2.24619 | 1.259 | -2.27686 |
| O | 4.02703 | -0.40874 | -1.46783 | C | -1.54389 | 0.06779 | -2.42366 |
| C | -2.1351 | 0.7053 | 0.99794 | C | -0.32058 | -0.10662 | -1.75553 |
| C | -2.24888 | 2.10601 | 1.02864 | H | -2.28283 | 3.25484 | -1.46396 |
| C | -1.50365 | 2.87095 | 1.90871 | H | -3.19562 | 1.37953 | -2.79785 |
| C | -0.62045 | 2.19236 | 2.75184 | H | -1.96001 | -0.69871 | -3.0685 |
| C | -0.49508 | 0.80518 | 2.7321 | C | 1.44827 | 3.2082 | 0.1147 |
| C | -1.25107 | 0.03613 | 1.84511 | O | 2.02591 | 4.01156 | 0.80361 |
| H | -1.58562 | 3.95599 | 1.93472 | N | 0.08468 | 3.18074 | -0.1064 |
| H | 0.00001 | 2.76305 | 3.44098 | C | -0.68626 | 4.32962 | 0.33692 |
| H | 0.23009 | 0.31669 | 3.37746 | H | -0.9099 | 5.00575 | -0.49971 |
| C | -2.96272 | 0.2301 | -0.10294 | H | -1.62613 | 3.99046 | 0.7888 |
| C | -3.57189 | 1.51117 | -0.73856 | H | -0.09081 | 4.86798 | 1.07801 |
| O | -3.19003 | -0.89177 | -0.50491 | C | 0.63762 | -1.20822 | -1.8994 |
| O | -4.26965 | 1.57285 | -1.72356 | C | 0.48194 | -2.41465 | -2.60825 |
| N | -3.14787 | 2.55858 | 0.05316 | C | 1.5836 | -3.26666 | -2.68029 |
| C | -3.40138 | 3.94298 | -0.24909 | C | 2.88503 | -1.75364 | -1.38913 |
| H | -3.9091 | 4.44404 | 0.58506 | C | 2.79688 | -2.94238 | -2.09185 |
| H | -2.46132 | 4.47109 | -0.46573 | H | 1.47795 | -4.20607 | -3.22272 |
| H | -4.04537 | 3.97245 | -1.13358 | H | 3.78799 | -1.41964 | -0.8787 |
| C | -1.08909 | -1.44249 | 1.84199 | H | 3.66028 | -3.59792 | -2.1646 |
| C | -2.11475 | -2.28391 | 2.3053 | C | -0.79088 | -2.82012 | -3.28698 |
| C | -1.83416 | -3.64477 | 2.38911 | H | -1.65561 | -2.75669 | -2.61541 |
| C | 0.35119 | -3.22311 | 1.55714 | H | -0.99716 | -2.19795 | -4.16892 |
| C | -0.58668 | -4.1299 | 2.0229 | H | -0.71707 | -3.85704 | -3.6343 |
| H | -2.60335 | -4.32409 | 2.75695 | N | 1.83215 | -0.93731 | -1.28945 |
| H | 1.34627 | -3.5499 | 1.24998 | Rh | 1.86475 | 0.65449 | 0.01276 |
| H | -0.34389 | -5.18708 | 2.09686 | Cl | 4.10784 | 0.52752 | 1.01872 |
| C | -3.46108 | -1.75801 | 2.69292 | C | 2.30591 | 2.22142 | -0.91252 |
| H | -3.38918 | -0.82423 | 3.26394 | O | 2.88849 | 2.69253 | -1.8246 |
| H | -4.06267 | -1.55387 | 1.79627 | C | -2.23265 | -0.42509 | 1.03443 |
| H | -4.0061 | -2.48995 | 3.30023 | C | -3.1855 | 0.60771 | 0.99516 |
| N | 0.10963 | -1.91327 | 1.46273 | C | -3.04858 | 1.74516 | 1.77324 |
| | | | | C | -1.89598 | 1.84837 | 2.55755 |
| | | | | C | -0.92282 | 0.85311 | 2.57393 |
| | | | | C | -1.08925 | -0.31813 | 1.82564 |
| | | | | H | -3.79482 | 2.53783 | 1.76532 |
| | | | | H | -1.7528 | 2.73665 | 3.17182 |
| | | | | H | -0.02963 | 0.96599 | 3.1865 |

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MeTS_{B1-C}

| | | | | | | | |
|---|----------|----------|----------|----|----------|----------|----------|
| C | -2.63376 | -1.42033 | 0.04382 | H | -1.83417 | 3.97556 | -0.66286 |
| C | -3.92001 | -0.84504 | -0.61016 | H | -0.26537 | 4.76 | -0.3225 |
| O | -2.14038 | -2.48299 | -0.26604 | C | 0.76384 | -1.87637 | -1.41889 |
| O | -4.54018 | -1.31413 | -1.53359 | C | 0.58038 | -3.25582 | -1.65244 |
| N | -4.20565 | 0.31764 | 0.083 | C | 1.66275 | -4.09687 | -1.38689 |
| C | -5.24533 | 1.23551 | -0.30394 | C | 2.96207 | -2.24773 | -0.67444 |
| H | -5.90999 | 1.46031 | 0.53956 | C | 2.87114 | -3.61014 | -0.91379 |
| H | -4.81267 | 2.17336 | -0.68287 | H | 1.54092 | -5.16608 | -1.56207 |
| H | -5.82339 | 0.75737 | -1.10071 | H | 3.86689 | -1.7713 | -0.28952 |
| C | -0.08381 | -1.40173 | 1.96063 | H | 3.71587 | -4.26726 | -0.72364 |
| C | -0.43516 | -2.63126 | 2.54412 | C | -0.69256 | -3.87709 | -2.14438 |
| C | 0.59583 | -3.53935 | 2.77426 | H | -1.55979 | -3.57276 | -1.54474 |
| C | 2.14876 | -1.97584 | 1.87103 | H | -0.89657 | -3.62791 | -3.19469 |
| C | 1.90175 | -3.2135 | 2.44644 | H | -0.62095 | -4.96943 | -2.08414 |
| H | 0.36317 | -4.50054 | 3.23345 | N | 1.94073 | -1.43039 | -0.9076 |
| H | 3.15654 | -1.6458 | 1.61522 | Rh | 1.84245 | 0.7876 | -0.28087 |
| H | 2.72313 | -3.89927 | 2.63969 | Cl | 4.25806 | 0.97725 | 0.44008 |
| C | -1.84037 | -2.97719 | 2.93239 | C | 2.57974 | 1.483 | -1.83343 |
| H | -2.3602 | -2.13456 | 3.40508 | O | 3.04014 | 1.90003 | -2.79595 |
| H | -2.42489 | -3.2791 | 2.0525 | C | -2.24731 | -0.0507 | 1.00072 |
| H | -1.84826 | -3.81608 | 3.6382 | C | -3.35352 | 0.71528 | 0.60137 |
| N | 1.1784 | -1.0888 | 1.62275 | C | -3.46359 | 2.05369 | 0.94178 |
| | | | | C | -2.40683 | 2.62007 | 1.65839 |
| | | | | C | -1.28048 | 1.88362 | 2.02376 |
| | | | | C | -1.18984 | 0.52686 | 1.70096 |
| | | | | H | -4.33095 | 2.64676 | 0.65682 |
| | | | | H | -2.45831 | 3.67266 | 1.93405 |
| | | | | H | -0.45748 | 2.3644 | 2.55109 |
| | | | | C | -2.44948 | -1.40421 | 0.48944 |
| | | | | C | -3.76314 | -1.33059 | -0.33831 |
| | | | | O | -1.81739 | -2.4223 | 0.66661 |
| | | | | O | -4.26054 | -2.20761 | -1.00251 |
| | | | | N | -4.25379 | -0.0516 | -0.14528 |
| | | | | C | -5.41122 | 0.46984 | -0.82403 |
| | | | | H | -6.17802 | 0.79692 | -0.10992 |
| | | | | H | -5.13547 | 1.31975 | -1.46479 |
| | | | | H | -5.81733 | -0.33538 | -1.44404 |
| | | | | C | -0.05067 | -0.27072 | 2.22257 |
| | | | | C | -0.28562 | -1.08542 | 3.34342 |

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MeC

| | | | | | | | |
|---|----------|----------|----------|---|----------|----------|----------|
| C | 0.13695 | 0.47052 | -1.21064 | H | -4.33095 | 2.64676 | 0.65682 |
| C | -0.62105 | 1.61641 | -1.44895 | H | -2.45831 | 3.67266 | 1.93405 |
| C | -1.79308 | 1.52074 | -2.19491 | H | -0.45748 | 2.3644 | 2.55109 |
| C | -2.17501 | 0.2587 | -2.65856 | C | -2.44948 | -1.40421 | 0.48944 |
| C | -1.41832 | -0.88244 | -2.4134 | C | -3.76314 | -1.33059 | -0.33831 |
| C | -0.21034 | -0.79175 | -1.68964 | O | -1.81739 | -2.4223 | 0.66661 |
| H | -2.40394 | 2.39713 | -2.41129 | O | -4.26054 | -2.20761 | -1.00251 |
| H | -3.09572 | 0.15953 | -3.23368 | N | -4.25379 | -0.0516 | -0.14528 |
| H | -1.77612 | -1.82663 | -2.80872 | C | -5.41122 | 0.46984 | -0.82403 |
| C | 1.00676 | 2.62917 | -0.02144 | H | -6.17802 | 0.79692 | -0.10992 |
| O | 1.38561 | 3.49967 | 0.71897 | H | -5.13547 | 1.31975 | -1.46479 |
| N | -0.11329 | 2.77722 | -0.86063 | H | -5.81733 | -0.33538 | -1.44404 |
| C | -0.78397 | 4.0531 | -0.97543 | C | -0.05067 | -0.27072 | 2.22257 |
| H | -0.75079 | 4.41947 | -2.01065 | C | -0.28562 | -1.08542 | 3.34342 |

| | | | | | | | |
|---|----------|----------|---------|----|----------|----------|----------|
| C | 0.80359 | -1.7353 | 3.91322 | H | -4.82054 | 1.68264 | 0.84714 |
| C | 2.21247 | -0.73964 | 2.27378 | H | -4.74761 | 2.31914 | -0.80552 |
| C | 2.06823 | -1.55631 | 3.38067 | H | -5.96533 | 1.11147 | -0.37283 |
| H | 0.65003 | -2.36958 | 4.78621 | N | -1.8496 | -0.69097 | -0.94216 |
| H | 3.19105 | -0.54557 | 1.8352 | Rh | 0.40846 | -0.28362 | -0.95761 |
| H | 2.94425 | -2.03161 | 3.81437 | Cl | 0.97381 | -2.65797 | -1.50782 |
| C | -1.65502 | -1.25777 | 3.9284 | C | 0.25228 | -0.76936 | 1.40949 |
| H | -2.19075 | -0.30476 | 4.02008 | C | 1.47093 | -0.79531 | 1.2313 |
| H | -2.26789 | -1.92447 | 3.3069 | C | -1.05933 | -0.87695 | 1.97675 |
| H | -1.59044 | -1.707 | 4.92627 | C | -1.76968 | -2.081 | 1.88051 |
| N | 1.17782 | -0.10938 | 1.68834 | C | -1.62982 | 0.21721 | 2.63975 |

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MeC1

| | | | | | | | |
|---|----------|----------|----------|---|----------|----------|----------|
| C | -0.39452 | 1.43985 | -0.42762 | H | -1.0735 | 1.15194 | 2.70257 |
| C | 0.5179 | 2.45379 | -0.15227 | C | -3.60423 | -1.09046 | 3.09261 |
| C | 0.06518 | 3.66757 | 0.35563 | H | -3.58572 | -3.11884 | 2.35974 |
| C | -1.30746 | 3.82154 | 0.56744 | H | -3.33675 | 0.95719 | 3.71368 |
| C | -2.21685 | 2.81189 | 0.28023 | H | -4.59812 | -1.17558 | 3.52928 |
| C | -1.77192 | 1.57788 | -0.23991 | C | 2.89753 | -0.80895 | 1.29326 |
| H | 0.75215 | 4.48085 | 0.58519 | C | 3.64968 | -1.76962 | 0.60644 |
| H | -1.67653 | 4.76382 | 0.96905 | C | 3.54063 | 0.17886 | 2.05492 |
| H | -3.2649 | 2.99833 | 0.48296 | C | 5.03422 | -1.73351 | 0.68604 |
| C | 2.11558 | 0.87399 | -0.97157 | H | 3.1289 | -2.50156 | -0.00927 |
| O | 3.19595 | 0.54658 | -1.38673 | C | 4.92508 | 0.20671 | 2.12208 |
| N | 1.84974 | 2.13427 | -0.43176 | H | 2.93916 | 0.91753 | 2.58397 |
| C | 2.90913 | 3.11445 | -0.30786 | C | 5.67203 | -0.74796 | 1.43482 |
| H | 2.71348 | 3.98547 | -0.94867 | H | 5.62139 | -2.47293 | 0.1452 |
| H | 3.00268 | 3.45291 | 0.73314 | H | 5.42515 | 0.97419 | 2.71029 |
| H | 3.84191 | 2.63763 | -0.61793 | H | 6.75949 | -0.72167 | 1.48301 |
| C | -2.58987 | 0.39066 | -0.58582 | C | 0.35452 | 0.03302 | -2.79777 |
| C | -3.99792 | 0.29675 | -0.59443 | O | 0.31176 | 0.19328 | -3.93085 |
| C | -4.56122 | -0.9165 | -0.99371 | | | | |
| C | -2.40354 | -1.83696 | -1.32493 | 57 | | | |
| C | -3.77981 | -1.99689 | -1.36979 | Me^eTS_{C1-D1} | | | |
| H | -5.64818 | -1.00089 | -1.0118 | C | 0.71979 | -1.02227 | 0.76655 |
| H | -1.6998 | -2.63014 | -1.5905 | C | 0.40738 | -1.54084 | 2.03329 |
| H | -4.22078 | -2.93791 | -1.68841 | C | 1.44544 | -1.93989 | 2.87999 |
| C | -4.92333 | 1.41219 | -0.21292 | C | 2.74786 | -1.90602 | 2.38538 |

| | | | | | | | |
|----|----------|----------|----------|-------------|----------|----------|----------|
| C | 3.04962 | -1.48488 | 1.08597 | H | 4.33269 | 3.96643 | 1.48611 |
| C | 2.02996 | -1.03121 | 0.24704 | C | -2.29151 | 1.79232 | 0.14006 |
| H | 1.24693 | -2.32626 | 3.87833 | C | -2.08635 | 3.17093 | 0.31169 |
| H | 3.55949 | -2.24917 | 3.02503 | C | -3.58827 | 1.31099 | -0.06947 |
| H | 4.07921 | -1.54651 | 0.74705 | C | -3.15697 | 4.0504 | 0.25964 |
| C | -1.8557 | -1.52195 | 1.21816 | H | -1.07625 | 3.5432 | 0.48503 |
| O | -3.04009 | -1.67028 | 1.36904 | C | -4.65708 | 2.19856 | -0.10973 |
| N | -0.94422 | -1.67632 | 2.29451 | H | -3.74478 | 0.24272 | -0.19606 |
| C | -1.43365 | -2.00431 | 3.62004 | C | -4.44615 | 3.56424 | 0.04859 |
| H | -1.11799 | -3.01432 | 3.91558 | H | -2.9876 | 5.11849 | 0.38765 |
| H | -1.06362 | -1.2813 | 4.35844 | H | -5.66281 | 1.81513 | -0.27118 |
| H | -2.52441 | -1.9687 | 3.58675 | H | -5.28767 | 4.25445 | 0.0094 |
| C | 2.15266 | -0.54379 | -1.14599 | C | -0.77027 | -2.94504 | -1.01798 |
| C | 3.32024 | -0.02924 | -1.74296 | O | -0.80836 | -4.03597 | -1.36045 |
| C | 3.22088 | 0.40306 | -3.0671 | | | | |
| C | 0.90615 | -0.13537 | -3.09093 | 57 | | | |
| C | 2.02357 | 0.34267 | -3.76376 | MeD1 | | | |
| H | 4.10981 | 0.81182 | -3.54874 | C | -0.44919 | -1.05443 | -0.78667 |
| H | -0.08919 | -0.18545 | -3.53873 | C | 0.28421 | -1.66168 | -1.84451 |
| H | 1.94772 | 0.68438 | -4.79299 | C | -0.03022 | -2.96915 | -2.23922 |
| C | 4.62444 | 0.1429 | -1.02417 | C | -0.93632 | -3.70549 | -1.49116 |
| H | 4.48084 | 0.56282 | -0.01941 | C | -1.4761 | -3.20513 | -0.29621 |
| H | 5.17359 | -0.8026 | -0.91575 | C | -1.21271 | -1.89826 | 0.07023 |
| H | 5.27447 | 0.82701 | -1.58279 | H | 0.48742 | -3.42461 | -3.08135 |
| N | 0.98247 | -0.5526 | -1.83256 | H | -1.15329 | -4.73162 | -1.78366 |
| Rh | -0.8636 | -1.07095 | -0.47917 | H | -2.05338 | -3.85505 | 0.36044 |
| Cl | -2.52008 | -0.92711 | -2.30222 | C | 2.21784 | -0.35177 | -1.44647 |
| C | 0.04583 | 0.90319 | 0.69228 | O | 3.23032 | 0.20922 | -1.75734 |
| C | -1.14916 | 0.89987 | 0.22583 | N | 1.35439 | -0.94476 | -2.38755 |
| C | 1.23194 | 1.7013 | 0.92741 | C | 1.76623 | -1.07424 | -3.77377 |
| C | 1.63188 | 2.61097 | -0.06316 | H | 2.3368 | -1.99756 | -3.95091 |
| C | 1.96479 | 1.61525 | 2.11814 | H | 0.88583 | -1.05817 | -4.42579 |
| C | 2.74161 | 3.42312 | 0.14003 | H | 2.41011 | -0.22335 | -4.00985 |
| H | 1.06052 | 2.66162 | -0.99092 | C | -1.49732 | -1.34353 | 1.42079 |
| C | 3.0714 | 2.42772 | 2.31531 | C | -2.76566 | -1.18653 | 1.9804 |
| H | 1.65462 | 0.90005 | 2.87889 | C | -2.81711 | -0.64997 | 3.27148 |
| C | 3.46315 | 3.33096 | 1.32686 | C | -0.43838 | -0.46376 | 3.28224 |
| H | 3.04501 | 4.12805 | -0.63209 | C | -1.65617 | -0.29489 | 3.93759 |
| H | 3.63188 | 2.36228 | 3.24618 | H | -3.78938 | -0.50065 | 3.74294 |

| | | | | | | | |
|----|----------|----------|----------|----|----------|----------|----------|
| H | 0.51039 | -0.17326 | 3.73521 | C | 0.52916 | 2.27692 | 0.64293 |
| H | -1.68719 | 0.12702 | 4.93928 | C | 0.08911 | 3.28313 | 1.49692 |
| C | -4.02673 | -1.50681 | 1.23708 | C | -1.28086 | 3.37138 | 1.75986 |
| H | -4.68488 | -0.62762 | 1.20812 | C | -2.2007 | 2.50703 | 1.18072 |
| H | -3.82828 | -1.79535 | 0.19953 | C | -1.76415 | 1.48404 | 0.31168 |
| H | -4.58565 | -2.32042 | 1.7193 | H | 0.78269 | 3.99457 | 1.94349 |
| N | -0.36587 | -0.97189 | 2.05784 | H | -1.64023 | 4.15107 | 2.42961 |
| Rh | 1.41632 | -0.69057 | 0.37136 | H | -3.24782 | 2.64445 | 1.42316 |
| C | -0.64369 | 0.44592 | -0.70014 | C | 2.10598 | 1.05011 | -0.66885 |
| C | 0.42466 | 1.02981 | -0.14463 | O | 3.18068 | 0.85506 | -1.17702 |
| C | -1.96274 | 0.97393 | -1.08436 | N | 1.85479 | 2.07297 | 0.24253 |
| C | -2.43976 | 2.18493 | -0.5621 | C | 2.90596 | 3.00104 | 0.60308 |
| C | -2.80134 | 0.23768 | -1.93269 | H | 2.65104 | 4.02054 | 0.28277 |
| C | -3.70841 | 2.64341 | -0.88845 | H | 3.07084 | 2.99912 | 1.69035 |
| H | -1.80563 | 2.75997 | 0.11163 | H | 3.82033 | 2.68074 | 0.09801 |
| C | -4.0721 | 0.69894 | -2.2572 | C | -2.58691 | 0.49644 | -0.42419 |
| H | -2.44819 | -0.70937 | -2.34636 | C | -3.99729 | 0.42294 | -0.45818 |
| C | -4.53176 | 1.90403 | -1.73566 | C | -4.57747 | -0.55961 | -1.2595 |
| H | -4.06231 | 3.58511 | -0.47118 | C | -2.43333 | -1.30273 | -1.92116 |
| H | -4.70517 | 0.11346 | -2.92269 | C | -3.80876 | -1.43054 | -2.01457 |
| H | -5.52704 | 2.26665 | -1.98732 | H | -5.66519 | -0.6242 | -1.29651 |
| C | 0.77767 | 2.43167 | 0.00083 | H | -1.76183 | -1.94916 | -2.48676 |
| C | 0.99304 | 3.01944 | 1.25343 | H | -4.25824 | -2.18254 | -2.65784 |
| C | 0.89258 | 3.22481 | -1.15004 | C | -4.91171 | 1.34193 | 0.2934 |
| C | 1.28266 | 4.37428 | 1.35049 | H | -4.7828 | 1.25523 | 1.38064 |
| H | 0.94019 | 2.39846 | 2.14558 | H | -4.75039 | 2.39342 | 0.02318 |
| C | 1.19937 | 4.57512 | -1.04853 | H | -5.95748 | 1.10179 | 0.06819 |
| H | 0.73718 | 2.76242 | -2.12546 | N | -1.85497 | -0.39253 | -1.14473 |
| C | 1.38856 | 5.1555 | 0.20259 | Rh | 0.41052 | -0.04976 | -0.98227 |
| H | 1.44054 | 4.82173 | 2.33068 | Cl | 0.14186 | 1.36867 | -2.8818 |
| H | 1.2892 | 5.17787 | -1.95102 | C | 0.1912 | -1.27714 | 0.98909 |
| H | 1.6279 | 6.21474 | 0.28289 | C | 1.41712 | -1.17466 | 0.84659 |
| C | 2.31514 | -2.46853 | 0.71241 | C | -1.09895 | -1.56759 | 1.54356 |
| O | 2.89828 | -3.43732 | 0.88653 | C | -1.85517 | -2.64949 | 1.07551 |
| Cl | 3.03086 | 0.41851 | 1.69511 | C | -1.61276 | -0.75092 | 2.55943 |
| | | | | C | -3.10858 | -2.90534 | 1.61229 |
| | | | | H | -1.45106 | -3.27406 | 0.27942 |
| | | | | C | -2.86766 | -1.01498 | 3.09317 |
| C | -0.38935 | 1.3825 | 0.10242 | H | -1.02398 | 0.09711 | 2.90734 |

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MeC2

| | | | | | | | |
|---|----------|----------|----------|----|----------|----------|----------|
| C | -3.61879 | -2.08674 | 2.61834 | C | -0.90529 | 0.38877 | 3.10804 |
| H | -3.69321 | -3.74626 | 1.24342 | C | -2.01146 | 0.96771 | 3.71372 |
| H | -3.26168 | -0.37613 | 3.88199 | H | -4.08937 | 1.44104 | 3.42774 |
| H | -4.60375 | -2.28811 | 3.0364 | H | 0.07423 | 0.39454 | 3.58607 |
| C | 2.83914 | -1.2089 | 1.01252 | H | -1.92822 | 1.43598 | 4.69128 |
| C | 3.63878 | -2.04351 | 0.22435 | C | -4.60369 | 0.4423 | 1.01554 |
| C | 3.43307 | -0.36889 | 1.96392 | H | -4.44219 | 0.66341 | -0.04784 |
| C | 5.01634 | -2.03311 | 0.38469 | H | -5.19555 | -0.48122 | 1.07786 |
| H | 3.17267 | -2.68268 | -0.524 | H | -5.21866 | 1.24685 | 1.43715 |
| C | 4.81203 | -0.36091 | 2.11398 | N | -0.97052 | -0.19412 | 1.91574 |
| H | 2.79748 | 0.28238 | 2.56383 | Rh | 0.8679 | -0.92826 | 0.61048 |
| C | 5.60449 | -1.18925 | 1.32284 | Cl | 0.3981 | -3.2074 | 1.35393 |
| H | 5.63681 | -2.67716 | -0.23528 | C | 0.03338 | 0.8863 | -0.7464 |
| H | 5.27216 | 0.29761 | 2.84864 | C | 1.22812 | 0.91935 | -0.29125 |
| H | 6.68695 | -1.17493 | 1.43661 | C | -1.14816 | 1.62239 | -1.14291 |
| C | 1.32457 | -1.40257 | -2.23884 | C | -1.664 | 2.58827 | -0.26682 |
| O | 1.88884 | -2.03974 | -3.00105 | C | -1.77301 | 1.40812 | -2.37784 |

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Me^eTS_{C2-D}

| | | | | | | | |
|---|----------|----------|----------|---|----------|----------|----------|
| C | -0.76078 | -1.05383 | -0.58974 | H | -1.37975 | 0.64032 | -3.04283 |
| C | -0.47379 | -1.77072 | -1.75564 | C | -3.39287 | 3.11705 | -1.85864 |
| C | -1.5255 | -2.2931 | -2.50849 | H | -3.183 | 4.0733 | 0.06305 |
| C | -2.8213 | -2.16268 | -2.01062 | H | -3.36037 | 1.9936 | -3.69911 |
| C | -3.09408 | -1.53823 | -0.79264 | H | -4.26895 | 3.69902 | -2.14028 |
| C | -2.0534 | -0.96273 | -0.05805 | C | 2.39281 | 1.78827 | -0.27413 |
| H | -1.34526 | -2.84344 | -3.43047 | C | 2.2039 | 3.17648 | -0.34243 |
| H | -3.64493 | -2.60062 | -2.57209 | C | 3.69366 | 1.27629 | -0.20557 |
| H | -4.11413 | -1.54551 | -0.42128 | C | 3.29425 | 4.03417 | -0.32214 |
| C | 1.80191 | -1.67965 | -1.00675 | H | 1.19105 | 3.57366 | -0.40797 |
| O | 2.98695 | -1.87322 | -1.13313 | C | 4.78131 | 2.14146 | -0.19586 |
| N | 0.87795 | -1.96431 | -2.01951 | H | 3.84417 | 0.19713 | -0.20007 |
| C | 1.32853 | -2.56409 | -3.26086 | C | 4.58588 | 3.51835 | -0.24573 |
| H | 0.99554 | -3.60833 | -3.33204 | H | 3.13649 | 5.11054 | -0.36716 |
| H | 0.94253 | -2.00167 | -4.12087 | H | 5.78944 | 1.73368 | -0.14864 |
| H | 2.4198 | -2.53765 | -3.26526 | H | 5.44153 | 4.19139 | -0.22955 |
| C | -2.14772 | -0.27109 | 1.24463 | C | 2.45993 | -1.04253 | 1.77676 |
| C | -3.3065 | 0.34487 | 1.76106 | O | 3.36991 | -1.18359 | 2.45427 |
| C | -3.20619 | 0.95579 | 3.0109 | | | | |

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MeD

| | | | |
|----|----------|----------|----------|
| C | -0.28685 | -1.12292 | -0.7824 |
| C | 0.6021 | -1.77294 | -1.67427 |
| C | 0.46188 | -3.13658 | -1.92805 |
| C | -0.4625 | -3.87226 | -1.2022 |
| C | -1.20213 | -3.28817 | -0.1692 |
| C | -1.1 | -1.92829 | 0.05763 |
| H | 1.13333 | -3.6329 | -2.62537 |
| H | -0.53827 | -4.94441 | -1.37344 |
| H | -1.79897 | -3.91209 | 0.49403 |
| C | 2.41901 | -0.31177 | -1.25411 |
| O | 3.43248 | 0.28199 | -1.50756 |
| N | 1.6792 | -1.02578 | -2.18505 |
| C | 2.26076 | -1.29386 | -3.49064 |
| H | 2.92942 | -2.16569 | -3.46942 |
| H | 1.45797 | -1.46352 | -4.21605 |
| H | 2.84382 | -0.41907 | -3.78838 |
| C | -1.63636 | -1.27032 | 1.27576 |
| C | -2.99361 | -1.22267 | 1.6145 |
| C | -3.32074 | -0.56109 | 2.79884 |
| C | -1.01234 | -0.08072 | 3.14998 |
| C | -2.33026 | 0.00967 | 3.58414 |
| H | -4.3679 | -0.4871 | 3.09335 |
| H | -0.19455 | 0.35935 | 3.72189 |
| H | -2.57181 | 0.52982 | 4.50813 |
| C | -4.05644 | -1.79803 | 0.72863 |
| H | -3.8691 | -1.55674 | -0.32649 |
| H | -4.11713 | -2.89192 | 0.80907 |
| H | -5.04096 | -1.3963 | 0.99666 |
| N | -0.67334 | -0.70042 | 2.02372 |
| Rh | 1.51273 | -0.49621 | 0.5395 |
| Cl | 2.24589 | -2.68936 | 1.3091 |
| C | -0.53008 | 0.37032 | -0.79913 |
| C | 0.45631 | 1.06756 | -0.21925 |
| C | -1.8755 | 0.80886 | -1.21189 |
| C | -2.54232 | 1.82242 | -0.51192 |
| C | -2.54849 | 0.15869 | -2.25432 |
| C | -3.83784 | 2.18437 | -0.85643 |

| | | | |
|---|----------|----------|----------|
| H | -2.03759 | 2.3036 | 0.32662 |
| C | -3.84369 | 0.52551 | -2.60164 |
| H | -2.04459 | -0.64456 | -2.79525 |
| C | -4.49327 | 1.53974 | -1.90322 |
| H | -4.34485 | 2.9692 | -0.29703 |
| H | -4.34898 | 0.01599 | -3.421 |
| H | -5.5102 | 1.82295 | -2.16973 |
| C | 0.66056 | 2.50195 | -0.09727 |
| C | 0.92589 | 3.09873 | 1.1425 |
| C | 0.5963 | 3.3164 | -1.23696 |
| C | 1.10184 | 4.47284 | 1.24247 |
| H | 0.97712 | 2.47228 | 2.03434 |
| C | 0.78746 | 4.68812 | -1.13567 |
| H | 0.39845 | 2.85187 | -2.2027 |
| C | 1.03715 | 5.27138 | 0.1037 |
| H | 1.29721 | 4.92286 | 2.21456 |
| H | 0.74462 | 5.30631 | -2.03103 |
| H | 1.18806 | 6.34666 | 0.18176 |
| C | 2.90435 | 0.42255 | 1.34933 |
| O | 3.77675 | 0.98659 | 1.8349 |

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MeD2

| | | | |
|---|----------|----------|----------|
| C | 0.89337 | -1.19983 | 0.567 |
| C | 0.16206 | -2.14859 | 1.30412 |
| C | 0.61094 | -3.46433 | 1.42111 |
| C | 1.78272 | -3.8583 | 0.79469 |
| C | 2.49649 | -2.94298 | 0.02836 |
| C | 2.05808 | -1.62844 | -0.09909 |
| H | 0.02439 | -4.1809 | 1.99334 |
| H | 2.12355 | -4.8882 | 0.87793 |
| H | 3.38837 | -3.25882 | -0.51206 |
| C | -2.01522 | -1.0737 | 1.3869 |
| O | -3.01887 | -0.62525 | 1.90683 |
| N | -1.03076 | -1.78023 | 1.98122 |
| C | -1.23331 | -2.19373 | 3.36986 |
| H | -1.65492 | -3.20499 | 3.43362 |
| H | -0.27294 | -2.16693 | 3.89445 |
| H | -1.93161 | -1.49475 | 3.83752 |

| | | | |
|----|----------|----------|----------|
| C | 2.76401 | -0.70166 | -1.02634 |
| C | 4.10052 | -0.31801 | -0.82587 |
| C | 4.65047 | 0.55336 | -1.76494 |
| C | 2.58141 | 0.54457 | -2.94199 |
| C | 3.89431 | 0.99117 | -2.84199 |
| H | 5.67849 | 0.89454 | -1.63638 |
| H | 1.94669 | 0.86323 | -3.77084 |
| H | 4.30751 | 1.67166 | -3.5835 |
| C | 4.91276 | -0.77018 | 0.35085 |
| H | 5.41223 | -1.73144 | 0.16301 |
| H | 5.69336 | -0.03398 | 0.58164 |
| H | 4.29652 | -0.89509 | 1.24942 |
| N | 2.0226 | -0.27589 | -2.05686 |
| Rh | -2.28989 | -0.61773 | -0.5181 |
| Cl | -4.08298 | -0.79386 | -2.05012 |
| C | -0.77812 | 0.54528 | 0.14167 |
| C | 0.4737 | 0.21756 | 0.49753 |
| C | 1.49302 | 1.24144 | 0.83443 |
| C | 2.32473 | 1.05473 | 1.94505 |
| C | 1.65839 | 2.39422 | 0.05922 |
| C | 3.30123 | 1.98993 | 2.26785 |
| H | 2.20068 | 0.16015 | 2.55735 |
| C | 2.63818 | 3.32558 | 0.37858 |
| H | 1.02943 | 2.53778 | -0.81859 |
| C | 3.46516 | 3.12649 | 1.48135 |
| H | 3.93813 | 1.82832 | 3.13657 |
| H | 2.76278 | 4.21029 | -0.24384 |
| H | 4.23483 | 3.85635 | 1.7269 |
| C | -1.49165 | 1.81721 | 0.19185 |
| C | -2.05779 | 2.36915 | -0.97188 |
| C | -1.72787 | 2.4441 | 1.42858 |
| C | -2.82413 | 3.52737 | -0.89784 |
| H | -1.87916 | 1.88529 | -1.93275 |
| C | -2.48078 | 3.60426 | 1.49168 |
| H | -1.30799 | 2.00014 | 2.331 |
| C | -3.03186 | 4.14623 | 0.32929 |
| H | -3.25797 | 3.94452 | -1.80423 |
| H | -2.65088 | 4.08752 | 2.45211 |
| H | -3.63155 | 5.05308 | 0.38503 |

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Me^eTS_{D2-A}

| | | | |
|----|----------|----------|----------|
| C | -1.24289 | -1.84008 | -1.40338 |
| O | -0.6317 | -2.62082 | -1.98201 |
| C | 0.8596 | -1.19133 | 0.65534 |
| C | 0.09168 | -2.08291 | 1.43078 |
| C | 0.53415 | -3.38987 | 1.65073 |
| C | 1.71565 | -3.82731 | 1.0753 |
| C | 2.45795 | -2.97283 | 0.26504 |
| C | 2.0388 | -1.66543 | 0.04664 |
| H | -0.06468 | -4.06998 | 2.25294 |
| H | 2.0439 | -4.85276 | 1.23252 |
| H | 3.35395 | -3.33605 | -0.23684 |
| C | -1.93362 | -0.7646 | 1.37649 |
| O | -2.94005 | -0.25596 | 1.84534 |
| N | -1.10962 | -1.64532 | 2.01245 |
| C | -1.54967 | -2.17615 | 3.29829 |
| H | -2.04251 | -3.15036 | 3.18211 |
| H | -0.68624 | -2.2817 | 3.96339 |
| H | -2.26543 | -1.47281 | 3.72934 |
| C | 2.76942 | -0.80241 | -0.92136 |
| C | 4.11894 | -0.45267 | -0.74519 |
| C | 4.68463 | 0.3726 | -1.71672 |
| C | 2.60966 | 0.38019 | -2.88113 |
| C | 3.93492 | 0.79359 | -2.8047 |
| H | 5.7226 | 0.6892 | -1.60595 |
| H | 1.97812 | 0.68644 | -3.71708 |
| H | 4.36205 | 1.43625 | -3.57151 |
| C | 4.93594 | -0.88814 | 0.43471 |
| H | 5.4531 | -1.83991 | 0.24613 |
| H | 5.70477 | -0.13904 | 0.66336 |
| H | 4.32448 | -1.027 | 1.334 |
| N | 2.03441 | -0.38953 | -1.96239 |
| Rh | -2.32165 | -0.6317 | -0.59356 |
| Cl | -4.04701 | -0.97572 | -2.12845 |
| C | -0.85679 | 0.50885 | 0.28114 |
| C | 0.44161 | 0.20997 | 0.52112 |
| C | 1.46654 | 1.25661 | 0.74404 |

| | | | | | | | |
|---|----------|----------|----------|----|----------|----------|----------|
| C | 2.32213 | 1.1603 | 1.84753 | C | 3.23526 | 1.72183 | -2.4921 |
| C | 1.615 | 2.33622 | -0.13278 | H | 3.68027 | 0.7207 | -2.53119 |
| C | 3.3095 | 2.11387 | 2.06463 | H | 2.90858 | 2.02956 | -3.49459 |
| H | 2.20755 | 0.32461 | 2.53897 | H | 3.98693 | 2.42089 | -2.11574 |
| C | 2.61182 | 3.28015 | 0.07634 | C | -2.61426 | 1.68545 | -0.33426 |
| H | 0.96155 | 2.40599 | -1.00165 | C | -3.0739 | 2.99822 | -0.2446 |
| C | 3.46206 | 3.17258 | 1.17411 | C | -4.2691 | 3.17765 | 0.45911 |
| H | 3.96352 | 2.02885 | 2.93134 | C | -4.41389 | 0.82625 | 0.89519 |
| H | 2.73014 | 4.10206 | -0.6279 | C | -4.94048 | 2.104 | 1.03164 |
| H | 4.24138 | 3.91565 | 1.33563 | H | -4.67846 | 4.18417 | 0.54872 |
| C | -1.48852 | 1.83763 | 0.28627 | H | -4.85743 | -0.07162 | 1.32173 |
| C | -1.99332 | 2.39013 | -0.90132 | H | -5.86981 | 2.25256 | 1.57589 |
| C | -1.65923 | 2.53823 | 1.48884 | C | -2.35455 | 4.15122 | -0.8662 |
| C | -2.64161 | 3.62141 | -0.88412 | H | -3.05275 | 4.95902 | -1.11546 |
| H | -1.85469 | 1.85475 | -1.84198 | H | -1.59999 | 4.54855 | -0.1749 |
| C | -2.29669 | 3.76884 | 1.49866 | H | -1.83121 | 3.85526 | -1.78431 |
| H | -1.28228 | 2.09982 | 2.41244 | N | -3.27924 | 0.65249 | 0.21853 |
| C | -2.79235 | 4.31102 | 0.31308 | Rh | -1.99542 | -0.88293 | -0.11821 |
| H | -3.02764 | 4.03923 | -1.81184 | Cl | -3.1039 | -2.30667 | 1.44179 |
| H | -2.41755 | 4.30751 | 2.43691 | H | -2.73299 | -0.00277 | -2.42663 |
| H | -3.3002 | 5.2739 | 0.32677 | C | 2.10766 | -0.64638 | 0.93908 |
| C | -1.24719 | -1.87213 | -1.39873 | C | 2.44395 | 0.36553 | 1.86027 |
| O | -0.61397 | -2.68597 | -1.90604 | C | 1.64055 | 0.65205 | 2.94805 |

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| | | | | | | | |
|---|----------|----------|----------|---|----------|----------|----------|
| C | -0.11357 | 1.61061 | -0.9533 | H | 1.88813 | 1.44803 | 3.64655 |
| C | 0.88831 | 1.11923 | -1.79071 | H | -0.17124 | 0.08405 | 3.95081 |
| C | 0.65196 | 0.10313 | -2.72504 | H | -0.76677 | -1.71356 | 2.37668 |
| C | -0.64315 | -0.35207 | -2.85516 | C | 3.1231 | -0.61873 | -0.10923 |
| C | -1.71561 | 0.12979 | -2.05534 | C | 4.13017 | 0.48322 | 0.32425 |
| C | -1.44056 | 1.1053 | -1.03696 | O | 3.23278 | -1.25775 | -1.13558 |
| H | 1.46271 | -0.29799 | -3.32864 | O | 5.12927 | 0.82055 | -0.2667 |
| H | -0.86528 | -1.10431 | -3.61194 | N | 3.64211 | 0.99635 | 1.50475 |
| C | 0.49548 | 2.59586 | -0.08245 | C | 4.20223 | 2.14464 | 2.17683 |
| C | 1.9607 | 2.72636 | -0.59032 | H | 3.49446 | 2.98353 | 2.15069 |
| O | 0.05378 | 3.24097 | 0.84665 | H | 4.46151 | 1.9003 | 3.21481 |
| O | 2.78967 | 3.525 | -0.22545 | H | 5.10609 | 2.42923 | 1.63076 |
| N | 2.11819 | 1.75327 | -1.56665 | C | 0.58181 | -2.52124 | 0.19134 |

| | | | | | | | |
|---|----------|----------|----------|----|----------|----------|----------|
| C | 1.40047 | -3.65431 | 0.04437 | H | 0.39463 | -3.47838 | 1.59854 |
| C | 0.94871 | -4.67354 | -0.78908 | H | -1.59957 | -5.00259 | 1.92 |
| C | -1.03227 | -3.42984 | -1.21371 | C | -4.2849 | -2.22508 | -0.66337 |
| C | -0.27509 | -4.56538 | -1.43205 | H | -5.02341 | -1.7502 | -0.00686 |
| H | 1.56228 | -5.56523 | -0.91582 | H | -4.136 | -1.56249 | -1.52362 |
| H | -2.01721 | -3.29954 | -1.65797 | H | -4.70847 | -3.16655 | -1.03414 |
| H | -0.65199 | -5.35556 | -2.07621 | N | -0.68516 | -2.10986 | 0.51348 |
| C | 2.70685 | -3.80728 | 0.76029 | Rh | 1.00452 | -1.13713 | -0.09986 |
| H | 3.51904 | -3.33204 | 0.19428 | Cl | 0.37215 | -2.58939 | -2.92763 |
| H | 2.68541 | -3.35775 | 1.75966 | C | 1.7467 | 0.97559 | 1.51608 |
| H | 2.95886 | -4.86843 | 0.87189 | C | 0.77561 | 1.72371 | 2.20173 |
| N | -0.61352 | -2.42694 | -0.42688 | C | 0.69009 | 3.09854 | 2.06283 |

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MeTS_{A1}'

| | | | | | | | |
|---|----------|----------|----------|---|----------|----------|----------|
| C | -2.67973 | 0.61696 | -0.8198 | H | -0.06298 | 3.67831 | 2.59337 |
| C | -2.39309 | 1.77086 | -1.58144 | H | 1.55436 | 4.79953 | 1.07127 |
| C | -1.17877 | 1.94722 | -2.21883 | H | 3.18317 | 3.4958 | -0.22883 |
| C | -0.19787 | 0.97547 | -2.00688 | C | 1.50418 | -0.45274 | 1.81693 |
| C | -0.42258 | -0.17188 | -1.23653 | C | 0.33804 | -0.44772 | 2.81388 |
| C | -1.71982 | -0.39434 | -0.69814 | O | 2.27645 | -1.45603 | 1.67642 |
| H | -0.97361 | 2.83342 | -2.81695 | O | -0.15318 | -1.38836 | 3.39812 |
| H | 0.78977 | 1.12126 | -2.44821 | N | -0.04295 | 0.87911 | 2.95212 |
| H | 0.10175 | -1.45423 | -2.03146 | C | -1.16961 | 1.30165 | 3.74317 |
| C | -3.93858 | 0.88712 | -0.1202 | H | -0.86315 | 2.02013 | 4.51483 |
| C | -4.43639 | 2.25231 | -0.66967 | H | -1.94397 | 1.75795 | 3.11096 |
| O | -4.50747 | 0.28535 | 0.7621 | H | -1.58135 | 0.40953 | 4.22408 |
| O | -5.46195 | 2.82334 | -0.38799 | C | 3.42428 | 0.77074 | -0.30236 |
| N | -3.45589 | 2.68176 | -1.53911 | C | 4.7606 | 1.06702 | -0.61962 |
| C | -3.49687 | 3.93997 | -2.23766 | C | 5.39147 | 0.27242 | -1.57467 |
| H | -2.6661 | 4.58926 | -1.92975 | C | 3.41224 | -1.02726 | -1.79227 |
| H | -3.44648 | 3.78811 | -3.32373 | C | 4.71453 | -0.77061 | -2.18657 |
| H | -4.44538 | 4.42252 | -1.98363 | H | 6.43236 | 0.47704 | -1.82675 |
| C | -1.87186 | -1.67689 | 0.00434 | H | 2.83109 | -1.84548 | -2.21921 |
| C | -3.00537 | -2.50093 | 0.05983 | H | 5.18689 | -1.39387 | -2.94098 |
| C | -2.88319 | -3.7026 | 0.76563 | C | 5.53615 | 2.15941 | 0.05698 |
| C | -0.58934 | -3.2498 | 1.19383 | H | 5.49549 | 3.10333 | -0.50442 |
| C | -1.69247 | -4.0738 | 1.36407 | H | 5.16495 | 2.36395 | 1.0669 |
| H | -3.75062 | -4.36041 | 0.82097 | H | 6.59418 | 1.87984 | 0.13214 |

N 2.78614 -0.28314 -0.8705

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Me^eTS_{AI'}-B'

C 2.37987 0.64161 -0.67147
C 2.52398 -0.58701 -1.34999
C 1.45969 -1.18801 -1.99821
C 0.20368 -0.58735 -1.85538
C 0.01498 0.60702 -1.15471
C 1.14506 1.31578 -0.67712
H 1.56782 -2.1381 -2.52027
H -0.66497 -1.09602 -2.27497
C 3.57307 0.77666 0.16719
C 4.51773 -0.38102 -0.25814
O 3.81595 1.51704 1.09481
O 5.63138 -0.59607 0.16051
N 3.81607 -1.11296 -1.18589
C 4.33588 -2.28811 -1.84719
H 3.74991 -3.17812 -1.58706
H 4.33199 -2.15003 -2.93624
H 5.36654 -2.41808 -1.50329
C 0.88287 2.69455 -0.24265
C 1.79134 3.76837 -0.22508
C 1.30686 5.00964 0.19997
C -0.88205 4.10881 0.41021
C -0.01759 5.18554 0.55256
H 1.99772 5.85246 0.22769
H -1.95118 4.17087 0.60948
H -0.39678 6.14717 0.8881
C 3.20483 3.70719 -0.71083
H 3.47687 4.66674 -1.16714
H 3.90596 3.5086 0.10814
H 3.35109 2.9222 -1.46198
N -0.44094 2.91647 0.00992
Rh -1.7078 1.34725 -0.40103
Cl -3.55546 2.227 0.91347
H -1.26358 1.45932 -1.90167
C -0.47211 -2.07677 0.94281
C 0.61937 -1.84008 1.7991

C 0.55361 -0.91171 2.82186
C -0.65144 -0.22248 2.9787
C -1.73357 -0.41848 2.12195
C -1.64658 -1.33387 1.06607
H 1.40264 -0.71842 3.4743
H -0.74413 0.50976 3.77861
H -2.63683 0.17859 2.2383
C -0.04551 -3.08257 -0.02858
C 1.43635 -3.38749 0.32681
O -0.64122 -3.63082 -0.92884
O 2.18117 -4.13914 -0.25989
N 1.72439 -2.6238 1.4355
C 3.02946 -2.54147 2.04666
H 3.40473 -1.50785 2.038
H 3.00258 -2.89769 3.08446
H 3.70869 -3.17411 1.4666
C -2.74462 -1.42487 0.06448
C -3.58395 -2.54025 -0.03575
C -4.601 -2.49404 -0.98664
C -3.89479 -0.30915 -1.62279
C -4.76301 -1.37451 -1.78931
H -5.27456 -3.34512 -1.08439
H -3.98065 0.60851 -2.1998
H -5.55798 -1.31567 -2.52798
C -3.39791 -3.7405 0.83732
H -2.59319 -4.37552 0.4427
H -3.13003 -3.46186 1.86378
H -4.31304 -4.3427 0.87374
N -2.90395 -0.33846 -0.7218

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Me^eB'

C -2.33264 -0.62921 -0.77259
C -2.50773 0.58443 -1.46725
C -1.44774 1.22571 -2.08213
C -0.16969 0.68452 -1.88822
C 0.05582 -0.4916 -1.1669
C -1.06363 -1.23868 -0.72194
H -1.58046 2.16737 -2.61394

| | | | | | | | |
|----|----------|----------|----------|-------------|----------|----------|----------|
| H | 0.68366 | 1.24308 | -2.276 | N | -1.91497 | 2.14346 | 1.60052 |
| C | -3.5335 | -0.79357 | 0.04374 | C | -3.20323 | 1.90099 | 2.21107 |
| C | -4.52115 | 0.30909 | -0.42913 | H | -3.53303 | 0.86467 | 2.05251 |
| O | -3.74992 | -1.50168 | 1.00563 | H | -3.16771 | 2.1016 | 3.28942 |
| O | -5.65357 | 0.47847 | -0.04047 | H | -3.92214 | 2.5796 | 1.74066 |
| N | -3.82491 | 1.06063 | -1.34311 | C | 2.6501 | 1.56005 | 0.13442 |
| C | -4.35027 | 2.2358 | -1.99517 | C | 3.38286 | 2.74817 | 0.13536 |
| H | -3.77151 | 3.12529 | -1.71883 | C | 4.39309 | 2.8683 | -0.81974 |
| H | -4.33797 | 2.11306 | -3.08599 | C | 3.87995 | 0.68742 | -1.64086 |
| H | -5.38304 | 2.35809 | -1.65563 | C | 4.64614 | 1.84008 | -1.71459 |
| C | -0.75744 | -2.59876 | -0.25934 | H | 4.99089 | 3.7792 | -0.84558 |
| C | -1.62201 | -3.70859 | -0.21562 | H | 4.04569 | -0.16954 | -2.2887 |
| C | -1.09116 | -4.91727 | 0.24736 | H | 5.4378 | 1.91803 | -2.45508 |
| C | 1.06261 | -3.93307 | 0.42869 | C | 3.11112 | 3.84903 | 1.11012 |
| C | 0.23826 | -5.03533 | 0.60635 | H | 2.35673 | 4.53615 | 0.70466 |
| H | -1.74978 | -5.78471 | 0.29645 | H | 2.73252 | 3.46641 | 2.06545 |
| H | 2.13782 | -3.94764 | 0.61004 | H | 4.0209 | 4.42644 | 1.31173 |
| H | 0.65175 | -5.97305 | 0.96794 | N | 2.90088 | 0.56134 | -0.7401 |
| C | -3.03217 | -3.72059 | -0.71521 | | | | |
| H | -3.26032 | -4.70519 | -1.14116 | 88 | | | |
| H | -3.75145 | -3.52075 | 0.08758 | MeC' | | | |
| H | -3.19878 | -2.96845 | -1.4951 | C | -3.17425 | 0.65417 | 0.03771 |
| N | 0.57356 | -2.77061 | -0.00178 | C | -3.46002 | -0.031 | -1.16071 |
| Rh | 1.78812 | -1.16603 | -0.42102 | C | -2.50306 | -0.76501 | -1.83486 |
| Cl | 3.86238 | -2.1453 | 0.54472 | C | -1.19533 | -0.71347 | -1.34719 |
| H | 2.04592 | -1.76021 | -1.8063 | C | -0.8509 | -0.01706 | -0.18498 |
| C | 0.32328 | 1.88385 | 1.07269 | C | -1.87652 | 0.58796 | 0.58491 |
| C | -0.75654 | 1.39646 | 1.83218 | H | -2.73864 | -1.32269 | -2.74034 |
| C | -0.63093 | 0.28186 | 2.64789 | H | -0.42295 | -1.24095 | -1.90805 |
| C | 0.6232 | -0.32332 | 2.70878 | C | -4.33225 | 1.5184 | 0.28998 |
| C | 1.7101 | 0.13578 | 1.95704 | C | -5.37285 | 1.16351 | -0.80783 |
| C | 1.55781 | 1.23251 | 1.09183 | O | -4.51594 | 2.41501 | 1.08358 |
| H | -1.47475 | -0.11147 | 3.21075 | O | -6.4712 | 1.64895 | -0.9491 |
| H | 0.76457 | -1.19297 | 3.34856 | N | -4.77574 | 0.20679 | -1.5911 |
| H | 2.67639 | -0.36301 | 2.03635 | C | -5.3564 | -0.32769 | -2.79384 |
| C | -0.18284 | 2.99635 | 0.26884 | H | -4.76367 | -0.0457 | -3.67612 |
| C | -1.68406 | 3.12043 | 0.65203 | H | -5.42255 | -1.42239 | -2.74853 |
| O | 0.36533 | 3.72196 | -0.5296 | H | -6.36228 | 0.09304 | -2.88556 |
| O | -2.48273 | 3.91258 | 0.21179 | C | -1.42863 | 1.15822 | 1.86234 |

| | | | | | | | |
|----|----------|----------|----------|--------------|----------|----------|----------|
| C | -2.19143 | 1.4353 | 3.01079 | C | 0.63301 | -3.7655 | 0.18293 |
| C | -1.55438 | 2.11962 | 4.05128 | C | 0.21369 | -4.45366 | 1.33535 |
| C | 0.52352 | 1.95825 | 2.91634 | C | 0.92573 | -4.37666 | 2.51921 |
| C | -0.21026 | 2.43908 | 3.99332 | C | 2.07414 | -3.5804 | 2.52607 |
| H | -2.13961 | 2.37178 | 4.93652 | C | 2.49724 | -2.87564 | 1.40101 |
| H | 1.61119 | 2.01239 | 2.85843 | C | 1.76714 | -2.95237 | 0.21229 |
| H | 0.28646 | 2.9732 | 4.79906 | H | 0.6076 | -4.9096 | 3.41307 |
| C | -3.57787 | 0.92733 | 3.26114 | H | 2.64955 | -3.49319 | 3.44584 |
| H | -3.63054 | 0.52996 | 4.2835 | H | 3.35196 | -2.20296 | 1.45797 |
| H | -4.33219 | 1.71442 | 3.16022 | C | -0.33354 | -4.06231 | -0.87366 |
| H | -3.85368 | 0.12032 | 2.57399 | C | -1.3911 | -4.9905 | -0.20952 |
| N | -0.07114 | 1.3264 | 1.90634 | O | -0.37298 | -3.7283 | -2.03693 |
| Rh | 1.00117 | 0.26522 | 0.50474 | O | -2.37612 | -5.46075 | -0.72374 |
| Cl | 3.23695 | 0.53418 | 1.58134 | N | -0.96368 | -5.1711 | 1.09154 |
| H | 0.63895 | -0.97276 | 1.30828 | C | -1.66907 | -5.96225 | 2.06671 |
| C | 0.86691 | 3.06019 | -0.89805 | H | -1.05063 | -6.79917 | 2.41707 |
| C | 2.07099 | 3.07166 | -0.70448 | H | -1.96529 | -5.35034 | 2.92899 |
| C | -0.52035 | 3.23683 | -1.17656 | H | -2.56573 | -6.35709 | 1.57987 |
| C | -1.32081 | 3.9944 | -0.30711 | C | 2.18599 | -2.18042 | -0.9858 |
| C | -1.09032 | 2.70063 | -2.33988 | C | 2.8225 | -2.82645 | -2.05598 |
| C | -2.6535 | 4.22893 | -0.61119 | C | 3.19764 | -2.05403 | -3.14976 |
| H | -0.87824 | 4.39791 | 0.60329 | C | 2.29999 | -0.13347 | -2.06874 |
| C | -2.42654 | 2.93696 | -2.63482 | C | 2.93165 | -0.69252 | -3.16317 |
| H | -0.47175 | 2.0941 | -3.00147 | H | 3.69806 | -2.53045 | -3.9925 |
| C | -3.20973 | 3.70626 | -1.77743 | H | 2.05645 | 0.92815 | -2.02372 |
| H | -3.27212 | 4.80716 | 0.07168 | H | 3.20969 | -0.06626 | -4.00737 |
| H | -2.86039 | 2.51478 | -3.54115 | C | 3.07753 | -4.30128 | -2.0342 |
| H | -4.25922 | 3.88889 | -2.00687 | H | 3.81032 | -4.58007 | -2.80009 |
| C | 3.4817 | 3.16972 | -0.54105 | H | 3.45362 | -4.63913 | -1.06083 |
| C | 4.34372 | 2.85953 | -1.60231 | H | 2.15263 | -4.85579 | -2.24284 |
| C | 4.0236 | 3.59969 | 0.67778 | N | 1.93741 | -0.85695 | -0.9968 |
| C | 5.71807 | 2.96446 | -1.44054 | | | | |
| H | 3.92341 | 2.5459 | -2.55765 | 88 | | | |
| C | 5.39687 | 3.71246 | 0.82953 | MeC1' | | | |
| H | 3.35216 | 3.82772 | 1.50306 | C | 1.36743 | -1.55087 | 1.13672 |
| C | 6.24665 | 3.38946 | -0.22471 | C | 1.95237 | -0.85195 | 2.21385 |
| H | 6.38037 | 2.71792 | -2.26869 | C | 1.47715 | 0.37423 | 2.63541 |
| H | 5.8084 | 4.04124 | 1.78186 | C | 0.4233 | 0.9356 | 1.91389 |
| H | 7.32509 | 3.47064 | -0.09922 | C | -0.17877 | 0.28878 | 0.83301 |

| | | | | | | | |
|----|----------|----------|----------|---|----------|----------|----------|
| C | 0.24977 | -1.00964 | 0.46404 | H | -5.92234 | -1.97864 | -3.00228 |
| H | 1.95423 | 0.91952 | 3.44736 | H | -5.72144 | -4.24859 | -2.01718 |
| H | 0.07932 | 1.93112 | 2.19292 | C | -3.01187 | 0.94555 | 2.624 |
| C | 2.31175 | -2.61871 | 0.80321 | C | -2.60067 | 2.173 | 3.15362 |
| C | 3.42372 | -2.55846 | 1.88765 | C | -3.63521 | 0.01694 | 3.47318 |
| O | 2.3803 | -3.37481 | -0.14459 | C | -2.8107 | 2.46542 | 4.49538 |
| O | 4.39075 | -3.28127 | 1.9616 | H | -2.12508 | 2.90368 | 2.49984 |
| N | 3.10084 | -1.499 | 2.69803 | C | -3.84283 | 0.31311 | 4.81163 |
| C | 3.98946 | -0.94869 | 3.69448 | H | -3.9594 | -0.9374 | 3.05927 |
| H | 4.33428 | 0.04819 | 3.38623 | C | -3.42803 | 1.53817 | 5.32901 |
| H | 3.49504 | -0.89305 | 4.6723 | H | -2.48782 | 3.42644 | 4.89201 |
| H | 4.85584 | -1.61329 | 3.75628 | H | -4.32895 | -0.41696 | 5.45648 |
| C | -0.43144 | -1.62946 | -0.68955 | H | -3.5873 | 1.76921 | 6.38083 |
| C | -0.59877 | -3.00113 | -0.94777 | C | 2.89013 | 0.70512 | -1.04764 |
| C | -1.18169 | -3.34921 | -2.17156 | C | 3.4279 | -0.52406 | -1.47046 |
| C | -1.59779 | -1.06292 | -2.64143 | C | 2.90711 | -1.21229 | -2.55345 |
| C | -1.64092 | -2.38999 | -3.05548 | C | 1.82624 | -0.63244 | -3.21634 |
| H | -1.31279 | -4.40842 | -2.39747 | C | 1.2786 | 0.58314 | -2.81061 |
| H | -2.07561 | -0.25121 | -3.19564 | C | 1.79601 | 1.26985 | -1.70938 |
| H | -2.11132 | -2.66071 | -3.99768 | H | 3.31025 | -2.17406 | -2.86126 |
| C | -0.35157 | -4.09593 | 0.04336 | H | 1.38476 | -1.15164 | -4.06627 |
| H | -1.20992 | -4.78211 | 0.03626 | H | 0.42908 | 1.01122 | -3.34183 |
| H | 0.54802 | -4.6735 | -0.1952 | C | 3.64655 | 1.11716 | 0.13477 |
| H | -0.24021 | -3.71254 | 1.06382 | C | 4.71773 | 0.00801 | 0.33987 |
| N | -1.01152 | -0.71088 | -1.50446 | O | 3.54733 | 2.08825 | 0.85092 |
| Rh | -1.56247 | 1.13375 | -0.34721 | O | 5.56848 | -0.02513 | 1.19804 |
| Cl | -3.11812 | 2.0237 | -2.1167 | N | 4.49764 | -0.92021 | -0.65528 |
| H | -1.93212 | 2.33323 | 0.57118 | C | 5.30737 | -2.10177 | -0.8636 |
| C | -3.1985 | -0.16747 | 0.27263 | H | 4.69396 | -3.00771 | -0.77622 |
| C | -2.86316 | 0.56103 | 1.24119 | H | 5.79037 | -2.06393 | -1.84884 |
| C | -3.86984 | -1.24895 | -0.39462 | H | 6.0693 | -2.11677 | -0.07943 |
| C | -3.76026 | -2.53423 | 0.15938 | C | 1.22976 | 2.60629 | -1.40288 |
| C | -4.64955 | -1.05572 | -1.54325 | C | 2.02203 | 3.75056 | -1.61499 |
| C | -4.42335 | -3.607 | -0.42193 | C | 1.40711 | 4.99363 | -1.50502 |
| H | -3.14605 | -2.67409 | 1.05019 | C | -0.65723 | 3.90364 | -1.05326 |
| C | -5.31126 | -2.13487 | -2.11488 | C | 0.05243 | 5.07667 | -1.23593 |
| H | -4.71029 | -0.05381 | -1.96719 | H | 1.99814 | 5.89505 | -1.66708 |
| C | -5.19902 | -3.40877 | -1.56135 | H | -1.73074 | 3.91597 | -0.89064 |
| H | -4.33449 | -4.60003 | 0.0172 | H | -0.46227 | 6.03238 | -1.18009 |

| | | | | | | | |
|----|----------|----------|----------|----|----------|----------|----------|
| C | 3.47247 | 3.67867 | -1.98559 | Cl | 3.26603 | -1.25654 | -2.44484 |
| H | 3.79234 | 4.61538 | -2.45675 | H | 2.264 | -1.91515 | 0.27332 |
| H | 4.09624 | 3.5268 | -1.09496 | C | 3.03331 | 0.50962 | 0.25872 |
| H | 3.6826 | 2.86008 | -2.68428 | C | 3.07605 | -0.55231 | 0.95549 |
| N | -0.08627 | 2.68611 | -1.1065 | C | 3.39123 | 1.85931 | -0.0926 |
| | | | | C | 3.09191 | 2.91151 | 0.78478 |
| | | | | C | 4.02741 | 2.1305 | -1.3123 |
| | | | | C | 3.43083 | 4.21643 | 0.44842 |
| | | | | H | 2.58523 | 2.6905 | 1.7252 |
| | | | | C | 4.37262 | 3.4374 | -1.63211 |
| | | | | H | 4.23775 | 1.29677 | -1.98419 |
| | | | | C | 4.07178 | 4.48119 | -0.75955 |
| | | | | H | 3.19737 | 5.0292 | 1.13511 |
| | | | | H | 4.87681 | 3.64358 | -2.57503 |
| | | | | H | 4.34229 | 5.50379 | -1.0186 |
| | | | | C | 3.59533 | -1.23644 | 2.11694 |
| | | | | C | 3.36845 | -2.58857 | 2.39053 |
| | | | | C | 4.37304 | -0.48473 | 3.01265 |
| | | | | C | 3.90668 | -3.17778 | 3.52788 |
| | | | | H | 2.76506 | -3.18203 | 1.70147 |
| | | | | C | 4.9112 | -1.07817 | 4.14387 |
| | | | | H | 4.55012 | 0.56951 | 2.80077 |
| | | | | C | 4.67826 | -2.42656 | 4.40804 |
| | | | | H | 3.72063 | -4.23189 | 3.72608 |
| | | | | H | 5.51553 | -0.48336 | 4.82665 |
| | | | | H | 5.09748 | -2.88909 | 5.29977 |
| | | | | C | -2.87198 | -1.04225 | -0.8734 |
| | | | | C | -3.64534 | 0.10622 | -1.11604 |
| | | | | C | -3.39112 | 0.93815 | -2.19312 |
| | | | | C | -2.33363 | 0.58648 | -3.03277 |
| | | | | C | -1.55626 | -0.54789 | -2.80505 |
| | | | | C | -1.80875 | -1.38107 | -1.71225 |
| | | | | H | -3.96947 | 1.84352 | -2.35994 |
| | | | | H | -2.09827 | 1.22489 | -3.88344 |
| | | | | H | -0.73378 | -0.79622 | -3.47452 |
| | | | | C | -3.36334 | -1.63987 | 0.36616 |
| | | | | C | -4.53518 | -0.72388 | 0.82151 |
| | | | | O | -3.01312 | -2.63268 | 0.96319 |
| Rh | 1.6145 | -0.75813 | -0.59657 | O | -5.22606 | -0.86329 | 1.80392 |

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Me^eTS_{Cl^r-D^r}

| | | | | | | | |
|---|----------|----------|----------|----|----------|----------|----------|
| N | -4.62712 | 0.2736 | -0.1275 | C | -0.07133 | 1.08985 | 2.8292 |
| C | -5.66849 | 1.27906 | -0.15158 | C | 0.36176 | 0.02721 | 3.62792 |
| H | -5.2344 | 2.28627 | -0.16051 | C | 0.61532 | -1.34741 | 1.70479 |
| H | -6.31348 | 1.13987 | -1.02919 | C | 0.76509 | -1.17454 | 3.07403 |
| H | -6.25697 | 1.16041 | 0.76275 | H | 0.33779 | 0.15002 | 4.71092 |
| C | -1.0037 | -2.62031 | -1.57564 | H | 0.76237 | -2.30432 | 1.20363 |
| C | -1.61504 | -3.87086 | -1.78371 | H | 1.08974 | -2.0108 | 3.68846 |
| C | -0.79037 | -4.99001 | -1.8338 | C | -0.68726 | 2.27705 | 3.4999 |
| C | 1.10146 | -3.58141 | -1.52271 | H | -1.2678 | 1.93617 | 4.36737 |
| C | 0.58268 | -4.84896 | -1.71855 | H | 0.06307 | 2.99529 | 3.84796 |
| H | -1.23632 | -5.97167 | -1.99481 | H | -1.3706 | 2.81313 | 2.83074 |
| H | 2.17404 | -3.40649 | -1.47505 | N | 0.19524 | -0.34347 | 0.93225 |
| H | 1.25234 | -5.70216 | -1.79063 | Rh | -0.48036 | -0.7419 | -0.90576 |
| C | -3.09207 | -4.02646 | -1.98227 | H | -2.89082 | -0.38194 | -2.04259 |
| H | -3.31851 | -5.01267 | -2.40399 | C | -2.31954 | -1.00799 | -0.13729 |
| H | -3.62616 | -3.94411 | -1.02663 | C | -3.24427 | -0.79261 | -1.08377 |
| H | -3.50169 | -3.26885 | -2.66172 | C | -2.54606 | -1.42343 | 1.24757 |
| N | 0.32914 | -2.48473 | -1.42519 | C | -3.05233 | -0.50298 | 2.17569 |

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| | | | | | | | |
|---|----------|---------|----------|---|----------|----------|----------|
| C | -0.24599 | 3.2626 | 0.39959 | C | -2.27279 | -2.73417 | 1.66643 |
| C | -0.63984 | 4.01181 | -0.72728 | C | -3.29476 | -0.88496 | 3.49031 |
| C | -1.10457 | 3.40954 | -1.88348 | H | -3.26641 | 0.51409 | 1.84141 |
| C | -1.11247 | 2.01256 | -1.92536 | C | -2.52998 | -3.11342 | 2.9791 |
| C | -0.72267 | 1.23207 | -0.83773 | H | -1.86816 | -3.43931 | 0.93892 |
| C | -0.35605 | 1.8582 | 0.37424 | C | -3.03659 | -2.1926 | 3.89409 |
| H | -1.40278 | 3.99867 | -2.7494 | H | -3.69751 | -0.16198 | 4.1993 |
| H | -1.41253 | 1.52313 | -2.85509 | H | -2.33316 | -4.13851 | 3.29046 |
| C | 0.46383 | 4.20018 | 1.27165 | H | -3.23728 | -2.49607 | 4.9207 |
| C | 0.2547 | 5.60595 | 0.64383 | C | -4.69198 | -1.04748 | -1.07664 |
| O | 1.18735 | 4.013 | 2.22717 | C | -5.35184 | -1.8211 | -0.10897 |
| O | 0.62341 | 6.66404 | 1.09384 | C | -5.46223 | -0.49383 | -2.10966 |
| N | -0.41463 | 5.38521 | -0.53703 | C | -6.72589 | -2.01018 | -0.17112 |
| C | -0.74815 | 6.42072 | -1.47965 | H | -4.78469 | -2.29048 | 0.69193 |
| H | -0.23842 | 6.26043 | -2.43952 | C | -6.83643 | -0.68229 | -2.16962 |
| H | -1.83123 | 6.46243 | -1.6539 | H | -4.96306 | 0.09903 | -2.87785 |
| H | -0.41426 | 7.37003 | -1.05025 | C | -7.4777 | -1.44095 | -1.19549 |
| C | -0.03829 | 0.90892 | 1.43771 | H | -7.21475 | -2.61781 | 0.58925 |
| | | | | H | -7.4081 | -0.23634 | -2.98248 |
| | | | | H | -8.55469 | -1.59494 | -1.23849 |
| | | | | C | 3.45876 | -0.93492 | -0.04942 |

| | | | | | | | |
|----|----------|----------|----------|----|----------|----------|----------|
| C | 3.75018 | -0.59832 | 1.28256 | C | -0.29735 | 0.963 | -1.27329 |
| C | 3.57646 | 0.69146 | 1.75485 | C | 0.32842 | 1.50312 | -0.12623 |
| C | 3.09574 | 1.64614 | 0.85597 | H | 0.55989 | 3.31078 | -3.61385 |
| C | 2.77896 | 1.32079 | -0.46293 | H | -0.80012 | 1.23798 | -3.34014 |
| C | 2.94128 | 0.01303 | -0.9273 | C | 2.2698 | 3.16444 | 0.47914 |
| H | 3.7973 | 0.95945 | 2.78637 | C | 2.93005 | 4.25526 | -0.4077 |
| H | 2.94355 | 2.66433 | 1.21101 | O | 2.74047 | 2.83322 | 1.54728 |
| H | 2.37223 | 2.0785 | -1.13326 | O | 3.89715 | 4.92417 | -0.12728 |
| C | 3.78058 | -2.35384 | -0.22743 | N | 2.21167 | 4.26732 | -1.57796 |
| C | 4.24958 | -2.83722 | 1.17722 | C | 2.55555 | 5.06457 | -2.72637 |
| O | 3.7664 | -3.04711 | -1.21485 | H | 2.85491 | 4.42922 | -3.57224 |
| O | 4.60268 | -3.94395 | 1.49916 | H | 1.71127 | 5.69322 | -3.03669 |
| N | 4.20219 | -1.71542 | 1.99138 | H | 3.39675 | 5.70291 | -2.44022 |
| C | 4.60238 | -1.71074 | 3.37468 | C | 0.1665 | 0.71885 | 1.09923 |
| H | 5.47253 | -1.0599 | 3.53351 | C | 0.29924 | 1.12474 | 2.43567 |
| H | 3.78068 | -1.36668 | 4.01709 | C | 0.31495 | 0.11514 | 3.40774 |
| H | 4.86746 | -2.73836 | 3.64119 | C | -0.2308 | -1.50185 | 1.75987 |
| C | 2.53564 | -0.36304 | -2.30628 | C | 0.1093 | -1.2117 | 3.0761 |
| C | 3.47916 | -0.49322 | -3.33426 | H | 0.47649 | 0.39974 | 4.44775 |
| C | 3.0014 | -0.82672 | -4.59745 | H | -0.53615 | -2.50055 | 1.44501 |
| C | 0.7945 | -0.91107 | -3.71418 | H | 0.16136 | -2.00498 | 3.81629 |
| C | 1.6445 | -1.0388 | -4.79907 | N | -0.21318 | -0.56357 | 0.81871 |
| H | 3.70609 | -0.93311 | -5.42221 | Rh | -1.11315 | -0.79812 | -1.03104 |
| H | -0.2745 | -1.11062 | -3.81114 | H | -2.62772 | 2.04991 | -0.96994 |
| H | 1.2516 | -1.31603 | -5.77385 | C | -2.75771 | 0.07589 | -0.29634 |
| C | 4.94257 | -0.3199 | -3.07416 | C | -3.22893 | 1.32424 | -0.41708 |
| H | 5.14996 | 0.55543 | -2.44578 | C | -3.2898 | -1.03787 | 0.49652 |
| H | 5.34061 | -1.20204 | -2.55342 | C | -3.32392 | -0.95643 | 1.90003 |
| H | 5.49816 | -0.20893 | -4.01251 | C | -3.62836 | -2.25864 | -0.1136 |
| N | 1.22578 | -0.56765 | -2.49439 | C | -3.68251 | -2.05573 | 2.66463 |
| Cl | -0.20148 | -3.16278 | -1.22202 | H | -3.04812 | -0.01275 | 2.37336 |
| | | | | C | -3.97894 | -3.36248 | 0.66201 |
| | | | | H | -3.63721 | -2.31356 | -1.2034 |
| | | | | C | -4.00322 | -3.26701 | 2.04901 |
| | | | | H | -3.70722 | -1.97421 | 3.75069 |
| | | | | H | -4.2464 | -4.29917 | 0.17464 |
| | | | | H | -4.27841 | -4.13047 | 2.65252 |
| | | | | C | -4.48872 | 1.86907 | 0.10908 |
| | | | | C | -5.614 | 1.08772 | 0.4087 |

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MeD1'

| | | | | | | | |
|---|----------|---------|----------|---|----------|----------|---------|
| C | 1.15699 | 2.63137 | -0.30212 | H | -4.2464 | -4.29917 | 0.17464 |
| C | 1.23695 | 3.25358 | -1.56196 | H | -4.27841 | -4.13047 | 2.65252 |
| C | 0.50601 | 2.80831 | -2.64911 | C | -4.48872 | 1.86907 | 0.10908 |
| C | -0.25142 | 1.64609 | -2.49295 | C | -5.614 | 1.08772 | 0.4087 |

| | | | | | | | |
|----|----------|----------|----------|---|----------|----------|----------|
| C | -4.58288 | 3.25499 | 0.30028 | H | 0.03784 | 3.23987 | 2.07538 |
| C | -6.77193 | 1.67088 | 0.90607 | H | -0.45152 | 2.67327 | 3.67965 |
| H | -5.5849 | 0.01418 | 0.23098 | C | 3.67376 | -4.20831 | -0.82732 |
| C | -5.73971 | 3.83869 | 0.80018 | H | 4.32084 | -3.41322 | -1.21657 |
| H | -3.72204 | 3.87768 | 0.05188 | H | 3.79795 | -4.23566 | 0.26323 |
| C | -6.84088 | 3.04673 | 1.11081 | H | 4.03635 | -5.16352 | -1.22501 |
| H | -7.63495 | 1.04428 | 1.12779 | | | | |
| H | -5.78352 | 4.91764 | 0.94365 | | | | |
| H | -7.7523 | 3.49892 | 1.49889 | | | | |
| C | 3.06642 | -1.23782 | 0.25383 | | | | |
| C | 3.87468 | -0.09642 | 0.41667 | | | | |
| C | 4.09424 | 0.78625 | -0.62907 | | | | |
| C | 3.43289 | 0.52657 | -1.83113 | | | | |
| C | 2.60092 | -0.58079 | -1.99703 | | | | |
| C | 2.42514 | -1.50124 | -0.95894 | | | | |
| H | 4.73559 | 1.65876 | -0.51046 | | | | |
| H | 3.56403 | 1.21636 | -2.66503 | | | | |
| H | 2.08648 | -0.74511 | -2.94308 | | | | |
| C | 3.01743 | -1.91215 | 1.54933 | | | | |
| C | 3.87069 | -1.02804 | 2.50204 | | | | |
| O | 2.46601 | -2.93422 | 1.89439 | | | | |
| O | 4.06062 | -1.21047 | 3.68021 | | | | |
| N | 4.37027 | -0.00807 | 1.71946 | | | | |
| C | 5.2421 | 1.03537 | 2.21081 | | | | |
| H | 6.21498 | 0.99599 | 1.70336 | | | | |
| H | 4.78436 | 2.02091 | 2.06393 | | | | |
| H | 5.3883 | 0.85498 | 3.27978 | | | | |
| C | 1.6302 | -2.73082 | -1.21182 | | | | |
| C | 2.2365 | -3.99879 | -1.19143 | | | | |
| C | 1.44681 | -5.08949 | -1.54974 | | | | |
| C | -0.37904 | -3.61899 | -1.94639 | | | | |
| C | 0.12816 | -4.90867 | -1.9347 | | | | |
| H | 1.88888 | -6.08597 | -1.54395 | | | | |
| H | -1.39294 | -3.40402 | -2.28481 | | | | |
| H | -0.49577 | -5.74588 | -2.23741 | | | | |
| N | 0.3477 | -2.55431 | -1.58092 | | | | |
| Cl | -2.16209 | -1.00959 | -3.14799 | | | | |
| C | 0.29825 | 2.55196 | 2.88628 | | | | |
| H | 1.27006 | 2.85845 | 3.28664 | | | | |
| | | | | 88 | | | |
| | | | | Me^eTS_{D1'}-A | | | |
| | | | | C | 0.58555 | 2.46267 | -0.38865 |
| | | | | C | 0.35271 | 2.964 | -1.67847 |
| | | | | C | -0.57016 | 2.37792 | -2.5298 |
| | | | | C | -1.19798 | 1.21326 | -2.10184 |
| | | | | C | -0.93948 | 0.63886 | -0.8459 |
| | | | | C | -0.09334 | 1.31741 | 0.0676 |
| | | | | H | -0.75549 | 2.77213 | -3.52778 |
| | | | | H | -1.86679 | 0.69003 | -2.78138 |
| | | | | C | 1.81528 | 3.09623 | 0.0784 |
| | | | | C | 2.23387 | 4.08089 | -1.04831 |
| | | | | O | 2.50141 | 2.91175 | 1.06139 |
| | | | | O | 3.24282 | 4.74932 | -1.08262 |
| | | | | N | 1.2536 | 3.9956 | -2.00562 |
| | | | | C | 1.3524 | 4.61394 | -3.30242 |
| | | | | H | 1.50337 | 3.85713 | -4.08664 |
| | | | | H | 0.44827 | 5.18986 | -3.53536 |
| | | | | H | 2.21451 | 5.28715 | -3.28064 |
| | | | | C | 0.18649 | 0.62936 | 1.33131 |
| | | | | C | 0.49021 | 1.2067 | 2.57371 |
| | | | | C | 0.83052 | 0.33787 | 3.61424 |
| | | | | C | 0.36184 | -1.52768 | 2.22038 |
| | | | | C | 0.8081 | -1.03461 | 3.43792 |
| | | | | H | 1.09477 | 0.76292 | 4.58254 |
| | | | | H | 0.24601 | -2.5956 | 2.04043 |
| | | | | H | 1.09393 | -1.71824 | 4.23221 |
| | | | | C | 0.34473 | 2.66444 | 2.87792 |
| | | | | H | -0.25445 | 2.77764 | 3.79194 |
| | | | | H | 1.31767 | 3.14217 | 3.03798 |
| | | | | H | -0.17131 | 3.20469 | 2.07687 |
| | | | | N | 0.04881 | -0.71868 | 1.2085 |

| | | | | | | | |
|----|----------|----------|----------|-------------|----------|----------|----------|
| Rh | -0.87176 | -1.34519 | -0.5468 | N | 4.62037 | 0.9263 | 0.40513 |
| H | -3.43167 | -0.54603 | -1.91597 | C | 5.38598 | 2.15107 | 0.32634 |
| C | -2.59039 | -0.2255 | -0.03899 | H | 6.08587 | 2.11077 | -0.51832 |
| C | -3.6461 | -0.2526 | -0.887 | H | 4.72798 | 3.02356 | 0.23049 |
| C | -2.75266 | 0.24085 | 1.35772 | H | 5.95107 | 2.23175 | 1.25943 |
| C | -2.92814 | 1.60388 | 1.62375 | C | 1.82092 | -2.85062 | -0.74722 |
| C | -2.81789 | -0.66347 | 2.42323 | C | 2.6845 | -3.95487 | -0.65925 |
| C | -3.16253 | 2.05176 | 2.91904 | C | 2.10706 | -5.20744 | -0.46586 |
| H | -2.90233 | 2.30913 | 0.79164 | C | -0.05335 | -4.21305 | -0.51057 |
| C | -3.05653 | -0.21754 | 3.71862 | C | 0.72916 | -5.34819 | -0.38982 |
| H | -2.69753 | -1.72737 | 2.21551 | H | 2.75397 | -6.08177 | -0.39577 |
| C | -3.22581 | 1.14215 | 3.9714 | H | -1.14107 | -4.25495 | -0.5046 |
| H | -3.3056 | 3.11553 | 3.10637 | H | 0.26311 | -6.32158 | -0.2605 |
| H | -3.11442 | -0.93576 | 4.53555 | C | 4.17102 | -3.82279 | -0.77478 |
| H | -3.41571 | 1.49039 | 4.98559 | H | 4.4606 | -3.08349 | -1.53104 |
| C | -5.06357 | 0.05314 | -0.67701 | H | 4.60494 | -3.50715 | 0.18334 |
| C | -5.72507 | 0.14255 | 0.56087 | H | 4.62438 | -4.78365 | -1.04442 |
| C | -5.83268 | 0.25123 | -1.83769 | N | 0.48546 | -2.9958 | -0.66618 |
| C | -7.08026 | 0.43892 | 0.62192 | Cl | -1.68461 | -2.14146 | -2.6617 |
| H | -5.18346 | -0.03692 | 1.48606 | | | | |
| C | -7.18431 | 0.55697 | -1.7747 | 34 | | | |
| H | -5.34475 | 0.16072 | -2.80879 | PPh3 | | | |
| C | -7.8169 | 0.65647 | -0.53938 | P | -0.00206 | -0.00199 | 1.27864 |
| H | -7.56809 | 0.49798 | 1.5941 | C | -1.5784 | -0.46657 | 0.44613 |
| H | -7.7468 | 0.71198 | -2.69435 | C | -2.75535 | 0.05652 | 0.99329 |
| H | -8.87853 | 0.89156 | -0.4814 | C | -1.66557 | -1.28319 | -0.68443 |
| C | 3.21054 | -0.80356 | -0.20907 | C | -3.99036 | -0.21609 | 0.41696 |
| C | 3.77581 | 0.43072 | -0.58881 | H | -2.69793 | 0.68688 | 1.88243 |
| C | 3.47626 | 1.00792 | -1.81335 | C | -2.90347 | -1.56737 | -1.25422 |
| C | 2.57274 | 0.32929 | -2.63751 | H | -0.75788 | -1.69904 | -1.12258 |
| C | 2.0052 | -0.89185 | -2.27645 | C | -4.06626 | -1.03302 | -0.708 |
| C | 2.33745 | -1.49023 | -1.05445 | H | -4.89732 | 0.20216 | 0.8512 |
| H | 3.92248 | 1.95247 | -2.12291 | H | -2.95838 | -2.20739 | -2.13387 |
| H | 2.29699 | 0.77261 | -3.59413 | H | -5.03312 | -1.25535 | -1.15705 |
| H | 1.2943 | -1.38727 | -2.9377 | C | 1.1903 | -1.1329 | 0.44539 |
| C | 3.67024 | -1.08195 | 1.14956 | C | 1.94585 | -0.79567 | -0.68063 |
| C | 4.59083 | 0.1142 | 1.52114 | C | 1.32544 | -2.41544 | 0.989 |
| O | 3.439 | -2.01448 | 1.88822 | C | 2.81479 | -1.72266 | -1.2494 |
| O | 5.18058 | 0.27612 | 2.56141 | H | 1.85284 | 0.19915 | -1.11691 |

| | | | | | | | |
|---|----------|----------|----------|---|---------|----------|----------|
| C | 2.18394 | -3.34531 | 0.41432 | C | 3.08395 | -3.60958 | -2.66772 |
| H | 0.7472 | -2.68472 | 1.87482 | H | 1.35677 | -2.56298 | -1.90466 |
| C | 2.93393 | -2.99792 | -0.70615 | C | 4.46989 | -3.63603 | -2.75613 |
| H | 3.40003 | -1.44666 | -2.12563 | H | 6.31512 | -2.66544 | -2.19721 |
| H | 2.27565 | -4.34055 | 0.84693 | H | 2.4899 | -4.38452 | -3.14869 |
| H | 3.61448 | -3.72077 | -1.15354 | H | 4.9666 | -4.43344 | -3.30738 |
| C | 0.38387 | 1.59608 | 0.44631 | C | 3.24955 | -0.54633 | 1.25584 |
| C | -0.28106 | 2.08259 | -0.6824 | C | 3.96976 | 0.4179 | 1.9623 |
| C | 1.42631 | 2.35283 | 0.99355 | C | 3.12926 | -1.83059 | 1.80512 |
| C | 0.09292 | 3.29687 | -1.25163 | C | 4.52564 | 0.11926 | 3.20437 |
| H | -1.09643 | 1.50737 | -1.12159 | H | 4.12741 | 1.40743 | 1.54085 |
| C | 1.80791 | 3.55922 | 0.41847 | C | 3.68879 | -2.12713 | 3.04111 |
| H | 1.94423 | 1.98587 | 1.8816 | H | 2.60267 | -2.61345 | 1.25686 |
| C | 1.13824 | 4.03512 | -0.70567 | C | 4.3792 | -1.14834 | 3.75169 |
| H | -0.43443 | 3.66623 | -2.13023 | H | 5.08333 | 0.88655 | 3.73915 |
| H | 2.62415 | 4.13419 | 0.85333 | H | 3.59358 | -3.13381 | 3.44683 |
| H | 1.4295 | 4.98392 | -1.15373 | H | 4.81469 | -1.38008 | 4.72239 |

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| | | | | | | | |
|----|---------|----------|----------|---|----------|----------|----------|
| Rh | 0.02171 | -0.2046 | -0.29995 | C | 0.04532 | 0.41558 | 1.55669 |
| P | 2.40356 | -0.27257 | -0.35944 | C | 0.11238 | -0.58345 | 2.52794 |
| Cl | 0.04893 | -0.40319 | -2.82888 | C | 0.20768 | -0.24728 | 3.87312 |
| C | 3.0585 | 1.28129 | -1.06847 | C | 0.20882 | 1.10787 | 4.21586 |
| C | 3.00602 | 2.48265 | -0.34922 | C | 0.10258 | 2.10739 | 3.25766 |
| C | 3.45312 | 1.31532 | -2.40922 | C | 0.00689 | 1.7768 | 1.88707 |
| C | 3.39364 | 3.67907 | -0.94007 | H | 0.28291 | -1.01171 | 4.6457 |
| H | 2.63097 | 2.49227 | 0.67387 | H | 0.29388 | 1.38888 | 5.26452 |
| C | 3.82521 | 2.51773 | -3.00295 | H | 0.11313 | 3.13803 | 3.59392 |
| H | 3.45614 | 0.39932 | -2.99751 | C | 0.03114 | -2.01558 | 0.61556 |
| C | 3.80707 | 3.69861 | -2.26924 | O | 0.00685 | -3.1209 | 0.1038 |
| H | 3.35288 | 4.60198 | -0.36292 | N | 0.06574 | -1.87695 | 2.01364 |
| H | 4.12832 | 2.52748 | -4.04854 | C | -0.01847 | -3.02724 | 2.88278 |
| H | 4.10454 | 4.63686 | -2.73526 | H | 0.8844 | -3.11693 | 3.50587 |
| C | 3.19612 | -1.59471 | -1.34833 | H | -0.89846 | -2.94771 | 3.5386 |
| C | 4.59482 | -1.63326 | -1.42666 | H | -0.11352 | -3.91407 | 2.25148 |
| C | 2.44152 | -2.5898 | -1.96834 | C | -0.10335 | 2.70498 | 0.74134 |
| C | 5.22825 | -2.64512 | -2.13452 | C | -0.28088 | 4.10529 | 0.79438 |
| H | 5.18922 | -0.86471 | -0.92996 | C | -0.27682 | 4.80228 | -0.41459 |
| | | | | C | 0.0154 | 2.77409 | -1.60286 |
| | | | | C | -0.10015 | 4.15506 | -1.62621 |
| | | | | H | -0.4127 | 5.88431 | -0.38911 |

| | | | | | | | |
|---|----------|----------|----------|-------------|----------|----------|----------|
| H | 0.12488 | 2.17382 | -2.50983 | H | -3.33334 | -0.06603 | 4.54398 |
| H | -0.07658 | 4.69927 | -2.56728 | H | -4.2777 | -2.36355 | 4.7264 |
| C | -0.50319 | 4.88664 | 2.05583 | | | | |
| H | -1.29504 | 4.44972 | 2.67745 | | | | |
| H | 0.40142 | 4.95211 | 2.67629 | | | | |
| H | -0.80152 | 5.91383 | 1.81372 | | | | |
| N | -0.0034 | 2.08588 | -0.46558 | | | | |
| P | -2.35741 | -0.42487 | -0.30526 | | | | |
| C | -3.08704 | -1.58066 | -1.52404 | | | | |
| C | -2.33976 | -2.64197 | -2.03791 | | | | |
| C | -4.43195 | -1.44072 | -1.88504 | | | | |
| C | -2.93822 | -3.55185 | -2.90513 | | | | |
| H | -1.29802 | -2.76148 | -1.75049 | | | | |
| C | -5.02195 | -2.35071 | -2.7534 | | | | |
| H | -5.0206 | -0.61474 | -1.48442 | | | | |
| C | -4.2731 | -3.40679 | -3.26608 | | | | |
| H | -2.34967 | -4.3754 | -3.30553 | | | | |
| H | -6.06806 | -2.23316 | -3.03199 | | | | |
| H | -4.73304 | -4.11813 | -3.95081 | | | | |
| C | -3.23733 | 1.1367 | -0.69148 | | | | |
| C | -4.18196 | 1.7421 | 0.13898 | | | | |
| C | -2.93377 | 1.72193 | -1.92779 | | | | |
| C | -4.7982 | 2.92904 | -0.25092 | | | | |
| H | -4.45433 | 1.28127 | 1.0872 | | | | |
| C | -3.55299 | 2.90403 | -2.31144 | | | | |
| H | -2.2088 | 1.23705 | -2.58697 | | | | |
| C | -4.48206 | 3.51401 | -1.47154 | | | | |
| H | -5.53556 | 3.3915 | 0.40371 | | | | |
| H | -3.30783 | 3.35203 | -3.27354 | | | | |
| H | -4.96633 | 4.4414 | -1.77399 | | | | |
| C | -3.05213 | -1.01842 | 1.28549 | | | | |
| C | -3.56804 | -2.31361 | 1.40075 | | | | |
| C | -2.96752 | -0.22218 | 2.43499 | | | | |
| C | -4.00362 | -2.79315 | 2.63233 | | | | |
| H | -3.6248 | -2.95634 | 0.52323 | | | | |
| C | -3.41095 | -0.70108 | 3.66255 | | | | |
| H | -2.53854 | 0.77869 | 2.37766 | | | | |
| C | -3.93148 | -1.98761 | 3.76471 | | | | |
| H | -4.40428 | -3.80311 | 2.70383 | | | | |
| | | | | 89 | | | |
| | | | | P-C2 | | | |
| | | | | C | 0.86958 | 0.28507 | 1.36817 |
| | | | | C | 0.28116 | 0.98883 | 2.41983 |
| | | | | C | 0.83819 | 0.93761 | 3.69239 |
| | | | | C | 2.00355 | 0.18569 | 3.87235 |
| | | | | C | 2.61228 | -0.48767 | 2.82293 |
| | | | | C | 2.05424 | -0.44632 | 1.52534 |
| | | | | H | 0.38578 | 1.46154 | 4.53345 |
| | | | | H | 2.45064 | 0.13192 | 4.86381 |
| | | | | H | 3.52488 | -1.03254 | 3.03328 |
| | | | | C | -1.35484 | 1.50241 | 0.75554 |
| | | | | O | -2.4405 | 1.931 | 0.42403 |
| | | | | N | -0.87559 | 1.68385 | 2.06335 |
| | | | | C | -1.63534 | 2.43595 | 3.03446 |
| | | | | H | -2.03945 | 1.77881 | 3.82017 |
| | | | | H | -1.00135 | 3.19805 | 3.50865 |
| | | | | H | -2.45657 | 2.92713 | 2.50551 |
| | | | | C | 2.59671 | -1.05418 | 0.28853 |
| | | | | C | 3.76627 | -1.83747 | 0.16179 |
| | | | | C | 4.08584 | -2.32252 | -1.10723 |
| | | | | C | 2.16484 | -1.2711 | -2.01214 |
| | | | | C | 3.29026 | -2.05545 | -2.20964 |
| | | | | H | 4.98763 | -2.92592 | -1.21857 |
| | | | | H | 1.47961 | -1.00026 | -2.819 |
| | | | | H | 3.53389 | -2.43833 | -3.19759 |
| | | | | C | 4.69878 | -2.16257 | 1.28978 |
| | | | | H | 5.13791 | -1.25459 | 1.72588 |
| | | | | H | 4.20366 | -2.71347 | 2.10037 |
| | | | | H | 5.52596 | -2.78498 | 0.92815 |
| | | | | N | 1.84239 | -0.79625 | -0.81283 |
| | | | | Rh | 0.0079 | 0.4978 | -0.37515 |
| | | | | Cl | -0.58487 | 0.51477 | -2.8465 |
| | | | | C | 1.65511 | 2.30422 | -0.66018 |
| | | | | C | 0.56585 | 2.86774 | -0.7747 |
| | | | | C | 3.05272 | 2.00001 | -0.62055 |

| | | | | | | | |
|----|----------|----------|----------|------------|----------|----------|----------|
| C | 0.54082 | -3.79072 | -2.17611 | C | -3.01095 | 3.60134 | -2.16094 |
| H | 1.11312 | -5.67762 | -1.3208 | H | -1.22126 | 2.59825 | -1.49136 |
| H | 0.05315 | -1.72244 | -2.65627 | C | -5.08875 | 2.44348 | -1.76276 |
| H | 0.39419 | -4.16751 | -3.1849 | H | -4.9369 | 0.54868 | -0.75827 |
| C | 1.55911 | -5.08564 | 1.21965 | C | -4.39524 | 3.54454 | -2.2635 |
| H | 2.50902 | -4.773 | 1.67326 | H | -2.46746 | 4.46241 | -2.54548 |
| H | 0.8238 | -5.19157 | 2.02844 | H | -6.17438 | 2.39887 | -1.83595 |
| H | 1.71384 | -6.08142 | 0.7878 | H | -4.94105 | 4.3622 | -2.73267 |
| N | 0.50626 | -1.96098 | -0.66704 | C | -2.93574 | 0.15151 | 1.41992 |
| Rh | 0.36041 | 0.12968 | -0.24264 | C | -3.82863 | -0.81505 | 1.88689 |
| Cl | 0.30583 | 0.75058 | -2.70022 | C | -2.69152 | 1.28239 | 2.21086 |
| C | 2.38082 | 0.45767 | -0.13901 | C | -4.44135 | -0.67117 | 3.12962 |
| C | 2.01627 | 1.67357 | 0.13918 | H | -4.06828 | -1.68388 | 1.27581 |
| C | 3.45747 | -0.45653 | -0.4066 | C | -3.31214 | 1.42712 | 3.44539 |
| C | 3.64631 | -0.94915 | -1.70724 | H | -2.03168 | 2.07056 | 1.84233 |
| C | 4.27052 | -0.91937 | 0.63744 | C | -4.18153 | 0.44527 | 3.91437 |
| C | 4.654 | -1.87057 | -1.95554 | H | -5.13474 | -1.4354 | 3.4781 |
| H | 2.9875 | -0.59374 | -2.50121 | H | -3.12288 | 2.32016 | 4.04055 |
| C | 5.26341 | -1.85589 | 0.37959 | H | -4.66389 | 0.55836 | 4.88408 |
| H | 4.09959 | -0.54816 | 1.64798 | C | -2.66897 | -1.43627 | -1.01709 |
| C | 5.45949 | -2.33046 | -0.91489 | C | -3.11434 | -1.43662 | -2.34152 |
| H | 4.80663 | -2.24151 | -2.96782 | C | -2.50014 | -2.66288 | -0.3598 |
| H | 5.89072 | -2.21447 | 1.19425 | C | -3.41666 | -2.63561 | -2.98183 |
| H | 6.24176 | -3.06153 | -1.11335 | H | -3.21365 | -0.49413 | -2.87872 |
| C | 2.52792 | 2.98552 | -0.28052 | C | -2.81459 | -3.85692 | -0.9963 |
| C | 2.79309 | 3.20619 | -1.63515 | H | -2.10704 | -2.68336 | 0.65841 |
| C | 2.79252 | 3.99258 | 0.65181 | C | -3.2775 | -3.84537 | -2.31001 |
| C | 3.32697 | 4.42327 | -2.04545 | H | -3.76309 | -2.62019 | -4.01396 |
| H | 2.54285 | 2.42484 | -2.35272 | H | -2.68387 | -4.8013 | -0.46921 |
| C | 3.33658 | 5.19967 | 0.23817 | H | -3.52102 | -4.78067 | -2.81193 |
| H | 2.57444 | 3.81969 | 1.70602 | | | | |
| C | 3.60221 | 5.41756 | -1.11264 | 89 | | | |
| H | 3.52487 | 4.5948 | -3.10227 | P-D | | | |
| H | 3.54881 | 5.97749 | 0.96999 | C | 0.50923 | 0.53121 | 1.33231 |
| H | 4.0202 | 6.36921 | -1.43784 | C | 0.99428 | 1.7764 | 1.73442 |
| P | -2.09093 | 0.10433 | -0.21862 | C | 1.00311 | 2.08523 | 3.0972 |
| C | -2.99482 | 1.44942 | -1.07294 | C | 0.59973 | 1.14602 | 4.04096 |
| C | -2.30529 | 2.55634 | -1.56874 | C | 0.25018 | -0.13744 | 3.64855 |
| C | -4.39242 | 1.40402 | -1.16199 | C | 0.23392 | -0.47385 | 2.28594 |

| | | | | | | | |
|----|----------|----------|----------|---|----------|----------|----------|
| H | 1.35192 | 3.06783 | 3.41408 | C | 5.18498 | 0.43125 | -1.43496 |
| H | 0.60078 | 1.40659 | 5.09756 | C | 5.23747 | 1.37697 | 0.7733 |
| H | -0.02562 | -0.86039 | 4.4083 | C | 6.5711 | 0.32503 | -1.41932 |
| C | 2.53427 | 2.45959 | -0.06866 | H | 4.62262 | 0.12293 | -2.31502 |
| O | 3.09563 | 3.39752 | -0.60776 | C | 6.62201 | 1.26963 | 0.79236 |
| N | 1.46823 | 2.7095 | 0.79152 | H | 4.70962 | 1.79752 | 1.63156 |
| C | 1.07899 | 4.10435 | 0.91458 | C | 7.29443 | 0.73939 | -0.3054 |
| H | 0.10838 | 4.15473 | 1.42073 | H | 7.08978 | -0.07754 | -2.28846 |
| H | 1.81957 | 4.69873 | 1.46936 | H | 7.17983 | 1.60211 | 1.667 |
| H | 0.996 | 4.53499 | -0.08929 | H | 8.38033 | 0.65667 | -0.29508 |
| C | -0.03655 | -1.78112 | 1.69479 | P | -2.33568 | 0.35005 | -0.47757 |
| C | -0.19708 | -3.03213 | 2.32709 | C | -3.01154 | 1.98326 | 0.01657 |
| C | -0.36286 | -4.15041 | 1.51496 | C | -2.25224 | 3.12988 | -0.23539 |
| C | -0.22615 | -2.79374 | -0.42408 | C | -4.26741 | 2.11703 | 0.62306 |
| C | -0.38154 | -4.04869 | 0.13019 | C | -2.74618 | 4.38619 | 0.10586 |
| H | -0.47769 | -5.12558 | 1.98821 | H | -1.27667 | 3.03295 | -0.71313 |
| H | -0.21213 | -2.62981 | -1.50109 | C | -4.75502 | 3.37289 | 0.96348 |
| H | -0.50504 | -4.91971 | -0.50693 | H | -4.86066 | 1.23261 | 0.85623 |
| C | -0.18538 | -3.21772 | 3.81248 | C | -3.99499 | 4.51052 | 0.70375 |
| H | 0.72719 | -2.81668 | 4.27205 | H | -2.14515 | 5.27074 | -0.1011 |
| H | -1.04505 | -2.72493 | 4.28865 | H | -5.73177 | 3.4637 | 1.43645 |
| H | -0.2414 | -4.28348 | 4.0627 | H | -4.37767 | 5.49397 | 0.97246 |
| N | -0.05449 | -1.71075 | 0.33786 | C | -3.08041 | -0.77786 | 0.76169 |
| Rh | 0.15845 | 0.1204 | -0.55998 | C | -3.61075 | -2.02174 | 0.40651 |
| Cl | 0.27709 | 1.79224 | -2.23056 | C | -2.98207 | -0.44931 | 2.12025 |
| C | 2.19827 | 0.02776 | -0.59499 | C | -4.05189 | -2.90778 | 1.38519 |
| C | 3.01512 | 1.05649 | -0.30096 | H | -3.68692 | -2.29829 | -0.64551 |
| C | 2.63914 | -1.32773 | -0.95158 | C | -3.42365 | -1.33498 | 3.09632 |
| C | 2.42239 | -1.81953 | -2.2474 | H | -2.56714 | 0.51565 | 2.41503 |
| C | 3.18862 | -2.18764 | 0.00905 | C | -3.95977 | -2.56796 | 2.73144 |
| C | 2.75378 | -3.13052 | -2.57388 | H | -4.47051 | -3.86923 | 1.09128 |
| H | 2.00163 | -1.14476 | -2.99662 | H | -3.35216 | -1.05595 | 4.14756 |
| C | 3.50516 | -3.50133 | -0.31662 | H | -4.3106 | -3.26033 | 3.49543 |
| H | 3.36998 | -1.80451 | 1.01442 | C | -3.20251 | -0.08683 | -2.0338 |
| C | 3.28823 | -3.97928 | -1.60751 | C | -4.59393 | -0.01561 | -2.16619 |
| H | 2.59578 | -3.49157 | -3.58968 | C | -2.4384 | -0.53364 | -3.1143 |
| H | 3.93433 | -4.15664 | 0.4406 | C | -5.20688 | -0.39482 | -3.35301 |
| H | 3.54429 | -5.00695 | -1.86114 | H | -5.2036 | 0.33736 | -1.3344 |
| C | 4.49839 | 0.95178 | -0.33584 | C | -3.0532 | -0.91296 | -4.30455 |

| | | | |
|---|----------|----------|----------|
| H | -1.3499 | -0.55093 | -3.03258 |
| C | -4.43638 | -0.84567 | -4.42325 |
| H | -6.29 | -0.33526 | -3.44669 |
| H | -2.44646 | -1.24926 | -5.14343 |
| H | -4.91873 | -1.13894 | -5.3544 |

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2a

| | | | |
|---|----------|----------|----------|
| C | 4.68926 | -0.07531 | -0.00008 |
| C | 5.70739 | -0.72434 | -0.00015 |
| H | 6.60981 | -1.29667 | -0.00019 |
| C | 3.4428 | 0.678 | -0.00001 |
| H | 3.41156 | 1.34267 | -0.87844 |
| H | 3.41168 | 1.34273 | 0.87838 |
| C | 2.20566 | -0.22157 | 0.0001 |
| H | 2.23992 | -0.88327 | 0.87956 |
| H | 2.23986 | -0.88341 | -0.87925 |
| C | 0.91215 | 0.57627 | 0.00008 |
| H | 0.89035 | 1.24226 | -0.88005 |
| H | 0.89038 | 1.24237 | 0.88012 |
| C | -0.32881 | -0.30243 | 0.00016 |
| H | -0.30602 | -0.96851 | 0.87988 |
| H | -0.30597 | -0.96872 | -0.87941 |
| C | -1.62663 | 0.49016 | 0.00002 |
| H | -1.64888 | 1.15646 | -0.87984 |
| H | -1.64894 | 1.15667 | 0.87972 |
| C | -2.86768 | -0.3882 | 0.00008 |
| H | -2.84601 | -1.05486 | 0.87978 |
| H | -2.84589 | -1.05515 | -0.8794 |
| C | -4.16688 | 0.40349 | -0.00015 |
| H | -4.18532 | 1.06806 | -0.87925 |
| H | -4.18544 | 1.06837 | 0.87871 |
| C | -5.3963 | -0.48928 | -0.00008 |
| H | -5.41004 | -1.14054 | 0.88508 |
| H | -6.32687 | 0.09167 | -0.00028 |
| H | -5.40989 | -1.1409 | -0.88496 |

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2b

| | | | |
|---|----------|----------|----------|
| C | 0.84727 | 0.10764 | 0.21752 |
| C | 2.0518 | 0.17609 | 0.33577 |
| C | -0.57309 | 0.03933 | 0.09839 |
| C | -1.23618 | -1.19595 | 0.13173 |
| C | -1.32451 | 1.21343 | -0.05418 |
| C | -2.61832 | -1.2505 | 0.01418 |
| H | -0.65127 | -2.10631 | 0.25048 |
| C | -2.70618 | 1.15187 | -0.16836 |
| H | -0.8071 | 2.17091 | -0.08064 |
| C | -3.35643 | -0.07918 | -0.1348 |
| H | -3.12402 | -2.21428 | 0.0414 |
| H | -3.27996 | 2.06969 | -0.28476 |
| H | -4.44029 | -0.12657 | -0.2252 |
| C | 3.50803 | 0.27159 | 0.40201 |
| H | 3.79802 | 1.33802 | 0.41914 |
| H | 3.87639 | -0.16312 | 1.341 |
| O | 4.16398 | -0.42736 | -0.63097 |
| H | 3.762 | -0.15532 | -1.4672 |

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2c

| | | | |
|---|----------|----------|----------|
| C | -0.50129 | -0.05111 | -0.00002 |
| C | -1.71471 | -0.11237 | -0.00007 |
| C | 0.92107 | -0.01229 | -0.00002 |
| C | 1.60306 | 1.21373 | 0.00002 |
| C | 1.65386 | -1.20865 | -0.00003 |
| C | 2.9902 | 1.23809 | 0.00004 |
| H | 1.02893 | 2.13855 | 0.00002 |
| C | 3.04063 | -1.17576 | -0.00003 |
| H | 1.11689 | -2.1553 | -0.00007 |
| C | 3.71028 | 0.04579 | 0.00002 |
| H | 3.5144 | 2.19201 | 0.00008 |
| H | 3.60411 | -2.1069 | -0.00004 |
| H | 4.79856 | 0.06917 | 0.00005 |
| C | -3.16226 | -0.1837 | -0.00006 |
| C | -3.86802 | 1.14559 | -0.00005 |
| H | -3.5767 | 1.73106 | 0.88201 |
| H | -3.57643 | 1.73151 | -0.88169 |
| H | -4.95035 | 0.98679 | -0.00016 |

| | | | | | | | |
|-----------|----------|----------|----------|------------------------|-----------|----------|----------|
| O | -3.74956 | -1.24785 | 0.00011 | H | -1.20731 | -0.85559 | 0.61493 |
| 61 | | | | C | -2.59855 | -0.77176 | -1.05228 |
| 2A | | | | H | -2.63581 | -0.33091 | -2.06041 |
| C | 1.44947 | -0.21812 | 1.17554 | H | -2.66461 | -1.86191 | -1.19173 |
| C | 1.41491 | -1.38951 | 1.9252 | C | -3.7772 | -0.28335 | -0.2261 |
| C | 0.81913 | -1.38281 | 3.18317 | H | -3.69891 | 0.80798 | -0.08128 |
| C | 0.27092 | -0.18337 | 3.64586 | H | -3.72612 | -0.72558 | 0.78371 |
| C | 0.31583 | 0.98639 | 2.89819 | C | -5.11864 | -0.61726 | -0.85998 |
| C | 0.92891 | 0.99598 | 1.62735 | H | -5.17079 | -0.16803 | -1.86658 |
| H | 0.76878 | -2.28309 | 3.79412 | H | -5.18826 | -1.7076 | -1.01543 |
| H | -0.2081 | -0.16546 | 4.62328 | C | -6.30687 | -0.14907 | -0.03471 |
| H | -0.14562 | 1.87506 | 3.31327 | H | -6.23851 | 0.94156 | 0.12147 |
| C | 2.4787 | -2.34086 | 0.00078 | H | -6.25339 | -0.59919 | 0.97183 |
| O | 2.92866 | -3.24242 | -0.65637 | C | -7.64711 | -0.48666 | -0.66866 |
| N | 1.97294 | -2.50513 | 1.29199 | H | -7.71236 | -1.57679 | -0.8299 |
| C | 1.98698 | -3.80866 | 1.92424 | H | -7.70338 | -0.03331 | -1.67362 |
| H | 2.56677 | -3.78267 | 2.85671 | C | -8.83873 | -0.02829 | 0.1585 |
| H | 0.96513 | -4.14352 | 2.14959 | H | -8.77247 | 1.06049 | 0.31657 |
| H | 2.45067 | -4.51066 | 1.22785 | H | -8.77844 | -0.48136 | 1.1615 |
| C | 1.03246 | 2.13327 | 0.68073 | C | -10.1685 | -0.3778 | -0.48801 |
| C | 0.72558 | 3.48557 | 0.93708 | H | -10.26474 | -1.46341 | -0.62933 |
| C | 0.88472 | 4.39144 | -0.11446 | H | -11.02069 | -0.04511 | 0.11733 |
| C | 1.64296 | 2.65075 | -1.53362 | H | -10.26115 | 0.08933 | -1.47847 |
| C | 1.33395 | 3.99236 | -1.36249 | C | 3.95481 | -0.0349 | 0.00494 |
| H | 0.65484 | 5.44158 | 0.0685 | O | 5.01546 | 0.19622 | 0.369 |
| H | 2.03982 | 2.2412 | -2.46545 | | | | |
| H | 1.46034 | 4.70173 | -2.17614 | 61 | | | |
| C | 0.27185 | 4.01739 | 2.264 | TS_{2A} | | | |
| H | -0.74616 | 3.69229 | 2.51873 | C | 1.24208 | -0.23609 | 1.01329 |
| H | 0.93238 | 3.70398 | 3.08221 | C | 1.13171 | -1.40914 | 1.77606 |
| H | 0.2641 | 5.11345 | 2.24797 | C | 0.72699 | -1.31596 | 3.10903 |
| N | 1.49088 | 1.77307 | -0.54802 | C | 0.54888 | -0.0439 | 3.65186 |
| Rh | 2.23953 | -0.4075 | -0.6288 | C | 0.75525 | 1.12908 | 2.9196 |
| Cl | 3.29282 | -0.15212 | -2.88333 | C | 1.11034 | 1.05054 | 1.56842 |
| C | -0.14542 | -0.92508 | -1.20076 | H | 0.60057 | -2.20124 | 3.73007 |
| C | 0.63018 | -1.43795 | -1.99644 | H | 0.2665 | 0.03991 | 4.70025 |
| H | 1.21008 | -1.92144 | -2.75979 | H | 0.66752 | 2.08147 | 3.43287 |
| C | -1.25794 | -0.42744 | -0.39903 | C | 2.08857 | -2.46416 | -0.17387 |
| H | -1.16695 | 0.6628 | -0.27188 | O | 2.40207 | -3.43933 | -0.79924 |

| | | | | | | | |
|----|----------|----------|----------|------------|-----------|----------|----------|
| N | 1.48396 | -2.57086 | 1.11261 | H | -7.73461 | -1.36357 | -1.19526 |
| C | 1.22369 | -3.8786 | 1.68378 | H | -7.69284 | 0.30736 | -1.74385 |
| H | 1.78369 | -4.01159 | 2.61917 | C | -9.03504 | -0.04337 | -0.09382 |
| H | 0.15248 | -4.01344 | 1.88581 | H | -9.03741 | 1.00244 | 0.25426 |
| H | 1.5554 | -4.62564 | 0.95937 | H | -9.06913 | -0.66264 | 0.81741 |
| C | 1.38309 | 2.16711 | 0.63199 | C | -10.26494 | -0.30826 | -0.94544 |
| C | 0.94737 | 3.49865 | 0.77814 | H | -10.29796 | -1.356 | -1.27522 |
| C | 1.30141 | 4.39988 | -0.22879 | H | -11.19433 | -0.10154 | -0.40063 |
| C | 2.40036 | 2.6644 | -1.42181 | H | -10.26224 | 0.31807 | -1.84851 |
| C | 2.03972 | 4.00307 | -1.33212 | C | 4.10869 | -0.54967 | 0.04902 |
| H | 0.972 | 5.43555 | -0.13922 | O | 5.20226 | -0.57096 | 0.38863 |
| H | 2.94474 | 2.24594 | -2.27189 | | | | |
| H | 2.31088 | 4.70525 | -2.11636 | 61 | | | |
| C | 0.10492 | 3.99018 | 1.91754 | 2A' | | | |
| H | -0.70756 | 3.29382 | 2.16192 | C | 2.44911 | 1.00299 | -0.19815 |
| H | 0.69178 | 4.14205 | 2.83418 | C | 2.23265 | 2.37392 | -0.27387 |
| H | -0.34706 | 4.95658 | 1.66481 | C | 3.28975 | 3.22031 | -0.59028 |
| N | 2.07961 | 1.79482 | -0.4718 | C | 4.54488 | 2.64982 | -0.8144 |
| Rh | 2.31566 | -0.52141 | -0.67405 | C | 4.76099 | 1.28138 | -0.71859 |
| Cl | 3.33242 | -0.50025 | -2.90587 | C | 3.69615 | 0.4134 | -0.39274 |
| C | -0.2033 | -0.37345 | -0.43762 | H | 3.15544 | 4.29879 | -0.6598 |
| C | 0.40888 | -0.56664 | -1.52851 | H | 5.38205 | 3.29807 | -1.06764 |
| H | 0.28735 | -0.71881 | -2.59149 | H | 5.76345 | 0.91288 | -0.90067 |
| C | -1.45369 | -0.18658 | 0.32255 | C | -0.01227 | 1.80046 | 0.32529 |
| H | -1.47072 | 0.81806 | 0.77709 | O | -1.17385 | 2.04049 | 0.56168 |
| H | -1.50863 | -0.90108 | 1.15841 | N | 0.91632 | 2.77699 | -0.01721 |
| C | -2.65986 | -0.36365 | -0.59973 | C | 0.53678 | 4.17477 | -0.0357 |
| H | -2.57686 | 0.33053 | -1.4505 | H | 1.11188 | 4.74093 | 0.70933 |
| H | -2.64549 | -1.37816 | -1.02734 | H | 0.70843 | 4.61289 | -1.02848 |
| C | -3.96694 | -0.12506 | 0.14088 | H | -0.5261 | 4.23479 | 0.20738 |
| H | -3.97726 | 0.9019 | 0.5451 | C | 3.73671 | -1.05852 | -0.22154 |
| H | -4.01947 | -0.79307 | 1.01786 | C | 4.87857 | -1.88855 | -0.29657 |
| C | -5.19571 | -0.33875 | -0.72923 | C | 4.69891 | -3.25799 | -0.10434 |
| H | -5.13787 | 0.31392 | -1.61711 | C | 2.38281 | -2.91996 | 0.22388 |
| H | -5.19505 | -1.37195 | -1.11644 | C | 3.4499 | -3.79949 | 0.15367 |
| C | -6.49782 | -0.07466 | 0.01091 | H | 5.57245 | -3.90834 | -0.15555 |
| H | -6.50482 | 0.96619 | 0.37875 | H | 1.3718 | -3.26921 | 0.43638 |
| H | -6.54044 | -0.70981 | 0.91291 | H | 3.3081 | -4.86623 | 0.3063 |
| C | -7.73612 | -0.31971 | -0.83634 | C | 6.27156 | -1.39684 | -0.55271 |

| | | | | | | | |
|----|-----------|----------|----------|----|----------|----------|----------|
| H | 6.37551 | -0.93788 | -1.54491 | C | 2.2408 | 0.87597 | -0.55809 |
| H | 6.58826 | -0.65404 | 0.19063 | C | 2.07176 | 2.2593 | -0.65097 |
| H | 6.98057 | -2.2316 | -0.50513 | C | 3.13863 | 3.04496 | -1.077 |
| N | 2.52399 | -1.61103 | 0.04448 | C | 4.36298 | 2.42129 | -1.31821 |
| Rh | 0.83625 | -0.03334 | 0.31605 | C | 4.55097 | 1.05366 | -1.12938 |
| Cl | 1.58315 | 0.37594 | 2.54448 | C | 3.47468 | 0.24331 | -0.7394 |
| C | 0.69395 | -0.08523 | -1.9176 | H | 3.04499 | 4.12518 | -1.17352 |
| C | -0.38908 | -0.62385 | -1.67815 | H | 5.21217 | 3.03075 | -1.62244 |
| C | -1.71199 | -1.2445 | -1.64747 | H | 5.55154 | 0.65024 | -1.24516 |
| H | -1.90443 | -1.65066 | -2.65428 | C | -0.0266 | 1.8817 | 0.46137 |
| H | -1.70094 | -2.11641 | -0.97502 | O | -1.1023 | 2.22705 | 0.88363 |
| C | -2.84146 | -0.2886 | -1.25328 | N | 0.82872 | 2.73819 | -0.23867 |
| H | -2.95729 | 0.4702 | -2.0427 | C | 0.4709 | 4.13467 | -0.40181 |
| H | -2.56655 | 0.27178 | -0.34776 | H | 1.11509 | 4.77454 | 0.21642 |
| C | -4.1486 | -1.03272 | -1.0369 | H | 0.56485 | 4.43512 | -1.45328 |
| H | -4.40372 | -1.61745 | -1.93855 | H | -0.56472 | 4.25286 | -0.07737 |
| H | -4.01326 | -1.77068 | -0.22606 | C | 3.51169 | -1.19647 | -0.39881 |
| C | -5.30285 | -0.10764 | -0.68629 | C | 4.50746 | -2.11342 | -0.79576 |
| H | -5.43771 | 0.63397 | -1.49245 | C | 4.39994 | -3.42315 | -0.32789 |
| H | -5.04101 | 0.47397 | 0.2135 | C | 2.38509 | -2.86428 | 0.78652 |
| C | -6.61156 | -0.84581 | -0.45304 | C | 3.34847 | -3.815 | 0.48474 |
| H | -6.8749 | -1.42277 | -1.35692 | H | 5.16069 | -4.14679 | -0.62206 |
| H | -6.47297 | -1.59296 | 0.34772 | H | 1.51483 | -3.11086 | 1.39552 |
| C | -7.76405 | 0.07619 | -0.08844 | H | 3.26361 | -4.83213 | 0.85868 |
| H | -7.90099 | 0.82723 | -0.88612 | C | 5.64615 | -1.77627 | -1.71175 |
| H | -7.50172 | 0.64981 | 0.81734 | H | 5.33202 | -1.12659 | -2.53732 |
| C | -9.07569 | -0.65915 | 0.14192 | H | 6.46537 | -1.26685 | -1.1854 |
| H | -9.3365 | -1.22821 | -0.76544 | H | 6.06602 | -2.6924 | -2.14428 |
| H | -8.93502 | -1.4105 | 0.93604 | N | 2.46248 | -1.60999 | 0.35687 |
| C | -10.21405 | 0.27677 | 0.51129 | Rh | 0.80728 | 0.05414 | 0.63409 |
| H | -11.15493 | -0.26287 | 0.67561 | Cl | 2.04095 | 0.92023 | 2.55894 |
| H | -9.98363 | 0.83273 | 1.43084 | C | 0.79262 | -0.04683 | -1.67072 |
| H | -10.38876 | 1.01752 | -0.28168 | C | -0.17644 | -0.6199 | -1.09074 |
| C | -0.74328 | -0.93686 | 1.24568 | H | 1.27871 | 0.26008 | -2.58162 |
| O | -1.60304 | -1.34738 | 1.87636 | C | -1.46743 | -1.32951 | -1.19195 |
| H | 1.5237 | 0.32105 | -2.46544 | H | -1.58992 | -1.72484 | -2.21323 |
| | | | | H | -1.46522 | -2.19827 | -0.51435 |
| | | | | C | -2.64659 | -0.41813 | -0.84754 |
| | | | | H | -2.63586 | 0.45344 | -1.52167 |

61
TS_{2A}'

| | | | | | | | |
|-----------|-----------|----------|----------|-----------|----------|----------|----------|
| H | -2.51494 | -0.00488 | 0.16393 | H | 3.23862 | 3.47938 | 0.8925 |
| C | -3.98002 | -1.14049 | -0.9474 | H | 4.40137 | 2.35405 | 0.13267 |
| H | -4.1113 | -1.54397 | -1.96668 | C | -1.91713 | 0.09274 | -1.05578 |
| H | -3.97464 | -2.01692 | -0.27595 | C | -3.30543 | -0.03617 | -1.27334 |
| C | -5.15883 | -0.24542 | -0.59895 | C | -3.8243 | -1.32783 | -1.377 |
| H | -5.16063 | 0.63379 | -1.26608 | C | -1.67089 | -2.25066 | -1.02342 |
| H | -5.0233 | 0.15548 | 0.41972 | C | -3.02084 | -2.45133 | -1.26534 |
| C | -6.50084 | -0.95405 | -0.6919 | H | -4.89465 | -1.44272 | -1.55093 |
| H | -6.6379 | -1.35085 | -1.71309 | H | -0.95489 | -3.06668 | -0.8982 |
| H | -6.49695 | -1.83598 | -0.02772 | H | -3.42772 | -3.4553 | -1.35449 |
| C | -7.6769 | -0.05905 | -0.33503 | C | -4.25733 | 1.11602 | -1.3884 |
| H | -7.67991 | 0.82484 | -0.99674 | H | -4.25641 | 1.73559 | -0.48054 |
| H | -7.54026 | 0.3362 | 0.68647 | H | -4.02347 | 1.7677 | -2.24038 |
| C | -9.02226 | -0.76285 | -0.42823 | H | -5.27956 | 0.74697 | -1.53218 |
| H | -9.15629 | -1.15546 | -1.44949 | N | -1.15944 | -1.02788 | -0.91987 |
| H | -9.01623 | -1.645 | 0.23272 | Rh | 1.02864 | -0.60408 | -0.46234 |
| C | -10.1845 | 0.14629 | -0.06635 | Cl | 1.63727 | -3.02326 | -0.35587 |
| H | -11.14972 | -0.37016 | -0.13798 | C | 0.20386 | -0.45047 | 1.86173 |
| H | -10.08393 | 0.52454 | 0.96054 | C | 1.37786 | -0.81253 | 1.92419 |
| H | -10.22378 | 1.01981 | -0.73226 | C | -1.18194 | -0.14332 | 2.05018 |
| C | -0.50905 | -0.54711 | 1.97185 | C | -2.10963 | -1.19397 | 2.08786 |
| O | -1.26301 | -0.84303 | 2.77895 | C | -1.62217 | 1.17731 | 2.19888 |
| | | | | C | -3.45875 | -0.92292 | 2.26017 |
| 51 | | | | H | -1.75125 | -2.216 | 1.96825 |
| 2B | | | | C | -2.97467 | 1.43978 | 2.37859 |
| C | 0.21907 | 1.18693 | -0.64532 | H | -0.89593 | 1.98811 | 2.15836 |
| C | 1.08961 | 2.25305 | -0.45345 | C | -3.8941 | 0.39356 | 2.4043 |
| C | 0.61011 | 3.55698 | -0.52495 | H | -4.17558 | -1.742 | 2.28192 |
| C | -0.74534 | 3.74269 | -0.80794 | H | -3.31219 | 2.46866 | 2.49352 |
| C | -1.61213 | 2.67498 | -1.00406 | H | -4.95373 | 0.60386 | 2.54217 |
| C | -1.14076 | 1.34827 | -0.91916 | C | 1.50697 | -0.71281 | -2.26659 |
| H | 1.26342 | 4.41452 | -0.37207 | O | 1.8016 | -0.8114 | -3.36807 |
| H | -1.13551 | 4.75656 | -0.87733 | C | 2.70751 | -1.27064 | 2.38942 |
| H | -2.65099 | 2.89695 | -1.21761 | H | 2.52242 | -1.85287 | 3.30408 |
| C | 2.71945 | 0.52955 | -0.19025 | H | 3.12471 | -1.95936 | 1.6399 |
| O | 3.84781 | 0.1147 | -0.01722 | O | 3.57097 | -0.22143 | 2.71787 |
| N | 2.41791 | 1.88342 | -0.20475 | H | 4.02944 | 0.01148 | 1.89213 |
| C | 3.45278 | 2.87811 | -0.00076 | | | | |
| H | 3.52644 | 3.54225 | -0.87219 | 51 | | | |

TS_{2B}

| | | | |
|----|----------|----------|----------|
| C | -0.1015 | 0.66024 | -0.81679 |
| C | 0.18359 | 2.00249 | -1.11842 |
| C | -0.73476 | 2.73426 | -1.87863 |
| C | -1.84496 | 2.06437 | -2.385 |
| C | -2.0815 | 0.70128 | -2.16251 |
| C | -1.20152 | -0.03265 | -1.36694 |
| H | -0.56899 | 3.7839 | -2.11605 |
| H | -2.54881 | 2.61829 | -3.00442 |
| H | -2.93821 | 0.24214 | -2.64483 |
| C | 2.31483 | 1.51035 | -0.10749 |
| O | 3.40093 | 1.84313 | 0.27853 |
| N | 1.39901 | 2.46003 | -0.65638 |
| C | 1.73702 | 3.87013 | -0.67103 |
| H | 1.81397 | 4.24418 | -1.70081 |
| H | 0.98147 | 4.45626 | -0.13001 |
| H | 2.70548 | 3.98091 | -0.17845 |
| C | -1.29247 | -1.45675 | -0.97179 |
| C | -2.45409 | -2.25465 | -1.00737 |
| C | -2.34909 | -3.55615 | -0.51045 |
| C | -0.06041 | -3.1923 | 0.01574 |
| C | -1.15761 | -4.04432 | 0.00201 |
| H | -3.23696 | -4.18907 | -0.5183 |
| H | 0.91268 | -3.47959 | 0.42112 |
| H | -1.08007 | -5.05429 | 0.39661 |
| C | -3.78974 | -1.77631 | -1.49158 |
| H | -4.05124 | -0.79823 | -1.0652 |
| H | -3.82764 | -1.68241 | -2.58561 |
| H | -4.57305 | -2.48764 | -1.20411 |
| N | -0.13773 | -1.95385 | -0.45648 |
| Rh | 1.50756 | -0.33665 | -0.15752 |
| Cl | 3.17255 | -1.8204 | 0.93664 |
| C | -0.47395 | 0.65706 | 1.21324 |
| C | 0.61768 | 0.17646 | 1.66877 |
| C | -1.88075 | 0.94107 | 1.3517 |
| C | -2.73147 | -0.09987 | 1.75654 |
| C | -2.41527 | 2.21083 | 1.10106 |
| C | -4.0935 | 0.12946 | 1.90147 |
| H | -2.30238 | -1.08429 | 1.94635 |

| | | | |
|---|----------|----------|----------|
| C | -3.7782 | 2.43149 | 1.24066 |
| H | -1.74869 | 3.01397 | 0.7894 |
| C | -4.61849 | 1.39207 | 1.63514 |
| H | -4.74825 | -0.67973 | 2.22069 |
| H | -4.18994 | 3.42014 | 1.04658 |
| H | -5.68727 | 1.56941 | 1.74259 |
| C | 2.38102 | -0.70515 | -1.85803 |
| O | 2.95598 | -0.94047 | -2.81981 |
| C | 1.23919 | -0.11387 | 3.00852 |
| H | 0.63153 | 0.35449 | 3.79579 |
| H | 1.18295 | -1.21081 | 3.14055 |
| O | 2.53008 | 0.37148 | 3.13838 |
| H | 3.09085 | -0.15546 | 2.53362 |

**51
2B'**

| | | | |
|---|----------|----------|----------|
| C | 1.4288 | 0.97179 | -0.21056 |
| C | 1.28249 | 2.33329 | -0.44802 |
| C | 2.30687 | 3.03895 | -1.06943 |
| C | 3.46433 | 2.34079 | -1.42303 |
| C | 3.62658 | 0.9914 | -1.13743 |
| C | 2.60038 | 0.27141 | -0.49017 |
| H | 2.21945 | 4.10365 | -1.28093 |
| H | 4.26925 | 2.87283 | -1.92721 |
| H | 4.55312 | 0.51799 | -1.43876 |
| C | -0.83671 | 2.03013 | 0.61338 |
| O | -1.89939 | 2.40603 | 1.05448 |
| N | 0.06117 | 2.87351 | -0.02742 |
| C | -0.21425 | 4.29182 | -0.14019 |
| H | 0.53973 | 4.87425 | 0.40624 |
| H | -0.21478 | 4.60573 | -1.19279 |
| H | -1.19851 | 4.47678 | 0.29491 |
| C | 2.60684 | -1.15344 | -0.08135 |
| C | 3.71739 | -2.02651 | -0.08635 |
| C | 3.51319 | -3.33538 | 0.35029 |
| C | 1.23784 | -2.85188 | 0.77613 |
| C | 2.27199 | -3.77373 | 0.78138 |
| H | 4.36249 | -4.01893 | 0.35649 |
| H | 0.23725 | -3.11776 | 1.11725 |

| | | | |
|---|----------|----------|----------|
| H | 1.19833 | -1.315 | -2.49654 |
| H | 0.75882 | 0.29817 | -3.07827 |
| O | -0.55321 | -1.28047 | -3.48686 |
| H | -1.31118 | -0.69416 | -3.62712 |

**52
2C**

| | | | |
|----|----------|----------|----------|
| C | 0.20934 | 1.33903 | -0.50956 |
| C | 1.1497 | 2.30577 | -0.16719 |
| C | 0.72983 | 3.60083 | 0.12018 |
| C | -0.63717 | 3.88082 | 0.04913 |
| C | -1.57226 | 2.91539 | -0.30124 |
| C | -1.16039 | 1.5986 | -0.59856 |
| H | 1.43839 | 4.37934 | 0.39858 |
| H | -0.98067 | 4.88808 | 0.27838 |
| H | -2.61753 | 3.20077 | -0.31584 |
| C | 2.70745 | 0.52069 | -0.44928 |
| O | 3.80419 | 0.03169 | -0.54168 |
| N | 2.47203 | 1.85298 | -0.13744 |
| C | 3.57133 | 2.72749 | 0.22229 |
| H | 3.6688 | 3.55105 | -0.49784 |
| H | 3.41374 | 3.13636 | 1.22849 |
| H | 4.4859 | 2.13121 | 0.21944 |
| C | -2.01473 | 0.44115 | -0.95637 |
| C | -3.39509 | 0.45853 | -1.2491 |
| C | -3.99567 | -0.75271 | -1.59705 |
| C | -1.92411 | -1.87774 | -1.35648 |
| C | -3.27558 | -1.93474 | -1.66011 |
| H | -5.06004 | -0.75324 | -1.8338 |
| H | -1.2679 | -2.75201 | -1.37323 |
| H | -3.74423 | -2.87467 | -1.94029 |
| C | -4.2528 | 1.68751 | -1.22332 |
| H | -4.35645 | 2.09335 | -0.20729 |
| H | -3.85394 | 2.48682 | -1.86084 |
| H | -5.2614 | 1.45246 | -1.58272 |
| N | -1.33682 | -0.73471 | -1.01562 |
| Rh | 0.92508 | -0.49428 | -0.66635 |
| Cl | 1.33964 | -2.94847 | -0.77986 |
| C | 0.16768 | -0.65063 | 1.76518 |

| | | | |
|---|----------|----------|----------|
| C | 1.38812 | -0.71473 | 1.59788 |
| C | -1.22373 | -0.57696 | 2.03722 |
| C | -2.0197 | -1.72747 | 1.9303 |
| C | -1.7991 | 0.648 | 2.40833 |
| C | -3.37718 | -1.6501 | 2.20105 |
| H | -1.55067 | -2.6614 | 1.62122 |
| C | -3.15971 | 0.71386 | 2.67578 |
| H | -1.16757 | 1.53389 | 2.46751 |
| C | -3.94619 | -0.43144 | 2.57077 |
| H | -3.99816 | -2.54 | 2.11899 |
| H | -3.609 | 1.66182 | 2.9669 |
| H | -5.01276 | -0.37596 | 2.78289 |
| C | 1.24506 | -0.41437 | -2.50708 |
| O | 1.44951 | -0.39928 | -3.63336 |
| C | 2.7892 | -0.81035 | 2.08366 |
| C | 3.45811 | -2.12811 | 1.89291 |
| H | 2.84088 | -2.93792 | 2.30227 |
| H | 3.54687 | -2.32761 | 0.81565 |
| H | 4.44384 | -2.10874 | 2.36632 |
| O | 3.28612 | 0.16073 | 2.61055 |

**52
TS_{2C}**

| | | | |
|---|----------|----------|----------|
| C | 0.13244 | -0.67462 | -0.90127 |
| C | -0.04906 | -2.04429 | -1.16387 |
| C | 0.9403 | -2.73484 | -1.87118 |
| C | 2.0223 | -2.0069 | -2.35677 |
| C | 2.16195 | -0.625 | -2.16935 |
| C | 1.20331 | 0.07567 | -1.43652 |
| H | 0.85463 | -3.80055 | -2.07727 |
| H | 2.7868 | -2.53021 | -2.92923 |
| H | 3.01135 | -0.12959 | -2.62675 |
| C | -2.21691 | -1.67909 | -0.17808 |
| O | -3.27274 | -2.07887 | 0.2229 |
| N | -1.23384 | -2.57375 | -0.70418 |
| C | -1.46998 | -4.00474 | -0.67788 |
| H | -1.51671 | -4.41206 | -1.69668 |
| H | -0.67638 | -4.51951 | -0.11903 |
| H | -2.42939 | -4.16923 | -0.18268 |

| | | | | | | | |
|----|----------|----------|----------|----|----------|----------|----------|
| C | 1.18581 | 1.51547 | -1.08721 | C | 1.46222 | 1.06082 | 0.1844 |
| C | 2.27876 | 2.40439 | -1.15624 | C | 1.30573 | 2.43622 | 0.04404 |
| C | 2.06776 | 3.71076 | -0.70802 | C | 2.38585 | 3.21527 | -0.36051 |
| C | -0.18513 | 3.18572 | -0.16875 | C | 3.59922 | 2.57065 | -0.61314 |
| C | 0.84019 | 4.12207 | -0.21408 | C | 3.74719 | 1.195 | -0.48446 |
| H | 2.90087 | 4.41324 | -0.74407 | C | 2.66022 | 0.3938 | -0.07688 |
| H | -1.18352 | 3.40712 | 0.21747 | H | 2.29982 | 4.29434 | -0.47979 |
| H | 0.68129 | 5.13777 | 0.13916 | H | 4.45729 | 3.16465 | -0.92299 |
| C | 3.64732 | 2.02592 | -1.63637 | H | 4.71989 | 0.76775 | -0.69604 |
| H | 4.01789 | 1.11766 | -1.14168 | C | -0.96741 | 1.95677 | 0.62105 |
| H | 3.67365 | 1.84794 | -2.72005 | O | -2.1368 | 2.23683 | 0.72603 |
| H | 4.35865 | 2.83358 | -1.42758 | N | 0.00855 | 2.90103 | 0.28975 |
| N | -0.00497 | 1.93999 | -0.59005 | C | -0.34859 | 4.28842 | 0.07895 |
| Rh | -1.54262 | 0.22134 | -0.26361 | H | 0.2345 | 4.94368 | 0.73955 |
| Cl | -3.31239 | 1.64087 | 0.71218 | H | -0.16674 | 4.58446 | -0.96446 |
| C | 0.53454 | -0.6455 | 1.13436 | H | -1.41127 | 4.3975 | 0.30591 |
| C | -0.59056 | -0.22545 | 1.56699 | C | 2.61469 | -1.08065 | 0.0753 |
| C | 1.94571 | -0.88083 | 1.28357 | C | 3.62908 | -2.00042 | -0.25744 |
| C | 2.76893 | 0.2023 | 1.63155 | C | 3.35396 | -3.35567 | -0.07459 |
| C | 2.51215 | -2.14662 | 1.09089 | C | 1.17845 | -2.83317 | 0.70575 |
| C | 4.13706 | 0.01782 | 1.77627 | C | 2.13268 | -3.79358 | 0.40977 |
| H | 2.31186 | 1.18152 | 1.78233 | H | 4.12635 | -4.0805 | -0.33303 |
| C | 3.88155 | -2.323 | 1.23351 | H | 0.18302 | -3.07543 | 1.08448 |
| H | 1.86534 | -2.98195 | 0.82641 | H | 1.91895 | -4.85048 | 0.54633 |
| C | 4.69432 | -1.24261 | 1.56867 | C | 4.95856 | -1.62193 | -0.83636 |
| H | 4.77116 | 0.85828 | 2.05322 | H | 4.84312 | -1.05423 | -1.76926 |
| H | 4.319 | -3.30868 | 1.08664 | H | 5.56189 | -1.01622 | -0.14738 |
| H | 5.76807 | -1.38531 | 1.67765 | H | 5.53864 | -2.52215 | -1.0701 |
| C | -2.42416 | 0.48439 | -1.95551 | N | 1.42509 | -1.5375 | 0.54446 |
| O | -3.00374 | 0.66122 | -2.92711 | Rh | -0.1464 | 0.08926 | 0.80223 |
| C | -1.19354 | -0.04173 | 2.9181 | Cl | -1.81678 | -1.47726 | 1.81234 |
| C | -1.17316 | 1.37156 | 3.41578 | C | -0.56365 | -0.25337 | -1.41933 |
| H | -0.20149 | 1.84556 | 3.21803 | C | -1.78667 | -0.37127 | -1.24145 |
| H | -1.93997 | 1.92853 | 2.85401 | C | -3.17318 | -0.54264 | -1.0571 |
| H | -1.40449 | 1.39084 | 4.48514 | C | -3.68753 | -1.8395 | -0.87719 |
| O | -1.65848 | -0.981 | 3.51778 | C | -4.0372 | 0.5659 | -1.06791 |
| | | | | C | -5.05267 | -2.02198 | -0.73602 |
| | | | | H | -2.99758 | -2.67897 | -0.84204 |
| | | | | C | -5.39993 | 0.37008 | -0.91655 |

52
2C'

| | | | | | | | |
|---|----------|----------|----------|----|----------|----------|----------|
| H | -3.61666 | 1.56366 | -1.16289 | H | -3.3465 | 2.93408 | -2.24122 |
| C | -5.90481 | -0.9193 | -0.75543 | C | 0.26042 | 4.72251 | 0.09877 |
| H | -5.45626 | -3.02224 | -0.59529 | H | 0.74186 | 4.4015 | 1.03085 |
| H | -6.07313 | 1.22458 | -0.91446 | H | 1.03497 | 5.19494 | -0.52155 |
| H | -6.97715 | -1.06571 | -0.63498 | H | -0.47087 | 5.50204 | 0.34386 |
| C | 0.2232 | 0.48722 | 2.59275 | N | -0.5863 | 1.29015 | -1.28526 |
| O | 0.45657 | 0.71747 | 3.68992 | Rh | 0.29371 | -0.84523 | -0.78014 |
| C | 0.54855 | -0.2512 | -2.39329 | Cl | -1.40808 | -2.08929 | -2.08289 |
| C | 0.69675 | 1.02311 | -3.17474 | C | 0.10725 | -0.11609 | 1.36792 |
| H | 1.51802 | 0.92037 | -3.89049 | C | -1.00558 | -0.51687 | 0.88617 |
| H | -0.23771 | 1.25386 | -3.70286 | C | -2.42438 | -0.68322 | 0.99707 |
| H | 0.90069 | 1.85997 | -2.49169 | C | -3.19317 | 0.41685 | 1.41478 |
| O | 1.25822 | -1.22034 | -2.54417 | C | -3.05296 | -1.90345 | 0.70969 |

52 TS_{2C'}

| | | | | | | | |
|---|----------|----------|----------|---|----------|----------|----------|
| C | 1.56433 | 0.46505 | 0.07089 | H | -2.69643 | 1.36484 | 1.62566 |
| C | 2.77211 | -0.13442 | 0.43935 | C | -4.42718 | -2.01828 | 0.86729 |
| C | 3.87721 | 0.67222 | 0.695 | H | -2.45411 | -2.74026 | 0.35874 |
| C | 3.74794 | 2.04938 | 0.52182 | C | -5.18665 | -0.92525 | 1.27694 |
| C | 2.56124 | 2.63769 | 0.08453 | H | -5.16058 | 1.15109 | 1.86262 |
| C | 1.43297 | 1.84526 | -0.16359 | H | -4.91126 | -2.96903 | 0.65301 |
| H | 4.82888 | 0.2457 | 1.00612 | H | -6.26564 | -1.02271 | 1.38418 |
| H | 4.61217 | 2.68465 | 0.707 | C | 1.27582 | -1.11264 | -2.42746 |
| H | 2.54935 | 3.70672 | -0.1055 | O | 1.79501 | -1.26612 | -3.43373 |
| C | 1.58832 | -2.18554 | 0.0455 | C | 0.71392 | 0.00266 | 2.71505 |
| O | 1.40113 | -3.3659 | 0.15836 | C | -0.29534 | 0.474 | 3.73277 |
| N | 2.75059 | -1.52931 | 0.4668 | H | -0.51424 | 1.53698 | 3.56129 |
| C | 3.7825 | -2.27095 | 1.17204 | H | -1.24325 | -0.07086 | 3.63971 |
| H | 4.75044 | -2.15663 | 0.66778 | H | 0.12252 | 0.3502 | 4.73597 |
| H | 3.85891 | -1.91111 | 2.20602 | O | 1.86424 | -0.24136 | 2.99921 |
| H | 3.50003 | -3.32565 | 1.1674 | | | | |
| C | 0.12868 | 2.28513 | -0.7005 | | | | |
| C | -0.41245 | 3.58304 | -0.60719 | | | | |
| C | -1.66924 | 3.79401 | -1.1777 | | | | |
| C | -1.78667 | 1.50854 | -1.81205 | | | | |
| C | -2.36751 | 2.76924 | -1.79835 | | | | |
| H | -2.10821 | 4.79041 | -1.11423 | | | | |
| H | -2.27616 | 0.63035 | -2.24039 | | | | |

19 NoDG1

| | | | |
|---|----------|----------|----------|
| C | -0.53314 | -0.7738 | 0.00021 |
| C | -0.36686 | 0.62053 | 0.00005 |
| C | -1.46196 | 1.46816 | -0.00019 |
| C | -2.72974 | 0.87905 | -0.00014 |
| C | -2.90623 | -0.50489 | 0.00003 |
| C | -1.79519 | -1.34552 | 0.0001 |
| H | -1.34903 | 2.55058 | -0.00042 |

| | | | | | | | |
|---|----------|----------|----------|----|----------|----------|----------|
| H | -3.60628 | 1.52521 | -0.00026 | Cl | -0.66049 | 0.51279 | 2.54544 |
| H | -3.91049 | -0.92236 | 0.00012 | H | -2.3805 | 2.09879 | 1.04894 |
| C | 0.79943 | -1.37847 | 0. | H | -3.5078 | 0.1516 | 1.80947 |
| C | 1.78664 | -0.17322 | -0.00015 | H | -0.69215 | -0.33727 | -2.18781 |
| O | 1.13669 | -2.53726 | 0.00001 | H | -1.51489 | -2.33678 | -1.16666 |
| O | 2.99216 | -0.20762 | -0.00018 | H | -1.87753 | 2.64246 | -1.2123 |
| N | 0.98993 | 0.96101 | -0.00012 | H | 0.44288 | 1.78386 | 0.07973 |
| C | 1.51068 | 2.30372 | 0.00029 | H | 5.40623 | 1.42492 | -0.5569 |
| H | 1.188 | 2.85325 | -0.89409 | C | 1.63453 | -0.86538 | 0.05824 |
| H | 1.18632 | 2.85317 | 0.8941 | O | 0.5028 | -1.31119 | 0.19923 |
| H | 2.60226 | 2.22888 | 0.00127 | C | 2.8614 | -1.8018 | -0.03927 |
| H | -1.89295 | -2.43013 | 0.0002 | O | 2.86865 | -3.00571 | 0.01949 |

41
NoDGA

| | | | |
|----|----------|----------|----------|
| C | 3.54123 | 0.37102 | -0.2538 |
| C | 4.32838 | 1.49523 | -0.42701 |
| C | 3.68439 | 2.73633 | -0.42456 |
| C | 2.30475 | 2.85858 | -0.25549 |
| C | 1.52077 | 1.7232 | -0.08099 |
| C | 2.14524 | 0.47993 | -0.08404 |
| H | 4.28427 | 3.63551 | -0.55613 |
| H | 1.84587 | 3.84424 | -0.24983 |
| C | -2.70346 | 1.39221 | 0.28002 |
| C | -3.38756 | 0.24856 | 0.72794 |
| C | -1.68541 | -0.28466 | -1.72995 |
| C | -4.32555 | -0.57505 | -0.13297 |
| C | -2.16684 | -1.45894 | -1.12936 |
| C | -3.60725 | -1.75668 | -0.79498 |
| H | -5.14822 | -0.95225 | 0.48829 |
| H | -4.79541 | 0.0712 | -0.88722 |
| H | -3.60885 | -2.60787 | -0.10015 |
| H | -4.15581 | -2.09403 | -1.69151 |
| C | -2.71866 | 1.93836 | -1.12624 |
| H | -3.62975 | 2.53776 | -1.29769 |
| C | -2.56875 | 0.85441 | -2.20034 |
| H | -3.5506 | 0.46236 | -2.50022 |
| H | -2.14004 | 1.29884 | -3.10846 |
| Rh | -1.33908 | -0.21952 | 0.39075 |

| | | | |
|---|----------|----------|----------|
| H | -2.3805 | 2.09879 | 1.04894 |
| H | -3.5078 | 0.1516 | 1.80947 |
| H | -0.69215 | -0.33727 | -2.18781 |
| H | -1.51489 | -2.33678 | -1.16666 |
| H | -1.87753 | 2.64246 | -1.2123 |
| H | 0.44288 | 1.78386 | 0.07973 |
| H | 5.40623 | 1.42492 | -0.5569 |
| C | 1.63453 | -0.86538 | 0.05824 |
| O | 0.5028 | -1.31119 | 0.19923 |
| C | 2.8614 | -1.8018 | -0.03927 |
| O | 2.86865 | -3.00571 | 0.01949 |
| N | 3.94696 | -0.96585 | -0.22109 |
| C | 5.30368 | -1.43308 | -0.35498 |
| H | 5.72442 | -1.14405 | -1.32692 |
| H | 5.93756 | -1.03121 | 0.44593 |
| H | 5.28163 | -2.52432 | -0.28227 |

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NoDGA1

| | | | |
|---|----------|----------|----------|
| C | -3.12293 | 0.85535 | 0.36433 |
| C | -3.5294 | -0.47861 | 0.23321 |
| C | -4.80671 | -0.80383 | -0.17933 |
| C | -5.67768 | 0.25655 | -0.45399 |
| C | -5.28718 | 1.58781 | -0.3201 |
| C | -3.99262 | 1.89757 | 0.0942 |
| H | -5.12983 | -1.83669 | -0.29176 |
| H | -6.69091 | 0.02938 | -0.78123 |
| H | -5.99494 | 2.38257 | -0.54433 |
| C | -1.72417 | 0.84922 | 0.79638 |
| C | -1.34757 | -0.65562 | 0.84364 |
| O | -0.9909 | 1.74959 | 1.12814 |
| O | -0.25225 | -1.13515 | 1.13611 |
| N | -2.47807 | -1.35537 | 0.57405 |
| C | -2.48732 | -2.7752 | 0.3091 |
| H | -3.28494 | -3.26944 | 0.87618 |
| H | -2.62715 | -2.95516 | -0.76511 |
| H | -1.51901 | -3.17826 | 0.61638 |
| C | 2.84812 | -0.93692 | 1.17903 |

| | | | | | | | |
|----|----------|----------|----------|----|----------|----------|----------|
| C | 2.52949 | 0.38693 | 1.52618 | C | -2.7427 | -2.67869 | -0.12809 |
| C | 2.98324 | 0.01234 | -1.4428 | H | -3.76308 | -2.76156 | 0.26492 |
| C | 3.39444 | 1.58524 | 1.19507 | H | -2.7606 | -2.6758 | -1.22706 |
| C | 2.41815 | 1.26587 | -1.12321 | H | -2.1516 | -3.52792 | 0.22268 |
| C | 2.93526 | 2.25187 | -0.10625 | C | 2.15458 | -0.43985 | 1.38602 |
| H | 3.34027 | 2.31347 | 2.01491 | C | 2.04366 | 0.94881 | 1.28823 |
| H | 4.44839 | 1.28143 | 1.13375 | C | 2.50238 | -0.33336 | -1.43123 |
| H | 2.10526 | 2.93553 | 0.12342 | C | 3.02158 | 1.88203 | 0.60589 |
| H | 3.73815 | 2.87398 | -0.5391 | C | 2.06443 | 0.97853 | -1.55723 |
| C | 4.05319 | -1.37355 | 0.38136 | C | 2.62904 | 2.17383 | -0.84321 |
| H | 4.95766 | -1.40012 | 1.01376 | H | 3.05138 | 2.82668 | 1.16471 |
| C | 4.28643 | -0.5106 | -0.86549 | H | 4.03922 | 1.47513 | 0.66578 |
| H | 4.95566 | 0.33169 | -0.63977 | H | 1.85647 | 2.95565 | -0.85204 |
| H | 4.8071 | -1.10558 | -1.62726 | H | 3.48218 | 2.5861 | -1.40913 |
| Rh | 1.34499 | -0.23968 | -0.13384 | C | 3.21966 | -1.30631 | 0.77163 |
| Cl | -0.35047 | -0.24168 | -1.84639 | H | 4.08478 | -1.39221 | 1.45106 |
| H | 2.36852 | -1.72942 | 1.76264 | C | 3.66859 | -0.82806 | -0.61344 |
| H | 1.79753 | 0.53004 | 2.32608 | H | 4.43686 | -0.04885 | -0.5354 |
| H | 2.66926 | -0.42744 | -2.39306 | H | 4.14058 | -1.664 | -1.14631 |
| H | 1.72626 | 1.68799 | -1.85702 | Rh | 0.67948 | -0.06414 | -0.16245 |
| H | 3.87297 | -2.41042 | 0.06444 | Cl | -0.57985 | -0.57909 | -2.15322 |
| H | -3.65179 | 2.92622 | 0.19803 | H | 1.57846 | -0.91689 | 2.18179 |

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NoDGTS_{A1-B}

| | | | |
|---|----------|----------|----------|
| C | -1.97677 | 0.83495 | 0.77512 |
| C | -2.67499 | -0.20517 | 0.14909 |
| C | -3.83799 | 0.06205 | -0.55576 |
| C | -4.27083 | 1.38491 | -0.63854 |
| C | -3.57498 | 2.42428 | -0.02293 |
| C | -2.41832 | 2.14831 | 0.69959 |
| H | -4.39084 | -0.73363 | -1.04966 |
| H | -5.17664 | 1.60745 | -1.19989 |
| H | -3.94253 | 3.44522 | -0.09789 |
| C | -0.79557 | 0.33046 | 1.47674 |
| C | -0.80975 | -1.48972 | 0.79236 |
| O | -0.46631 | 0.48925 | 2.62167 |
| O | -0.21349 | -2.44951 | 1.21145 |
| N | -2.11653 | -1.46795 | 0.36084 |

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NoDGB

| | | | |
|---|---------|----------|----------|
| C | 2.02179 | 0.96879 | 0.05613 |
| C | 2.6333 | -0.2634 | -0.27719 |
| C | 4.00543 | -0.23975 | -0.58379 |
| C | 4.74115 | 0.93331 | -0.56412 |
| C | 4.14146 | 2.14389 | -0.23256 |
| C | 2.79555 | 2.14145 | 0.07358 |
| H | 4.5162 | -1.15898 | -0.84852 |
| H | 5.80034 | 0.89293 | -0.81303 |
| H | 4.71488 | 3.06765 | -0.20983 |

| | | | | | | | |
|------------------------------------|----------|----------|----------|-----------|----------|----------|----------|
| C | 0.60727 | 1.18436 | 0.41064 | C | -3.08848 | -2.37884 | 0.73289 |
| C | 0.60956 | -1.66112 | -0.18736 | C | -1.85888 | -2.04957 | 0.16876 |
| O | 0.17529 | 2.23995 | 0.79602 | H | -4.42161 | 0.73138 | 1.00944 |
| O | 0.07177 | -2.74853 | -0.30479 | H | -4.95684 | -1.63243 | 1.50925 |
| N | 1.97274 | -1.49604 | -0.31713 | H | -3.33618 | -3.4244 | 0.90723 |
| C | 2.75121 | -2.71595 | -0.52426 | C | -0.59457 | 0.41708 | -1.47133 |
| H | 3.20377 | -2.7354 | -1.52376 | C | -1.15202 | 1.76549 | -1.01211 |
| H | 3.53629 | -2.7989 | 0.23588 | O | -0.47861 | 0.10596 | -2.61419 |
| H | 2.06474 | -3.55711 | -0.42883 | O | -0.68448 | 2.81599 | -1.40216 |
| C | -1.52346 | -0.588 | -1.75599 | N | -2.15196 | 1.60378 | -0.10571 |
| C | -1.20367 | 0.75947 | -1.68342 | C | -2.83773 | 2.75476 | 0.43985 |
| C | -3.12868 | -0.0315 | 0.71221 | H | -3.85365 | 2.85012 | 0.03533 |
| C | -2.19074 | 1.90599 | -1.54431 | H | -2.89279 | 2.67519 | 1.53292 |
| C | -2.64032 | 1.21961 | 0.89969 | H | -2.26347 | 3.64314 | 0.16037 |
| C | -2.65019 | 2.31539 | -0.12825 | Rh | 0.65586 | -0.50647 | -0.09513 |
| H | -1.74266 | 2.78829 | -2.01949 | Cl | 0.92348 | -2.47548 | -1.41797 |
| H | -3.06528 | 1.65705 | -2.16297 | H | -1.16222 | -2.83854 | -0.10495 |
| H | -2.00509 | 3.11929 | 0.23647 | C | 0.79001 | 0.32506 | 1.9178 |
| H | -3.66387 | 2.74273 | -0.2027 | C | 0.79863 | 1.43759 | 1.08135 |
| C | -2.85376 | -1.24482 | -1.5031 | C | 2.91233 | -0.65181 | 0.21352 |
| H | -3.35677 | -1.42827 | -2.46825 | C | 1.98832 | 2.2576 | 0.62427 |
| C | -3.80312 | -0.50661 | -0.54837 | C | 2.67079 | 0.25536 | -0.79949 |
| H | -4.28034 | 0.34056 | -1.05821 | C | 2.6051 | 1.75096 | -0.68384 |
| H | -4.61716 | -1.19334 | -0.28061 | H | 1.64428 | 3.2865 | 0.46072 |
| Rh | -0.7177 | -0.29406 | 0.28016 | H | 2.73803 | 2.31342 | 1.42422 |
| Cl | -0.21842 | -0.77969 | 2.53868 | H | 1.99286 | 2.12158 | -1.51874 |
| H | -0.80347 | -1.24262 | -2.25051 | H | 3.60999 | 2.18191 | -0.8308 |
| H | -0.23394 | 1.03232 | -2.10701 | C | 1.97979 | -0.36783 | 2.52588 |
| H | -3.11028 | -0.72019 | 1.56114 | H | 2.1799 | 0.06583 | 3.52099 |
| H | -2.26119 | 1.47731 | 1.88945 | C | 3.23628 | -0.33104 | 1.65206 |
| H | -2.63334 | -2.2426 | -1.09066 | H | 3.74344 | 0.63746 | 1.73384 |
| H | 2.2845 | 3.06076 | 0.34958 | H | 3.94965 | -1.07639 | 2.02701 |
| | | | | H | -0.16433 | 0.09063 | 2.39826 |
| | | | | H | -0.15252 | 1.96158 | 1.0299 |
| | | | | H | 3.06981 | -1.68637 | -0.09647 |
| | | | | H | 2.67507 | -0.14204 | -1.81787 |
| | | | | H | 1.70239 | -1.41735 | 2.7095 |
| 41 NoDGTS _{A-C} | | | | | | | |
| C | -1.47904 | -0.71154 | -0.0127 | | | | |
| C | -2.44808 | 0.27505 | 0.26611 | | | | |
| C | -3.68721 | -0.04788 | 0.81328 | | | | |
| C | -3.99293 | -1.37863 | 1.07153 | 41 | | | |

| | | | | | | | |
|-------|----------|----------|----------|-------------------------------|----------|----------|----------|
| NoDGC | | | H | -2.91971 | -1.83388 | 0.6026 | |
| C | 1.45023 | -0.76514 | -0.10096 | H | -2.75257 | 0.16479 | 1.81194 |
| C | 2.42798 | 0.23764 | -0.16175 | H | -1.45468 | -2.18453 | -2.08677 |
| C | 3.76476 | -0.09337 | -0.41328 | | | | |
| C | 4.13446 | -1.41081 | -0.63974 | 64 | | | |
| C | 3.17242 | -2.41294 | -0.60108 | MeTS_{A1-B(1)} | | | |
| C | 1.85089 | -2.08708 | -0.31328 | C | 1.89818 | 0.85694 | 0.27297 |
| H | 4.52403 | 0.68589 | -0.42777 | C | 1.92091 | 2.25351 | 0.44228 |
| H | 5.17729 | -1.65012 | -0.83966 | C | 2.33131 | 3.08227 | -0.59998 |
| H | 3.44753 | -3.45142 | -0.77817 | C | 2.80671 | 2.49563 | -1.76871 |
| C | 0.09003 | 1.05831 | 1.31048 | C | 2.94994 | 1.11379 | -1.88709 |
| C | 0.98685 | 2.07635 | 0.60583 | C | 2.52424 | 0.27452 | -0.8521 |
| O | -0.34208 | 1.22321 | 2.40435 | H | 2.3016 | 4.16497 | -0.48996 |
| O | 0.59792 | 3.23175 | 0.61694 | H | 3.11513 | 3.13243 | -2.59643 |
| N | 2.09659 | 1.61919 | -0.02493 | H | 3.33839 | 0.70539 | -2.81534 |
| C | 2.94053 | 2.62163 | -0.66095 | C | 1.96635 | 0.33677 | 1.98897 |
| H | 3.85883 | 2.79565 | -0.08646 | C | 1.63282 | 1.6819 | 2.66877 |
| H | 3.20764 | 2.28845 | -1.67016 | O | 2.79185 | -0.4348 | 2.42421 |
| H | 2.37651 | 3.55563 | -0.70928 | O | 1.44114 | 1.8177 | 3.85084 |
| Rh | -0.53298 | -0.47378 | 0.21675 | N | 1.6137 | 2.68805 | 1.72135 |
| Cl | -0.468 | -2.04233 | 1.97524 | C | 1.15223 | 4.01688 | 2.04127 |
| H | 1.11039 | -2.88397 | -0.24325 | H | 0.87173 | 4.01088 | 3.09851 |
| C | -0.79378 | -0.18041 | -1.94696 | H | 1.93678 | 4.76831 | 1.88126 |
| C | -0.93276 | 1.09896 | -1.42899 | H | 0.26745 | 4.2603 | 1.43827 |
| C | -2.92297 | -0.90829 | 0.02333 | C | 2.57263 | -1.19473 | -0.85687 |
| C | -2.22253 | 1.85873 | -1.19521 | C | 3.47071 | -2.00222 | -1.58158 |
| C | -2.81238 | 0.25258 | 0.7252 | C | 3.38594 | -3.38165 | -1.40097 |
| C | -2.86066 | 1.65556 | 0.18635 | C | 1.62486 | -3.07979 | 0.16546 |
| H | -2.006 | 2.92863 | -1.30876 | C | 2.46258 | -3.93606 | -0.52611 |
| H | -2.9332 | 1.61493 | -1.9957 | H | 4.07617 | -4.02536 | -1.94596 |
| H | -2.34035 | 2.3059 | 0.90328 | H | 0.88847 | -3.44502 | 0.87896 |
| H | -3.90346 | 2.01257 | 0.16763 | H | 2.40434 | -5.00939 | -0.36563 |
| C | -1.87647 | -1.17946 | -2.26178 | C | 4.53029 | -1.46088 | -2.49383 |
| H | -2.0908 | -1.14264 | -3.34369 | H | 4.12611 | -1.1635 | -3.47176 |
| C | -3.17459 | -1.03973 | -1.4564 | H | 5.03048 | -0.58429 | -2.06501 |
| H | -3.76877 | -0.19378 | -1.82222 | H | 5.29217 | -2.22622 | -2.68224 |
| H | -3.78437 | -1.93527 | -1.6333 | N | 1.67196 | -1.75627 | -0.00624 |
| H | 0.17882 | -0.42794 | -2.3798 | Rh | 0.38692 | -0.40992 | 0.89908 |
| H | -0.04185 | 1.72156 | -1.51392 | C | -2.24665 | 0.25077 | -1.26759 |

| | | | | | | | |
|---|----------|----------|----------|----|----------|----------|----------|
| C | -1.67337 | 1.1936 | -2.13223 | C | 2.57223 | 0.44317 | 0.49306 |
| C | -0.67066 | 0.83396 | -3.02002 | H | 1.15761 | 3.70507 | 2.09434 |
| C | -0.24197 | -0.49538 | -3.00366 | H | 3.50588 | 3.61833 | 1.29363 |
| C | -0.7458 | -1.41973 | -2.09112 | H | 4.43583 | 1.54386 | 0.38424 |
| C | -1.73816 | -1.03745 | -1.18083 | C | -0.08129 | -0.71759 | 1.6031 |
| H | -0.21784 | 1.55839 | -3.69444 | C | -1.04136 | 0.35133 | 2.16948 |
| H | 0.5385 | -0.80745 | -3.69797 | O | 0.28322 | -1.67316 | 2.23314 |
| H | -0.33393 | -2.4284 | -2.04959 | O | -2.07811 | 0.0666 | 2.72235 |
| C | -3.30702 | 0.93186 | -0.50808 | N | -0.5767 | 1.62174 | 1.93702 |
| C | -3.18438 | 2.42477 | -0.91557 | C | -1.29831 | 2.76732 | 2.44237 |
| O | -4.19713 | 0.47562 | 0.1685 | H | -0.86038 | 3.14464 | 3.37739 |
| O | -3.80975 | 3.36441 | -0.49478 | H | -1.29601 | 3.56682 | 1.69103 |
| N | -2.22824 | 2.45624 | -1.92529 | H | -2.32561 | 2.4488 | 2.64109 |
| C | -1.72948 | 3.67411 | -2.50776 | C | 3.02678 | -0.87948 | 0.04458 |
| H | -0.66078 | 3.80073 | -2.28162 | C | 4.33469 | -1.3947 | 0.13571 |
| H | -1.87064 | 3.68343 | -3.59674 | C | 4.53383 | -2.71101 | -0.27956 |
| H | -2.29377 | 4.50088 | -2.06593 | C | 2.22741 | -2.91978 | -0.80585 |
| C | -2.10752 | -1.87738 | -0.00914 | C | 3.49019 | -3.48449 | -0.7604 |
| C | -3.25402 | -2.67401 | 0.03965 | H | 5.53559 | -3.13455 | -0.20577 |
| C | -3.50375 | -3.36027 | 1.22582 | H | 1.35446 | -3.45127 | -1.17843 |
| C | -1.5392 | -2.40091 | 2.18242 | H | 3.64234 | -4.51111 | -1.08199 |
| C | -2.64702 | -3.22297 | 2.30967 | C | 5.50531 | -0.6431 | 0.69677 |
| H | -4.38987 | -3.99052 | 1.29954 | H | 5.91183 | 0.09125 | -0.01242 |
| H | -0.84114 | -2.23111 | 3.00054 | H | 5.24659 | -0.10515 | 1.61687 |
| H | -2.83764 | -3.73429 | 3.24973 | H | 6.31781 | -1.34006 | 0.93298 |
| C | -4.19534 | -2.73034 | -1.12058 | N | 2.01435 | -1.66326 | -0.409 |
| H | -3.66211 | -2.77812 | -2.07816 | Rh | 0.09737 | -0.78352 | -0.40832 |
| H | -4.8626 | -3.59727 | -1.05122 | Cl | -0.54787 | -2.10191 | -2.27022 |
| H | -4.81812 | -1.82491 | -1.13553 | C | -1.31557 | 0.79757 | -0.90651 |
| N | -1.27166 | -1.75414 | 1.04032 | C | -2.00752 | -0.15749 | -0.48996 |
| Cl | -1.16422 | 1.27064 | 1.6292 | C | -0.91247 | 2.10246 | -1.33653 |
| | | | | C | 0.28089 | 2.31823 | -2.03818 |
| | | | | C | -1.73033 | 3.197 | -1.01647 |
| | | | | C | 0.65383 | 3.60647 | -2.39542 |
| | | | | H | 0.90477 | 1.46115 | -2.29103 |
| | | | | C | -1.34827 | 4.48288 | -1.37365 |
| | | | | H | -2.66138 | 3.01733 | -0.4774 |
| | | | | C | -0.15256 | 4.69096 | -2.05784 |
| | | | | H | 1.58301 | 3.76643 | -2.93946 |
| 57 | | | | | | | |
| Me^eTS_{AI-B}(2) | | | | | | | |
| C | 1.1856 | 0.571 | 0.72844 | H | 0.90477 | 1.46115 | -2.29103 |
| C | 0.71835 | 1.70477 | 1.40856 | C | -1.34827 | 4.48288 | -1.37365 |
| C | 1.5408 | 2.81037 | 1.60735 | H | -2.66138 | 3.01733 | -0.4774 |
| C | 2.86299 | 2.74749 | 1.18284 | C | -0.15256 | 4.69096 | -2.05784 |
| C | 3.39085 | 1.56651 | 0.67407 | H | 1.58301 | 3.76643 | -2.93946 |

| | | | |
|---|----------|----------|----------|
| H | -1.98642 | 5.32758 | -1.11872 |
| H | 0.14685 | 5.70026 | -2.3351 |
| C | -3.17191 | -0.93264 | -0.17878 |
| C | -3.09516 | -2.22801 | 0.34408 |
| C | -4.42803 | -0.34343 | -0.38741 |
| C | -4.25802 | -2.92049 | 0.6488 |
| H | -2.11781 | -2.68151 | 0.50234 |
| C | -5.58533 | -1.04374 | -0.08285 |
| H | -4.47803 | 0.66547 | -0.79652 |
| C | -5.50252 | -2.33304 | 0.43751 |
| H | -4.19153 | -3.92712 | 1.05717 |
| H | -6.55704 | -0.58207 | -0.25033 |
| H | -6.41127 | -2.88151 | 0.68002 |

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MeTS_{A1-B}(3)

| | | | |
|---|----------|----------|----------|
| C | 0.96233 | 1.13903 | -0.12059 |
| C | 0.48011 | 2.45791 | -0.17246 |
| C | 1.01799 | 3.39071 | -1.05246 |
| C | 2.10528 | 3.01327 | -1.834 |
| C | 2.71346 | 1.77302 | -1.66492 |
| C | 2.18292 | 0.83816 | -0.76932 |
| H | 0.61079 | 4.39816 | -1.11477 |
| H | 2.51882 | 3.71765 | -2.55318 |
| H | 3.5811 | 1.52858 | -2.26916 |
| C | 0.52981 | 0.76232 | 1.64618 |
| C | -0.41401 | 1.95317 | 1.91273 |
| O | 1.33946 | 0.38465 | 2.45803 |
| O | -1.04498 | 2.10514 | 2.93294 |
| N | -0.47384 | 2.76886 | 0.80359 |
| C | -1.28921 | 3.95979 | 0.7866 |
| H | -0.67832 | 4.87096 | 0.84705 |
| H | -1.8952 | 3.99216 | -0.12848 |
| H | -1.94529 | 3.91752 | 1.66068 |
| C | 2.77415 | -0.46715 | -0.44519 |
| C | 4.13452 | -0.81413 | -0.54949 |
| C | 4.50744 | -2.07702 | -0.08919 |
| C | 2.25865 | -2.53657 | 0.52971 |
| C | 3.57816 | -2.95086 | 0.44853 |

| | | | |
|----|----------|----------|----------|
| H | 5.55753 | -2.36392 | -0.14486 |
| H | 1.46801 | -3.16699 | 0.93003 |
| H | 3.86564 | -3.93195 | 0.81667 |
| C | 5.20478 | 0.09904 | -1.06938 |
| H | 5.20356 | 0.16554 | -2.16607 |
| H | 5.1045 | 1.11785 | -0.67581 |
| H | 6.19158 | -0.27679 | -0.77508 |
| N | 1.88115 | -1.33309 | 0.09696 |
| C | -4.84029 | -0.07347 | -1.66892 |
| C | -5.07761 | -0.82303 | -0.58778 |
| C | -1.94797 | 0.25787 | -0.66718 |
| C | -4.16957 | -1.7898 | 0.12008 |
| C | -2.32943 | -0.04177 | 0.63288 |
| C | -3.25878 | -1.11251 | 1.14989 |
| H | -4.78857 | -2.51725 | 0.6641 |
| H | -3.56577 | -2.38179 | -0.57468 |
| H | -3.89699 | -0.61505 | 1.89818 |
| H | -2.69547 | -1.8802 | 1.69547 |
| C | -3.61099 | 0.04454 | -2.52282 |
| H | -3.78674 | -0.45734 | -3.48942 |
| C | -2.2917 | -0.46899 | -1.93769 |
| H | -2.30761 | -1.55098 | -1.79379 |
| H | -1.4923 | -0.27788 | -2.66981 |
| Rh | -0.10641 | -0.61686 | 0.25943 |
| Cl | -0.86332 | -2.86749 | 0.04179 |
| H | -5.66397 | 0.56199 | -2.00649 |
| H | -6.06452 | -0.70318 | -0.13199 |
| H | -1.65774 | 1.2981 | -0.84539 |
| H | -2.23994 | 0.78045 | 1.34016 |
| H | -3.48556 | 1.11055 | -2.78095 |

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MeTS_{A1-B}(4)

| | | | |
|---|----------|---------|----------|
| C | 0.43112 | 1.3006 | -0.01311 |
| C | -0.16034 | 2.57697 | 0.0091 |
| C | 0.39608 | 3.61775 | 0.74681 |
| C | 1.60572 | 3.39856 | 1.3985 |
| C | 2.30543 | 2.20826 | 1.22411 |
| C | 1.75233 | 1.16644 | 0.46839 |

| | | | | | | | |
|---|----------|----------|----------|-------------------------------|----------|----------|----------|
| H | -0.09235 | 4.58973 | 0.79272 | H | -2.57621 | 1.30305 | 2.69153 |
| H | 2.03864 | 4.18879 | 2.00879 | Rh | -0.47955 | -0.62918 | -0.10539 |
| H | 3.26808 | 2.09237 | 1.71093 | Cl | -1.0025 | -2.50472 | -1.73133 |
| C | -0.21639 | 0.7478 | -1.68279 | H | 0.86053 | -1.15341 | 2.26144 |
| C | -1.37745 | 1.74762 | -1.80568 | H | -0.10727 | -3.03504 | 1.20388 |
| O | 0.53973 | 0.52569 | -2.59828 | H | -2.39653 | 1.29912 | 0.36773 |
| O | -2.28946 | 1.66114 | -2.5955 | H | -3.03943 | -0.53656 | -1.00024 |
| N | -1.25918 | 2.73301 | -0.84067 | H | -0.2897 | 0.8179 | 2.91057 |
| C | -2.21323 | 3.81063 | -0.74023 | | | | |
| H | -2.65316 | 3.84782 | 0.26698 | 53 | | | |
| H | -1.74899 | 4.78066 | -0.96259 | MeTS_{A1-B}(5) | | | |
| H | -2.99853 | 3.61467 | -1.47673 | C | -0.43768 | 1.32816 | -0.0001 |
| C | 2.42316 | -0.09277 | 0.11925 | C | 0.14437 | 2.60769 | 0.03173 |
| C | 3.81376 | -0.3141 | 0.07656 | C | -0.39949 | 3.62911 | 0.80552 |
| C | 4.25272 | -1.55992 | -0.37035 | C | -1.58208 | 3.38152 | 1.49537 |
| C | 2.00426 | -2.24536 | -0.72961 | C | -2.2756 | 2.18698 | 1.32258 |
| C | 3.35738 | -2.53635 | -0.77104 | C | -1.74023 | 1.16951 | 0.52254 |
| H | 5.32503 | -1.74936 | -0.41896 | H | 0.07938 | 4.60567 | 0.8548 |
| H | 1.23353 | -2.93279 | -1.07893 | H | -2.00123 | 4.15387 | 2.13748 |
| H | 3.69351 | -3.50187 | -1.13931 | H | -3.21856 | 2.05012 | 1.84173 |
| C | 4.84687 | 0.71374 | 0.43207 | C | 0.18646 | 0.79977 | -1.67682 |
| H | 5.82913 | 0.39611 | 0.06357 | C | 1.34126 | 1.80482 | -1.80475 |
| H | 4.62504 | 1.69217 | -0.01108 | O | -0.57897 | 0.57803 | -2.58556 |
| H | 4.9448 | 0.85545 | 1.51719 | O | 2.25218 | 1.72085 | -2.59563 |
| N | 1.56271 | -1.06337 | -0.29339 | N | 1.22523 | 2.78542 | -0.83408 |
| C | -0.22728 | -1.15828 | 2.15684 | C | 2.19863 | 3.84223 | -0.70476 |
| C | -0.79158 | -2.26661 | 1.56615 | H | 1.75212 | 4.82748 | -0.89354 |
| C | -2.32994 | 0.31246 | 0.81642 | H | 2.64342 | 3.83796 | 0.30154 |
| C | -2.24498 | -2.67335 | 1.65603 | H | 2.97742 | 3.65532 | -1.4508 |
| C | -2.73495 | -0.75136 | 0.02635 | C | -2.41509 | -0.0826 | 0.15205 |
| C | -3.15578 | -2.09248 | 0.56012 | C | -3.80543 | -0.31095 | 0.13637 |
| H | -2.29723 | -3.76796 | 1.59826 | C | -4.25005 | -1.52959 | -0.37495 |
| H | -2.6271 | -2.4136 | 2.65402 | C | -2.00901 | -2.17849 | -0.83391 |
| H | -3.1934 | -2.78738 | -0.28372 | C | -3.36157 | -2.4716 | -0.86526 |
| H | -4.18741 | -2.00031 | 0.94381 | H | -5.32223 | -1.72354 | -0.40489 |
| C | -0.93708 | -0.07242 | 2.91818 | H | -1.24146 | -2.83988 | -1.23781 |
| H | -1.04612 | -0.35514 | 3.9799 | H | -3.70398 | -3.41206 | -1.28851 |
| C | -2.29831 | 0.30253 | 2.33131 | C | -4.8312 | 0.68625 | 0.58643 |
| H | -3.07871 | -0.3753 | 2.70364 | H | -4.87772 | 0.77814 | 1.6802 |

| | | | | | | | |
|----|----------|----------|----------|----|----------|----------|----------|
| H | -4.63966 | 1.68618 | 0.17809 | O | 0.03333 | 0.65912 | -2.53084 |
| H | -5.82689 | 0.37422 | 0.25076 | O | -2.27007 | 2.432 | -2.04627 |
| N | -1.56236 | -1.02686 | -0.32769 | N | -0.95306 | 2.98661 | -0.25039 |
| C | 0.6067 | -2.35729 | 1.50201 | C | -1.6272 | 4.23625 | 0.01719 |
| C | 0.40021 | -1.21563 | 2.22625 | H | -1.85459 | 4.32434 | 1.08681 |
| C | 2.71367 | -0.85456 | 0.12251 | H | -1.01932 | 5.09788 | -0.29208 |
| C | 1.49444 | -0.50296 | 2.97921 | H | -2.55558 | 4.23792 | -0.5609 |
| C | 2.33951 | 0.34123 | 0.71608 | C | 2.40918 | -0.34126 | -0.19842 |
| C | 2.13569 | 0.63133 | 2.18065 | C | 3.73584 | -0.74675 | -0.45484 |
| H | 1.08733 | -0.09507 | 3.91441 | C | 3.92296 | -1.89541 | -1.22038 |
| H | 2.25705 | -1.23355 | 3.28191 | C | 1.57878 | -2.15616 | -1.42839 |
| H | 1.49937 | 1.52731 | 2.25604 | C | 2.84984 | -2.60607 | -1.73203 |
| H | 3.10406 | 0.91531 | 2.63022 | H | 4.94115 | -2.21988 | -1.43373 |
| C | 1.92772 | -3.04116 | 1.2888 | H | 0.69628 | -2.66376 | -1.81109 |
| H | 2.21082 | -3.60133 | 2.19662 | H | 2.98841 | -3.48275 | -2.35839 |
| C | 3.08478 | -2.1169 | 0.87415 | C | 4.95328 | -0.01223 | 0.01863 |
| H | 3.67018 | -1.81689 | 1.75752 | H | 5.85423 | -0.46203 | -0.41414 |
| H | 3.76809 | -2.69471 | 0.23982 | H | 4.93713 | 1.04592 | -0.27122 |
| Rh | 0.48055 | -0.60648 | -0.13475 | H | 5.06159 | -0.05771 | 1.11033 |
| Cl | 1.049 | -2.45314 | -1.7673 | N | 1.37402 | -1.08137 | -0.67064 |
| H | -0.26998 | -2.92952 | 1.19279 | C | -1.26326 | -2.61804 | 0.04454 |
| H | -0.62755 | -0.9177 | 2.44394 | C | -1.80912 | -1.97973 | -1.06071 |
| H | 3.07207 | -0.78686 | -0.90528 | C | -2.21422 | -0.39438 | 1.55913 |
| H | 2.54615 | 1.23253 | 0.12889 | C | -3.27075 | -1.59372 | -1.11989 |
| H | 1.78259 | -3.77995 | 0.49356 | C | -2.59969 | 0.31342 | 0.43311 |
| | | | | C | -3.53825 | -0.16409 | -0.64621 |
| | | | | H | -3.62907 | -1.70115 | -2.15182 |
| | | | | H | -3.85154 | -2.31462 | -0.52654 |
| | | | | H | -3.44222 | 0.52233 | -1.49609 |
| | | | | H | -4.57938 | -0.06251 | -0.29347 |
| | | | | C | -2.0108 | -2.94816 | 1.30742 |
| | | | | H | -2.71381 | -3.77777 | 1.11898 |
| | | | | C | -2.75771 | -1.75711 | 1.92543 |
| | | | | H | -3.82179 | -1.77893 | 1.64324 |
| | | | | H | -2.72328 | -1.85284 | 3.01742 |
| | | | | Rh | -0.51145 | -0.50103 | 0.07109 |
| | | | | Cl | 0.58994 | -1.35758 | 2.3298 |
| | | | | H | -0.3249 | -3.16282 | -0.06703 |
| | | | | H | -1.27751 | -2.00866 | -2.01536 |

53

MeTS_{A1-B}(6)

| | | | | | | | |
|---|----------|---------|----------|----|----------|----------|----------|
| C | 0.63116 | 1.27144 | 0.18604 | H | -3.44222 | 0.52233 | -1.49609 |
| C | 0.2331 | 2.59658 | 0.39157 | H | -4.57938 | -0.06251 | -0.29347 |
| C | 1.04588 | 3.4927 | 1.08095 | C | -2.0108 | -2.94816 | 1.30742 |
| C | 2.29746 | 3.06091 | 1.50468 | H | -2.71381 | -3.77777 | 1.11898 |
| C | 2.78677 | 1.81274 | 1.13579 | C | -2.75771 | -1.75711 | 1.92543 |
| C | 1.97977 | 0.92509 | 0.41445 | H | -3.82179 | -1.77893 | 1.64324 |
| H | 0.71754 | 4.51317 | 1.27024 | H | -2.72328 | -1.85284 | 3.01742 |
| H | 2.9285 | 3.7304 | 2.08594 | Rh | -0.51145 | -0.50103 | 0.07109 |
| H | 3.7845 | 1.53345 | 1.45174 | Cl | 0.58994 | -1.35758 | 2.3298 |
| C | -0.45451 | 0.94089 | -1.46209 | H | -0.3249 | -3.16282 | -0.06703 |
| C | -1.32725 | 2.2046 | -1.31713 | H | -1.27751 | -2.00866 | -2.01536 |

| | | | |
|---|----------|----------|---------|
| H | -1.72905 | 0.16109 | 2.36125 |
| H | -2.49008 | 1.39429 | 0.50054 |
| H | -1.27125 | -3.30501 | 2.03083 |

53
MeTS_{A1-B}(7)

| | | | |
|---|----------|----------|----------|
| C | -1.04872 | 1.01923 | 0.24119 |
| C | -2.39626 | 1.08373 | 0.63884 |
| C | -2.75559 | 1.78443 | 1.78954 |
| C | -1.77261 | 2.48051 | 2.48229 |
| C | -0.46781 | 2.57762 | 1.99861 |
| C | -0.10296 | 1.88129 | 0.84317 |
| H | -3.78896 | 1.79371 | 2.13045 |
| H | -2.03814 | 3.00562 | 3.39817 |
| H | 0.25627 | 3.16471 | 2.55461 |
| C | -1.2706 | 0.56834 | -1.50991 |
| C | -2.75873 | 0.16146 | -1.45826 |
| O | -0.8185 | 1.20573 | -2.43536 |
| O | -3.35385 | -0.34109 | -2.3782 |
| N | -3.30085 | 0.50829 | -0.23639 |
| C | -4.63832 | 0.11031 | 0.13008 |
| H | -4.60344 | -0.57871 | 0.98424 |
| H | -5.26272 | 0.97968 | 0.37407 |
| H | -5.06526 | -0.40734 | -0.73368 |
| C | 1.17654 | 1.9664 | 0.12518 |
| C | 2.02869 | 3.08853 | 0.09021 |
| C | 3.04717 | 3.09175 | -0.86064 |
| C | 2.32722 | 0.96934 | -1.64404 |
| C | 3.1873 | 2.0462 | -1.75978 |
| H | 3.70956 | 3.95518 | -0.91782 |
| H | 2.37183 | 0.13535 | -2.33878 |
| H | 3.93555 | 2.06733 | -2.54742 |
| C | 1.86301 | 4.29234 | 0.96776 |
| H | 2.51828 | 5.10132 | 0.62516 |
| H | 0.83225 | 4.66812 | 0.95706 |
| H | 2.1265 | 4.08578 | 2.01375 |
| N | 1.38988 | 0.9038 | -0.69653 |
| C | 1.05629 | -1.66718 | 2.17582 |
| C | 2.24127 | -1.17492 | 1.79781 |

| | | | |
|----|----------|----------|----------|
| C | 0.81794 | -2.92628 | -0.61753 |
| C | 3.28598 | -1.97838 | 1.08948 |
| C | 1.82828 | -2.12685 | -1.07297 |
| C | 3.17582 | -1.89758 | -0.44086 |
| H | 4.28946 | -1.62678 | 1.36861 |
| H | 3.23508 | -3.02454 | 1.41674 |
| H | 3.56321 | -0.92141 | -0.76574 |
| H | 3.86858 | -2.63504 | -0.88326 |
| C | 0.59402 | -3.08749 | 2.00823 |
| H | 1.05777 | -3.71807 | 2.78533 |
| C | 0.8388 | -3.76637 | 0.63985 |
| H | 1.79942 | -4.30353 | 0.65567 |
| H | 0.06701 | -4.53745 | 0.52599 |
| Rh | -0.00131 | -0.66021 | -0.40836 |
| H | 0.35305 | -0.99372 | 2.67294 |
| H | 2.4536 | -0.11676 | 1.97178 |
| H | 0.04117 | -3.17936 | -1.33785 |
| H | 1.76287 | -1.83792 | -2.12587 |
| H | -0.48429 | -3.10755 | 2.197 |
| Cl | -1.86614 | -2.11998 | 0.14761 |

53
MeTS_{A1-B}(8)

| | | | |
|---|----------|---------|----------|
| C | 1.02309 | 1.43561 | 0.1726 |
| C | 0.34781 | 2.64302 | -0.04873 |
| C | 0.82774 | 3.55315 | -0.97609 |
| C | 1.96174 | 3.20546 | -1.71017 |
| C | 2.61088 | 1.98801 | -1.52209 |
| C | 2.15205 | 1.08422 | -0.5627 |
| H | 0.31756 | 4.49711 | -1.15415 |
| H | 2.34128 | 3.90219 | -2.45552 |
| H | 3.48537 | 1.73009 | -2.11735 |
| C | 0.30588 | 0.62354 | 1.16736 |
| C | -1.33563 | 1.62992 | 1.24516 |
| O | 0.68487 | 0.21148 | 2.23607 |
| O | -2.22227 | 1.53596 | 2.05251 |
| N | -0.79651 | 2.79564 | 0.74068 |
| C | -1.59601 | 4.00343 | 0.71484 |

| | | | | | | | |
|----|----------|----------|----------|-------------------------------|----------|----------|----------|
| H | -0.97438 | 4.87223 | 0.96143 | 53 | | | |
| H | -2.05201 | 4.12962 | -0.2778 | MeTS_{A1-B(9)} | | | |
| H | -2.38402 | 3.898 | 1.46443 | C | 1.20697 | 1.29898 | 0.03258 |
| C | 2.82476 | -0.22511 | -0.33849 | C | 0.59551 | 2.51949 | -0.27296 |
| C | 3.62894 | -0.43008 | 0.79706 | C | 1.13739 | 3.34922 | -1.24638 |
| C | 4.20023 | -1.69257 | 0.94159 | C | 2.26601 | 2.90637 | -1.93736 |
| C | 3.18572 | -2.35245 | -1.10873 | C | 2.84242 | 1.66899 | -1.66979 |
| C | 3.97783 | -2.67489 | -0.01435 | C | 2.32243 | 0.84765 | -0.66494 |
| H | 4.82804 | -1.89742 | 1.80935 | H | 0.6839 | 4.30991 | -1.48103 |
| H | 2.99414 | -3.08906 | -1.89269 | H | 2.69551 | 3.54207 | -2.70961 |
| H | 4.41813 | -3.6653 | 0.08079 | H | 3.71049 | 1.33093 | -2.2337 |
| C | 3.86883 | 0.65268 | 1.80319 | C | 0.52647 | 0.59216 | 1.12705 |
| H | 4.13414 | 1.60123 | 1.31819 | C | -1.12893 | 1.72335 | 1.17057 |
| H | 2.96542 | 0.83247 | 2.40128 | O | 1.02235 | 0.15564 | 2.11742 |
| H | 4.68171 | 0.37859 | 2.48617 | O | -2.01122 | 1.87424 | 1.98166 |
| N | 2.61588 | -1.15857 | -1.27337 | N | -0.5696 | 2.77503 | 0.44888 |
| C | -1.56398 | -1.67167 | 1.53911 | C | -1.19469 | 4.08129 | 0.46078 |
| C | -0.41466 | -2.08769 | 0.86015 | H | -0.45498 | 4.85656 | 0.69571 |
| C | -2.74621 | -1.62766 | -1.03691 | H | -1.65697 | 4.30802 | -0.51096 |
| C | -0.30735 | -3.22116 | -0.13861 | H | -1.9668 | 4.06848 | 1.23434 |
| C | -1.54301 | -1.68823 | -1.72721 | C | 2.92193 | -0.49022 | -0.38984 |
| C | -0.48234 | -2.74047 | -1.5804 | C | 3.8658 | -0.65972 | 0.63391 |
| H | 0.68554 | -3.68003 | -0.03382 | C | 4.37861 | -1.9434 | 0.80454 |
| H | -1.02683 | -4.01337 | 0.10658 | C | 3.01219 | -2.69664 | -0.99556 |
| H | 0.46243 | -2.29282 | -1.92371 | C | 3.95103 | -2.98092 | -0.01275 |
| H | -0.69394 | -3.5871 | -2.25635 | H | 5.11417 | -2.12344 | 1.58895 |
| C | -2.95365 | -2.22452 | 1.38687 | H | 2.64909 | -3.48012 | -1.6634 |
| H | -3.10705 | -3.07072 | 2.07824 | H | 4.33741 | -3.99038 | 0.10938 |
| C | -3.28603 | -2.63153 | -0.0514 | C | 4.28097 | 0.47706 | 1.51431 |
| H | -2.9052 | -3.63476 | -0.27759 | H | 4.58704 | 1.35611 | 0.93169 |
| H | -4.37631 | -2.68664 | -0.16788 | H | 3.44484 | 0.78419 | 2.15702 |
| Rh | -1.27576 | -0.2321 | -0.06537 | H | 5.11771 | 0.18917 | 2.16152 |
| Cl | -2.08903 | 1.39521 | -1.65541 | N | 2.5073 | -1.47821 | -1.18918 |
| H | -1.40164 | -1.08499 | 2.44605 | C | -1.21759 | 0.34548 | -1.66294 |
| H | 0.53209 | -1.80652 | 1.31788 | C | -2.55169 | 0.48713 | -1.29278 |
| H | -3.45666 | -0.87781 | -1.39054 | C | -1.43328 | -2.28527 | -0.6213 |
| H | -1.45052 | -1.03772 | -2.59874 | C | -3.6473 | -0.44818 | -1.75944 |
| H | -3.65073 | -1.43639 | 1.70743 | C | -2.69765 | -2.08258 | -0.06774 |
| | | | | C | -3.92688 | -1.57979 | -0.77086 |

| | | | | | | | |
|--------------------------------|----------|----------|----------|----|----------|----------|----------|
| H | -4.56739 | 0.12789 | -1.92292 | C | -5.46713 | 2.97334 | -1.02737 |
| H | -3.36734 | -0.85548 | -2.74139 | C | -4.10477 | 2.04924 | -2.75207 |
| H | -4.61446 | -1.21598 | 0.00556 | C | -4.80542 | 3.13348 | -2.23852 |
| H | -4.44958 | -2.41329 | -1.27113 | H | -6.03451 | 3.79765 | -0.59321 |
| C | -0.61755 | -0.76565 | -2.47801 | H | -3.56462 | 2.12455 | -3.69632 |
| H | -0.79016 | -0.58005 | -3.55283 | H | -4.83259 | 4.07878 | -2.77624 |
| C | -1.10184 | -2.16447 | -2.08935 | C | -6.07811 | 1.55714 | 0.9733 |
| H | -1.97987 | -2.46059 | -2.68233 | H | -6.70715 | 0.65688 | 0.97683 |
| H | -0.31132 | -2.88737 | -2.33259 | H | -5.32052 | 1.43456 | 1.7584 |
| Rh | -1.4725 | -0.34512 | 0.45073 | H | -6.70874 | 2.41635 | 1.23165 |
| Cl | -1.39295 | -1.43923 | 2.55951 | N | -4.0401 | 0.87198 | -2.13043 |
| H | -0.61748 | 1.25191 | -1.6663 | Rh | -0.70203 | 0.23218 | 0.06215 |
| H | -2.87773 | 1.4785 | -0.96412 | Cl | -0.02195 | 1.02897 | -2.00751 |
| H | -0.72769 | -2.84465 | -0.00291 | C | 2.81692 | 2.17589 | 0.22826 |
| H | -2.88065 | -2.54422 | 0.90307 | C | 4.05288 | 1.51564 | 0.14962 |
| H | 0.46995 | -0.72962 | -2.32756 | C | 4.39127 | 0.53761 | 1.06977 |
| | | | | C | 3.43949 | 0.20187 | 2.0386 |
| | | | | C | 2.19327 | 0.82257 | 2.10891 |
| | | | | C | 1.88251 | 1.84232 | 1.20637 |
| 95 | | | | H | 5.36873 | 0.05824 | 1.04416 |
| MeTS_{A1-B}(10) | | | | H | 3.68249 | -0.56816 | 2.77058 |
| C | -3.46542 | -0.76452 | 0.64224 | H | 1.45884 | 0.52884 | 2.85666 |
| C | -3.24202 | -2.0075 | 1.23676 | C | 2.81216 | 3.21493 | -0.81073 |
| C | -4.01573 | -3.10948 | 0.91376 | C | 4.17089 | 3.04553 | -1.54972 |
| C | -5.02936 | -2.93502 | -0.03372 | O | 2.01929 | 4.09186 | -1.05513 |
| C | -5.25626 | -1.69976 | -0.63186 | O | 4.58852 | 3.69743 | -2.4742 |
| C | -4.47593 | -0.58797 | -0.29156 | N | 4.82951 | 2.01708 | -0.89633 |
| H | -3.8517 | -4.07845 | 1.38287 | C | 6.16353 | 1.58328 | -1.23487 |
| H | -5.65187 | -3.78557 | -0.30662 | H | 6.85678 | 1.76445 | -0.40156 |
| H | -6.04546 | -1.58522 | -1.37433 | H | 6.17367 | 0.5192 | -1.50264 |
| C | -2.5139 | 0.23751 | 1.19984 | H | 6.48132 | 2.17462 | -2.09874 |
| C | -1.50824 | -0.74431 | 2.16331 | C | 0.66193 | 2.68381 | 1.27305 |
| O | -2.89268 | 1.28247 | 1.73395 | C | 0.75539 | 3.97812 | 1.80349 |
| O | -0.67886 | -0.42177 | 2.98753 | C | -0.32269 | 4.83214 | 1.60554 |
| N | -2.1755 | -1.96312 | 2.1545 | C | -1.45563 | 3.0894 | 0.44551 |
| C | -2.09613 | -2.8601 | 3.28575 | C | -1.42 | 4.40219 | 0.87634 |
| H | -3.02689 | -2.83191 | 3.86967 | H | -0.27719 | 5.84916 | 1.99541 |
| H | -1.91936 | -3.89687 | 2.96788 | H | -2.30838 | 2.69906 | -0.09931 |
| H | -1.26227 | -2.52615 | 3.91191 | H | -2.25505 | 5.06199 | 0.65619 |
| C | -4.65967 | 0.73598 | -0.95329 | | | | |
| C | -5.40593 | 1.75866 | -0.34767 | | | | |

| | | | | | | | |
|---|----------|----------|----------|----|----------|----------|----------|
| C | 1.99484 | 4.45658 | 2.49674 | C | -2.91392 | -1.14529 | -0.64826 |
| H | 2.47071 | 3.66601 | 3.08915 | C | -2.51764 | -2.13618 | -1.56202 |
| H | 2.73804 | 4.8153 | 1.77064 | C | -3.18834 | -2.33638 | -2.75554 |
| H | 1.76236 | 5.29364 | 3.16611 | C | -4.25405 | -1.49262 | -3.06146 |
| N | -0.45438 | 2.22927 | 0.68463 | C | -4.66642 | -0.51663 | -2.16782 |
| C | 2.24648 | -2.47763 | -0.15996 | C | -4.02771 | -0.34691 | -0.93189 |
| C | 3.30855 | -2.74073 | 0.71995 | H | -2.87394 | -3.10984 | -3.45259 |
| C | 3.09522 | -3.25489 | 1.9871 | H | -4.7761 | -1.61284 | -4.00908 |
| C | 1.77266 | -3.51669 | 2.35226 | H | -5.51376 | 0.12474 | -2.40191 |
| C | 0.71726 | -3.30252 | 1.47239 | C | -1.981 | -1.03707 | 0.50661 |
| C | 0.93489 | -2.77026 | 0.1988 | C | -0.84044 | -2.52839 | 0.03052 |
| H | 3.91951 | -3.45944 | 2.66811 | O | -2.29299 | -0.8503 | 1.66683 |
| H | 1.56576 | -3.92709 | 3.33981 | O | -0.20816 | -3.26093 | 0.76567 |
| H | -0.29469 | -3.5811 | 1.74947 | N | -1.45326 | -2.93405 | -1.12534 |
| C | 2.82337 | -1.96893 | -1.40974 | C | -1.13933 | -4.20192 | -1.74271 |
| C | 4.35651 | -1.91436 | -1.14325 | H | -2.03559 | -4.83099 | -1.82731 |
| O | 2.30805 | -1.68572 | -2.46149 | H | -0.71362 | -4.04441 | -2.74322 |
| O | 5.22422 | -1.52204 | -1.88692 | H | -0.40769 | -4.70834 | -1.10706 |
| N | 4.53623 | -2.43436 | 0.12543 | C | -4.62018 | 0.66523 | -0.01314 |
| C | 5.82196 | -2.61216 | 0.74529 | C | -5.21622 | 0.30053 | 1.20817 |
| H | 5.88304 | -2.063 | 1.69618 | C | -5.76599 | 1.33267 | 1.96738 |
| H | 6.02558 | -3.67382 | 0.93932 | C | -5.19608 | 2.87298 | 0.248 |
| H | 6.57547 | -2.22236 | 0.05286 | C | -5.74413 | 2.64008 | 1.50358 |
| C | -0.16233 | -2.73195 | -0.80355 | H | -6.2342 | 1.09471 | 2.92343 |
| C | -0.35061 | -3.87568 | -1.59565 | H | -5.19624 | 3.87613 | -0.18378 |
| C | -1.36304 | -3.84364 | -2.54926 | H | -6.17121 | 3.45421 | 2.08546 |
| C | -1.85608 | -1.60471 | -1.9027 | C | -5.33573 | -1.12286 | 1.65773 |
| C | -2.11551 | -2.6939 | -2.71488 | H | -5.61887 | -1.77911 | 0.82432 |
| H | -1.53823 | -4.72038 | -3.17298 | H | -4.38352 | -1.49296 | 2.05595 |
| H | -2.41101 | -0.67689 | -2.0234 | H | -6.099 | -1.21907 | 2.43978 |
| H | -2.89854 | -2.61989 | -3.46513 | N | -4.65144 | 1.91397 | -0.49587 |
| C | 0.53073 | -5.08211 | -1.46263 | Rh | -0.0094 | -0.38154 | 0.0366 |
| H | 1.53511 | -4.8857 | -1.86411 | Cl | -0.36956 | 0.00028 | -2.2864 |
| H | 0.65831 | -5.39848 | -0.41968 | C | 3.67561 | -0.31197 | -0.07966 |
| H | 0.11378 | -5.92587 | -2.0249 | C | 4.20067 | -0.40683 | -1.3806 |
| N | -0.92168 | -1.62969 | -0.93402 | C | 3.88471 | -1.46563 | -2.2129 |
| | | | | C | 3.02883 | -2.44175 | -1.70227 |
| | | | | C | 2.49195 | -2.36242 | -0.41831 |
| | | | | C | 2.78844 | -1.27216 | 0.41102 |

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MeTS_{Al-B}(11)

| | | | | | | | |
|---|----------|----------|----------|--|----------|----------|----------|
| H | 4.2821 | -1.53799 | -3.22284 | H | 2.37265 | 1.80447 | -1.28367 |
| H | 2.76662 | -3.29252 | -2.3289 | H | 1.2939 | 5.52282 | 0.60096 |
| H | 1.825 | -3.13936 | -0.05235 | H | -1.01168 | 5.41795 | 0.46825 |
| C | 4.20038 | 0.91833 | 0.50814 | H | 1.64541 | 1.47588 | 1.05915 |
| C | 5.09139 | 1.55338 | -0.59702 | H | -0.56231 | 1.48913 | 1.76551 |
| O | 4.02918 | 1.40826 | 1.6022 | H | 2.726 | 3.69592 | 0.21243 |
| O | 5.70525 | 2.59003 | -0.53499 | | | | |
| N | 5.03129 | 0.68203 | -1.66775 | | | | |
| C | 5.68204 | 0.91864 | -2.93186 | | | | |
| H | 6.40559 | 0.1246 | -3.15841 | | | | |
| H | 4.94563 | 0.97854 | -3.74378 | | | | |
| H | 6.20952 | 1.87378 | -2.8515 | | | | |
| C | 2.21245 | -1.19173 | 1.78602 | | | | |
| C | 2.9834 | -1.50633 | 2.90935 | | | | |
| C | 2.35474 | -1.46091 | 4.1521 | | | | |
| C | 0.3203 | -0.82095 | 3.0836 | | | | |
| C | 1.01491 | -1.12114 | 4.24464 | | | | |
| H | 2.92789 | -1.70501 | 5.04644 | | | | |
| H | -0.74155 | -0.5852 | 3.07702 | | | | |
| H | 0.50229 | -1.09269 | 5.20275 | | | | |
| C | 4.43163 | -1.86553 | 2.78724 | | | | |
| H | 4.61302 | -2.55803 | 1.95575 | | | | |
| H | 5.04124 | -0.9686 | 2.60989 | | | | |
| H | 4.79533 | -2.33528 | 3.70835 | | | | |
| N | 0.91172 | -0.84613 | 1.88386 | | | | |
| C | 0.87601 | 4.68976 | 0.02933 | | | | |
| C | -0.4568 | 4.63726 | -0.05899 | | | | |
| C | 0.91035 | 1.63902 | 0.26228 | | | | |
| C | -1.29511 | 3.62127 | -0.77973 | | | | |
| C | -0.41679 | 1.68577 | 0.69962 | | | | |
| C | -1.59388 | 2.35605 | 0.03844 | | | | |
| H | -2.26651 | 4.06634 | -1.04019 | | | | |
| H | -0.84167 | 3.33942 | -1.73694 | | | | |
| H | -2.31348 | 2.60169 | 0.83512 | | | | |
| H | -2.12032 | 1.66197 | -0.62817 | | | | |
| C | 1.92101 | 3.77149 | -0.53859 | | | | |
| H | 2.39744 | 4.25034 | -1.41137 | | | | |
| C | 1.48513 | 2.35191 | -0.92658 | | | | |
| H | 0.79755 | 2.34057 | -1.77427 | | | | |
| | | | | 84 | | | |
| | | | | Me^eTS_{A1-B}(12) | | | |
| | | | | C | 3.00412 | -0.20449 | 1.18097 |
| | | | | C | 2.63261 | 0.35445 | 2.41106 |
| | | | | C | 3.38706 | 1.33831 | 3.02419 |
| | | | | C | 4.53963 | 1.77453 | 2.36521 |
| | | | | C | 4.91568 | 1.23706 | 1.14075 |
| | | | | C | 4.1543 | 0.2317 | 0.52999 |
| | | | | H | 3.09073 | 1.76406 | 3.98094 |
| | | | | H | 5.14814 | 2.55436 | 2.81945 |
| | | | | H | 5.80681 | 1.5998 | 0.63119 |
| | | | | C | 1.9621 | -1.14552 | 0.6992 |
| | | | | C | 0.88259 | -1.13328 | 2.06902 |
| | | | | O | 2.15899 | -2.18579 | 0.08895 |
| | | | | O | 0.11072 | -2.00148 | 2.40583 |
| | | | | N | 1.4483 | -0.20357 | 2.91157 |
| | | | | C | 0.988 | -0.00103 | 4.26375 |
| | | | | H | 1.78679 | -0.21108 | 4.98752 |
| | | | | H | 0.64303 | 1.03385 | 4.40145 |
| | | | | H | 0.15565 | -0.68819 | 4.4405 |
| | | | | C | 4.53425 | -0.24753 | -0.82762 |
| | | | | C | 5.1175 | -1.50738 | -1.03086 |
| | | | | C | 5.44454 | -1.83804 | -2.34369 |
| | | | | C | 4.62763 | 0.28433 | -3.05293 |
| | | | | C | 5.19117 | -0.94362 | -3.37489 |
| | | | | H | 5.90169 | -2.80644 | -2.55021 |
| | | | | H | 4.42147 | 1.02515 | -3.82747 |
| | | | | H | 5.43355 | -1.18842 | -4.4068 |
| | | | | C | 5.38298 | -2.4482 | 0.10203 |
| | | | | H | 5.90092 | -1.94977 | 0.93234 |
| | | | | H | 4.43911 | -2.84841 | 0.49472 |
| | | | | H | 6.00121 | -3.29276 | -0.22528 |

| | | | | | | | |
|----|----------|----------|----------|---|----------|----------|----------|
| N | 4.31339 | 0.63546 | -1.80626 | C | -1.2217 | 2.60146 | 0.36808 |
| Rh | 0.0868 | -0.25337 | -0.04318 | H | -2.13835 | 4.28446 | -0.57592 |
| Cl | -1.0291 | 0.23939 | -2.04756 | H | -1.09038 | 3.3839 | -1.64274 |
| C | -3.73733 | -0.2991 | 0.08515 | H | -1.55988 | 2.98044 | 1.34619 |
| C | -4.29252 | 0.86703 | 0.63744 | H | -2.0024 | 1.90807 | 0.02776 |
| C | -4.07516 | 1.21523 | 1.95988 | C | 1.9565 | 3.72188 | -1.50906 |
| C | -3.25356 | 0.37376 | 2.71332 | H | 2.15117 | 4.1237 | -2.51819 |
| C | -2.65066 | -0.75696 | 2.16641 | C | 1.32801 | 2.33131 | -1.63886 |
| C | -2.87265 | -1.09894 | 0.8262 | H | 0.40459 | 2.34961 | -2.21733 |
| H | -4.51346 | 2.11181 | 2.39452 | H | 2.02874 | 1.6928 | -2.19554 |
| H | -3.06972 | 0.61498 | 3.75984 | H | 1.81733 | 5.59446 | -0.3919 |
| H | -1.98971 | -1.37559 | 2.76966 | H | -0.3881 | 5.63194 | 0.27236 |
| C | -4.22853 | -0.40387 | -1.29659 | H | 2.1203 | 1.59325 | 0.20774 |
| C | -5.02653 | 0.90955 | -1.5376 | H | 0.31674 | 1.72443 | 1.66434 |
| O | -4.1598 | -1.306 | -2.09463 | H | 2.95733 | 3.60457 | -1.05646 |
| O | -5.56246 | 1.27401 | -2.55403 | | | | |
| N | -5.03012 | 1.57044 | -0.31897 | | | | |
| C | -5.63048 | 2.86169 | -0.11142 | | | | |
| H | -6.4313 | 2.81327 | 0.63851 | | | | |
| H | -4.87802 | 3.59341 | 0.21582 | | | | |
| H | -6.05265 | 3.18182 | -1.06869 | | | | |
| C | -2.23019 | -2.27956 | 0.18405 | | | | |
| C | -2.95736 | -3.46387 | 0.0181 | | | | |
| C | -2.33413 | -4.5135 | -0.64981 | | | | |
| C | -0.39566 | -3.15543 | -0.9232 | | | | |
| C | -1.04854 | -4.35761 | -1.13986 | | | | |
| H | -2.87461 | -5.44878 | -0.79625 | | | | |
| H | 0.61967 | -2.98625 | -1.26498 | | | | |
| H | -0.54593 | -5.15406 | -1.68252 | | | | |
| C | -4.37064 | -3.58646 | 0.49808 | | | | |
| H | -4.50488 | -3.17328 | 1.50564 | | | | |
| H | -5.05195 | -3.04609 | -0.1742 | | | | |
| H | -4.68552 | -4.63648 | 0.51494 | | | | |
| N | -0.96619 | -2.14388 | -0.2578 | | | | |
| C | 1.204 | 4.7453 | -0.70759 | | | | |
| C | -0.07982 | 4.77511 | -0.3335 | | | | |
| C | 1.15413 | 1.7435 | -0.26798 | | | | |
| C | -1.16419 | 3.77427 | -0.62239 | | | | |
| C | 0.07673 | 1.8637 | 0.60367 | | | | |
| | | | | C | -3.09563 | -1.93644 | 0.554 |
| | | | | C | -2.35554 | -3.06448 | 0.94813 |
| | | | | C | -2.67532 | -4.32932 | 0.49125 |
| | | | | C | -3.73643 | -4.44709 | -0.40753 |
| | | | | C | -4.47333 | -3.33959 | -0.81117 |
| | | | | C | -4.1768 | -2.06402 | -0.31843 |
| | | | | H | -2.09619 | -5.19931 | 0.79254 |
| | | | | H | -3.99079 | -5.42972 | -0.80103 |
| | | | | H | -5.29625 | -3.45161 | -1.51489 |
| | | | | C | -2.47412 | -0.73393 | 1.12739 |
| | | | | C | -1.05278 | -1.39631 | 1.91383 |
| | | | | O | -2.99526 | 0.24046 | 1.63764 |
| | | | | O | -0.38591 | -0.85224 | 2.76838 |
| | | | | N | -1.33845 | -2.74567 | 1.84994 |
| | | | | C | -0.44583 | -3.72714 | 2.41824 |
| | | | | H | -1.01468 | -4.5025 | 2.94695 |
| | | | | H | 0.16838 | -4.17551 | 1.62389 |
| | | | | H | 0.20595 | -3.21128 | 3.12898 |
| | | | | C | -5.02292 | -0.91844 | -0.75013 |
| | | | | C | -5.90653 | -0.28822 | 0.1459 |
| | | | | C | -6.70288 | 0.7314 | -0.37143 |

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MeTS_{A1-B}(13)

| | | | | | | | |
|----|----------|----------|----------|---|----------|----------|----------|
| C | -5.72337 | 0.37501 | -2.51215 | H | -1.25846 | 4.92131 | 2.06345 |
| C | -6.61782 | 1.07771 | -1.71371 | H | -0.54887 | 5.53772 | 0.56572 |
| H | -7.40613 | 1.24178 | 0.2876 | H | -2.24573 | 5.87775 | 0.93781 |
| H | -5.63096 | 0.59867 | -3.5771 | N | -1.51352 | 1.5367 | -0.1999 |
| H | -7.24263 | 1.8626 | -2.13574 | C | 3.4633 | -1.6477 | -0.454 |
| C | -6.02236 | -0.71 | 1.57724 | C | 3.87283 | -2.51948 | 0.56763 |
| H | -6.12015 | -1.79997 | 1.6671 | C | 3.56688 | -2.27962 | 1.89637 |
| H | -5.12919 | -0.41153 | 2.14166 | C | 2.80159 | -1.14795 | 2.17725 |
| H | -6.89802 | -0.24899 | 2.0503 | C | 2.3524 | -0.29558 | 1.17088 |
| N | -4.9427 | -0.60034 | -2.04824 | C | 2.66982 | -0.53551 | -0.16585 |
| Rh | -0.57739 | -0.39234 | -0.09716 | H | 3.89079 | -2.95403 | 2.68706 |
| Cl | 0.28063 | -2.53657 | -0.70519 | H | 2.51095 | -0.93568 | 3.20565 |
| C | 1.23722 | 3.07899 | 0.9506 | H | 1.70386 | 0.5345 | 1.4296 |
| C | 2.34747 | 3.01369 | 1.80671 | C | 3.88789 | -2.24396 | -1.72353 |
| C | 2.22452 | 2.55342 | 3.10642 | C | 4.61314 | -3.56318 | -1.33291 |
| C | 0.96318 | 2.10505 | 3.5111 | O | 3.77644 | -1.86084 | -2.86453 |
| C | -0.1395 | 2.11745 | 2.6581 | O | 5.12779 | -4.36589 | -2.07245 |
| C | -0.01007 | 2.60951 | 1.35897 | N | 4.57124 | -3.61534 | 0.04713 |
| H | 3.07769 | 2.5083 | 3.78064 | C | 5.09082 | -4.7102 | 0.82239 |
| H | 0.84255 | 1.70192 | 4.51528 | H | 5.85106 | -4.36475 | 1.53584 |
| H | -1.09255 | 1.69937 | 2.97554 | H | 4.2877 | -5.21831 | 1.37364 |
| C | 1.69916 | 3.61979 | -0.32717 | H | 5.54836 | -5.41595 | 0.12238 |
| C | 3.23726 | 3.77303 | -0.16519 | C | 2.16642 | 0.33608 | -1.26048 |
| O | 1.09062 | 3.93568 | -1.32456 | C | 3.06872 | 1.0714 | -2.0463 |
| O | 4.03139 | 4.11746 | -1.00856 | C | 2.55925 | 1.80114 | -3.11767 |
| N | 3.51114 | 3.42991 | 1.14525 | C | 0.37538 | 1.04732 | -2.55386 |
| C | 4.8418 | 3.33254 | 1.68928 | C | 1.20668 | 1.76015 | -3.40118 |
| H | 4.97233 | 4.00893 | 2.54376 | H | 3.23794 | 2.40069 | -3.72299 |
| H | 5.05091 | 2.30206 | 2.01004 | H | -0.69812 | 1.01904 | -2.71952 |
| H | 5.54153 | 3.61524 | 0.8968 | H | 0.78279 | 2.3018 | -4.24209 |
| C | -1.1745 | 2.66435 | 0.4419 | C | 4.54399 | 1.07841 | -1.78501 |
| C | -1.87703 | 3.86843 | 0.2791 | H | 4.78217 | 0.95192 | -0.72151 |
| C | -2.95989 | 3.86912 | -0.5914 | H | 5.02863 | 0.26 | -2.33433 |
| C | -2.5594 | 1.56556 | -1.04521 | H | 4.98186 | 2.02531 | -2.12076 |
| C | -3.30416 | 2.70838 | -1.26986 | N | 0.82945 | 0.37912 | -1.48534 |
| H | -3.52913 | 4.78731 | -0.73626 | | | | |
| H | -2.80816 | 0.62457 | -1.53935 | | | | |
| H | -4.14989 | 2.67277 | -1.95257 | | | | |
| C | -1.46326 | 5.11276 | 1.00264 | C | -2.27531 | 1.14002 | -0.36342 |

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Me^eTS_{A1-B}(14)

| | | | | | | | |
|----|----------|----------|----------|--------------------------------|----------|----------|----------|
| C | -2.26079 | 2.44086 | 0.1555 | H | 4.37608 | 1.20513 | 3.11873 |
| C | -3.25487 | 2.88529 | 1.00975 | H | 4.60589 | 1.17366 | 0.66278 |
| C | -4.25719 | 1.98303 | 1.36272 | C | 1.09877 | -2.06303 | 0.561 |
| C | -4.27818 | 0.68772 | 0.85902 | C | 0.30845 | -2.48261 | 1.82821 |
| C | -3.2859 | 0.24216 | -0.02177 | O | 1.09582 | -2.68724 | -0.47443 |
| H | -3.24153 | 3.89442 | 1.41491 | O | -0.53064 | -3.34384 | 1.91925 |
| H | -5.03627 | 2.30017 | 2.0539 | N | 0.82602 | -1.72382 | 2.86508 |
| H | -5.06069 | -0.00168 | 1.1706 | C | 0.31506 | -1.75463 | 4.2127 |
| C | -1.13126 | 0.94023 | -1.26058 | H | 1.08185 | -2.09777 | 4.91989 |
| C | -0.25106 | 2.50461 | -1.0194 | H | -0.03344 | -0.7541 | 4.49819 |
| O | -1.08285 | 0.39788 | -2.33612 | H | -0.52425 | -2.45558 | 4.22595 |
| O | 0.63328 | 2.96975 | -1.7058 | C | 3.07895 | -0.25034 | -1.1224 |
| N | -1.19291 | 3.20853 | -0.31365 | C | 4.1974 | -0.61595 | -1.86457 |
| C | -0.97546 | 4.58106 | 0.07875 | C | 4.05027 | -0.57945 | -3.25474 |
| H | -1.8503 | 5.19582 | -0.1675 | C | 1.78804 | 0.1727 | -3.01125 |
| H | -0.77388 | 4.63228 | 1.1582 | C | 2.85219 | -0.18555 | -3.83068 |
| H | -0.1081 | 4.9526 | -0.47293 | H | 4.89111 | -0.87275 | -3.88373 |
| C | -3.26587 | -1.14921 | -0.53053 | H | 0.81955 | 0.49114 | -3.3857 |
| C | -4.40006 | -1.73908 | -1.11665 | H | 2.73176 | -0.15901 | -4.9107 |
| C | -4.26557 | -3.05833 | -1.54799 | C | 5.48453 | -1.03976 | -1.22662 |
| C | -1.99949 | -3.04436 | -0.81335 | H | 6.17303 | -0.19223 | -1.10227 |
| C | -3.06401 | -3.72882 | -1.39133 | H | 5.32601 | -1.47901 | -0.235 |
| H | -5.11647 | -3.55036 | -2.02181 | H | 5.99734 | -1.78341 | -1.84862 |
| H | -1.02958 | -3.52097 | -0.67201 | N | 1.91938 | 0.13192 | -1.68736 |
| H | -2.94374 | -4.75861 | -1.72071 | | | | |
| C | -5.69873 | -1.01812 | -1.33613 | 77 | | | |
| H | -6.36931 | -1.09346 | -0.46825 | MeTS_{A1-B}(15) | | | |
| H | -5.55063 | 0.04987 | -1.53443 | C | -1.61323 | 0.74347 | -1.34641 |
| H | -6.23356 | -1.45152 | -2.19065 | C | -1.24729 | 2.08802 | -1.48797 |
| N | -2.09372 | -1.78466 | -0.39691 | C | -2.17615 | 3.10811 | -1.35409 |
| Rh | 0.80363 | 0.75088 | -0.05152 | C | -3.49279 | 2.74611 | -1.06482 |
| Cl | -0.03776 | 1.49412 | 2.05638 | C | -3.86517 | 1.41452 | -0.91442 |
| C | 1.91935 | -0.9138 | 0.99955 | C | -2.92867 | 0.38072 | -1.05542 |
| C | 1.82663 | -0.8751 | 2.42313 | H | -1.88829 | 4.1506 | -1.47393 |
| C | 2.69614 | -0.13203 | 3.18935 | H | -4.24321 | 3.52551 | -0.94244 |
| C | 3.69264 | 0.59862 | 2.52692 | H | -4.89087 | 1.17386 | -0.6413 |
| C | 3.83284 | 0.581 | 1.1487 | C | -0.4451 | -0.10569 | -1.63707 |
| C | 2.95622 | -0.18186 | 0.35364 | C | 0.82128 | 1.07119 | -1.83806 |
| H | 2.60899 | -0.10185 | 4.27273 | O | -0.40204 | -1.13914 | -2.25885 |

| | | | | | | | |
|----|----------|----------|----------|--|----------|----------|----------|
| O | 1.8943 | 0.92794 | -2.38639 | H | 4.83328 | -4.82138 | -1.89587 |
| N | 0.09665 | 2.24695 | -1.82531 | H | 1.11551 | -4.45152 | 0.46479 |
| C | 0.6451 | 3.48889 | -2.32438 | C | 1.4248 | 5.40126 | 1.04453 |
| H | 0.05311 | 3.85264 | -3.17485 | C | 0.75917 | 4.18992 | 1.17827 |
| H | 0.66069 | 4.24942 | -1.53171 | C | 1.42374 | 2.98359 | 0.90381 |
| H | 1.66901 | 3.29025 | -2.65122 | C | 2.76301 | 3.0169 | 0.49414 |
| C | -3.2715 | -1.0418 | -0.81475 | C | 3.42102 | 4.23313 | 0.36218 |
| C | -4.44364 | -1.64894 | -1.30178 | C | 2.75626 | 5.42675 | 0.63274 |
| C | -4.63382 | -2.99223 | -0.97256 | H | 0.90344 | 6.33164 | 1.26536 |
| C | -2.56991 | -2.98012 | 0.20516 | H | -0.28196 | 4.15721 | 1.5009 |
| C | -3.70455 | -3.67362 | -0.20292 | H | 3.27306 | 2.07535 | 0.28947 |
| H | -5.52326 | -3.50433 | -1.34197 | H | 4.46304 | 4.24869 | 0.0474 |
| H | -1.79533 | -3.46535 | 0.80513 | H | 3.27535 | 6.37794 | 0.52701 |
| H | -3.84586 | -4.71956 | 0.06027 | C | 0.70829 | 1.74599 | 1.02359 |
| C | -5.44904 | -0.95853 | -2.17639 | C | -0.18604 | 0.96789 | 1.43669 |
| H | -6.22881 | -0.44993 | -1.59174 | C | -1.30259 | 0.39779 | 2.12916 |
| H | -4.98634 | -0.20495 | -2.82369 | C | -1.20504 | -0.82961 | 2.79992 |
| H | -5.95854 | -1.68831 | -2.81778 | C | -2.52333 | 1.08679 | 2.12764 |
| N | -2.35702 | -1.70812 | -0.09853 | C | -2.31173 | -1.3515 | 3.45242 |
| C | 1.46817 | -2.58667 | -0.41097 | H | -0.24798 | -1.34976 | 2.79801 |
| C | 2.35653 | -1.78612 | -1.07387 | C | -3.62991 | 0.54979 | 2.77271 |
| C | 3.80046 | -4.63438 | -0.11618 | H | -2.59548 | 2.03749 | 1.59915 |
| C | 3.83023 | -1.60834 | -0.83582 | C | -3.5284 | -0.67115 | 3.43314 |
| C | 4.42122 | -4.10788 | -1.1765 | H | -2.22809 | -2.30295 | 3.97584 |
| C | 4.65637 | -2.67635 | -1.55828 | H | -4.57639 | 1.08924 | 2.75931 |
| H | 4.11628 | -0.62444 | -1.23792 | H | -4.39685 | -1.09255 | 3.93723 |
| H | 4.06752 | -1.57592 | 0.2312 | | | | |
| H | 4.47394 | -2.58483 | -2.64233 | | | | |
| H | 5.72713 | -2.44146 | -1.43308 | | | | |
| C | 1.68231 | -3.54087 | 0.7259 | 81 | | | |
| H | 1.20641 | -3.14588 | 1.63649 | Me^eTS_{A1-B(16)} | | | |
| C | 3.12705 | -3.94067 | 1.03627 | C | 1.16592 | -1.38897 | -1.36174 |
| H | 3.68485 | -3.06343 | 1.37717 | C | 0.20578 | -2.38622 | -1.57597 |
| H | 3.10282 | -4.62719 | 1.89449 | C | 0.54041 | -3.73116 | -1.56643 |
| Rh | 1.16585 | -0.12802 | 0.13367 | C | 1.87741 | -4.06051 | -1.33782 |
| Cl | 2.29595 | -0.61364 | 2.1207 | C | 2.84185 | -3.07948 | -1.13997 |
| H | 0.47656 | -2.65563 | -0.86381 | C | 2.50571 | -1.71878 | -1.15549 |
| H | 2.00684 | -1.39194 | -2.03058 | H | -0.21273 | -4.49921 | -1.73274 |
| H | 3.74612 | -5.7262 | -0.08685 | H | 2.16924 | -5.10914 | -1.31033 |
| | | | | H | 3.86839 | -3.37217 | -0.92924 |

| | | | | | | | |
|----|----------|----------|----------|--------------------------------|----------|----------|----------|
| C | 0.52979 | -0.06162 | -1.49474 | C | 1.61745 | -2.83027 | 2.08518 |
| C | -1.13287 | -0.49126 | -1.75508 | C | 3.0758 | -0.78665 | 3.2802 |
| O | 0.95505 | 0.93315 | -2.03073 | H | 1.46089 | 0.51636 | 2.67281 |
| O | -1.99461 | 0.19667 | -2.25277 | C | 2.8454 | -3.1071 | 2.67055 |
| N | -1.06065 | -1.86511 | -1.84935 | H | 1.04629 | -3.61843 | 1.59404 |
| C | -2.13333 | -2.64763 | -2.42256 | C | 3.57857 | -2.08496 | 3.26759 |
| H | -1.7833 | -3.18256 | -3.31554 | H | 3.64685 | 0.01527 | 3.74593 |
| H | -2.52209 | -3.36734 | -1.68829 | H | 3.23197 | -4.1253 | 2.65915 |
| H | -2.93388 | -1.95735 | -2.70141 | H | 4.54239 | -2.30108 | 3.7263 |
| C | 3.50374 | -0.65285 | -0.90103 | C | -5.24274 | 2.31378 | -1.69586 |
| C | 4.76943 | -0.6241 | -1.5154 | C | -3.8571 | 2.38209 | -1.67021 |
| C | 5.59596 | 0.45312 | -1.19088 | C | -3.18351 | 2.46821 | -0.44324 |
| C | 3.89793 | 1.30212 | 0.24069 | C | -3.92025 | 2.49531 | 0.75212 |
| C | 5.17276 | 1.42749 | -0.3018 | C | -5.30586 | 2.42162 | 0.71389 |
| H | 6.57834 | 0.52426 | -1.66013 | C | -5.96983 | 2.32898 | -0.50754 |
| H | 3.50957 | 2.04679 | 0.93932 | H | -5.75953 | 2.24386 | -2.65161 |
| H | 5.80369 | 2.276 | -0.04396 | H | -3.27686 | 2.34966 | -2.58829 |
| C | 5.24621 | -1.63788 | -2.5145 | H | -3.38416 | 2.54758 | 1.6985 |
| H | 5.72639 | -2.50174 | -2.03309 | H | -5.87083 | 2.4363 | 1.64427 |
| H | 4.42977 | -2.02594 | -3.13447 | H | -7.05701 | 2.27131 | -0.53429 |
| H | 5.99331 | -1.19047 | -3.18184 | C | -1.75646 | 2.55561 | -0.39521 |
| N | 3.0846 | 0.29945 | -0.05868 | C | -0.54975 | 2.77915 | -0.30793 |
| Rh | -0.7555 | 0.50313 | 0.36062 | C | 0.74396 | 3.38053 | -0.14671 |
| Cl | -1.09651 | 1.33988 | 2.52253 | C | 1.53349 | 3.71257 | -1.25579 |
| C | -3.90191 | -4.11042 | 0.75915 | C | 1.1785 | 3.72726 | 1.14222 |
| C | -2.69107 | -3.46433 | 0.96954 | C | 2.72597 | 4.40069 | -1.07626 |
| C | -2.60393 | -2.06676 | 0.85199 | H | 1.19982 | 3.42113 | -2.24813 |
| C | -3.75088 | -1.33444 | 0.51518 | C | 2.37089 | 4.42028 | 1.30864 |
| C | -4.95591 | -1.99085 | 0.30067 | H | 0.56174 | 3.44885 | 1.99596 |
| C | -5.03681 | -3.37628 | 0.41876 | C | 3.14444 | 4.76364 | 0.20178 |
| H | -3.96123 | -5.19318 | 0.85961 | H | 3.33214 | 4.65896 | -1.94306 |
| H | -1.79607 | -4.02913 | 1.23287 | H | 2.69363 | 4.70032 | 2.31033 |
| H | -3.68522 | -0.24958 | 0.42556 | H | 4.07651 | 5.31144 | 0.33565 |
| H | -5.84003 | -1.41104 | 0.03966 | | | | |
| H | -5.98474 | -3.88449 | 0.24961 | | | | |
| C | -1.33112 | -1.44248 | 1.05802 | 53 | | | |
| C | -0.14892 | -1.27941 | 1.44232 | MeTS_{A1-B}(17) | | | |
| C | 1.11257 | -1.52132 | 2.0821 | C | 1.89746 | -0.24402 | -0.66882 |
| C | 1.85627 | -0.49802 | 2.68496 | C | 2.70712 | -1.34515 | -0.33516 |
| | | | | C | 3.95893 | -1.15497 | 0.22734 |

| | | | | | | | |
|---|----------|----------|----------|-------------|----------|----------|----------|
| C | 4.33032 | 0.14905 | 0.55015 | H | -2.74968 | 1.28908 | -0.7774 |
| C | 3.47482 | 1.23258 | 0.35894 | C | -4.10975 | -0.02168 | -1.85751 |
| C | 2.226 | 1.05124 | -0.24008 | H | -4.57599 | 0.83439 | -2.37459 |
| H | 4.60214 | -1.9959 | 0.47603 | H | -3.9932 | -0.79082 | -2.63806 |
| H | 5.29334 | 0.31719 | 1.02857 | Rh | -0.1464 | -0.46159 | 0.30224 |
| H | 3.75656 | 2.20815 | 0.74914 | Cl | 0.80476 | -0.91705 | 2.57975 |
| C | 0.6753 | -0.69362 | -1.46389 | H | -1.80339 | -1.58718 | -1.36335 |
| C | 0.72537 | -2.43759 | -0.86886 | H | -1.95871 | -2.17778 | 0.89275 |
| O | 0.37096 | -0.50134 | -2.61881 | H | -5.85452 | -1.18859 | -1.2553 |
| O | -0.03493 | -3.33965 | -1.10838 | H | -5.87024 | -0.9344 | 1.04283 |
| N | 2.07231 | -2.55889 | -0.55818 | H | -2.10369 | 0.64156 | -2.27487 |
| C | 2.67785 | -3.83969 | -0.26109 | | | | |
| H | 3.61963 | -3.95908 | -0.81019 | 64 | | | |
| H | 2.86277 | -3.92571 | 0.81843 | MeB2 | | | |
| H | 1.97376 | -4.61608 | -0.57115 | C | 2.24462 | -0.05071 | -0.69768 |
| C | 1.17903 | 2.10035 | -0.16459 | C | 2.75005 | 0.55676 | -1.8496 |
| C | 1.41257 | 3.45408 | -0.44434 | C | 3.89686 | 0.04898 | -2.46383 |
| C | 0.38534 | 4.3576 | -0.171 | C | 4.58721 | -1.00168 | -1.87098 |
| C | -0.98353 | 2.56188 | 0.57971 | C | 4.20399 | -1.48261 | -0.62532 |
| C | -0.81079 | 3.92225 | 0.37542 | C | 3.05097 | -0.98041 | -0.00884 |
| H | 0.53974 | 5.41455 | -0.38805 | H | 4.27667 | 0.49604 | -3.38127 |
| H | -1.90651 | 2.16104 | 0.99485 | H | 5.47855 | -1.39947 | -2.35199 |
| H | -1.60978 | 4.61548 | 0.62453 | H | 4.83222 | -2.21956 | -0.13778 |
| C | 2.69445 | 3.95009 | -1.04529 | C | 1.45599 | 2.24187 | 0.01144 |
| H | 3.38833 | 4.32252 | -0.2789 | C | 1.56117 | 2.64835 | -1.47934 |
| H | 3.21478 | 3.16911 | -1.60961 | O | 1.7832 | 2.99527 | 0.89019 |
| H | 2.49262 | 4.78585 | -1.72635 | O | 1.04883 | 3.69122 | -1.84615 |
| N | -0.03164 | 1.67417 | 0.28915 | N | 2.13245 | 1.73808 | -2.33705 |
| C | -2.02967 | -0.75545 | -0.68588 | C | 2.27077 | 2.12035 | -3.73017 |
| C | -2.13831 | -1.11979 | 0.67955 | H | 1.52345 | 2.88918 | -3.94387 |
| C | -5.0625 | -0.56697 | -0.82987 | H | 3.26557 | 2.53541 | -3.94373 |
| C | -2.87455 | -0.38155 | 1.77264 | H | 2.10743 | 1.24455 | -4.3704 |
| C | -5.08264 | -0.40921 | 0.49715 | C | 2.6546 | -1.15747 | 1.38982 |
| C | -4.13506 | 0.39064 | 1.34495 | C | 3.14778 | -2.07688 | 2.33263 |
| H | -3.15965 | -1.12758 | 2.52782 | C | 2.67914 | -1.98061 | 3.64028 |
| H | -2.18836 | 0.29477 | 2.30944 | C | 1.2661 | -0.18092 | 3.02228 |
| H | -4.65274 | 0.70904 | 2.26118 | C | 1.74897 | -1.02071 | 4.00774 |
| H | -3.86413 | 1.3219 | 0.8297 | H | 3.04722 | -2.69155 | 4.37992 |
| C | -2.70425 | 0.38339 | -1.39001 | H | 0.48014 | 0.54337 | 3.21653 |

| | | | |
|----|----------|----------|----------|
| H | 1.37279 | -0.94582 | 5.02394 |
| C | 4.10669 | -3.17593 | 1.99021 |
| H | 3.80496 | -3.70916 | 1.08032 |
| H | 5.12989 | -2.80459 | 1.83914 |
| H | 4.14586 | -3.90761 | 2.80533 |
| N | 1.71299 | -0.24656 | 1.76943 |
| Rh | 0.57812 | 0.50855 | 0.23827 |
| Cl | -0.44057 | -1.90419 | 0.53679 |
| C | -2.79596 | -0.54452 | -0.85034 |
| C | -2.33733 | -1.38768 | -1.8885 |
| C | -1.3528 | -0.98915 | -2.7819 |
| C | -0.77106 | 0.25203 | -2.56915 |
| C | -1.13471 | 1.07412 | -1.48705 |
| C | -2.18421 | 0.6688 | -0.61847 |
| H | -1.00719 | -1.64676 | -3.57552 |
| H | 0.0019 | 0.60457 | -3.24952 |
| H | -0.81441 | 2.11595 | -1.46765 |
| C | -3.69012 | -1.34609 | -0.00762 |
| C | -3.71809 | -2.74417 | -0.67384 |
| O | -4.31692 | -1.05676 | 0.98355 |
| O | -4.3028 | -3.72765 | -0.30247 |
| N | -2.93719 | -2.63044 | -1.82345 |
| C | -2.47415 | -3.78247 | -2.56021 |
| H | -2.6367 | -3.65194 | -3.63676 |
| H | -1.40581 | -3.94688 | -2.36045 |
| H | -3.04722 | -4.64586 | -2.21127 |
| C | -2.36148 | 1.4644 | 0.61507 |
| C | -3.5452 | 2.08424 | 1.02922 |
| C | -3.46274 | 2.87622 | 2.17467 |
| C | -1.13542 | 2.3864 | 2.3473 |
| C | -2.25588 | 3.04102 | 2.83884 |
| H | -4.35873 | 3.38573 | 2.5292 |
| H | -0.14815 | 2.52021 | 2.79125 |
| H | -2.17676 | 3.68199 | 3.71322 |
| C | -4.83319 | 1.93092 | 0.2862 |
| H | -4.67753 | 1.90168 | -0.79944 |
| H | -5.32225 | 0.99062 | 0.57472 |
| H | -5.51631 | 2.75831 | 0.51065 |
| N | -1.19614 | 1.59842 | 1.27392 |

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MeTS_{B2-B3}

| | | | |
|----|----------|----------|----------|
| C | -2.50001 | 0.70611 | 0.25263 |
| C | -2.81449 | 2.0561 | 0.14128 |
| C | -3.96159 | 2.54922 | 0.75855 |
| C | -4.79787 | 1.66421 | 1.43575 |
| C | -4.5274 | 0.30245 | 1.47884 |
| C | -3.36381 | -0.20242 | 0.87732 |
| H | -4.21979 | 3.60549 | 0.70468 |
| H | -5.69923 | 2.04425 | 1.91214 |
| H | -5.2411 | -0.34766 | 1.97158 |
| C | -1.57447 | 0.78698 | -2.15442 |
| C | -1.19735 | 2.37069 | -1.66292 |
| O | -2.02713 | 0.63477 | -3.23725 |
| O | -0.4495 | 3.01876 | -2.36107 |
| N | -1.95593 | 2.87323 | -0.63855 |
| C | -1.9409 | 4.31273 | -0.42822 |
| H | -1.05901 | 4.72086 | -0.92606 |
| H | -2.83557 | 4.78677 | -0.8535 |
| H | -1.89463 | 4.52014 | 0.64637 |
| C | -2.91494 | -1.59236 | 0.76929 |
| C | -3.45054 | -2.72542 | 1.41287 |
| C | -2.83649 | -3.95466 | 1.19048 |
| C | -1.22983 | -2.91536 | -0.21038 |
| C | -1.71769 | -4.06541 | 0.37968 |
| H | -3.23828 | -4.83773 | 1.68678 |
| H | -0.32954 | -2.92287 | -0.81961 |
| H | -1.21532 | -5.01578 | 0.22321 |
| C | -4.61766 | -2.66878 | 2.35102 |
| H | -4.45685 | -1.94369 | 3.15906 |
| H | -5.5506 | -2.39771 | 1.83869 |
| H | -4.77534 | -3.64905 | 2.8151 |
| N | -1.8263 | -1.73301 | -0.04588 |
| Rh | -0.86926 | 0.03395 | -0.58153 |
| Cl | 0.20647 | -0.1992 | 1.69551 |
| C | 3.08043 | 0.33297 | 0.53729 |
| C | 3.19636 | 1.37637 | 1.46643 |
| C | 2.81195 | 2.66951 | 1.15136 |

| | | | | | | | |
|-------------|----------|----------|----------|----|----------|----------|----------|
| C | 2.26086 | 2.88327 | -0.11271 | H | 5.31862 | 1.49152 | 0.8531 |
| C | 2.09679 | 1.84673 | -1.03019 | C | 1.75241 | -1.52942 | -1.93632 |
| C | 2.49847 | 0.54873 | -0.70365 | C | 0.90816 | -2.50182 | 0.42082 |
| H | 2.89975 | 3.48131 | 1.87035 | O | 2.32018 | -2.05943 | -2.78513 |
| H | 1.93595 | 3.88494 | -0.39151 | O | 0.02603 | -3.32517 | 0.39623 |
| H | 1.63055 | 2.04467 | -1.99396 | N | 2.11454 | -2.68788 | 1.0953 |
| C | 3.47378 | -0.90416 | 1.21168 | C | 2.35905 | -3.89412 | 1.85656 |
| C | 3.82337 | -0.47552 | 2.66351 | H | 1.48681 | -4.5416 | 1.7443 |
| O | 3.57665 | -2.03373 | 0.79111 | H | 3.25033 | -4.41715 | 1.48346 |
| O | 4.18343 | -1.18105 | 3.57313 | H | 2.5026 | -3.65958 | 2.92007 |
| N | 3.67358 | 0.90129 | 2.69005 | C | 2.70622 | 1.7948 | -0.39738 |
| C | 3.76616 | 1.68524 | 3.89401 | C | 3.13646 | 3.13866 | -0.41636 |
| H | 4.50268 | 2.49207 | 3.78459 | C | 2.28654 | 4.08169 | -0.9958 |
| H | 2.78901 | 2.11689 | 4.1502 | C | 0.71042 | 2.38635 | -1.48853 |
| H | 4.08544 | 1.01354 | 4.69634 | C | 1.05862 | 3.72698 | -1.52833 |
| C | 2.20621 | -0.54879 | -1.65477 | H | 2.59923 | 5.12616 | -1.00294 |
| C | 3.22037 | -1.20756 | -2.36816 | H | -0.25212 | 2.03414 | -1.86151 |
| C | 2.82773 | -2.13308 | -3.3294 | H | 0.37834 | 4.464 | -1.9461 |
| C | 0.55089 | -1.68599 | -2.80525 | C | 4.4234 | 3.62626 | 0.17878 |
| C | 1.48045 | -2.37327 | -3.56522 | H | 4.49414 | 3.3903 | 1.24847 |
| H | 3.59055 | -2.65485 | -3.90743 | H | 5.30331 | 3.19342 | -0.31538 |
| H | -0.52047 | -1.82349 | -2.95661 | H | 4.49695 | 4.71523 | 0.07659 |
| H | 1.15296 | -3.07283 | -4.33022 | N | 1.51409 | 1.46662 | -0.96405 |
| C | 4.66712 | -0.92986 | -2.11299 | Rh | 0.90128 | -0.68119 | -0.50207 |
| H | 4.85752 | 0.13964 | -1.96282 | Cl | 0.05194 | 0.25308 | 1.54251 |
| H | 4.99491 | -1.45525 | -1.20635 | C | -2.94675 | 0.20671 | 0.69243 |
| H | 5.28649 | -1.277 | -2.94816 | C | -3.22799 | 0.12629 | 2.06178 |
| N | 0.90205 | -0.80661 | -1.85525 | C | -3.35109 | -1.09907 | 2.69302 |
| | | | | C | -3.14086 | -2.24285 | 1.91885 |
| | | | | C | -2.83171 | -2.17663 | 0.56074 |
| | | | | C | -2.72093 | -0.93578 | -0.06308 |
| | | | | H | -3.56707 | -1.17576 | 3.75682 |
| | | | | H | -3.20809 | -3.21956 | 2.39498 |
| | | | | H | -2.62393 | -3.08431 | -0.00101 |
| | | | | C | -2.791 | 1.61744 | 0.35073 |
| | | | | C | -3.00975 | 2.37752 | 1.69095 |
| | | | | O | -2.55616 | 2.15614 | -0.70866 |
| | | | | O | -2.95323 | 3.56875 | 1.87633 |
| | | | | N | -3.30181 | 1.4029 | 2.62875 |
| 64 | | | | | | | |
| MeB3 | | | | | | | |
| C | 2.64445 | -0.51559 | 0.36281 | H | -3.56707 | -1.17576 | 3.75682 |
| C | 3.04086 | -1.63856 | 1.0772 | H | -3.20809 | -3.21956 | 2.39498 |
| C | 4.28364 | -1.63278 | 1.70272 | H | -2.62393 | -3.08431 | -0.00101 |
| C | 5.07691 | -0.48916 | 1.584 | C | -2.791 | 1.61744 | 0.35073 |
| C | 4.6504 | 0.63999 | 0.8968 | C | -3.00975 | 2.37752 | 1.69095 |
| C | 3.38397 | 0.6607 | 0.27496 | O | -2.55616 | 2.15614 | -0.70866 |
| H | 4.63718 | -2.49125 | 2.2717 | O | -2.95323 | 3.56875 | 1.87633 |
| H | 6.05866 | -0.47837 | 2.05429 | N | -3.30181 | 1.4029 | 2.62875 |

| | | | | | | | |
|---|----------|----------|----------|----|----------|----------|----------|
| C | -3.43782 | 1.66658 | 4.03738 | C | -2.63314 | 0.1403 | 2.28936 |
| H | -4.40442 | 1.30882 | 4.41597 | C | -3.90556 | 0.66003 | 2.44112 |
| H | -2.62804 | 1.18208 | 4.59993 | H | -5.65873 | 1.28878 | 1.36845 |
| H | -3.37599 | 2.75012 | 4.1749 | H | -1.9792 | -0.03395 | 3.14103 |
| C | -2.40642 | -0.778 | -1.50401 | H | -4.28478 | 0.91306 | 3.42734 |
| C | -3.46955 | -0.70099 | -2.42046 | C | -5.05961 | 0.72661 | -1.15534 |
| C | -3.1582 | -0.46417 | -3.75287 | H | -5.94206 | 1.31072 | -0.86928 |
| C | -0.85652 | -0.40298 | -3.15823 | H | -4.53805 | 1.27649 | -1.94879 |
| C | -1.83335 | -0.30236 | -4.13222 | H | -5.42053 | -0.21666 | -1.58718 |
| H | -3.95951 | -0.39131 | -4.48831 | N | -2.13555 | -0.16593 | 1.09024 |
| H | 0.19263 | -0.27393 | -3.42283 | Rh | -0.09833 | -0.76399 | 0.79683 |
| H | -1.55658 | -0.1015 | -5.1642 | Cl | -0.83616 | -3.02791 | 1.4425 |
| C | -4.89174 | -0.81789 | -1.96637 | C | 0.66397 | 0.92028 | -0.07799 |
| H | -5.05074 | -1.7032 | -1.33841 | C | 1.74095 | 0.18638 | -0.17654 |
| H | -5.18266 | 0.05487 | -1.36505 | C | 0.19733 | 2.24379 | -0.3908 |
| H | -5.57234 | -0.87507 | -2.8238 | C | -0.87843 | 2.82716 | 0.29569 |
| N | -1.12101 | -0.64398 | -1.86405 | C | 0.84156 | 2.98191 | -1.39969 |

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Me^cTS_{C2-D}(1)

| | | | | | | | |
|---|----------|----------|----------|---|----------|----------|----------|
| C | -0.88451 | -0.97391 | -0.99688 | H | 1.67066 | 2.52227 | -1.93629 |
| C | -0.10403 | -1.58459 | -1.97153 | C | -0.64059 | 4.84019 | -1.00877 |
| C | -0.62437 | -1.77098 | -3.25131 | H | -2.11912 | 4.56365 | 0.53409 |
| C | -1.92747 | -1.35046 | -3.51109 | H | 0.93012 | 4.82955 | -2.487 |
| C | -2.71647 | -0.75953 | -2.53103 | H | -0.96762 | 5.85017 | -1.2502 |
| C | -2.19871 | -0.56477 | -1.23812 | C | 3.15954 | 0.50713 | 0.01446 |
| H | -0.04042 | -2.25509 | -4.03254 | C | 3.49362 | 1.52357 | 0.91834 |
| H | -2.34439 | -1.50055 | -4.50528 | C | 4.1758 | -0.09846 | -0.73252 |
| H | -3.73214 | -0.48334 | -2.78895 | C | 4.81414 | 1.92931 | 1.06786 |
| C | 1.60905 | -1.67624 | -0.28384 | H | 2.7015 | 1.99071 | 1.50395 |
| O | 2.49558 | -2.25927 | 0.29377 | C | 5.49215 | 0.31274 | -0.58619 |
| N | 1.15336 | -2.02642 | -1.55637 | H | 3.92871 | -0.8953 | -1.43185 |
| C | 1.82278 | -3.10529 | -2.26037 | C | 5.81555 | 1.32461 | 0.3155 |
| H | 1.13254 | -3.9455 | -2.41117 | H | 5.06034 | 2.71629 | 1.77857 |
| H | 2.1947 | -2.76359 | -3.23606 | H | 6.27429 | -0.16295 | -1.17517 |
| H | 2.66107 | -3.43834 | -1.6445 | H | 6.85152 | 1.63768 | 0.43406 |
| C | -2.88579 | -0.05597 | -0.04256 | C | 0.67752 | -0.66086 | 2.70862 |
| C | -4.1819 | 0.49659 | 0.03684 | O | 1.06488 | -0.71969 | 3.78084 |
| C | -4.66098 | 0.85607 | 1.29394 | | | | |

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MeTS_{C2-D}(2)

| | | | | | | | |
|----|----------|----------|----------|---|----------|----------|----------|
| | | | | H | -3.32748 | 2.35832 | 0.20026 |
| | | | | C | -5.58295 | 0.33414 | -2.213 |
| C | -1.82832 | -1.37235 | -0.59546 | H | -3.80016 | -0.80048 | -2.66284 |
| C | -1.35122 | -2.15092 | -1.66971 | C | -6.12981 | 1.37249 | -1.45965 |
| C | -2.1257 | -3.20274 | -2.15559 | H | -5.7473 | 2.91105 | 0.00096 |
| C | -3.28644 | -3.54406 | -1.46284 | H | -6.21266 | -0.23551 | -2.89443 |
| C | -3.68934 | -2.8675 | -0.31017 | H | -7.18856 | 1.61055 | -1.54912 |
| C | -2.96455 | -1.76608 | 0.14965 | C | -0.1908 | 2.29871 | -1.52683 |
| H | -1.7961 | -3.79971 | -3.00403 | C | -0.95856 | 3.4355 | -1.83126 |
| H | -3.87248 | -4.3957 | -1.80445 | C | 1.20491 | 2.38186 | -1.60097 |
| H | -4.54866 | -3.24318 | 0.23538 | C | -0.33765 | 4.62692 | -2.17964 |
| C | 0.70529 | -1.03187 | -1.23678 | H | -2.04603 | 3.37526 | -1.78228 |
| O | 1.88219 | -0.85367 | -1.46511 | C | 1.82026 | 3.57605 | -1.95245 |
| N | -0.07854 | -1.82802 | -2.09643 | H | 1.81507 | 1.50824 | -1.38633 |
| C | 0.5169 | -2.45639 | -3.2587 | C | 1.05329 | 4.70234 | -2.23537 |
| H | 0.66348 | -3.53262 | -3.09032 | H | -0.94254 | 5.50316 | -2.40955 |
| H | -0.12088 | -2.31276 | -4.13973 | H | 2.90724 | 3.61045 | -1.9978 |
| H | 1.48835 | -1.98799 | -3.42921 | H | 1.5366 | 5.64062 | -2.50448 |
| C | -3.23752 | -0.97572 | 1.36403 | C | 3.91454 | -0.41928 | 0.5308 |
| C | -4.48373 | -0.89134 | 2.02336 | C | 4.47855 | -1.7013 | 0.46891 |
| C | -4.54078 | -0.13831 | 3.19411 | C | 4.31357 | -2.61393 | 1.49605 |
| C | -2.25334 | 0.43121 | 2.94524 | C | 3.52599 | -2.22196 | 2.57802 |
| C | -3.4186 | 0.50662 | 3.69241 | C | 2.90777 | -0.97517 | 2.62406 |
| H | -5.49479 | -0.05503 | 3.71591 | C | 3.0842 | -0.05888 | 1.58866 |
| H | -1.34201 | 0.94444 | 3.2557 | H | 4.7539 | -3.60818 | 1.4548 |
| H | -3.45254 | 1.08076 | 4.6151 | H | 3.35181 | -2.92705 | 3.38839 |
| C | -5.75311 | -1.49541 | 1.50044 | H | 2.23651 | -0.73192 | 3.44483 |
| H | -5.83132 | -1.39226 | 0.41023 | C | 4.29481 | 0.28241 | -0.69194 |
| H | -5.84367 | -2.56355 | 1.74206 | C | 5.07695 | -0.76278 | -1.53451 |
| H | -6.61828 | -0.99199 | 1.9491 | O | 4.14419 | 1.43761 | -1.02503 |
| N | -2.17598 | -0.25709 | 1.81176 | O | 5.53583 | -0.61898 | -2.642 |
| Rh | -0.3693 | -0.37347 | 0.31082 | N | 5.17313 | -1.88391 | -0.73429 |
| Cl | 0.26401 | -2.36518 | 1.56791 | C | 5.79276 | -3.11338 | -1.15055 |
| C | -1.98688 | 0.46508 | -1.11814 | H | 6.60057 | -3.40027 | -0.46416 |
| C | -0.8562 | 1.08883 | -1.08607 | H | 5.05766 | -3.92846 | -1.19676 |
| C | -3.41374 | 0.7574 | -1.23329 | H | 6.21101 | -2.9467 | -2.14794 |
| C | -3.96971 | 1.80058 | -0.483 | C | 2.36719 | 1.24008 | 1.62794 |
| C | -4.23606 | 0.02056 | -2.09403 | C | 3.06391 | 2.42712 | 1.91592 |
| C | -5.32264 | 2.10385 | -0.59355 | C | 2.324 | 3.59893 | 2.02452 |

| | | | | | | | |
|---|----------|---------|---------|----|----------|----------|----------|
| C | 0.3518 | 2.35543 | 1.57095 | H | -4.48331 | -0.09155 | -2.14868 |
| C | 0.94598 | 3.56879 | 1.8669 | H | -5.22869 | -1.39259 | -1.20118 |
| H | 2.83652 | 4.5355 | 2.24538 | N | -1.99096 | -0.00797 | 1.15428 |
| H | -0.72515 | 2.29128 | 1.40789 | Rh | 0.09385 | -0.51823 | 1.06877 |
| H | 0.34159 | 4.46839 | 1.95471 | Cl | 0.77974 | 1.1807 | 2.78507 |
| C | 4.54903 | 2.43671 | 2.0974 | C | 0.51803 | 0.78279 | -0.46288 |
| H | 4.88827 | 1.60518 | 2.72757 | C | 1.71082 | 0.27976 | -0.39819 |
| H | 5.05 | 2.34095 | 1.12503 | C | -0.37004 | 1.74644 | -1.05587 |
| H | 4.88126 | 3.37545 | 2.55619 | C | -0.84365 | 2.82326 | -0.29093 |
| N | 1.03557 | 1.20824 | 1.43815 | C | -0.84728 | 1.55426 | -2.35959 |

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MeTSCl-D1(1)

| | | | | | | | |
|---|----------|----------|----------|---|----------|----------|----------|
| C | -0.66326 | -1.52912 | -0.45472 | H | -0.49357 | 0.6971 | -2.93314 |
| C | 0.20174 | -2.28555 | -1.24097 | C | -2.24385 | 3.50662 | -2.13364 |
| C | -0.28335 | -2.94319 | -2.37154 | H | -2.1231 | 4.54493 | -0.2474 |
| C | -1.63416 | -2.81553 | -2.68796 | H | -2.15334 | 2.27973 | -3.9035 |
| C | -2.49351 | -2.03254 | -1.92503 | H | -2.97467 | 4.1958 | -2.55388 |
| C | -2.01355 | -1.35753 | -0.78781 | C | 3.05957 | 0.8496 | -0.49429 |
| H | 0.37068 | -3.55358 | -2.99265 | C | 3.37955 | 1.96457 | 0.28429 |
| H | -2.02602 | -3.33374 | -3.56124 | C | 4.00381 | 0.31441 | -1.37404 |
| H | -3.53128 | -1.96815 | -2.22986 | C | 4.63817 | 2.54443 | 0.1676 |
| C | 1.94758 | -1.44479 | 0.19121 | H | 2.64196 | 2.33771 | 0.99507 |
| O | 2.93804 | -1.62834 | 0.85855 | C | 5.25171 | 0.9075 | -1.4965 |
| N | 1.52201 | -2.33631 | -0.80221 | H | 3.74701 | -0.56529 | -1.96562 |
| C | 2.42596 | -3.37835 | -1.2485 | C | 5.57024 | 2.02272 | -0.72323 |
| H | 1.96438 | -4.36674 | -1.12408 | H | 4.89146 | 3.408 | 0.78006 |
| H | 2.69126 | -3.24192 | -2.30669 | H | 5.98193 | 0.49762 | -2.1923 |
| H | 3.32953 | -3.32331 | -0.63694 | H | 6.55359 | 2.48179 | -0.81372 |
| C | -2.74623 | -0.4474 | 0.10767 | C | 0.0189 | -1.88324 | 2.52029 |
| C | -4.06862 | 0.02028 | -0.03273 | O | -0.01519 | -2.65542 | 3.36229 |
| C | -4.56025 | 0.8792 | 0.94909 | | | | |
| C | -2.47789 | 0.8127 | 2.08591 | | | | |
| C | -3.78189 | 1.27284 | 2.0261 | | | | |
| H | -5.58128 | 1.24884 | 0.85283 | | | | |
| H | -1.77082 | 1.11622 | 2.85952 | | | | |
| H | -4.16305 | 1.94252 | 2.7923 | | | | |
| C | -4.95816 | -0.32834 | -1.18725 | | | | |
| H | -5.89208 | 0.24269 | -1.13044 | | | | |

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MeTSCl-D1(2)

| | | | |
|---|----------|---------|---------|
| C | -0.20049 | 0.59943 | 0.89487 |
| C | 0.02577 | -0.0615 | 2.13428 |
| C | 0.72121 | 0.58643 | 3.14771 |
| C | 1.30337 | 1.82868 | 2.86999 |
| C | 1.265 | 2.38825 | 1.5945 |

| | | | | | | | |
|----|----------|----------|----------|---|----------|----------|----------|
| C | 0.54148 | 1.77345 | 0.56317 | C | -3.79021 | -1.03966 | 0.74058 |
| H | 0.87431 | 0.11654 | 4.11773 | C | -4.64724 | -0.51164 | 1.72725 |
| H | 1.85869 | 2.33543 | 3.65868 | C | -4.14853 | -2.22317 | 0.0753 |
| H | 1.83739 | 3.2928 | 1.41496 | C | -5.83907 | -1.14797 | 2.02835 |
| C | -0.8668 | -1.94576 | 0.98384 | H | -4.3567 | 0.40399 | 2.24234 |
| O | -1.15235 | -3.11542 | 0.90734 | C | -5.34471 | -2.85177 | 0.38977 |
| N | -0.47636 | -1.34268 | 2.19554 | H | -3.48961 | -2.61142 | -0.69846 |
| C | -0.34618 | -2.15122 | 3.397 | C | -6.19005 | -2.3221 | 1.36186 |
| H | 0.71443 | -2.29833 | 3.64294 | H | -6.49917 | -0.73137 | 2.78747 |
| H | -0.86197 | -1.66829 | 4.23617 | H | -5.62172 | -3.76546 | -0.13306 |
| H | -0.80226 | -3.12161 | 3.19231 | H | -7.12537 | -2.82502 | 1.60288 |
| C | 0.46147 | 2.18262 | -0.8463 | C | 3.08523 | -0.52732 | 0.2952 |
| C | 0.8023 | 3.44863 | -1.37674 | C | 3.81869 | 0.57434 | 0.7683 |
| C | 0.67907 | 3.62308 | -2.75277 | C | 4.1805 | 1.61484 | -0.07165 |
| C | -0.14749 | 1.40923 | -2.98227 | C | 3.78169 | 1.52736 | -1.40758 |
| C | 0.21975 | 2.60525 | -3.57868 | C | 3.07279 | 0.43077 | -1.89447 |
| H | 0.93315 | 4.59469 | -3.17861 | C | 2.71094 | -0.61635 | -1.04393 |
| H | -0.58758 | 0.57415 | -3.53361 | H | 4.7507 | 2.46911 | 0.28973 |
| H | 0.11111 | 2.74736 | -4.65104 | H | 4.03801 | 2.33653 | -2.09051 |
| C | 1.2512 | 4.61292 | -0.54718 | H | 2.7861 | 0.38633 | -2.94487 |
| H | 0.61297 | 4.75004 | 0.335 | C | 2.83506 | -1.40915 | 1.43983 |
| H | 2.28746 | 4.49997 | -0.1953 | C | 3.50524 | -0.69501 | 2.6485 |
| H | 1.21026 | 5.53653 | -1.13702 | O | 2.25091 | -2.46467 | 1.52352 |
| N | -0.02505 | 1.21581 | -1.67106 | O | 3.51462 | -1.05627 | 3.80102 |
| Rh | -0.81702 | -0.63288 | -0.55904 | N | 4.09947 | 0.44115 | 2.13044 |
| Cl | -2.13953 | -1.32186 | -2.65055 | C | 4.78188 | 1.42306 | 2.92999 |
| C | -1.948 | 0.80748 | 0.55477 | H | 5.83203 | 1.52276 | 2.62522 |
| C | -2.58978 | -0.32888 | 0.45769 | H | 4.28969 | 2.40223 | 2.84451 |
| C | -2.36317 | 2.1838 | 0.25827 | H | 4.73871 | 1.08507 | 3.97015 |
| C | -2.9954 | 2.45992 | -0.95907 | C | 2.07627 | -1.8556 | -1.56301 |
| C | -2.13805 | 3.21699 | 1.17239 | C | 2.90397 | -2.8034 | -2.18358 |
| C | -3.37505 | 3.76127 | -1.26447 | C | 2.31534 | -3.99463 | -2.59832 |
| H | -3.15757 | 1.64351 | -1.66462 | C | 0.22394 | -3.21942 | -1.76073 |
| C | -2.53646 | 4.51444 | 0.86871 | C | 0.9673 | -4.21378 | -2.37544 |
| H | -1.65083 | 2.99315 | 2.12168 | H | 2.92987 | -4.75479 | -3.08115 |
| C | -3.1431 | 4.78975 | -0.35427 | H | -0.83544 | -3.34858 | -1.56289 |
| H | -3.85457 | 3.97245 | -2.21885 | H | 0.48381 | -5.14142 | -2.66964 |
| H | -2.37209 | 5.31356 | 1.59042 | C | 4.37591 | -2.57202 | -2.35915 |
| H | -3.44293 | 5.8087 | -0.59503 | H | 4.87689 | -2.40979 | -1.39477 |

| | | | | | | | |
|------------|----------|----------|----------|---|----------|----------|----------|
| H | 4.84679 | -3.43922 | -2.83667 | C | 2.29645 | 0.83374 | -1.0036 |
| H | 4.58916 | -1.69119 | -2.9784 | C | 2.06027 | -0.32368 | -1.40355 |
| N | 0.76123 | -2.05231 | -1.37516 | C | 2.14356 | -1.62073 | -2.01197 |
| | | | | C | 3.07902 | -2.54085 | -1.5201 |
| 88 | | | | C | 1.26382 | -2.01217 | -3.03032 |
| MeE | | | | C | 3.11207 | -3.83618 | -2.02075 |
| C | 1.64838 | -1.12329 | 1.25607 | H | 3.74707 | -2.23645 | -0.71449 |
| C | 2.71496 | -0.71155 | 2.06624 | C | 1.30085 | -3.30762 | -3.52367 |
| C | 3.4778 | -1.69331 | 2.71837 | H | 0.52411 | -1.30286 | -3.40069 |
| C | 3.2159 | -3.04072 | 2.53256 | C | 2.21899 | -4.22478 | -3.01534 |
| C | 2.16793 | -3.44699 | 1.72593 | H | 3.83271 | -4.54837 | -1.62151 |
| C | 1.34609 | -2.50014 | 1.10019 | H | 0.60188 | -3.60811 | -4.30226 |
| H | 4.28646 | -1.41032 | 3.38486 | H | 2.23882 | -5.2439 | -3.39798 |
| H | 3.83946 | -3.7816 | 3.02935 | C | 3.05275 | 2.05693 | -0.91553 |
| H | 2.0157 | -4.50742 | 1.5769 | C | 2.45985 | 3.314 | -1.07834 |
| C | 2.32395 | 1.78537 | 2.09975 | C | 4.42745 | 1.96655 | -0.65301 |
| O | 2.6845 | 2.86721 | 2.51915 | C | 3.23686 | 4.46057 | -0.98833 |
| N | 3.0962 | 0.6478 | 2.25323 | H | 1.38658 | 3.38037 | -1.24882 |
| C | 4.40663 | 0.90353 | 2.83935 | C | 5.19479 | 3.11847 | -0.55717 |
| H | 4.42294 | 0.69754 | 3.91837 | H | 4.87083 | 0.97999 | -0.51261 |
| H | 5.15915 | 0.28114 | 2.34173 | C | 4.60043 | 4.36682 | -0.72528 |
| H | 4.64133 | 1.95875 | 2.69495 | H | 2.7707 | 5.43642 | -1.1093 |
| C | 0.19604 | -2.86418 | 0.23838 | H | 6.26039 | 3.04277 | -0.34731 |
| C | -0.40068 | -4.13661 | 0.07528 | H | 5.20179 | 5.27055 | -0.64458 |
| C | -1.53431 | -4.21627 | -0.73695 | C | -3.67388 | 0.94318 | 0.30686 |
| C | -1.39153 | -1.90993 | -1.20724 | C | -4.27428 | 0.7703 | 1.56419 |
| C | -2.05944 | -3.10875 | -1.38237 | C | -4.09331 | 1.69063 | 2.57881 |
| H | -2.02285 | -5.18506 | -0.84449 | C | -3.25828 | 2.77827 | 2.31094 |
| H | -1.72014 | -0.99133 | -1.69166 | C | -2.60997 | 2.93453 | 1.08821 |
| H | -2.96895 | -3.15114 | -1.9768 | C | -2.79243 | 1.99441 | 0.07419 |
| C | 0.05063 | -5.40719 | 0.73357 | H | -4.55763 | 1.56754 | 3.555 |
| H | 1.01936 | -5.75507 | 0.34601 | H | -3.08772 | 3.51529 | 3.0937 |
| H | 0.14211 | -5.30407 | 1.82194 | H | -1.91798 | 3.75879 | 0.93611 |
| H | -0.67651 | -6.2047 | 0.54075 | C | -4.10915 | -0.15912 | -0.53774 |
| N | -0.32115 | -1.81186 | -0.42877 | C | -4.93921 | -1.08264 | 0.39625 |
| Rh | 0.53763 | 0.11865 | 0.20875 | O | -3.9412 | -0.37742 | -1.71969 |
| Cl | -1.04973 | -0.13645 | 2.00491 | O | -5.41343 | -2.15917 | 0.11918 |
| C | 1.04529 | 1.73893 | 1.23331 | N | -5.01976 | -0.41696 | 1.60115 |
| O | 0.38298 | 2.73904 | 1.16791 | C | -5.62489 | -0.97021 | 2.785 |

| | | | | | | | |
|---|----------|----------|----------|----|----------|----------|----------|
| H | -4.87116 | -1.12334 | 3.56917 | C | 0.31045 | -2.83806 | -3.13379 |
| H | -6.41535 | -0.31179 | 3.16847 | H | 1.57701 | -4.56683 | -3.28227 |
| H | -6.06172 | -1.93449 | 2.50869 | H | -0.72188 | -0.99572 | -2.64318 |
| C | -2.11727 | 2.12865 | -1.2435 | H | -0.13367 | -2.94438 | -4.11998 |
| C | -2.75955 | 2.88168 | -2.243 | C | 2.85777 | -4.59312 | -0.97313 |
| C | -2.13342 | 2.98473 | -3.47929 | H | 3.66871 | -4.10812 | -0.4155 |
| C | -0.36886 | 1.6271 | -2.64214 | H | 2.47353 | -5.41657 | -0.35537 |
| C | -0.91949 | 2.34885 | -3.68822 | H | 3.29652 | -5.04842 | -1.8697 |
| H | -2.60775 | 3.55864 | -4.27564 | N | 0.49461 | -1.62089 | -1.10479 |
| H | 0.5915 | 1.12882 | -2.76632 | Rh | 0.18175 | 0.13026 | 0.35806 |
| H | -0.40187 | 2.40761 | -4.64279 | Cl | -1.42447 | -1.42051 | 1.38537 |
| C | -4.09104 | 3.52327 | -1.99843 | C | -0.02377 | 1.37534 | 1.85248 |
| H | -4.87382 | 2.76484 | -1.85916 | O | -1.05489 | 1.96125 | 2.04528 |
| H | -4.08736 | 4.14608 | -1.09511 | C | 1.71566 | 1.48716 | -0.1288 |
| H | -4.38307 | 4.1513 | -2.84827 | C | 2.37789 | 0.3846 | -0.06361 |
| N | -0.93935 | 1.50893 | -1.43437 | C | 3.44829 | -0.31469 | -0.7661 |

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MeTS_{E-E1}

| | | | | | | | |
|---|----------|----------|----------|---|----------|----------|----------|
| C | 1.64338 | -0.91945 | 1.277 | H | 4.43926 | -1.03297 | 1.00566 |
| C | 2.0894 | -0.59357 | 2.5712 | C | 4.49622 | -0.89949 | -2.86973 |
| C | 2.59081 | -1.60424 | 3.40111 | H | 2.68666 | 0.2658 | -2.69151 |
| C | 2.63449 | -2.91592 | 2.95968 | C | 5.50141 | -1.57382 | -2.18268 |
| C | 2.22765 | -3.24272 | 1.66974 | H | 6.28238 | -2.1252 | -0.25046 |
| C | 1.75488 | -2.25937 | 0.80604 | H | 4.50168 | -0.8681 | -3.95779 |
| H | 2.9047 | -1.36366 | 4.41458 | H | 6.29961 | -2.07015 | -2.73222 |
| H | 2.98351 | -3.69767 | 3.63137 | C | 1.84446 | 2.90373 | -0.37653 |
| H | 2.23939 | -4.28366 | 1.36446 | C | 0.78345 | 3.80636 | -0.22001 |
| C | 1.18242 | 1.71939 | 2.75404 | C | 3.09379 | 3.38938 | -0.80199 |
| O | 1.2894 | 2.8568 | 3.16746 | C | 0.97086 | 5.15651 | -0.48692 |
| N | 2.10003 | 0.73305 | 3.04683 | H | -0.18338 | 3.44567 | 0.12677 |
| C | 3.17127 | 1.12146 | 3.95711 | C | 3.27105 | 4.73709 | -1.07139 |
| H | 2.94228 | 0.85259 | 4.99712 | H | 3.91997 | 2.68812 | -0.91897 |
| H | 4.10076 | 0.62829 | 3.65209 | C | 2.20854 | 5.62581 | -0.91516 |
| H | 3.28375 | 2.20587 | 3.90055 | H | 0.14232 | 5.84925 | -0.35126 |
| C | 1.33337 | -2.54155 | -0.58223 | H | 4.24313 | 5.09894 | -1.40276 |
| C | 1.78902 | -3.61787 | -1.3741 | H | 2.3494 | 6.68557 | -1.12152 |
| C | 1.24523 | -3.74002 | -2.65324 | C | -3.8902 | -0.26621 | -0.09219 |
| C | -0.02016 | -1.76387 | -2.32106 | C | -4.67143 | -0.90296 | 0.88318 |

| | | | | | | | |
|---|----------|----------|----------|----|----------|----------|----------|
| C | -5.07287 | -0.23771 | 2.02574 | H | 0.92299 | -4.95032 | 1.81588 |
| C | -4.64732 | 1.085 | 2.17965 | H | 0.82335 | -4.47271 | -0.60774 |
| C | -3.84809 | 1.71947 | 1.23369 | C | 1.50154 | 0.62264 | 2.71561 |
| C | -3.43905 | 1.03425 | 0.08912 | O | 2.00464 | 1.59929 | 3.2264 |
| H | -5.67413 | -0.72547 | 2.79024 | N | 2.04618 | -0.63963 | 2.80666 |
| H | -4.9363 | 1.63066 | 3.07629 | C | 3.2537 | -0.77245 | 3.61929 |
| H | -3.49138 | 2.73232 | 1.40834 | H | 3.16953 | -0.10892 | 4.48339 |
| C | -3.63035 | -1.24016 | -1.15111 | H | 3.3542 | -1.80973 | 3.95241 |
| C | -4.28965 | -2.55677 | -0.65571 | H | 4.14552 | -0.48857 | 3.04137 |
| O | -3.08218 | -1.12471 | -2.22482 | C | 1.09475 | -2.10272 | -1.80986 |
| O | -4.27531 | -3.63354 | -1.20204 | C | 1.56396 | -2.82049 | -2.91658 |
| N | -4.92062 | -2.23453 | 0.53046 | C | 1.02333 | -2.48331 | -4.15862 |
| C | -5.5206 | -3.21121 | 1.40097 | C | -0.33734 | -0.83096 | -3.10945 |
| H | -4.95685 | -3.28661 | 2.3412 | C | 0.05004 | -1.50262 | -4.26338 |
| H | -6.56489 | -2.95614 | 1.62502 | H | 1.36833 | -3.01338 | -5.04719 |
| H | -5.4882 | -4.1739 | 0.88206 | H | -1.11457 | -0.06711 | -3.12619 |
| C | -2.6072 | 1.65266 | -0.97336 | H | -0.4048 | -1.25621 | -5.21952 |
| C | -3.22767 | 2.53986 | -1.87173 | C | 2.59931 | -3.90018 | -2.80909 |
| C | -2.4819 | 2.99754 | -2.95218 | H | 3.28915 | -3.72848 | -1.975 |
| C | -0.64811 | 1.70033 | -2.18107 | H | 2.14427 | -4.88907 | -2.65643 |
| C | -1.17987 | 2.55672 | -3.12852 | H | 3.19149 | -3.95897 | -3.73068 |
| H | -2.93844 | 3.68082 | -3.66859 | N | 0.1897 | -1.11106 | -1.91984 |
| H | 0.3792 | 1.34718 | -2.2709 | Rh | -0.03981 | -0.0446 | 0.21768 |
| H | -0.57842 | 2.87475 | -3.97637 | Cl | -1.71082 | -1.82825 | 0.79291 |
| C | -4.6647 | 2.93549 | -1.71061 | C | 0.12476 | 0.77544 | 1.97783 |
| H | -5.32438 | 2.05783 | -1.74608 | O | -0.68268 | 1.49167 | 2.50462 |
| H | -4.85237 | 3.42909 | -0.74911 | C | 1.74947 | 0.86107 | -0.18387 |
| H | -4.96997 | 3.62019 | -2.51052 | C | 2.57573 | -0.16116 | 0.06933 |
| N | -1.32401 | 1.26883 | -1.10717 | C | 4.04194 | -0.20668 | 0.21282 |
| | | | | C | 4.78121 | 0.95048 | 0.50094 |
| | | | | C | 4.72001 | -1.43258 | 0.16247 |
| | | | | C | 6.15216 | 0.88076 | 0.70685 |
| C | 1.799 | -1.38838 | 0.50192 | H | 4.26758 | 1.9057 | 0.59855 |
| C | 1.73379 | -1.66428 | 1.89215 | C | 6.09321 | -1.49886 | 0.36604 |
| C | 1.43018 | -2.94177 | 2.36004 | H | 4.15752 | -2.34987 | -0.02038 |
| C | 1.17722 | -3.95597 | 1.45433 | C | 6.81683 | -0.34188 | 0.63672 |
| C | 1.14939 | -3.69598 | 0.08196 | H | 6.70506 | 1.78893 | 0.94231 |
| C | 1.42289 | -2.42753 | -0.40093 | H | 6.59925 | -2.46228 | 0.31949 |
| H | 1.36482 | -3.11683 | 3.43233 | H | 7.89134 | -0.39341 | 0.80411 |

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MeE1

| | | | | | | | |
|---|----------|----------|----------|------------|----------|----------|----------|
| C | 2.05193 | 2.22414 | -0.60504 | H | -4.27221 | 4.02397 | 0.99154 |
| C | 1.6749 | 3.32727 | 0.17432 | H | -4.64243 | 4.64976 | -0.62584 |
| C | 2.68679 | 2.44892 | -1.83617 | N | -1.29088 | 1.56654 | -0.5703 |
| C | 1.94063 | 4.61788 | -0.26583 | | | | |
| H | 1.17995 | 3.16541 | 1.13245 | 88 | | | |
| C | 2.9369 | 3.74262 | -2.27715 | MeF | | | |
| H | 2.97385 | 1.58763 | -2.44163 | C | -0.12584 | 0.02141 | -0.81238 |
| C | 2.56467 | 4.83197 | -1.49281 | C | 0.04942 | -1.02633 | -1.73109 |
| H | 1.65362 | 5.46567 | 0.35432 | C | -0.76838 | -1.09061 | -2.87029 |
| H | 3.42715 | 3.90133 | -3.23684 | C | -1.70884 | -0.10283 | -3.1203 |
| H | 2.76225 | 5.84602 | -1.83677 | C | -1.86594 | 0.95475 | -2.23884 |
| C | -3.93059 | 0.13462 | 0.27949 | C | -1.08599 | 1.03354 | -1.07465 |
| C | -4.77326 | -0.67614 | 1.05236 | H | -0.68328 | -1.91719 | -3.57172 |
| C | -5.03554 | -0.37256 | 2.37464 | H | -2.32846 | -0.15655 | -4.01533 |
| C | -4.40834 | 0.75795 | 2.90989 | H | -2.58203 | 1.72632 | -2.48943 |
| C | -3.55068 | 1.55616 | 2.16018 | C | 1.57512 | -2.48508 | -0.37032 |
| C | -3.28475 | 1.23319 | 0.82797 | O | 2.1673 | -3.54324 | -0.28802 |
| H | -5.6817 | -0.99653 | 2.98908 | N | 1.02797 | -2.04479 | -1.56153 |
| H | -4.59003 | 1.01456 | 3.95235 | C | 1.35837 | -2.88289 | -2.70527 |
| H | -3.04987 | 2.40452 | 2.61995 | H | 0.60379 | -3.66538 | -2.87891 |
| C | -3.82347 | -0.4761 | -1.04833 | H | 1.44441 | -2.25968 | -3.60171 |
| C | -4.64799 | -1.78676 | -0.95002 | H | 2.31351 | -3.37237 | -2.50463 |
| O | -3.29718 | -0.07823 | -2.06381 | C | -1.14778 | 2.20163 | -0.1595 |
| O | -4.79994 | -2.62544 | -1.80517 | C | -2.13023 | 3.22224 | -0.13723 |
| N | -5.21893 | -1.77421 | 0.31013 | C | -1.93433 | 4.26951 | 0.76458 |
| C | -5.95634 | -2.8828 | 0.85414 | C | 0.04958 | 3.26031 | 1.56272 |
| H | -5.39941 | -3.35523 | 1.6755 | C | -0.84265 | 4.31662 | 1.61588 |
| H | -6.93947 | -2.56097 | 1.22231 | H | -2.67905 | 5.06517 | 0.79705 |
| H | -6.09407 | -3.61002 | 0.04828 | H | 0.932 | 3.19218 | 2.20317 |
| C | -2.45995 | 2.0504 | -0.09534 | H | -0.69567 | 5.13761 | 2.31316 |
| C | -3.03395 | 3.23109 | -0.6012 | C | -3.37876 | 3.27455 | -0.97026 |
| C | -2.40166 | 3.87156 | -1.66072 | H | -3.17039 | 3.55242 | -2.01338 |
| C | -0.74503 | 2.17303 | -1.63592 | H | -3.93378 | 2.3282 | -0.96786 |
| C | -1.26057 | 3.31691 | -2.21378 | H | -4.05284 | 4.04123 | -0.57024 |
| H | -2.83348 | 4.78449 | -2.07087 | N | -0.11477 | 2.25363 | 0.70977 |
| H | 0.15738 | 1.72461 | -2.03537 | Rh | 1.06211 | 0.32696 | 0.7571 |
| H | -0.75348 | 3.76302 | -3.06556 | Cl | 2.6796 | 1.24006 | 2.49568 |
| C | -4.33499 | 3.75615 | -0.07014 | C | 1.51267 | -1.58403 | 0.88475 |
| H | -5.13363 | 3.00786 | -0.15996 | O | 1.68236 | -2.1003 | 1.95657 |

| | | | | | | | |
|---|----------|----------|----------|----------------------------|----------|----------|----------|
| C | 2.96224 | 0.29973 | -0.45856 | H | -3.50408 | -2.59173 | -3.71496 |
| C | 2.33481 | 1.30082 | -0.84636 | H | -4.84136 | -3.49478 | -2.93809 |
| C | 1.9528 | 2.56803 | -1.39592 | H | -5.1058 | -1.82218 | -3.50884 |
| C | 1.23223 | 2.6415 | -2.5944 | C | -1.55946 | -1.03718 | 2.26818 |
| C | 2.27993 | 3.74369 | -0.70572 | C | -2.44484 | -1.20619 | 3.34653 |
| C | 0.82079 | 3.87624 | -3.08045 | C | -2.23039 | -0.44597 | 4.49079 |
| H | 0.98464 | 1.72266 | -3.12487 | C | -0.33827 | 0.54012 | 3.43512 |
| C | 1.86185 | 4.97167 | -1.19733 | C | -1.16499 | 0.43447 | 4.53972 |
| H | 2.83995 | 3.66501 | 0.22595 | H | -2.90098 | -0.56019 | 5.34245 |
| C | 1.12672 | 5.03991 | -2.3798 | H | 0.54329 | 1.17809 | 3.44906 |
| H | 0.25375 | 3.92893 | -4.00857 | H | -0.95325 | 1.0295 | 5.42428 |
| H | 2.10799 | 5.88236 | -0.65384 | C | -3.59454 | -2.16733 | 3.28213 |
| H | 0.79448 | 6.00524 | -2.75861 | H | -4.39119 | -1.79779 | 2.62152 |
| C | 3.98793 | -0.70869 | -0.46414 | H | -3.29056 | -3.1521 | 2.90591 |
| C | 4.58524 | -1.16715 | 0.71616 | H | -4.03354 | -2.30583 | 4.27707 |
| C | 4.38154 | -1.24128 | -1.7012 | N | -0.52643 | -0.16918 | 2.3094 |
| C | 5.55684 | -2.15661 | 0.64939 | | | | |
| H | 4.26909 | -0.74008 | 1.6675 | | | | |
| C | 5.35318 | -2.22956 | -1.75446 | | | | |
| H | 3.90681 | -0.87156 | -2.61014 | | | | |
| C | 5.93756 | -2.69224 | -0.57763 | | | | |
| H | 6.0142 | -2.51898 | 1.56791 | | | | |
| H | 5.65505 | -2.64248 | -2.71571 | | | | |
| H | 6.69292 | -3.47526 | -0.61907 | | | | |
| C | -2.76439 | -1.6121 | 0.13804 | | | | |
| C | -3.01673 | -2.47354 | -0.94103 | | | | |
| C | -2.32713 | -3.66623 | -1.09059 | | | | |
| C | -1.36802 | -3.97266 | -0.12481 | | | | |
| C | -1.10076 | -3.12355 | 0.94989 | | | | |
| C | -1.78096 | -1.90902 | 1.08107 | | | | |
| H | -2.5163 | -4.3363 | -1.92717 | | | | |
| H | -0.79493 | -4.89473 | -0.21423 | | | | |
| H | -0.337 | -3.3956 | 1.67624 | | | | |
| C | -3.65164 | -0.4608 | -0.00864 | | | | |
| C | -4.39894 | -0.6982 | -1.35096 | | | | |
| O | -3.85986 | 0.48479 | 0.71857 | | | | |
| O | -5.16802 | 0.05259 | -1.903 | | | | |
| N | -4.0059 | -1.95089 | -1.78218 | | | | |
| C | -4.38067 | -2.50576 | -3.05635 | | | | |
| | | | | 88 | | | |
| | | | | MeTS_{F-F1} | | | |
| | | | | C | 0.16301 | 0.23572 | -0.86158 |
| | | | | C | 0.07268 | -0.72578 | -1.90591 |
| | | | | C | -0.82103 | -0.52826 | -2.9607 |
| | | | | C | -1.63954 | 0.59128 | -2.97849 |
| | | | | C | -1.61649 | 1.50749 | -1.93244 |
| | | | | C | -0.74282 | 1.35128 | -0.85234 |
| | | | | H | -0.8911 | -1.26181 | -3.76192 |
| | | | | H | -2.3338 | 0.74796 | -3.80397 |
| | | | | H | -2.31524 | 2.33032 | -1.98114 |
| | | | | C | 1.4259 | -2.57737 | -0.90209 |
| | | | | O | 2.10176 | -3.56974 | -1.07396 |
| | | | | N | 0.94789 | -1.82418 | -1.96593 |
| | | | | C | 1.33917 | -2.32726 | -3.27895 |
| | | | | H | 0.62175 | -3.06327 | -3.66887 |
| | | | | H | 1.41928 | -1.4874 | -3.97605 |
| | | | | H | 2.30898 | -2.81996 | -3.17486 |
| | | | | C | -0.63746 | 2.30823 | 0.27133 |
| | | | | C | -1.29227 | 3.56064 | 0.38787 |
| | | | | C | -0.97049 | 4.34431 | 1.4955 |
| | | | | C | 0.51045 | 2.67893 | 2.29045 |

| | | | | | | | |
|----|----------|----------|----------|-------------|----------|----------|----------|
| C | -0.06569 | 3.92593 | 2.45829 | C | -3.07378 | -2.96466 | -1.81747 |
| H | -1.45531 | 5.31549 | 1.59667 | C | -2.25561 | -3.63258 | -0.90306 |
| H | 1.23908 | 2.25901 | 2.98834 | C | -1.88795 | -3.06067 | 0.31427 |
| H | 0.18636 | 4.54733 | 3.31394 | C | -2.319 | -1.77315 | 0.6551 |
| C | -2.30958 | 4.11648 | -0.56426 | H | -3.36004 | -3.42785 | -2.7599 |
| H | -1.90036 | 4.25654 | -1.57454 | H | -1.89879 | -4.63303 | -1.14267 |
| H | -3.19927 | 3.47441 | -0.63628 | H | -1.2566 | -3.61232 | 1.0071 |
| H | -2.64737 | 5.09859 | -0.21354 | C | -3.72979 | 0.23801 | -0.22518 |
| N | 0.22567 | 1.91754 | 1.23873 | C | -4.43972 | 0.3878 | -1.60059 |
| Rh | 0.99612 | -0.21729 | 0.95157 | O | -3.73598 | 1.09919 | 0.62504 |
| Cl | 2.46183 | -0.10491 | 3.00699 | O | -4.98465 | 1.37387 | -2.03841 |
| C | 1.13597 | -2.11471 | 0.5393 | N | -4.31087 | -0.83719 | -2.22627 |
| O | 0.98151 | -2.94703 | 1.3939 | C | -4.74434 | -1.09355 | -3.57441 |
| C | 2.70882 | -0.13169 | -0.21895 | H | -3.88483 | -1.31565 | -4.22423 |
| C | 1.95465 | 0.77499 | -0.76565 | H | -5.44586 | -1.93663 | -3.61245 |
| C | 2.12808 | 2.18462 | -1.11703 | H | -5.24676 | -0.19023 | -3.93447 |
| C | 1.5974 | 2.72147 | -2.29469 | C | -2.07239 | -1.22399 | 2.01737 |
| C | 2.83 | 3.0166 | -0.23635 | C | -3.10406 | -1.38798 | 2.95843 |
| C | 1.75157 | 4.07306 | -2.57689 | C | -2.88477 | -0.91187 | 4.24633 |
| H | 1.06099 | 2.07306 | -2.98655 | C | -0.71642 | -0.19897 | 3.57101 |
| C | 2.96633 | 4.37058 | -0.51411 | C | -1.67908 | -0.30986 | 4.56008 |
| H | 3.23484 | 2.58581 | 0.67999 | H | -3.66444 | -1.02763 | 4.99959 |
| C | 2.42309 | 4.90137 | -1.68108 | H | 0.2662 | 0.21855 | 3.78366 |
| H | 1.34309 | 4.48282 | -3.49938 | H | -1.46893 | 0.06054 | 5.5603 |
| H | 3.49992 | 5.01395 | 0.18334 | C | -4.40394 | -2.04852 | 2.60723 |
| H | 2.52861 | 5.96351 | -1.89673 | H | -5.03234 | -1.39606 | 1.98558 |
| C | 3.91651 | -0.88687 | -0.34496 | H | -4.25621 | -2.98259 | 2.05042 |
| C | 4.42465 | -1.69193 | 0.68543 | H | -4.9728 | -2.28218 | 3.51482 |
| C | 4.58366 | -0.84784 | -1.58565 | N | -0.89982 | -0.63696 | 2.31565 |
| C | 5.58547 | -2.42338 | 0.47691 | | | | |
| H | 3.90102 | -1.71947 | 1.64031 | 88 | | | |
| C | 5.74339 | -1.57872 | -1.77896 | MeF1 | | | |
| H | 4.1627 | -0.24022 | -2.38791 | C | -0.66077 | 0.90106 | -0.78817 |
| C | 6.24675 | -2.37069 | -0.74674 | C | 0.46947 | 1.60779 | -0.32872 |
| H | 5.97368 | -3.04804 | 1.27908 | C | 1.54941 | 1.84766 | -1.19265 |
| H | 6.25395 | -1.5411 | -2.73999 | C | 1.5549 | 1.32195 | -2.47053 |
| H | 7.15272 | -2.95412 | -0.90286 | C | 0.50994 | 0.49083 | -2.89615 |
| C | -3.13761 | -1.10147 | -0.2512 | C | -0.57813 | 0.27551 | -2.07194 |
| C | -3.50388 | -1.69564 | -1.47055 | H | 2.37084 | 2.47458 | -0.84697 |

| | | | | | | | |
|----|----------|----------|----------|---|----------|----------|----------|
| H | 2.4058 | 1.50688 | -3.1245 | C | -3.38959 | -0.3859 | 1.46137 |
| H | 0.56957 | -0.01142 | -3.86067 | C | -4.56565 | -0.66404 | 0.74942 |
| C | 0.23176 | 1.52802 | 2.13561 | C | -3.37693 | -0.55342 | 2.85093 |
| O | 0.20976 | 2.11185 | 3.19456 | C | -5.71059 | -1.07977 | 1.41712 |
| N | 0.46333 | 2.1959 | 0.94622 | H | -4.56683 | -0.53742 | -0.33511 |
| C | 0.7903 | 3.61289 | 1.05289 | C | -4.52883 | -0.95478 | 3.51407 |
| H | 1.87034 | 3.7725 | 1.19442 | H | -2.45533 | -0.37679 | 3.40375 |
| H | 0.4613 | 4.12977 | 0.14588 | C | -5.69617 | -1.22034 | 2.80213 |
| H | 0.26898 | 4.01938 | 1.92291 | H | -6.61839 | -1.29392 | 0.85455 |
| C | -1.63382 | -0.71642 | -2.39005 | H | -4.51055 | -1.07467 | 4.5959 |
| C | -2.51862 | -0.63781 | -3.47026 | H | -6.59366 | -1.54389 | 3.32721 |
| C | -3.4744 | -1.65157 | -3.56386 | C | 3.89537 | 0.13132 | 0.29601 |
| C | -2.61809 | -2.64584 | -1.5697 | C | 4.21926 | 1.23918 | 1.09917 |
| C | -3.53246 | -2.6651 | -2.61652 | C | 3.88777 | 1.28261 | 2.44228 |
| H | -4.19285 | -1.62545 | -4.3837 | C | 3.21889 | 0.17558 | 2.97122 |
| H | -2.62548 | -3.37695 | -0.75815 | C | 2.87823 | -0.92455 | 2.18467 |
| H | -4.28599 | -3.4468 | -2.6751 | C | 3.19101 | -0.95167 | 0.82571 |
| C | -2.48596 | 0.50008 | -4.44533 | H | 4.12015 | 2.14522 | 3.06374 |
| H | -2.4998 | 1.46746 | -3.9244 | H | 2.91068 | 0.18736 | 4.01493 |
| H | -1.58814 | 0.48434 | -5.07698 | H | 2.31497 | -1.7492 | 2.61685 |
| H | -3.35628 | 0.46641 | -5.11123 | C | 4.37022 | 0.41814 | -1.05444 |
| N | -1.68666 | -1.69837 | -1.47486 | C | 4.95603 | 1.85826 | -0.98085 |
| Rh | -0.48988 | -0.97724 | 0.5085 | O | 4.37292 | -0.24852 | -2.06488 |
| Cl | -1.21878 | -2.94032 | 1.62574 | O | 5.39828 | 2.51249 | -1.8948 |
| C | 0.05549 | -0.05576 | 2.14604 | N | 4.84958 | 2.23887 | 0.34261 |
| O | 0.19841 | -0.55531 | 3.22635 | C | 5.28609 | 3.51578 | 0.84792 |
| C | -2.21093 | 0.04861 | 0.72701 | H | 4.44334 | 4.09192 | 1.25495 |
| C | -2.0008 | 1.0718 | -0.11212 | H | 6.04185 | 3.38966 | 1.63392 |
| C | -2.7941 | 2.26353 | -0.44848 | H | 5.72567 | 4.06458 | 0.00966 |
| C | -2.39575 | 3.10067 | -1.50334 | C | 2.76434 | -2.10751 | -0.00162 |
| C | -3.93982 | 2.62317 | 0.27941 | C | 3.72084 | -3.01585 | -0.48207 |
| C | -3.1301 | 4.23344 | -1.83843 | C | 3.2568 | -4.1133 | -1.19954 |
| H | -1.49356 | 2.86628 | -2.07245 | C | 1.02949 | -3.33431 | -0.88419 |
| C | -4.66665 | 3.75618 | -0.05553 | C | 1.89763 | -4.27733 | -1.40958 |
| H | -4.25458 | 2.00802 | 1.12051 | H | 3.97174 | -4.84192 | -1.58242 |
| C | -4.27243 | 4.56545 | -1.11935 | H | -0.04473 | -3.44018 | -1.0022 |
| H | -2.80126 | 4.86187 | -2.66525 | H | 1.50569 | -5.13085 | -1.95725 |
| H | -5.55004 | 4.01471 | 0.52667 | C | 5.18687 | -2.83353 | -0.23531 |
| H | -4.8475 | 5.45283 | -1.37837 | H | 5.60723 | -2.09219 | -0.92852 |

| | | | |
|---|---------|----------|----------|
| H | 5.39421 | -2.49121 | 0.78613 |
| H | 5.72428 | -3.77627 | -0.39175 |
| N | 1.44088 | -2.26237 | -0.19288 |

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MeTS_{A1'}-B'(1)

| | | | |
|----|----------|----------|----------|
| C | -3.06741 | -0.38809 | 0.26673 |
| C | -3.79136 | -1.48808 | -0.23669 |
| C | -3.28177 | -2.77383 | -0.20982 |
| C | -1.97228 | -2.94201 | 0.23943 |
| C | -1.20232 | -1.86545 | 0.69732 |
| C | -1.7904 | -0.5854 | 0.83308 |
| H | -3.85473 | -3.6205 | -0.58404 |
| H | -1.50657 | -3.92535 | 0.1962 |
| C | -3.76658 | 0.79932 | -0.21815 |
| C | -5.08444 | 0.28514 | -0.86129 |
| O | -3.4363 | 1.96662 | -0.26908 |
| O | -5.97549 | 0.95697 | -1.32295 |
| N | -5.00771 | -1.0862 | -0.81156 |
| C | -5.99021 | -1.96978 | -1.38416 |
| H | -5.56226 | -2.55309 | -2.21079 |
| H | -6.38795 | -2.66021 | -0.62926 |
| H | -6.80324 | -1.34594 | -1.76735 |
| C | -0.9517 | 0.41937 | 1.49472 |
| C | -1.36953 | 1.57417 | 2.18444 |
| C | -0.37468 | 2.42772 | 2.66879 |
| C | 1.29342 | 0.87625 | 2.00058 |
| C | 0.96722 | 2.10521 | 2.55615 |
| H | -0.67521 | 3.34873 | 3.1687 |
| H | 2.32379 | 0.5286 | 1.94676 |
| H | 1.75052 | 2.77335 | 2.90647 |
| C | -2.79157 | 1.89653 | 2.52435 |
| H | -2.83717 | 2.3 | 3.54355 |
| H | -3.21769 | 2.64369 | 1.84502 |
| H | -3.43595 | 1.01136 | 2.48343 |
| N | 0.36729 | 0.06693 | 1.48471 |
| Rh | 0.78717 | -1.82653 | 0.76135 |
| Cl | 1.16187 | -4.04248 | 0.02919 |
| H | -0.09304 | -2.39344 | 1.92898 |

| | | | |
|---|----------|----------|----------|
| C | 1.57859 | 1.57586 | -1.07539 |
| C | 0.31767 | 2.12386 | -1.37359 |
| C | -0.65032 | 1.39058 | -2.04189 |
| C | -0.33686 | 0.07205 | -2.37435 |
| C | 0.88352 | -0.50989 | -2.02786 |
| C | 1.86068 | 0.23904 | -1.36295 |
| H | -1.62681 | 1.81449 | -2.26637 |
| H | -1.08343 | -0.53702 | -2.8828 |
| H | 1.07398 | -1.55843 | -2.25468 |
| C | 2.31115 | 2.58009 | -0.30443 |
| C | 1.32581 | 3.77262 | -0.15232 |
| O | 3.42814 | 2.56868 | 0.16456 |
| O | 1.50925 | 4.78765 | 0.47616 |
| N | 0.19485 | 3.41857 | -0.85774 |
| C | -1.01762 | 4.20525 | -0.87672 |
| H | -1.27812 | 4.4969 | -1.90223 |
| H | -1.85213 | 3.63843 | -0.443 |
| H | -0.82566 | 5.10633 | -0.28661 |
| C | 3.07941 | -0.44325 | -0.85737 |
| C | 4.36854 | -0.15658 | -1.32207 |
| C | 5.41478 | -0.90927 | -0.79195 |
| C | 3.85864 | -2.12693 | 0.5414 |
| C | 5.16738 | -1.90113 | 0.14551 |
| H | 6.43166 | -0.71549 | -1.13342 |
| H | 3.59044 | -2.91417 | 1.24291 |
| H | 5.97241 | -2.50401 | 0.55757 |
| C | 4.62386 | 0.91183 | -2.33776 |
| H | 3.84552 | 0.93803 | -3.11006 |
| H | 4.64589 | 1.89802 | -1.85339 |
| H | 5.59035 | 0.75861 | -2.83187 |
| N | 2.84083 | -1.40261 | 0.05988 |

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MeTS_{A1'}-B'(2)

| | | | |
|---|---------|----------|----------|
| C | 2.57441 | -0.25637 | -0.00201 |
| C | 3.03264 | -1.55946 | -0.27291 |
| C | 2.17486 | -2.53784 | -0.72897 |
| C | 0.82752 | -2.19283 | -0.86536 |
| C | 0.32042 | -0.91384 | -0.59621 |

| | | | | | | | |
|---|----------|----------|----------|---|----------|----------|----------|
| C | 1.23201 | 0.09629 | -0.19191 | H | -3.71198 | -3.64883 | 0.076 |
| H | 2.51865 | -3.54575 | -0.95442 | Rh | -1.66676 | -0.28114 | -0.34036 |
| H | 0.14656 | -2.97065 | -1.21325 | Cl | -1.53513 | 1.31369 | -2.14454 |
| C | 3.70858 | 0.46675 | 0.59072 | H | -3.94932 | 0.18017 | -1.72623 |
| C | 4.89802 | -0.53485 | 0.5656 | H | -3.5549 | 1.5665 | 0.13048 |
| O | 3.80113 | 1.58081 | 1.05015 | H | -1.47542 | -2.92558 | 0.20748 |
| O | 6.02706 | -0.33681 | 0.94304 | H | -0.72545 | -1.41221 | 1.88292 |
| N | 4.39476 | -1.69676 | 0.01899 | H | -4.09328 | -2.18248 | -1.71632 |
| C | 5.16214 | -2.90214 | -0.15528 | H | -1.02933 | -1.13908 | -1.5078 |
| H | 4.75788 | -3.72024 | 0.4562 | | | | |
| H | 5.17093 | -3.21352 | -1.20804 | | | | |
| H | 6.18548 | -2.68513 | 0.16532 | | | | |
| C | 0.73779 | 1.4582 | 0.12431 | | | | |
| C | 1.31441 | 2.6319 | -0.38478 | | | | |
| C | 0.74072 | 3.83931 | 0.01344 | | | | |
| C | -0.9087 | 2.64703 | 1.23127 | | | | |
| C | -0.36217 | 3.86369 | 0.85058 | | | | |
| H | 1.16084 | 4.77041 | -0.368 | | | | |
| H | -1.819 | 2.6049 | 1.83288 | | | | |
| H | -0.81387 | 4.80015 | 1.16918 | | | | |
| C | 2.42228 | 2.65463 | -1.39044 | | | | |
| H | 2.2206 | 3.42265 | -2.14746 | | | | |
| H | 3.38387 | 2.89217 | -0.91841 | | | | |
| H | 2.52593 | 1.69679 | -1.91208 | | | | |
| N | -0.38074 | 1.47759 | 0.87857 | | | | |
| C | -3.88977 | -0.31448 | -0.75619 | | | | |
| C | -3.65641 | 0.49909 | 0.3416 | | | | |
| C | -2.20978 | -2.20637 | 0.57276 | | | | |
| C | -3.88412 | 0.10281 | 1.7868 | | | | |
| C | -1.76391 | -1.31927 | 1.55552 | | | | |
| C | -2.6413 | -0.49874 | 2.46521 | | | | |
| H | -4.19405 | 0.99186 | 2.35293 | | | | |
| H | -4.73337 | -0.59143 | 1.85112 | | | | |
| H | -2.01628 | 0.31392 | 2.85903 | | | | |
| H | -2.93936 | -1.10179 | 3.34068 | | | | |
| C | -4.33517 | -1.75125 | -0.7351 | | | | |
| H | -5.43391 | -1.80697 | -0.64188 | | | | |
| C | -3.66103 | -2.58733 | 0.35306 | | | | |
| H | -4.20417 | -2.50477 | 1.30427 | | | | |
| | | | | 53 | | | |
| | | | | Me^eTS_{A1'-B'}(3) | | | |
| | | | | C | -2.64356 | -0.06934 | 0.14314 |
| | | | | C | -3.23376 | -1.33472 | 0.30795 |
| | | | | C | -2.46204 | -2.46812 | 0.46059 |
| | | | | C | -1.07711 | -2.30951 | 0.4148 |
| | | | | C | -0.43983 | -1.06597 | 0.28199 |
| | | | | C | -1.24734 | 0.08627 | 0.15083 |
| | | | | H | -2.90566 | -3.45669 | 0.56269 |
| | | | | H | -0.4654 | -3.21073 | 0.45336 |
| | | | | C | -3.73482 | 0.85674 | -0.17847 |
| | | | | C | -5.03739 | 0.01247 | -0.08655 |
| | | | | O | -3.73554 | 2.02762 | -0.48315 |
| | | | | O | -6.16943 | 0.39806 | -0.24966 |
| | | | | N | -4.63008 | -1.26716 | 0.225 |
| | | | | C | -5.5243 | -2.39002 | 0.33836 |
| | | | | H | -5.32001 | -3.13878 | -0.43886 |
| | | | | H | -5.43555 | -2.86473 | 1.3243 |
| | | | | H | -6.54168 | -2.00799 | 0.21134 |
| | | | | C | -0.62575 | 1.39621 | -0.16124 |
| | | | | C | -0.94324 | 2.60607 | 0.47904 |
| | | | | C | -0.29037 | 3.75282 | 0.01831 |
| | | | | C | 0.91777 | 2.42935 | -1.54118 |
| | | | | C | 0.62296 | 3.68489 | -1.0215 |
| | | | | H | -0.51019 | 4.70851 | 0.49558 |
| | | | | H | 1.65915 | 2.30138 | -2.33181 |
| | | | | H | 1.11445 | 4.57626 | -1.40483 |
| | | | | C | -1.86653 | 2.7208 | 1.65264 |
| | | | | H | -1.45341 | 3.41679 | 2.39406 |

| | | | | | | | |
|----|----------|----------|----------|----|----------|----------|----------|
| H | -2.84529 | 3.1037 | 1.33833 | C | -4.83429 | -0.74029 | -0.67636 |
| H | -2.03066 | 1.75648 | 2.14698 | O | -3.87146 | 1.39192 | -1.34139 |
| N | 0.33294 | 1.31729 | -1.10751 | O | -5.95752 | -0.66932 | -1.11089 |
| C | 2.17773 | -0.27413 | 1.9156 | N | -4.26547 | -1.80797 | -0.01105 |
| C | 2.27355 | 0.92964 | 1.22559 | C | -4.94681 | -3.05261 | 0.23714 |
| C | 3.7435 | -1.36365 | -0.22275 | H | -4.44194 | -3.8855 | -0.27036 |
| C | 3.5748 | 1.57571 | 0.79266 | H | -4.99704 | -3.26645 | 1.31263 |
| C | 3.62313 | -0.22747 | -1.01481 | H | -5.96147 | -2.95102 | -0.15913 |
| C | 4.05244 | 1.15829 | -0.60641 | C | -0.78921 | 1.60062 | -0.08354 |
| H | 3.43967 | 2.66548 | 0.81236 | C | -1.48767 | 2.77864 | 0.22589 |
| H | 4.34755 | 1.35933 | 1.54463 | C | -0.88607 | 3.98803 | -0.1319 |
| H | 3.64891 | 1.8659 | -1.34241 | C | 1.02503 | 2.81316 | -0.89972 |
| H | 5.14946 | 1.2577 | -0.67433 | C | 0.3558 | 4.01754 | -0.73974 |
| C | 3.31819 | -1.19544 | 2.27225 | H | -1.41082 | 4.91706 | 0.0911 |
| H | 3.79658 | -0.84781 | 3.20444 | H | 2.03627 | 2.7831 | -1.30291 |
| C | 4.35837 | -1.36051 | 1.15957 | H | 0.82607 | 4.95179 | -1.03497 |
| H | 5.11535 | -0.56621 | 1.21948 | C | -2.77309 | 2.82075 | 0.99009 |
| H | 4.90084 | -2.30193 | 1.31621 | H | -3.63678 | 2.87601 | 0.31704 |
| Rh | 1.6096 | -0.67589 | -0.19414 | H | -2.89738 | 1.94124 | 1.63165 |
| Cl | 1.1977 | -2.08339 | -2.06088 | H | -2.78704 | 3.70731 | 1.63552 |
| H | 1.27222 | -0.4197 | 2.51026 | N | 0.48398 | 1.64614 | -0.55617 |
| H | 1.41912 | 1.60291 | 1.3117 | C | 3.60433 | 0.70502 | -0.34413 |
| H | 3.63803 | -2.32922 | -0.71839 | C | 3.28257 | 0.18696 | -1.59731 |
| H | 3.46248 | -0.38773 | -2.0837 | C | 2.74038 | -1.78187 | 0.68402 |
| H | 2.88708 | -2.17965 | 2.50301 | C | 3.83871 | -1.1119 | -2.14084 |
| H | 0.96538 | -1.72933 | 0.77452 | C | 2.18847 | -2.19981 | -0.53516 |
| | | | | C | 2.9133 | -2.29967 | -1.85408 |
| | | | | H | 3.98244 | -1.021 | -3.22573 |
| | | | | H | 4.83959 | -1.28792 | -1.72386 |
| | | | | H | 2.1476 | -2.35134 | -2.64133 |
| | | | | H | 3.47286 | -3.24994 | -1.91258 |
| | | | | C | 4.47593 | 0.058 | 0.70175 |
| | | | | H | 5.54233 | 0.23245 | 0.47514 |
| | | | | C | 4.20212 | -1.43831 | 0.88841 |
| | | | | H | 4.82427 | -2.04019 | 0.2111 |
| | | | | H | 4.49903 | -1.72943 | 1.90422 |
| | | | | Rh | 1.61671 | -0.16971 | -0.19673 |
| | | | | Cl | 1.03543 | 0.62311 | 2.99962 |
| | | | | H | 3.43949 | 1.77265 | -0.1732 |

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Me⁺TS_{AI'-B'}(4)

| | | | | | | | |
|---|----------|----------|----------|----|---------|----------|----------|
| C | -2.5753 | -0.21872 | -0.03936 | H | 2.1476 | -2.35134 | -2.64133 |
| C | -2.93391 | -1.53717 | 0.31528 | H | 3.47286 | -3.24994 | -1.91258 |
| C | -2.0265 | -2.41283 | 0.88254 | C | 4.47593 | 0.058 | 0.70175 |
| C | -0.70782 | -1.97136 | 1.002 | H | 5.54233 | 0.23245 | 0.47514 |
| C | -0.2806 | -0.69141 | 0.62246 | C | 4.20212 | -1.43831 | 0.88841 |
| C | -1.2636 | 0.22527 | 0.16985 | H | 4.82427 | -2.04019 | 0.2111 |
| H | -2.31689 | -3.41832 | 1.1823 | H | 4.49903 | -1.72943 | 1.90422 |
| H | 0.02505 | -2.66992 | 1.41263 | Rh | 1.61671 | -0.16971 | -0.19673 |
| H | 0.57716 | -0.04611 | 1.74494 | Cl | 1.03543 | 0.62311 | 2.99962 |
| C | -3.72603 | 0.34625 | -0.75015 | H | 3.43949 | 1.77265 | -0.1732 |

| | | | | | | | |
|-----------------------------|----------|----------|----------|---|----------|----------|----------|
| H | 2.87261 | 0.87667 | -2.34051 | H | 0.78189 | 0.003 | -1.41594 |
| H | 2.19609 | -2.03624 | 1.59778 | C | -1.22911 | -0.30821 | 2.58157 |
| H | 1.26757 | -2.78723 | -0.49692 | C | -0.65145 | 0.75442 | 2.74451 |
| H | 4.27448 | 0.57294 | 1.65081 | C | -1.97144 | -1.51927 | 2.45294 |
| 88 MeC'(1) | | | | C | -1.4929 | -2.72623 | 2.98473 |
| | | | | C | -3.19878 | -1.51531 | 1.77187 |
| | | | | C | -2.22323 | -3.89728 | 2.82922 |
| | | | | H | -0.54624 | -2.73501 | 3.52454 |
| C | -3.59045 | 0.76243 | -1.20131 | C | -3.91593 | -2.6914 | 1.60406 |
| C | -3.73194 | 2.15927 | -1.10287 | H | -3.57543 | -0.57505 | 1.37112 |
| C | -2.64975 | 2.98394 | -0.85154 | C | -3.43016 | -3.88511 | 2.13347 |
| C | -1.41416 | 2.38071 | -0.60326 | H | -1.84601 | -4.82738 | 3.2518 |
| C | -1.23655 | 0.99145 | -0.64996 | H | -4.85092 | -2.66661 | 1.04645 |
| C | -2.3162 | 0.1754 | -1.05838 | H | -3.99486 | -4.8074 | 2.00705 |
| H | -2.76317 | 4.0658 | -0.79117 | C | -0.04202 | 2.01214 | 3.01851 |
| H | -0.55866 | 2.99978 | -0.33335 | C | -0.73997 | 3.19932 | 2.75705 |
| C | -4.94666 | 0.21686 | -1.16078 | C | 1.25942 | 2.0762 | 3.53222 |
| C | -5.8981 | 1.44417 | -1.24124 | C | -0.13835 | 4.42556 | 3.00141 |
| O | -5.35104 | -0.91485 | -0.99313 | H | -1.74964 | 3.14139 | 2.35199 |
| O | -7.10434 | 1.42612 | -1.30538 | C | 1.85089 | 3.30552 | 3.78035 |
| N | -5.07833 | 2.5478 | -1.21076 | H | 1.81044 | 1.15292 | 3.70611 |
| C | -5.55351 | 3.90594 | -1.18743 | C | 1.15555 | 4.48137 | 3.51333 |
| H | -5.28626 | 4.40294 | -0.24473 | H | -0.68167 | 5.34538 | 2.79084 |
| H | -5.13722 | 4.48295 | -2.02355 | H | 2.86817 | 3.3466 | 4.16412 |
| H | -6.64329 | 3.87166 | -1.27863 | H | 1.6265 | 5.44557 | 3.69704 |
| C | -1.99798 | -1.24839 | -1.20474 | C | 3.77363 | -0.12685 | -1.39795 |
| C | -2.63094 | -2.19144 | -2.03431 | C | 3.74386 | 0.51051 | -2.6455 |
| C | -2.21206 | -3.5199 | -1.93082 | C | 3.13459 | -0.09055 | -3.73642 |
| C | -0.50621 | -2.87311 | -0.41386 | C | 2.54796 | -1.34392 | -3.53845 |
| C | -1.18092 | -3.88381 | -1.08261 | C | 2.53435 | -1.96515 | -2.29083 |
| H | -2.70494 | -4.26995 | -2.55003 | C | 3.13301 | -1.3377 | -1.19411 |
| H | 0.37239 | -3.07493 | 0.19663 | H | 3.10445 | 0.39189 | -4.71152 |
| H | -0.86496 | -4.91823 | -0.97487 | H | 2.06761 | -1.8381 | -4.38158 |
| C | -3.63712 | -1.85338 | -3.08981 | H | 2.02129 | -2.91765 | -2.15505 |
| H | -3.42497 | -2.43818 | -3.99408 | C | 4.51367 | 0.73769 | -0.46816 |
| H | -4.65813 | -2.08409 | -2.76596 | C | 4.83541 | 2.01383 | -1.29348 |
| H | -3.6095 | -0.79245 | -3.36117 | O | 4.92194 | 0.51502 | 0.6462 |
| N | -0.88414 | -1.59851 | -0.49755 | O | 5.40973 | 3.00813 | -0.92787 |
| Rh | 0.33415 | -0.00049 | 0.04056 | N | 4.37255 | 1.75309 | -2.57834 |
| Cl | 1.74676 | 1.90179 | 0.20996 | | | | |

| | | | | | | | |
|---|---------|----------|----------|----|----------|----------|----------|
| C | 4.4237 | 2.7118 | -3.65048 | C | -2.04082 | 3.00411 | -3.05787 |
| H | 4.97213 | 2.31129 | -4.51352 | C | 0.05569 | 2.19737 | -2.28776 |
| H | 3.4121 | 2.99923 | -3.9675 | C | -0.66113 | 3.07304 | -3.0923 |
| H | 4.94554 | 3.59547 | -3.27106 | H | -2.63997 | 3.73447 | -3.60247 |
| C | 3.02142 | -1.84715 | 0.19582 | H | 1.14034 | 2.23394 | -2.17853 |
| C | 3.95102 | -2.75618 | 0.71626 | H | -0.13871 | 3.82521 | -3.67784 |
| C | 3.81168 | -3.12042 | 2.05199 | C | -4.19651 | 2.13742 | -2.20732 |
| C | 1.9238 | -1.67531 | 2.21549 | H | -4.48171 | 3.19738 | -2.21516 |
| C | 2.7955 | -2.56789 | 2.81871 | H | -4.70379 | 1.64078 | -3.04188 |
| H | 4.51895 | -3.8241 | 2.49144 | H | -4.58366 | 1.6908 | -1.28352 |
| H | 1.10978 | -1.20886 | 2.77102 | N | -0.56129 | 1.25949 | -1.56936 |
| H | 2.67824 | -2.81815 | 3.87067 | Rh | 0.40458 | 0.26802 | -0.04645 |
| C | 5.08017 | -3.26617 | -0.12371 | Cl | 2.70179 | 0.86734 | -0.83494 |
| H | 5.60481 | -4.08767 | 0.37813 | H | 0.52851 | -0.94666 | -0.94665 |
| H | 4.73753 | -3.62356 | -1.10279 | C | -0.64101 | 2.52677 | 1.62386 |
| H | 5.81243 | -2.46842 | -0.31169 | C | 0.42374 | 2.96817 | 1.22102 |
| N | 2.01665 | -1.33009 | 0.9248 | C | -1.89679 | 2.10758 | 2.15523 |

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MeC'(2)

| | | | | | | | |
|---|----------|----------|----------|---|----------|----------|----------|
| C | -3.58376 | -0.74136 | -0.91823 | C | -3.06856 | 2.2629 | 1.39922 |
| C | -3.95852 | -1.66342 | 0.07744 | C | -3.21164 | 1.11279 | 3.92952 |
| C | -3.1543 | -1.92271 | 1.17031 | H | -1.08433 | 1.43051 | 4.03544 |
| C | -1.89314 | -1.31992 | 1.2008 | C | -4.29124 | 1.84411 | 1.90432 |
| C | -1.45909 | -0.41854 | 0.22375 | H | -2.99917 | 2.71176 | 0.40809 |
| C | -2.3691 | -0.03973 | -0.7971 | C | -4.36679 | 1.26082 | 3.16684 |
| H | -3.4627 | -2.61771 | 1.95029 | H | -3.26697 | 0.67004 | 4.92267 |
| H | -1.22367 | -1.57966 | 2.0232 | H | -5.19345 | 1.97172 | 1.30729 |
| C | -4.52567 | -0.93704 | -2.02458 | H | -5.3267 | 0.92905 | 3.55882 |
| C | -5.59655 | -1.93153 | -1.49533 | C | 1.61875 | 3.6202 | 0.79893 |
| O | -4.51489 | -0.53512 | -3.16664 | C | 1.54933 | 4.64683 | -0.15401 |
| O | -6.5888 | -2.30899 | -2.07222 | C | 2.86256 | 3.25074 | 1.327 |
| N | -5.17404 | -2.29488 | -0.23784 | C | 2.70736 | 5.28946 | -0.56795 |
| C | -5.85354 | -3.25126 | 0.59384 | H | 0.57797 | 4.93227 | -0.55712 |
| H | -5.21642 | -4.12295 | 0.79775 | C | 4.01382 | 3.90427 | 0.91472 |
| H | -6.15435 | -2.80129 | 1.54961 | H | 2.91973 | 2.4242 | 2.03357 |
| H | -6.74644 | -3.5766 | 0.05121 | C | 3.9397 | 4.91998 | -0.03377 |
| C | -1.91528 | 1.08071 | -1.63175 | H | 2.64877 | 6.08509 | -1.30888 |
| C | -2.70689 | 2.02499 | -2.31239 | H | 4.97761 | 3.59832 | 1.31594 |
| | | | | H | 4.84753 | 5.42229 | -0.36355 |
| | | | | C | 3.06413 | -2.29685 | -0.39465 |

| | | | | | | | |
|---|---------|----------|----------|----|----------|----------|----------|
| C | 3.31592 | -2.63245 | -1.73038 | H | -4.98621 | -0.05549 | -2.14025 |
| C | 2.41116 | -3.39988 | -2.44839 | H | -2.88172 | -1.37399 | -2.03687 |
| C | 1.24908 | -3.8154 | -1.7908 | C | -3.39991 | 3.34446 | 0.23181 |
| C | 0.97142 | -3.45275 | -0.47358 | C | -4.8181 | 3.62814 | -0.33783 |
| C | 1.87991 | -2.65349 | 0.22792 | O | -2.69724 | 4.21937 | 0.68917 |
| H | 2.5886 | -3.66945 | -3.48769 | O | -5.43672 | 4.66383 | -0.2666 |
| H | 0.52833 | -4.42367 | -2.33472 | N | -5.21162 | 2.46066 | -0.94773 |
| H | 0.03087 | -3.74579 | -0.00761 | C | -6.439 | 2.30934 | -1.68213 |
| C | 4.21086 | -1.52388 | 0.10331 | H | -6.24284 | 2.1143 | -2.74552 |
| C | 5.12896 | -1.34974 | -1.13617 | H | -7.04357 | 1.48716 | -1.27677 |
| O | 4.50042 | -1.20634 | 1.23278 | H | -6.99336 | 3.2478 | -1.58458 |
| O | 6.17765 | -0.76056 | -1.20748 | C | -0.86912 | 1.35315 | 1.0295 |
| N | 4.52553 | -2.08447 | -2.15293 | C | -0.82489 | 2.14452 | 2.19335 |
| C | 5.03473 | -2.13834 | -3.49789 | C | 0.42522 | 2.35995 | 2.78047 |
| H | 5.24549 | -3.17276 | -3.80095 | C | 1.39172 | 0.779 | 1.31014 |
| H | 4.32165 | -1.69325 | -4.20485 | C | 1.56002 | 1.71843 | 2.31752 |
| H | 5.96457 | -1.5618 | -3.51476 | H | 0.48058 | 3.01056 | 3.65417 |
| C | 1.62476 | -2.07722 | 1.56987 | H | 2.19975 | 0.11532 | 1.01371 |
| C | 1.9423 | -2.79488 | 2.7299 | H | 2.5407 | 1.86317 | 2.76596 |
| C | 1.7991 | -2.14981 | 3.95341 | C | -2.03149 | 2.64418 | 2.92641 |
| C | 1.09128 | -0.19017 | 2.79954 | H | -1.90305 | 2.43746 | 3.99852 |
| C | 1.38836 | -0.82485 | 3.99156 | H | -2.17915 | 3.72199 | 2.80004 |
| H | 2.04309 | -2.68262 | 4.87228 | H | -2.94955 | 2.14656 | 2.59525 |
| H | 0.76602 | 0.84837 | 2.7685 | N | 0.22658 | 0.61276 | 0.68597 |
| H | 1.30081 | -0.28295 | 4.93032 | Rh | -0.0983 | -0.92101 | -0.65601 |
| C | 2.48969 | -4.18535 | 2.63902 | Cl | -0.54679 | -2.5423 | -2.34538 |
| H | 2.58464 | -4.63542 | 3.63392 | H | 0.16294 | 0.03982 | -1.80847 |
| H | 1.86089 | -4.84043 | 2.02344 | C | -1.4257 | -2.74612 | 1.22813 |
| H | 3.48785 | -4.17324 | 2.179 | C | -0.54945 | -2.28264 | 1.94089 |
| N | 1.17392 | -0.80603 | 1.60946 | C | -2.53137 | -3.29996 | 0.52082 |

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MeC'(3)

| | | | | | | | |
|---|----------|----------|----------|---|----------|----------|----------|
| C | -3.14079 | 1.9273 | -0.03239 | H | -1.39515 | -4.84854 | -0.45384 |
| C | -4.19881 | 1.49014 | -0.85087 | C | -4.89151 | -3.23159 | -0.00471 |
| C | -4.15503 | 0.28134 | -1.52159 | H | -3.89985 | -1.83745 | 1.31217 |
| C | -2.97354 | -0.45864 | -1.45097 | C | -4.73532 | -4.33557 | -0.83949 |
| C | -1.88553 | -0.056 | -0.66612 | H | -3.35748 | -5.77853 | -1.65346 |
| C | -2.00485 | 1.10483 | 0.13582 | H | -5.86862 | -2.76529 | 0.11249 |

| | | | | | | | |
|---|----------|----------|----------|-----------------|----------|----------|----------|
| H | -5.5936 | -4.73929 | -1.37433 | H | 6.35997 | -2.09477 | -2.03113 |
| C | 0.29383 | -1.7577 | 2.96742 | H | 5.36705 | -0.84614 | -2.8112 |
| C | -0.27804 | -0.91256 | 3.93255 | H | 5.98209 | -0.59454 | -1.16974 |
| C | 1.65507 | -2.08051 | 3.0687 | N | 2.01308 | -1.85452 | -0.7052 |
| C | 0.49386 | -0.40601 | 4.9683 | | | | |
| H | -1.33645 | -0.66484 | 3.85422 | 88 | | | |
| C | 2.42159 | -1.56687 | 4.1066 | MeC1'(1) | | | |
| H | 2.1079 | -2.73526 | 2.32523 | C | -3.72977 | -1.21002 | 0.5203 |
| C | 1.84553 | -0.72978 | 5.05894 | C | -3.84746 | -1.44752 | 1.90365 |
| H | 0.03726 | 0.2493 | 5.70941 | C | -2.85172 | -1.0965 | 2.79375 |
| H | 3.47812 | -1.82065 | 4.16974 | C | -1.6647 | -0.58515 | 2.26103 |
| H | 2.45024 | -0.33081 | 5.87143 | C | -1.50111 | -0.36288 | 0.8959 |
| C | 3.40315 | 1.20118 | -1.3032 | C | -2.57961 | -0.57879 | 0.00545 |
| C | 3.13716 | 2.44606 | -1.903 | H | -2.95376 | -1.27435 | 3.863 |
| C | 2.48619 | 2.53477 | -3.12035 | H | -0.83592 | -0.37515 | 2.93585 |
| C | 2.09041 | 1.33791 | -3.7234 | C | -4.81967 | -1.96843 | -0.10894 |
| C | 2.30957 | 0.09935 | -3.12404 | C | -5.69324 | -2.49952 | 1.06091 |
| C | 2.96095 | 0.01647 | -1.88931 | O | -5.03374 | -2.2587 | -1.26332 |
| H | 2.28218 | 3.49447 | -3.59056 | O | -6.72888 | -3.11527 | 0.97514 |
| H | 1.57159 | 1.37587 | -4.6795 | N | -5.03837 | -2.12527 | 2.21135 |
| H | 1.93197 | -0.81139 | -3.58661 | C | -5.46127 | -2.49865 | 3.53473 |
| C | 4.10008 | 1.46859 | -0.04723 | H | -4.74031 | -3.18279 | 4.00338 |
| C | 4.17213 | 3.01808 | 0.0577 | H | -5.58046 | -1.61392 | 4.17396 |
| O | 4.55172 | 0.71749 | 0.78945 | H | -6.4258 | -3.00594 | 3.43574 |
| O | 4.6258 | 3.66347 | 0.97121 | C | -2.37295 | -0.18756 | -1.40144 |
| N | 3.60377 | 3.4978 | -1.10509 | C | -3.34912 | 0.12677 | -2.36642 |
| C | 3.42554 | 4.89931 | -1.39237 | C | -2.90374 | 0.30074 | -3.681 |
| H | 3.92944 | 5.17521 | -2.32765 | C | -0.65632 | 0.03758 | -2.97682 |
| H | 2.35983 | 5.15195 | -1.46806 | C | -1.56613 | 0.18555 | -4.01685 |
| H | 3.87054 | 5.46022 | -0.56529 | H | -3.64446 | 0.5258 | -4.4493 |
| C | 3.12087 | -1.31457 | -1.24231 | H | 0.42212 | 0.01515 | -3.14114 |
| C | 4.35189 | -1.98596 | -1.27924 | H | -1.22449 | 0.26384 | -5.04564 |
| C | 4.39314 | -3.27341 | -0.75234 | C | -4.78905 | 0.41251 | -2.07438 |
| C | 2.07759 | -3.1031 | -0.22458 | H | -5.07706 | 1.34057 | -2.58702 |
| C | 3.24541 | -3.84808 | -0.22561 | H | -5.44419 | -0.39353 | -2.42306 |
| H | 5.33144 | -3.82789 | -0.77222 | H | -4.97494 | 0.55233 | -1.00397 |
| H | 1.14468 | -3.50602 | 0.17123 | N | -1.05955 | -0.08287 | -1.71951 |
| H | 3.24803 | -4.86031 | 0.17133 | Rh | 0.2155 | 0.18252 | 0.06584 |
| C | 5.57623 | -1.3481 | -1.85809 | H | 1.04041 | -0.04253 | 1.3696 |

| | | | | | | | |
|---|----------|----------|----------|----|----------|----------|----------|
| C | -0.51434 | 2.22214 | 0.24132 | H | 4.53709 | -5.44951 | 1.06382 |
| C | 0.33039 | 2.00652 | 1.15374 | H | 2.7774 | -5.21112 | 1.3089 |
| C | -1.64993 | 2.83752 | -0.39755 | H | 3.38206 | -5.9325 | -0.21055 |
| C | -2.90309 | 2.76663 | 0.23407 | C | 3.47188 | 0.78668 | -0.77793 |
| C | -1.54744 | 3.51297 | -1.62086 | C | 4.5266 | 1.46267 | -1.41193 |
| C | -4.01685 | 3.35558 | -0.34898 | C | 4.19764 | 2.43902 | -2.34465 |
| H | -2.98517 | 2.24619 | 1.18775 | C | 1.89831 | 1.98488 | -1.94216 |
| C | -2.66798 | 4.09244 | -2.2027 | C | 2.86466 | 2.70603 | -2.62199 |
| H | -0.57678 | 3.60116 | -2.10588 | H | 4.99226 | 2.9755 | -2.86347 |
| C | -3.90564 | 4.01452 | -1.5707 | H | 0.83991 | 2.15552 | -2.13165 |
| H | -4.98142 | 3.29551 | 0.15312 | H | 2.57491 | 3.45516 | -3.35507 |
| H | -2.57099 | 4.61518 | -3.15279 | C | 5.952 | 1.09863 | -1.13102 |
| H | -4.7821 | 4.47257 | -2.0263 | H | 6.63729 | 1.71842 | -1.72077 |
| C | 1.09425 | 2.50668 | 2.2735 | H | 6.2082 | 1.22029 | -0.07071 |
| C | 1.79271 | 1.69009 | 3.16872 | H | 6.14299 | 0.04659 | -1.38464 |
| C | 1.10459 | 3.89664 | 2.48043 | N | 2.17988 | 1.04252 | -1.03544 |
| C | 2.48396 | 2.24608 | 4.239 | Cl | 0.65171 | -2.17797 | -0.21614 |
| H | 1.79908 | 0.61143 | 3.0128 | | | | |
| C | 1.79753 | 4.44741 | 3.54793 | | | | |
| H | 0.55742 | 4.53373 | 1.78636 | | | | |
| C | 2.492 | 3.62384 | 4.43182 | C | 1.76177 | -2.02301 | 1.14477 |
| H | 3.02257 | 1.59428 | 4.92596 | C | 1.45291 | -2.02899 | 2.51819 |
| H | 1.79725 | 5.52662 | 3.69135 | C | 0.20421 | -1.67045 | 2.98489 |
| H | 3.0379 | 4.05708 | 5.26812 | C | -0.7206 | -1.19193 | 2.05045 |
| C | 3.69155 | -1.61803 | -0.27476 | C | -0.42798 | -1.08231 | 0.68954 |
| C | 3.86879 | -2.6998 | 0.59808 | C | 0.79798 | -1.60664 | 0.20653 |
| C | 4.166 | -2.49216 | 1.93504 | H | -0.03923 | -1.70088 | 4.046 |
| C | 4.28626 | -1.16871 | 2.37077 | H | -1.69219 | -0.85596 | 2.41269 |
| C | 4.10005 | -0.08725 | 1.5123 | C | 3.20894 | -2.20311 | 1.05398 |
| C | 3.76781 | -0.31128 | 0.17331 | C | 3.7079 | -2.37622 | 2.51234 |
| H | 4.29298 | -3.32134 | 2.62822 | O | 3.97393 | -2.16253 | 0.11366 |
| H | 4.52462 | -0.97792 | 3.41708 | O | 4.85844 | -2.49084 | 2.87066 |
| H | 4.17551 | 0.93363 | 1.88722 | N | 2.58348 | -2.33616 | 3.29924 |
| C | 3.35958 | -2.15605 | -1.59969 | C | 2.61211 | -2.3168 | 4.73798 |
| C | 3.3088 | -3.69454 | -1.39401 | H | 2.30318 | -1.33336 | 5.12287 |
| O | 3.22126 | -1.59352 | -2.6606 | H | 1.94783 | -3.08404 | 5.15509 |
| O | 3.04963 | -4.54146 | -2.21168 | H | 3.64084 | -2.52053 | 5.04995 |
| N | 3.67013 | -3.9071 | -0.06913 | C | 1.00058 | -1.53269 | -1.24772 |
| C | 3.59054 | -5.19451 | 0.56971 | C | 1.82759 | -2.33024 | -2.05121 |

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MeC1'(2)

| | | | | | | | |
|----|----------|----------|----------|---|----------|----------|----------|
| C | 1.97748 | -1.94339 | -3.39133 | C | 3.76526 | 0.91588 | 0.3559 |
| C | 0.33121 | -0.25628 | -3.10881 | C | 3.77048 | 0.80561 | 1.73816 |
| C | 1.28195 | -0.8748 | -3.91719 | C | 2.61442 | 1.20619 | 2.41082 |
| H | 2.64615 | -2.52782 | -4.02408 | C | 1.51066 | 1.73129 | 1.74038 |
| H | -0.37269 | 0.48571 | -3.48282 | C | 1.51251 | 1.86405 | 0.34731 |
| H | 1.41411 | -0.55384 | -4.94617 | H | 4.63587 | 0.42333 | 2.27702 |
| C | 2.42028 | -3.63998 | -1.63146 | H | 2.58121 | 1.1208 | 3.49717 |
| H | 2.14821 | -4.40131 | -2.37531 | H | 0.65363 | 2.07936 | 2.31439 |
| H | 3.51285 | -3.59921 | -1.57323 | C | 2.9784 | 1.39656 | -1.75834 |
| H | 2.04507 | -3.97766 | -0.66012 | C | 4.40753 | 0.78556 | -1.83171 |
| N | 0.19719 | -0.59334 | -1.83189 | O | 2.34906 | 1.76589 | -2.72353 |
| Rh | -1.53789 | -0.18157 | -0.72332 | O | 5.05104 | 0.55835 | -2.82687 |
| Cl | -2.82809 | 0.50171 | -2.79099 | N | 4.79474 | 0.58251 | -0.52082 |
| H | -1.8615 | -1.65457 | -1.02874 | C | 6.06655 | 0.01765 | -0.12877 |
| C | -3.52022 | -0.68497 | 0.00568 | H | 6.63813 | 0.73426 | 0.47552 |
| C | -3.13336 | 0.30209 | 0.67744 | H | 5.9146 | -0.91319 | 0.43179 |
| C | -4.39818 | -1.76609 | -0.3534 | H | 6.61845 | -0.1986 | -1.048 |
| C | -5.31003 | -2.2018 | 0.62176 | C | 0.44489 | 2.66634 | -0.32144 |
| C | -4.39814 | -2.37319 | -1.61515 | C | 0.74477 | 4.02226 | -0.55081 |
| C | -6.19999 | -3.2281 | 0.34024 | C | -0.26798 | 4.82886 | -1.06067 |
| H | -5.29962 | -1.72865 | 1.60393 | C | -1.71404 | 2.94022 | -1.08336 |
| C | -5.29438 | -3.39817 | -1.88719 | C | -1.51454 | 4.28925 | -1.32362 |
| H | -3.71672 | -1.99909 | -2.3781 | H | -0.06823 | 5.88526 | -1.24234 |
| C | -6.19289 | -3.83081 | -0.91552 | H | -2.66767 | 2.46908 | -1.31094 |
| H | -6.89957 | -3.56225 | 1.10471 | H | -2.32839 | 4.89412 | -1.71494 |
| H | -5.29442 | -3.8601 | -2.87295 | C | 2.09669 | 4.60897 | -0.26745 |
| H | -6.89093 | -4.63651 | -1.13691 | H | 2.04782 | 5.70413 | -0.28341 |
| C | -3.3518 | 1.32518 | 1.66527 | H | 2.49331 | 4.30297 | 0.70909 |
| C | -2.33062 | 2.11246 | 2.20783 | H | 2.83168 | 4.30613 | -1.02581 |
| C | -4.66567 | 1.50693 | 2.13169 | N | -0.75988 | 2.13087 | -0.59447 |
| C | -2.60984 | 3.04991 | 3.19352 | | | | |
| H | -1.31999 | 1.97939 | 1.83249 | | | | |
| C | -4.93932 | 2.44578 | 3.11488 | | | | |
| H | -5.46392 | 0.90273 | 1.70119 | | | | |
| C | -3.91253 | 3.22004 | 3.65229 | | | | |
| H | -1.80248 | 3.65498 | 3.60442 | | | | |
| H | -5.96216 | 2.5766 | 3.46436 | | | | |
| H | -4.12924 | 3.9568 | 4.42381 | | | | |
| C | 2.64668 | 1.42211 | -0.33373 | | | | |

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MeC1'(3)

| | | | |
|---|---------|---------|----------|
| C | 3.34189 | 0.89072 | -0.7449 |
| C | 3.70147 | 0.96081 | -2.10568 |
| C | 2.76499 | 1.14781 | -3.10594 |
| C | 1.42097 | 1.22143 | -2.73746 |
| C | 1.01817 | 1.13695 | -1.40052 |
| C | 1.98678 | 1.04005 | -0.37391 |

| | | | | | | | |
|----|----------|----------|----------|---|----------|----------|----------|
| H | 3.05973 | 1.20091 | -4.1531 | C | -4.24188 | -0.2141 | 0.12995 |
| H | 0.65652 | 1.3424 | -3.50349 | C | -3.89829 | -1.41544 | 0.76175 |
| C | 4.52938 | 0.40123 | -0.04628 | C | -5.41303 | -0.15092 | -0.64111 |
| C | 5.66573 | 0.36947 | -1.10492 | C | -4.71691 | -2.52864 | 0.63953 |
| O | 4.6944 | -0.02667 | 1.07811 | H | -2.97445 | -1.48718 | 1.33156 |
| O | 6.82167 | 0.07125 | -0.91643 | C | -6.2278 | -1.269 | -0.75753 |
| N | 5.07566 | 0.72839 | -2.29132 | H | -5.66835 | 0.78407 | -1.13766 |
| C | 5.76687 | 0.78662 | -3.55264 | C | -5.88478 | -2.45832 | -0.11613 |
| H | 5.36533 | 0.04896 | -4.26099 | H | -4.42787 | -3.45519 | 1.1348 |
| H | 5.68706 | 1.7865 | -3.99876 | H | -7.13919 | -1.21242 | -1.35079 |
| H | 6.81935 | 0.56048 | -3.35635 | H | -6.53042 | -3.33065 | -0.20632 |
| C | 1.4396 | 0.97918 | 0.98346 | C | 0.70234 | -2.54837 | 0.75348 |
| C | 2.07322 | 1.29737 | 2.19894 | C | 2.03689 | -2.52536 | 1.19595 |
| C | 1.39688 | 0.97204 | 3.37895 | C | 3.0954 | -2.46928 | 0.3083 |
| C | -0.52028 | 0.36644 | 2.11965 | C | 2.7801 | -2.34553 | -1.04587 |
| C | 0.11466 | 0.45125 | 3.35261 | C | 1.46237 | -2.28218 | -1.49429 |
| H | 1.88887 | 1.16905 | 4.33227 | C | 0.39547 | -2.39224 | -0.59655 |
| H | -1.57646 | 0.11447 | 2.03599 | H | 4.12768 | -2.47801 | 0.6494 |
| H | -0.40874 | 0.15948 | 4.25919 | H | 3.59001 | -2.28453 | -1.77326 |
| C | 3.33803 | 2.0922 | 2.31079 | H | 1.25161 | -2.13305 | -2.55254 |
| H | 3.18889 | 2.88928 | 3.05115 | C | -0.13652 | -2.69368 | 1.9383 |
| H | 4.18909 | 1.48351 | 2.63457 | C | 0.84732 | -2.63654 | 3.14452 |
| H | 3.61145 | 2.56766 | 1.36336 | O | -1.33277 | -2.84937 | 2.05366 |
| N | 0.11475 | 0.63642 | 0.9799 | O | 0.55808 | -2.62218 | 4.31761 |
| Rh | -0.85631 | 1.07625 | -0.8051 | N | 2.10879 | -2.57429 | 2.59322 |
| H | -0.51697 | 2.53268 | -0.45398 | C | 3.3081 | -2.31131 | 3.354 |
| C | -2.94236 | 2.05209 | 0.51982 | H | 4.03146 | -3.13023 | 3.25321 |
| C | -3.4472 | 0.95964 | 0.30517 | H | 3.77145 | -1.37669 | 3.00793 |
| C | -2.54117 | 3.36722 | 0.92254 | H | 3.01249 | -2.22084 | 4.40379 |
| C | -2.51812 | 4.41896 | -0.00523 | C | -0.98364 | -2.37728 | -1.1536 |
| C | -2.19436 | 3.6121 | 2.25782 | C | -1.65502 | -3.59152 | -1.35923 |
| C | -2.15828 | 5.69352 | 0.40739 | C | -2.82489 | -3.55088 | -2.1144 |
| H | -2.75442 | 4.20519 | -1.04713 | C | -2.57828 | -1.19022 | -2.31404 |
| C | -1.83155 | 4.89131 | 2.65897 | C | -3.27972 | -2.34591 | -2.62371 |
| H | -2.21666 | 2.79046 | 2.97326 | H | -3.36639 | -4.47739 | -2.30922 |
| C | -1.81475 | 5.93373 | 1.73657 | H | -2.9061 | -0.21142 | -2.66616 |
| H | -2.13855 | 6.50649 | -0.31624 | H | -4.1799 | -2.28844 | -3.23091 |
| H | -1.56534 | 5.07668 | 3.69835 | C | -1.14086 | -4.882 | -0.79877 |
| H | -1.53142 | 6.93623 | 2.05317 | H | -1.70504 | -5.73241 | -1.1995 |

| | | | | | | | |
|-----------------|----------|----------|----------|---|----------|----------|----------|
| H | -0.0796 | -5.04218 | -1.02981 | C | -2.94394 | -0.16902 | -1.4291 |
| H | -1.2443 | -4.89954 | 0.29532 | C | -3.06626 | -2.75611 | -0.935 |
| N | -1.45327 | -1.19419 | -1.58655 | C | -3.538 | -3.16921 | 0.31841 |
| Cl | -1.82712 | 2.01385 | -2.76156 | C | -2.80781 | -3.70969 | -1.93117 |
| | | | | C | -3.7524 | -4.51975 | 0.56545 |
| 88 | | | | H | -3.7062 | -2.41569 | 1.08809 |
| MeC1'(4) | | | | C | -3.01648 | -5.05682 | -1.66996 |
| C | 3.82428 | 0.01022 | -0.43701 | H | -2.43747 | -3.37229 | -2.89864 |
| C | 4.46062 | -1.24505 | -0.46173 | C | -3.4896 | -5.46507 | -0.42304 |
| C | 3.79903 | -2.3792 | -0.88779 | H | -4.12035 | -4.8373 | 1.54013 |
| C | 2.44083 | -2.25321 | -1.19975 | H | -2.81724 | -5.79443 | -2.44567 |
| C | 1.76129 | -1.03262 | -1.13607 | H | -3.65919 | -6.52256 | -0.22547 |
| C | 2.48715 | 0.14653 | -0.85793 | C | -3.23266 | 1.21155 | -1.63929 |
| H | 4.29418 | -3.34798 | -0.93483 | C | -3.94341 | 1.90243 | -0.64396 |
| H | 1.8923 | -3.14894 | -1.48726 | C | -2.81842 | 1.88916 | -2.79571 |
| C | 4.71471 | 0.90149 | 0.30527 | C | -4.19601 | 3.2621 | -0.78384 |
| C | 6.01454 | 0.08573 | 0.55812 | H | -4.29647 | 1.36363 | 0.23492 |
| O | 4.54372 | 2.01485 | 0.75738 | C | -3.09383 | 3.24333 | -2.93174 |
| O | 7.0236 | 0.4753 | 1.09679 | H | -2.24171 | 1.34939 | -3.5458 |
| N | 5.76707 | -1.16833 | 0.05216 | C | -3.77072 | 3.9346 | -1.92754 |
| C | 6.69607 | -2.26465 | 0.12253 | H | -4.7311 | 3.78522 | 0.0079 |
| H | 6.30286 | -3.07843 | 0.74748 | H | -2.76485 | 3.76841 | -3.8271 |
| H | 6.91444 | -2.65969 | -0.87832 | H | -3.97452 | 4.99857 | -2.04209 |
| H | 7.61874 | -1.88167 | 0.56912 | C | -0.99786 | 1.00849 | 2.20961 |
| C | 1.7788 | 1.43218 | -0.9851 | C | -0.74202 | 2.38023 | 2.37146 |
| C | 2.35215 | 2.62529 | -1.46127 | C | 0.54984 | 2.87386 | 2.42086 |
| C | 1.52423 | 3.74976 | -1.51467 | C | 1.59395 | 1.95224 | 2.30757 |
| C | -0.30328 | 2.43079 | -0.77581 | C | 1.35322 | 0.58821 | 2.14355 |
| C | 0.19598 | 3.67565 | -1.14272 | C | 0.04753 | 0.10156 | 2.06309 |
| H | 1.94184 | 4.68731 | -1.88361 | H | 0.75326 | 3.93744 | 2.5278 |
| H | -1.36075 | 2.30353 | -0.54799 | H | 2.62326 | 2.30737 | 2.31253 |
| H | -0.46342 | 4.53982 | -1.18988 | H | 2.18842 | -0.10466 | 2.03723 |
| C | 3.74391 | 2.75788 | -1.99768 | C | -2.44513 | 0.82643 | 2.19862 |
| H | 3.74906 | 3.46393 | -2.83723 | C | -3.03008 | 2.25847 | 2.38671 |
| H | 4.43498 | 3.13769 | -1.23475 | O | -3.12413 | -0.16752 | 2.06583 |
| H | 4.14116 | 1.80459 | -2.36374 | O | -4.1958 | 2.57154 | 2.44353 |
| N | 0.45458 | 1.34423 | -0.71392 | N | -1.93969 | 3.10131 | 2.46046 |
| Rh | -0.20184 | -0.86021 | -1.2129 | C | -2.04372 | 4.5382 | 2.47057 |
| C | -2.87882 | -1.36433 | -1.18982 | H | -1.53856 | 4.96837 | 3.34465 |

| | | | | | | | |
|-----------------|----------|----------|----------|----|----------|----------|----------|
| H | -1.60678 | 4.96157 | 1.55495 | C | 2.89093 | -2.83866 | -3.07988 |
| H | -3.10838 | 4.78758 | 2.51113 | C | 0.82558 | -1.77867 | -2.57836 |
| C | -0.19909 | -1.3569 | 1.93333 | C | 1.60234 | -2.51512 | -3.46428 |
| C | -0.30295 | -2.11078 | 3.11351 | H | 3.49468 | -3.50801 | -3.69373 |
| C | -0.43391 | -3.48988 | 2.9952 | H | -0.22449 | -1.54957 | -2.76672 |
| C | -0.37982 | -3.24704 | 0.62712 | H | 1.17635 | -2.86812 | -4.39928 |
| C | -0.45688 | -4.0681 | 1.73713 | C | 4.78934 | -2.85984 | -1.47909 |
| H | -0.50999 | -4.10164 | 3.89393 | H | 4.80825 | -3.94577 | -1.64054 |
| H | -0.43126 | -3.66725 | -0.37286 | H | 5.61139 | -2.41575 | -2.05047 |
| H | -0.55932 | -5.14173 | 1.60046 | H | 4.98772 | -2.67669 | -0.41742 |
| C | -0.2837 | -1.45197 | 4.45963 | N | 1.34443 | -1.31817 | -1.44378 |
| H | -0.2895 | -2.20237 | 5.25839 | Rh | 0.18442 | -0.52569 | 0.09947 |
| H | 0.60086 | -0.81678 | 4.59516 | H | 0.44862 | -1.87376 | 0.85278 |
| H | -1.16415 | -0.80996 | 4.59984 | C | -0.98643 | -0.53588 | 1.91511 |
| N | -0.26308 | -1.90663 | 0.70398 | C | -0.81594 | 0.67597 | 1.61203 |
| H | -0.32598 | -2.24456 | -1.8771 | C | -1.56053 | -1.59756 | 2.70303 |
| Cl | -0.08262 | -0.12448 | -3.44579 | C | -2.46635 | -1.23497 | 3.71719 |
| | | | | C | -1.29161 | -2.95929 | 2.51494 |
| | | | | C | -3.07993 | -2.19791 | 4.5036 |
| | | | | H | -2.67202 | -0.1796 | 3.88864 |
| 88 | | | | C | -1.91066 | -3.9212 | 3.30243 |
| MeC1'(5) | | | | H | -0.58963 | -3.25924 | 1.7395 |
| C | 4.35557 | -0.14249 | 0.28061 | C | -2.80905 | -3.54853 | 4.29671 |
| C | 4.59456 | 0.58287 | 1.46378 | H | -3.77395 | -1.89136 | 5.28453 |
| C | 3.58391 | 0.8693 | 2.36033 | H | -1.68689 | -4.9735 | 3.13453 |
| C | 2.28237 | 0.50492 | 2.00754 | H | -3.29397 | -4.30549 | 4.91045 |
| C | 1.99894 | -0.17089 | 0.82192 | C | -0.95173 | 2.09227 | 1.84578 |
| C | 3.05834 | -0.60928 | -0.00964 | C | -0.12901 | 3.06248 | 1.2586 |
| H | 3.77775 | 1.4128 | 3.28358 | C | -1.94791 | 2.51044 | 2.74604 |
| H | 1.46929 | 0.77841 | 2.67665 | C | -0.31749 | 4.40792 | 1.5505 |
| C | 5.57373 | 0.00397 | -0.52894 | H | 0.63715 | 2.75106 | 0.55431 |
| C | 6.60639 | 0.71363 | 0.3893 | C | -2.12977 | 3.85506 | 3.03388 |
| O | 5.80163 | -0.24503 | -1.69016 | H | -2.59991 | 1.76603 | 3.20152 |
| O | 7.75951 | 0.96158 | 0.13089 | C | -1.31701 | 4.81164 | 2.43065 |
| N | 5.92965 | 1.00574 | 1.55091 | H | 0.32844 | 5.14822 | 1.08116 |
| C | 6.49676 | 1.74352 | 2.64819 | H | -2.9101 | 4.15725 | 3.73115 |
| H | 5.96903 | 2.69523 | 2.799 | H | -1.45962 | 5.86836 | 2.65185 |
| H | 6.45687 | 1.16185 | 3.57864 | C | -2.91623 | 0.9643 | -1.60617 |
| H | 7.54171 | 1.94854 | 2.39583 | C | -3.05178 | 2.3615 | -1.55901 |
| C | 2.66967 | -1.43731 | -1.15672 | | | | |
| C | 3.45698 | -2.32766 | -1.90677 | | | | |

| | | | | | | | |
|---|----------|----------|----------|-----------------|----------|----------|----------|
| H | -4.20179 | 0.17917 | 4.84095 | H | 6.63905 | 0.3584 | 2.86593 |
| C | 0.20018 | 3.63945 | -0.54353 | H | 5.76692 | -1.18291 | 2.76795 |
| C | -0.63 | 4.77001 | -0.48665 | H | 6.26658 | -0.36714 | 1.29026 |
| C | 1.41437 | 3.71278 | -1.23786 | N | 2.32992 | 0.79501 | 1.42226 |
| C | -0.25487 | 5.94744 | -1.11682 | | | | |
| H | -1.57313 | 4.70455 | 0.05519 | 88 | | | |
| C | 1.78477 | 4.89908 | -1.85992 | MeC1'(7) | | | |
| H | 2.06914 | 2.84153 | -1.2831 | C | -1.15604 | 1.95473 | 0.39492 |
| C | 0.95471 | 6.01493 | -1.80491 | C | -2.18403 | 1.89908 | -0.56771 |
| H | -0.90947 | 6.81642 | -1.07332 | C | -2.28814 | 0.86282 | -1.47819 |
| H | 2.73043 | 4.94546 | -2.39671 | C | -1.23466 | -0.05269 | -1.50608 |
| H | 1.24839 | 6.9384 | -2.30141 | C | -0.18813 | -0.02306 | -0.58407 |
| C | 3.83781 | -1.1918 | -0.58352 | C | -0.20873 | 0.90803 | 0.48362 |
| C | 3.96444 | -2.408 | -1.27282 | H | -3.10143 | 0.80775 | -2.20022 |
| C | 3.91572 | -3.62043 | -0.60722 | H | -1.22933 | -0.81607 | -2.28457 |
| C | 3.70576 | -3.58675 | 0.77297 | C | -1.14367 | 3.34159 | 0.86457 |
| C | 3.56203 | -2.3873 | 1.46547 | C | -2.43682 | 3.99474 | 0.29821 |
| C | 3.61615 | -1.16666 | 0.78455 | O | -0.28957 | 3.97343 | 1.44942 |
| H | 4.0035 | -4.56692 | -1.13666 | O | -2.85583 | 5.10356 | 0.53373 |
| H | 3.64851 | -4.52648 | 1.32046 | N | -2.98954 | 3.04885 | -0.53096 |
| H | 3.39632 | -2.39319 | 2.5437 | C | -4.16131 | 3.25128 | -1.34519 |
| C | 3.82484 | -0.11999 | -1.58332 | H | -3.89939 | 3.25814 | -2.41328 |
| C | 3.93962 | -0.84932 | -2.94907 | H | -4.89863 | 2.45787 | -1.16417 |
| O | 3.75799 | 1.08076 | -1.4592 | H | -4.5853 | 4.2223 | -1.07237 |
| O | 3.93071 | -0.3529 | -4.04798 | C | 0.74026 | 0.65813 | 1.58945 |
| N | 4.08124 | -2.19468 | -2.64619 | C | 0.67583 | 1.14868 | 2.91313 |
| C | 3.99586 | -3.23363 | -3.63982 | C | 1.69251 | 0.75184 | 3.78856 |
| H | 4.83047 | -3.93993 | -3.54579 | C | 2.63674 | -0.63368 | 2.114 |
| H | 3.0448 | -3.77754 | -3.54717 | C | 2.69887 | -0.11562 | 3.4012 |
| H | 4.04046 | -2.75145 | -4.62073 | H | 1.66652 | 1.13241 | 4.81065 |
| C | 3.48696 | 0.11871 | 1.516 | H | 3.35709 | -1.35619 | 1.72215 |
| C | 4.58655 | 0.56601 | 2.27015 | H | 3.49396 | -0.41048 | 4.08124 |
| C | 4.44651 | 1.76395 | 2.96233 | C | -0.43012 | 1.97486 | 3.49142 |
| C | 2.23469 | 1.94514 | 2.10269 | H | -0.56141 | 1.7202 | 4.55185 |
| C | 3.25371 | 2.46439 | 2.88598 | H | -0.22429 | 3.04891 | 3.4194 |
| H | 5.28093 | 2.1444 | 3.55207 | H | -1.38499 | 1.79352 | 2.98183 |
| H | 1.29117 | 2.47843 | 2.00872 | N | 1.68385 | -0.2634 | 1.26769 |
| H | 3.11117 | 3.40641 | 3.4101 | Rh | 1.52512 | -1.02255 | -0.80416 |
| C | 5.87824 | -0.19495 | 2.30288 | Cl | 3.75622 | -2.19833 | -0.81482 |

| | | | | | | | |
|---|----------|----------|----------|-----------------|----------|----------|----------|
| H | 1.31387 | -1.42829 | -2.30018 | C | -4.67789 | 0.79192 | 2.2837 |
| C | 1.92476 | 0.77859 | -1.9691 | H | -5.05756 | 0.46828 | 3.2607 |
| C | 2.80062 | 0.84267 | -1.08317 | H | -3.96047 | 1.61367 | 2.42903 |
| C | 1.06301 | 1.35693 | -2.97343 | H | -5.51397 | 1.14912 | 1.67501 |
| C | 0.57577 | 2.65087 | -2.73698 | C | -0.61595 | -3.36185 | 0.07777 |
| C | 0.64199 | 0.66411 | -4.11232 | C | -1.22796 | -4.6126 | -0.11305 |
| C | -0.34147 | 3.22433 | -3.60778 | C | -0.61222 | -5.513 | -0.97597 |
| H | 0.90728 | 3.18736 | -1.84715 | C | 1.11332 | -3.91817 | -1.35896 |
| C | -0.26173 | 1.2493 | -4.98916 | C | 0.57487 | -5.16986 | -1.59785 |
| H | 1.01574 | -0.34405 | -4.28736 | H | -1.06628 | -6.49052 | -1.13883 |
| C | -0.76612 | 2.52262 | -4.7333 | H | 2.05783 | -3.61235 | -1.80104 |
| H | -0.72906 | 4.2216 | -3.40301 | H | 1.09219 | -5.85667 | -2.26257 |
| H | -0.58422 | 0.70245 | -5.87351 | C | -2.4979 | -4.99478 | 0.58494 |
| H | -1.48776 | 2.96907 | -5.41564 | H | -2.65473 | -6.07816 | 0.52776 |
| C | 3.78467 | 1.33585 | -0.16448 | H | -2.49486 | -4.70923 | 1.64403 |
| C | 5.06851 | 0.78202 | -0.07267 | H | -3.36087 | -4.51004 | 0.10928 |
| C | 3.43091 | 2.41565 | 0.66266 | N | 0.53404 | -3.01438 | -0.54475 |
| C | 5.97713 | 1.30043 | 0.84033 | | | | |
| H | 5.31843 | -0.07185 | -0.69841 | | | | |
| C | 4.34738 | 2.92239 | 1.57319 | 88 | | | |
| H | 2.42638 | 2.83788 | 0.60216 | MeC1'(8) | | | |
| C | 5.62053 | 2.36483 | 1.66495 | C | 4.59402 | -0.31377 | -0.3428 |
| H | 6.97222 | 0.86482 | 0.91221 | C | 4.80236 | 0.04052 | -1.68929 |
| H | 4.06336 | 3.75496 | 2.21457 | C | 3.83743 | 0.69336 | -2.43098 |
| H | 6.33797 | 2.76278 | 2.38128 | C | 2.59461 | 0.90755 | -1.82888 |
| C | -2.40842 | -1.80182 | 0.96592 | C | 2.34163 | 0.54686 | -0.50753 |
| C | -2.8954 | -0.96006 | 1.97901 | C | 3.381 | 0.01428 | 0.2878 |
| C | -2.24147 | -0.83527 | 3.19298 | H | 4.00848 | 0.96526 | -3.4715 |
| C | -1.03811 | -1.52735 | 3.34459 | H | 1.79008 | 1.3254 | -2.43278 |
| C | -0.50352 | -2.30741 | 2.3215 | C | 5.68799 | -1.22968 | 0.00446 |
| C | -1.18206 | -2.45335 | 1.10848 | C | 6.65181 | -1.21591 | -1.21423 |
| H | -2.63325 | -0.20928 | 3.99258 | O | 5.85421 | -1.95334 | 0.95933 |
| H | -0.49338 | -1.4416 | 4.28414 | O | 7.71033 | -1.78959 | -1.31123 |
| H | 0.4537 | -2.80882 | 2.45796 | N | 6.04429 | -0.42013 | -2.15732 |
| C | -3.3558 | -1.72586 | -0.14833 | C | 6.55634 | -0.2117 | -3.48516 |
| C | -4.38507 | -0.63694 | 0.27265 | H | 5.87326 | -0.62491 | -4.24021 |
| O | -3.42257 | -2.35108 | -1.18157 | H | 6.7066 | 0.85716 | -3.68795 |
| O | -5.27356 | -0.16923 | -0.3997 | H | 7.51843 | -0.72929 | -3.54839 |
| N | -4.06536 | -0.30335 | 1.57446 | C | 3.02 | -0.23211 | 1.68592 |
| | | | | C | 3.87222 | -0.28116 | 2.80372 |

| | | | | | | | |
|----|----------|----------|----------|----|----------|----------|----------|
| C | 3.30014 | -0.62005 | 4.03253 | C | -2.62272 | -2.8897 | -2.45183 |
| C | 1.14328 | -0.61847 | 3.0431 | C | -1.46795 | -2.33494 | -2.99759 |
| C | 1.94074 | -0.84244 | 4.15589 | C | -1.1295 | -0.99554 | -2.80588 |
| H | 3.94835 | -0.68206 | 4.90694 | C | -1.94295 | -0.15868 | -2.04942 |
| H | 0.05769 | -0.66065 | 3.09374 | H | -2.86549 | -3.93965 | -2.60027 |
| H | 1.4881 | -1.11904 | 5.10426 | H | -0.79339 | -2.96829 | -3.56978 |
| C | 5.31327 | 0.12402 | 2.79297 | H | -0.19676 | -0.61121 | -3.2135 |
| H | 5.52587 | 0.72313 | 3.68791 | C | -4.20722 | -0.11082 | -0.74494 |
| H | 5.98026 | -0.74484 | 2.79582 | C | -5.20465 | -1.27516 | -0.48321 |
| H | 5.56682 | 0.7283 | 1.91514 | O | -4.40991 | 1.02898 | -0.38137 |
| N | 1.66888 | -0.29906 | 1.86261 | O | -6.25766 | -1.21289 | 0.10515 |
| Rh | 0.54277 | 0.42197 | 0.30441 | N | -4.65074 | -2.38004 | -1.09373 |
| H | 0.86059 | 1.8101 | 0.93559 | C | -5.23359 | -3.6958 | -1.06164 |
| C | -1.60131 | 1.16276 | 1.59019 | H | -5.45944 | -4.05315 | -2.07535 |
| C | -1.79493 | -0.04892 | 1.52508 | H | -4.55726 | -4.40713 | -0.56869 |
| C | -1.60611 | 2.5914 | 1.71894 | H | -6.16419 | -3.62566 | -0.49006 |
| C | -2.62204 | 3.3279 | 1.09492 | C | -1.57936 | 1.27518 | -1.9326 |
| C | -0.63476 | 3.26201 | 2.478 | C | -2.31305 | 2.22143 | -2.67464 |
| C | -2.64387 | 4.71367 | 1.20977 | C | -1.87898 | 3.54108 | -2.66362 |
| H | -3.37852 | 2.79773 | 0.51836 | C | -0.08383 | 2.90318 | -1.24125 |
| C | -0.66468 | 4.64412 | 2.58443 | C | -0.74537 | 3.88892 | -1.94595 |
| H | 0.14605 | 2.68413 | 2.97143 | H | -2.42862 | 4.2899 | -3.23383 |
| C | -1.66489 | 5.37486 | 1.94419 | H | 0.80408 | 3.13704 | -0.66141 |
| H | -3.43345 | 5.27874 | 0.71665 | H | -0.37503 | 4.91041 | -1.91889 |
| H | 0.09584 | 5.15654 | 3.17117 | C | -3.52169 | 1.83726 | -3.47167 |
| H | -1.68407 | 6.46033 | 2.02805 | H | -3.75933 | 2.61377 | -4.20803 |
| C | -2.43209 | -1.31864 | 1.75602 | H | -3.37924 | 0.89001 | -4.00548 |
| C | -1.80451 | -2.55523 | 1.56029 | H | -4.39467 | 1.72164 | -2.81567 |
| C | -3.7547 | -1.28224 | 2.23528 | N | -0.4836 | 1.61379 | -1.21549 |
| C | -2.48999 | -3.72822 | 1.85392 | Cl | 0.70416 | -2.00083 | -0.59351 |
| H | -0.79995 | -2.58458 | 1.13773 | | | | |
| C | -4.42737 | -2.46095 | 2.52673 | | | | |
| H | -4.24884 | -0.31863 | 2.35876 | | | | |
| C | -3.79379 | -3.68779 | 2.34295 | | | | |
| H | -1.99442 | -4.68528 | 1.69714 | | | | |
| H | -5.45679 | -2.4163 | 2.87741 | | | | |
| H | -4.32089 | -4.61292 | 2.57418 | | | | |
| C | -3.11871 | -0.6974 | -1.51432 | | | | |
| C | -3.43609 | -2.05299 | -1.70713 | | | | |

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MeC1'(9)

| | | | |
|---|---------|---------|----------|
| C | 2.87002 | 0.83208 | -1.3558 |
| C | 3.2964 | 1.87912 | -0.51295 |
| C | 2.45588 | 2.46641 | 0.41313 |
| C | 1.11877 | 2.06383 | 0.39929 |
| C | 0.66602 | 1.01577 | -0.40184 |
| C | 1.5722 | 0.28586 | -1.21483 |

| | | | | | | | |
|----|----------|----------|----------|---|----------|----------|----------|
| H | 2.79839 | 3.25069 | 1.08626 | C | -3.94014 | -1.82008 | -0.65509 |
| H | 0.41542 | 2.56909 | 1.0584 | C | -4.37338 | -2.48952 | -1.81005 |
| C | 3.88267 | 0.77029 | -2.42024 | C | -3.4681 | -2.57101 | 0.43274 |
| C | 5.06808 | 1.64891 | -1.93068 | C | -4.30728 | -3.87565 | -1.8828 |
| O | 3.85187 | 0.2755 | -3.52379 | H | -4.73876 | -1.90324 | -2.65116 |
| O | 6.15747 | 1.75215 | -2.44485 | C | -3.40508 | -3.95574 | 0.35112 |
| N | 4.61698 | 2.26863 | -0.79273 | H | -3.14386 | -2.05349 | 1.33542 |
| C | 5.38181 | 3.20407 | -0.00644 | C | -3.81603 | -4.61189 | -0.8076 |
| H | 4.93101 | 4.20528 | -0.03888 | H | -4.63915 | -4.3835 | -2.7867 |
| H | 5.4417 | 2.87137 | 1.0392 | H | -3.0362 | -4.52902 | 1.2008 |
| H | 6.38455 | 3.2499 | -0.44206 | H | -3.7621 | -5.6974 | -0.8684 |
| C | 1.08908 | -0.99912 | -1.759 | C | 1.78841 | -0.80727 | 2.08294 |
| C | 1.85929 | -2.06416 | -2.2843 | C | 2.97464 | -1.39712 | 1.61872 |
| C | 1.16845 | -3.1785 | -2.7732 | C | 2.95943 | -2.61912 | 0.9676 |
| C | -0.87338 | -2.23498 | -2.05734 | C | 1.71388 | -3.21055 | 0.741 |
| C | -0.20791 | -3.26501 | -2.70718 | C | 0.52362 | -2.61192 | 1.15155 |
| H | 1.75029 | -3.99707 | -3.19926 | C | 0.54951 | -1.39151 | 1.82973 |
| H | -1.94819 | -2.27051 | -1.90389 | H | 3.8757 | -3.09624 | 0.62498 |
| H | -0.75644 | -4.11924 | -3.09752 | H | 1.67247 | -4.16554 | 0.21851 |
| C | 3.35178 | -2.17624 | -2.28071 | H | -0.43322 | -3.09185 | 0.94347 |
| H | 3.63378 | -3.223 | -2.10069 | C | 2.16024 | 0.42084 | 2.79187 |
| H | 3.79313 | -1.86093 | -3.23245 | C | 3.69541 | 0.55552 | 2.57492 |
| H | 3.81003 | -1.56172 | -1.4985 | O | 1.50164 | 1.18222 | 3.46077 |
| N | -0.24627 | -1.17176 | -1.5777 | O | 4.40563 | 1.47351 | 2.91062 |
| Rh | -1.23723 | 0.57355 | -0.5074 | N | 4.08415 | -0.59667 | 1.91797 |
| Cl | -1.33742 | 1.4612 | -2.6842 | C | 5.42355 | -0.82497 | 1.43709 |
| C | -4.14064 | 0.8149 | -0.61972 | H | 5.82812 | -1.76809 | 1.82584 |
| C | -3.97606 | -0.39379 | -0.60602 | H | 5.44889 | -0.84847 | 0.33837 |
| C | -4.51779 | 2.18859 | -0.48762 | H | 6.04476 | 0.00343 | 1.7909 |
| C | -5.34592 | 2.55121 | 0.58709 | C | -0.68671 | -0.77808 | 2.37996 |
| C | -4.10124 | 3.16543 | -1.40226 | C | -1.02202 | -1.08064 | 3.71192 |
| C | -5.75032 | 3.86991 | 0.74379 | C | -2.15533 | -0.48463 | 4.25133 |
| H | -5.67325 | 1.78132 | 1.28674 | C | -2.48767 | 0.64843 | 2.18405 |
| C | -4.51474 | 4.48013 | -1.23647 | C | -2.89004 | 0.40443 | 3.48283 |
| H | -3.43176 | 2.87694 | -2.21199 | H | -2.44036 | -0.70453 | 5.27993 |
| C | -5.3357 | 4.83603 | -0.16892 | H | -3.03381 | 1.34865 | 1.56128 |
| H | -6.39259 | 4.14405 | 1.57903 | H | -3.76413 | 0.91668 | 3.87752 |
| H | -4.18482 | 5.23663 | -1.94614 | C | -0.16756 | -1.98511 | 4.54772 |
| H | -5.65285 | 5.87049 | -0.04697 | H | -0.68588 | -2.25756 | 5.4743 |

| | | | | | | | |
|------------------|----------|----------|----------|---|----------|----------|----------|
| H | 0.1026 | -2.90917 | 4.02208 | H | -3.21046 | 1.04858 | 0.04148 |
| H | 0.77014 | -1.48563 | 4.8279 | C | -3.29834 | -1.00933 | -0.24436 |
| N | -1.42364 | 0.04849 | 1.60997 | C | -2.22643 | -1.54852 | -0.6378 |
| H | -1.64018 | 1.99259 | -0.00261 | C | -4.72117 | -0.97004 | 0.00306 |
| | | | | C | -5.59652 | -0.66219 | -1.04561 |
| 88 | | | | C | -5.23457 | -1.26221 | 1.27127 |
| MeC1'(10) | | | | C | -6.96622 | -0.65536 | -0.82239 |
| C | 1.9514 | -1.64603 | 0.18489 | H | -5.17762 | -0.42253 | -2.02225 |
| C | 2.67771 | -1.43931 | -1.00674 | C | -6.60758 | -1.25016 | 1.48709 |
| C | 2.26211 | -0.55306 | -1.98612 | H | -4.54568 | -1.50914 | 2.07971 |
| C | 1.00797 | 0.03901 | -1.81301 | C | -7.47516 | -0.94779 | 0.44196 |
| C | 0.27088 | -0.10552 | -0.63888 | H | -7.64413 | -0.42137 | -1.64156 |
| C | 0.79813 | -0.8617 | 0.43132 | H | -7.00222 | -1.48365 | 2.47476 |
| H | 2.84939 | -0.38222 | -2.88752 | H | -8.55065 | -0.94141 | 0.61138 |
| H | 0.58483 | 0.63472 | -2.62454 | C | -1.39489 | -2.66502 | -1.01265 |
| C | 2.46559 | -2.90386 | 0.73437 | C | -1.09395 | -3.65575 | -0.06992 |
| C | 3.73337 | -3.24533 | -0.09742 | C | -0.85618 | -2.74805 | -2.30306 |
| O | 2.01033 | -3.65794 | 1.56747 | C | -0.28003 | -4.72649 | -0.41804 |
| O | 4.50798 | -4.15275 | 0.09831 | H | -1.49449 | -3.56783 | 0.94017 |
| N | 3.78328 | -2.3023 | -1.09493 | C | -0.03845 | -3.8181 | -2.64001 |
| C | 4.74847 | -2.28739 | -2.16507 | H | -1.08422 | -1.95991 | -3.01966 |
| H | 4.2683 | -2.50602 | -3.12909 | C | 0.25187 | -4.80773 | -1.70197 |
| H | 5.24119 | -1.3078 | -2.2312 | H | -0.04388 | -5.48784 | 0.32237 |
| H | 5.48965 | -3.06286 | -1.94942 | H | 0.37889 | -3.88003 | -3.64407 |
| C | 0.06766 | -0.72315 | 1.70499 | H | 0.8951 | -5.64402 | -1.97145 |
| C | 0.51882 | -1.02962 | 3.0111 | C | 2.2032 | 2.3136 | 0.31491 |
| C | -0.35697 | -0.8043 | 4.0753 | C | 3.17016 | 1.70766 | 1.13346 |
| C | -1.95492 | 0.12072 | 2.59864 | C | 2.96431 | 1.53707 | 2.49222 |
| C | -1.61123 | -0.25112 | 3.88689 | C | 1.73126 | 1.94151 | 3.00795 |
| H | -0.01839 | -1.05561 | 5.08105 | C | 0.74064 | 2.49235 | 2.19797 |
| H | -2.89964 | 0.608 | 2.36411 | C | 0.96314 | 2.68446 | 0.83124 |
| H | -2.29468 | -0.0762 | 4.71349 | H | 3.72442 | 1.09659 | 3.13504 |
| C | 1.89444 | -1.49139 | 3.37577 | H | 1.53714 | 1.81567 | 4.07296 |
| H | 2.18044 | -1.04886 | 4.33955 | H | -0.21543 | 2.79274 | 2.6256 |
| H | 1.94823 | -2.58114 | 3.46598 | C | 2.77235 | 2.39803 | -1.03492 |
| H | 2.64013 | -1.19263 | 2.63282 | C | 4.14043 | 1.66042 | -0.93993 |
| N | -1.1397 | -0.09362 | 1.56492 | O | 2.36788 | 2.94224 | -2.03442 |
| Rh | -1.71073 | 0.47271 | -0.3385 | O | 4.90782 | 1.41434 | -1.83994 |
| Cl | -2.17249 | 0.78732 | -2.67719 | N | 4.30234 | 1.34369 | 0.39555 |

| | | | | | | | |
|---|----------|---------|----------|----|----------|----------|----------|
| C | 5.39092 | 0.54532 | 0.89846 | C | -0.23784 | -0.38219 | 3.55531 |
| H | 5.9291 | 1.06799 | 1.69953 | C | -1.27285 | -1.51642 | 1.75126 |
| H | 5.02767 | -0.4196 | 1.28225 | C | -0.96833 | -1.46466 | 3.10596 |
| H | 6.07683 | 0.3644 | 0.06518 | H | -0.07394 | -0.23752 | 4.62343 |
| C | -0.07142 | 3.38023 | 0.02171 | H | -1.94637 | -2.26212 | 1.33569 |
| C | 0.12858 | 4.74368 | -0.25906 | H | -1.35305 | -2.22058 | 3.78389 |
| C | -0.88714 | 5.42284 | -0.92159 | C | 0.85565 | 1.82616 | 3.25066 |
| C | -2.15655 | 3.41014 | -0.96706 | H | 0.17964 | 2.18698 | 4.03848 |
| C | -2.04587 | 4.75372 | -1.2756 | H | 1.84226 | 1.66616 | 3.69804 |
| H | -0.76282 | 6.48187 | -1.14798 | H | 0.95411 | 2.62266 | 2.50391 |
| H | -3.03845 | 2.84469 | -1.24705 | N | -0.77055 | -0.63444 | 0.89252 |
| H | -2.86227 | 5.25607 | -1.78793 | Rh | -1.67979 | -0.26328 | -0.93715 |
| C | 1.38699 | 5.46258 | 0.12431 | Cl | -2.60694 | 0.38966 | -3.04263 |
| H | 1.22704 | 6.54713 | 0.10998 | H | -2.90582 | -1.36199 | -0.78189 |
| H | 1.74059 | 5.18678 | 1.12524 | C | -3.31682 | 0.48368 | 0.20929 |
| H | 2.19504 | 5.24083 | -0.58569 | C | -2.62528 | 1.48506 | -0.12741 |
| N | -1.19262 | 2.71968 | -0.32927 | C | -4.40213 | -0.03641 | 1.01049 |

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MeC1'(11)

| | | | | | | | |
|---|----------|---------|----------|---|----------|----------|----------|
| C | 1.92921 | 1.76173 | 0.19685 | C | -5.85459 | 0.32136 | 2.91785 |
| C | 2.35118 | 2.47376 | -0.94071 | H | -4.285 | 1.67395 | 2.31386 |
| C | 1.57795 | 2.55551 | -2.08487 | C | -6.11782 | -1.64902 | 1.55914 |
| C | 0.4063 | 1.79382 | -2.12266 | H | -4.7413 | -1.84211 | -0.09612 |
| C | -0.02158 | 1.01884 | -1.04407 | C | -6.51435 | -0.87453 | 2.64562 |
| C | 0.69325 | 1.08109 | 0.16891 | H | -6.15524 | 0.93138 | 3.76822 |
| H | 1.90125 | 3.13882 | -2.94656 | H | -6.62968 | -2.58491 | 1.34084 |
| H | -0.20053 | 1.7876 | -3.03145 | H | -7.33398 | -1.2037 | 3.28217 |
| C | 3.09262 | 1.65927 | 1.06852 | C | -2.20774 | 2.85709 | -0.23672 |
| C | 4.22696 | 2.44355 | 0.35744 | C | -2.3991 | 3.57139 | -1.4269 |
| O | 3.28131 | 1.04821 | 2.10131 | C | -1.55445 | 3.47098 | 0.83989 |
| O | 5.37719 | 2.53875 | 0.72463 | C | -1.93007 | 4.87382 | -1.53254 |
| N | 3.66418 | 2.96397 | -0.78159 | H | -2.88774 | 3.07161 | -2.26228 |
| C | 4.41629 | 3.6357 | -1.80849 | C | -1.07138 | 4.76699 | 0.7184 |
| H | 4.45274 | 3.03127 | -2.72715 | H | -1.41302 | 2.90963 | 1.76467 |
| H | 3.97538 | 4.61193 | -2.04651 | C | -1.2583 | 5.47142 | -0.4684 |
| H | 5.43267 | 3.77946 | -1.42968 | H | -2.08177 | 5.42496 | -2.45932 |
| C | 0.10882 | 0.33481 | 1.29376 | H | -0.55272 | 5.23162 | 1.55623 |
| C | 0.2867 | 0.56741 | 2.66888 | H | -0.88122 | 6.48855 | -0.56322 |
| | | | | C | 2.24572 | -2.01265 | 0.04573 |

| | | | | | | | |
|---|----------|----------|----------|----|----------|----------|----------|
| C | 3.50718 | -1.44412 | 0.30759 | H | -1.28411 | 4.35151 | -0.60625 |
| C | 4.16469 | -0.68297 | -0.64533 | H | 0.70826 | 2.97475 | -0.28626 |
| C | 3.50035 | -0.46704 | -1.85629 | C | -3.96973 | 0.91207 | -1.41391 |
| C | 2.25577 | -1.02995 | -2.13043 | C | -4.75276 | 2.24228 | -1.23637 |
| C | 1.61527 | -1.83692 | -1.18387 | O | -4.5345 | -0.16345 | -1.44213 |
| H | 5.14774 | -0.25428 | -0.45543 | O | -5.95415 | 2.37074 | -1.17253 |
| H | 3.9791 | 0.14894 | -2.61746 | N | -3.79844 | 3.22275 | -1.12865 |
| H | 1.77761 | -0.86655 | -3.0952 | C | -4.08815 | 4.59982 | -0.83193 |
| C | 1.8388 | -2.72519 | 1.25239 | H | -3.69619 | 4.88136 | 0.15676 |
| C | 2.98143 | -2.47369 | 2.27701 | H | -3.65118 | 5.26747 | -1.58559 |
| O | 0.85807 | -3.40093 | 1.47651 | H | -5.17636 | 4.71418 | -0.83423 |
| O | 3.0195 | -2.84376 | 3.42512 | C | -1.29929 | -0.9193 | -1.68611 |
| N | 3.94604 | -1.7611 | 1.59221 | C | -2.07434 | -1.58805 | -2.65187 |
| C | 5.18866 | -1.30995 | 2.17576 | C | -1.93674 | -2.97589 | -2.73349 |
| H | 6.04468 | -1.78234 | 1.67602 | C | -0.16837 | -2.90733 | -1.15974 |
| H | 5.26846 | -0.21824 | 2.10926 | C | -1.02935 | -3.66014 | -1.9446 |
| H | 5.17672 | -1.60663 | 3.2285 | H | -2.55013 | -3.51552 | -3.45555 |
| C | 0.4506 | -2.64111 | -1.64236 | H | 0.64419 | -3.36178 | -0.59968 |
| C | 0.69519 | -3.99429 | -1.95182 | H | -0.93655 | -4.74174 | -1.97939 |
| C | -0.30319 | -4.69487 | -2.61859 | C | -2.92687 | -0.90872 | -3.67862 |
| C | -1.6428 | -2.72917 | -2.6272 | H | -2.74339 | -1.37127 | -4.65693 |
| C | -1.47316 | -4.05212 | -2.99038 | H | -3.99494 | -1.00297 | -3.45318 |
| H | -0.13948 | -5.7423 | -2.87248 | H | -2.69291 | 0.15758 | -3.76594 |
| H | -2.53648 | -2.17199 | -2.89491 | N | -0.29198 | -1.58339 | -1.05643 |
| H | -2.25411 | -4.56331 | -3.54732 | Rh | 1.37993 | -0.35381 | -0.57413 |
| C | 1.98965 | -4.67395 | -1.6174 | C | 3.47718 | 0.05356 | -0.56207 |
| H | 2.0537 | -5.64302 | -2.1258 | C | 2.89131 | 1.06523 | -0.08112 |
| H | 2.86117 | -4.077 | -1.91628 | C | 4.70453 | -0.59756 | -0.95177 |
| H | 2.0739 | -4.86362 | -0.53892 | C | 5.90306 | 0.07659 | -0.66387 |
| N | -0.71648 | -2.03812 | -1.93558 | C | 4.75986 | -1.83732 | -1.59458 |
| | | | | C | 7.12463 | -0.48954 | -0.9951 |
| | | | | H | 5.85575 | 1.04973 | -0.1743 |
| | | | | C | 5.98727 | -2.39816 | -1.92673 |
| | | | | H | 3.82582 | -2.33811 | -1.84624 |
| | | | | C | 7.17078 | -1.73189 | -1.62544 |
| | | | | H | 8.04655 | 0.04031 | -0.76052 |
| | | | | H | 6.01761 | -3.3624 | -2.4313 |
| | | | | H | 8.1299 | -2.17628 | -1.88626 |
| | | | | C | 2.86037 | 2.39229 | 0.46952 |

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MeC1'(12)

| | | | | | | | |
|---|----------|---------|----------|---|---------|----------|----------|
| C | -2.5562 | 1.27064 | -1.39296 | H | 3.82582 | -2.33811 | -1.84624 |
| C | -2.51246 | 2.64893 | -1.11571 | C | 7.17078 | -1.73189 | -1.62544 |
| C | -1.33158 | 3.27749 | -0.78299 | H | 8.04655 | 0.04031 | -0.76052 |
| C | -0.20177 | 2.47054 | -0.60673 | H | 6.01761 | -3.3624 | -2.4313 |
| C | -0.19585 | 1.08337 | -0.79264 | H | 8.1299 | -2.17628 | -1.88626 |
| C | -1.3742 | 0.50217 | -1.31691 | C | 2.86037 | 2.39229 | 0.46952 |

| | | | | | | | |
|---|----------|----------|----------|------------------|----------|----------|----------|
| C | 2.35492 | 2.63734 | 1.75506 | H | -1.3646 | -1.2662 | 4.70452 |
| C | 3.33283 | 3.46646 | -0.29702 | N | 1.35487 | -0.77515 | 1.60041 |
| C | 2.318 | 3.93162 | 2.25551 | Cl | 1.64116 | -0.07192 | -2.90916 |
| H | 1.98846 | 1.80053 | 2.35209 | H | 2.31503 | -1.68994 | -0.65898 |
| C | 3.28838 | 4.75986 | 0.20905 | | | | |
| H | 3.71073 | 3.26705 | -1.2991 | 88 | | | |
| C | 2.77859 | 4.9964 | 1.48309 | MeC1'(13) | | | |
| H | 1.92651 | 4.11327 | 3.25551 | C | 3.55867 | -0.72681 | -0.13169 |
| H | 3.64898 | 5.5892 | -0.3971 | C | 3.90322 | 0.61954 | -0.3522 |
| H | 2.7413 | 6.01092 | 1.87627 | C | 2.93431 | 1.59312 | -0.47907 |
| C | -1.89441 | -1.17712 | 1.7551 | C | 1.59828 | 1.17504 | -0.50382 |
| C | -3.24572 | -0.89652 | 1.4911 | C | 1.18921 | -0.15772 | -0.38297 |
| C | -3.73552 | 0.39497 | 1.60042 | C | 2.19877 | -1.09824 | -0.07752 |
| C | -2.81974 | 1.40283 | 1.91925 | H | 3.18991 | 2.6439 | -0.62305 |
| C | -1.46957 | 1.13984 | 2.14962 | H | 0.85217 | 1.95613 | -0.64987 |
| C | -0.99091 | -0.16907 | 2.07209 | C | 4.80045 | -1.49195 | -0.26704 |
| H | -4.78296 | 0.62585 | 1.41101 | C | 5.92728 | -0.43713 | -0.45652 |
| H | -3.17492 | 2.43119 | 1.9894 | O | 5.01652 | -2.68375 | -0.29773 |
| H | -0.78149 | 1.95288 | 2.38263 | O | 7.11193 | -0.64836 | -0.56804 |
| C | -1.7159 | -2.62308 | 1.65008 | N | 5.29467 | 0.78434 | -0.46849 |
| C | -3.10234 | -3.16209 | 1.19414 | C | 5.96062 | 2.03119 | -0.7302 |
| O | -0.75285 | -3.31892 | 1.88014 | H | 5.59636 | 2.48301 | -1.6633 |
| O | -3.39065 | -4.30738 | 0.94442 | H | 5.80834 | 2.74444 | 0.09133 |
| N | -3.93883 | -2.06218 | 1.15556 | H | 7.0293 | 1.81644 | -0.8264 |
| C | -5.34822 | -2.13664 | 0.84076 | C | 1.73268 | -2.45211 | 0.25242 |
| H | -5.95365 | -1.84562 | 1.7098 | C | 2.3383 | -3.35691 | 1.14908 |
| H | -5.58508 | -1.48986 | -0.01179 | C | 1.78793 | -4.6346 | 1.2484 |
| H | -5.56483 | -3.17853 | 0.58718 | C | 0.04262 | -4.00546 | -0.22634 |
| C | 0.37703 | -0.55565 | 2.50145 | C | 0.66915 | -4.99349 | 0.51609 |
| C | 0.56207 | -0.75941 | 3.8826 | H | 2.25536 | -5.3515 | 1.9241 |
| C | 1.79906 | -1.21966 | 4.31547 | H | -0.88344 | -4.18694 | -0.76546 |
| C | 2.5291 | -1.25609 | 2.05176 | H | 0.25359 | -5.99678 | 0.55627 |
| C | 2.79193 | -1.48777 | 3.38813 | C | 3.46089 | -3.00586 | 2.07748 |
| H | 1.96804 | -1.3888 | 5.37876 | H | 3.26497 | -3.43655 | 3.06852 |
| H | 3.28685 | -1.45449 | 1.30104 | H | 4.41808 | -3.39919 | 1.71703 |
| H | 3.76264 | -1.87571 | 3.68523 | H | 3.57685 | -1.92158 | 2.18996 |
| C | -0.55091 | -0.54491 | 4.8648 | N | 0.53616 | -2.76846 | -0.30932 |
| H | -0.18799 | -0.67571 | 5.89066 | Rh | -0.63485 | -1.16872 | -1.00358 |
| H | -0.99411 | 0.45491 | 4.78351 | C | -2.46037 | -0.12261 | -1.64796 |

| | | | | | | | |
|---|----------|----------|----------|------------------|----------|----------|----------|
| C | -1.52305 | 0.69158 | -1.8095 | H | 2.03731 | 4.68423 | 1.11511 |
| C | -3.83089 | -0.54825 | -1.52278 | H | 0.70895 | 5.83237 | 1.45329 |
| C | -4.3328 | -1.6658 | -2.20188 | C | -1.73122 | -0.51929 | 2.01026 |
| C | -4.6751 | 0.18189 | -0.67397 | C | -2.69428 | -0.56617 | 3.03332 |
| C | -5.65724 | -2.04314 | -2.03631 | C | -3.7248 | -1.49159 | 2.9148 |
| H | -3.66324 | -2.2334 | -2.84757 | C | -2.78793 | -2.21056 | 0.85207 |
| C | -6.00042 | -0.20655 | -0.51143 | C | -3.76467 | -2.34005 | 1.82086 |
| H | -4.2736 | 1.0379 | -0.13015 | H | -4.48637 | -1.54831 | 3.69234 |
| C | -6.4938 | -1.31807 | -1.18759 | H | -2.80228 | -2.82899 | -0.04011 |
| H | -6.04223 | -2.9093 | -2.57222 | H | -4.54983 | -3.08146 | 1.69569 |
| H | -6.64913 | 0.36404 | 0.15133 | C | -2.62766 | 0.3528 | 4.21473 |
| H | -7.53123 | -1.62166 | -1.05585 | H | -3.33239 | 0.03478 | 4.99149 |
| C | -0.94841 | 1.9483 | -2.2175 | H | -1.62438 | 0.38713 | 4.6575 |
| C | 0.1117 | 2.01763 | -3.13298 | H | -2.89443 | 1.37778 | 3.92396 |
| C | -1.46338 | 3.13325 | -1.67135 | N | -1.79217 | -1.30593 | 0.91822 |
| C | 0.66052 | 3.2486 | -3.4637 | H | -1.70371 | -2.22203 | -1.61774 |
| H | 0.5073 | 1.09028 | -3.54384 | Cl | 0.37282 | -1.41723 | -3.11881 |
| C | -0.89605 | 4.36131 | -1.99704 | | | | |
| H | -2.32185 | 3.08598 | -1.00186 | 88 | | | |
| C | 0.1721 | 4.4201 | -2.8873 | MeC1'(14) | | | |
| H | 1.48607 | 3.29256 | -4.17247 | C | -3.62084 | -1.22377 | 0.06883 |
| H | -1.2963 | 5.26877 | -1.54807 | C | -3.74023 | -1.83147 | -1.19463 |
| H | 0.61692 | 5.38108 | -3.14227 | C | -2.63705 | -2.08897 | -1.98729 |
| C | -0.60863 | 1.73481 | 1.98518 | C | -1.40939 | -1.56146 | -1.56691 |
| C | 0.52066 | 2.54466 | 2.19815 | C | -1.2662 | -0.84499 | -0.37896 |
| C | 1.69727 | 2.02081 | 2.70331 | C | -2.3492 | -0.81858 | 0.52131 |
| C | 1.72562 | 0.64988 | 2.9681 | H | -2.72737 | -2.62225 | -2.93285 |
| C | 0.63202 | -0.1731 | 2.71168 | H | -0.53758 | -1.70768 | -2.2102 |
| C | -0.55245 | 0.36232 | 2.19862 | C | -4.98173 | -0.90842 | 0.50307 |
| H | 2.57263 | 2.64213 | 2.8799 | C | -5.91779 | -1.48247 | -0.59748 |
| H | 2.63864 | 0.20944 | 3.36721 | O | -5.40058 | -0.27086 | 1.44546 |
| H | 0.69655 | -1.2463 | 2.89169 | O | -7.1249 | -1.41691 | -0.63105 |
| C | -1.69459 | 2.6034 | 1.55049 | N | -5.08775 | -2.05855 | -1.52956 |
| C | -1.06551 | 4.02285 | 1.45748 | C | -5.5431 | -2.61718 | -2.77374 |
| O | -2.86182 | 2.36717 | 1.32826 | H | -5.19392 | -2.01672 | -3.62652 |
| O | -1.61194 | 5.04365 | 1.11674 | H | -5.18621 | -3.64784 | -2.89772 |
| N | 0.25005 | 3.87333 | 1.85352 | H | -6.63706 | -2.61275 | -2.75327 |
| C | 1.22301 | 4.93465 | 1.80931 | C | -2.0324 | -0.3061 | 1.86027 |
| H | 1.64489 | 5.13042 | 2.80371 | C | -2.68298 | -0.62995 | 3.06794 |

| | | | | | | | |
|----|----------|----------|----------|---|----------|----------|----------|
| C | -2.26735 | 0.0349 | 4.22252 | C | 4.50801 | -1.99234 | 0.98403 |
| C | -0.5106 | 1.07361 | 3.01861 | C | 5.13502 | -1.10373 | 1.83879 |
| C | -1.21241 | 0.93118 | 4.20423 | C | 5.00946 | 0.26059 | 1.5527 |
| H | -2.7765 | -0.19033 | 5.16001 | C | 4.28098 | 0.72852 | 0.46237 |
| H | 0.40402 | 1.65744 | 2.94523 | C | 3.64447 | -0.1816 | -0.38611 |
| H | -0.88756 | 1.45368 | 5.09991 | H | 5.69087 | -1.44059 | 2.71151 |
| C | -3.69305 | -1.72464 | 3.21846 | H | 5.48947 | 0.98082 | 2.21333 |
| H | -3.48976 | -2.27519 | 4.1457 | H | 4.17715 | 1.79947 | 0.28669 |
| H | -4.71529 | -1.33391 | 3.26621 | C | 3.22441 | -2.69192 | -0.81667 |
| H | -3.64964 | -2.43795 | 2.38851 | C | 3.64798 | -3.90994 | 0.05278 |
| N | -0.90346 | 0.45951 | 1.90258 | O | 2.61079 | -2.75879 | -1.85591 |
| Rh | 0.33761 | 0.36461 | 0.27766 | O | 3.3899 | -5.0741 | -0.12821 |
| Cl | 1.11259 | -1.70219 | 1.30446 | N | 4.43066 | -3.38438 | 1.07082 |
| H | 1.62727 | 1.0631 | 1.02284 | C | 4.97934 | -4.1762 | 2.14029 |
| C | -0.8417 | 2.07237 | -0.44797 | H | 6.07242 | -4.07882 | 2.18304 |
| C | 0.28311 | 2.49932 | -0.08059 | H | 4.5532 | -3.87577 | 3.10686 |
| C | -2.25046 | 2.07851 | -0.73738 | H | 4.71913 | -5.21996 | 1.94028 |
| C | -3.1377 | 2.42722 | 0.29403 | C | 2.86675 | 0.20458 | -1.58889 |
| C | -2.77305 | 1.68169 | -1.97453 | C | 3.56431 | 0.38787 | -2.79531 |
| C | -4.50905 | 2.36873 | 0.09292 | C | 2.83073 | 0.66848 | -3.9417 |
| H | -2.73048 | 2.72608 | 1.26053 | C | 0.84037 | 0.54333 | -2.64651 |
| C | -4.1468 | 1.61479 | -2.16632 | C | 1.44808 | 0.73628 | -3.87247 |
| H | -2.09876 | 1.4222 | -2.78887 | H | 3.34799 | 0.81315 | -4.89002 |
| C | -5.01922 | 1.95079 | -1.13394 | H | -0.23973 | 0.58815 | -2.54481 |
| H | -5.18579 | 2.61226 | 0.90893 | H | 0.84102 | 0.93794 | -4.75113 |
| H | -4.54024 | 1.28758 | -3.12812 | C | 5.05282 | 0.23022 | -2.85689 |
| H | -6.09599 | 1.87419 | -1.27792 | H | 5.437 | 0.54415 | -3.83429 |
| C | 1.24997 | 3.55087 | 0.13408 | H | 5.5642 | 0.81195 | -2.08044 |
| C | 2.36894 | 3.69426 | -0.69576 | H | 5.33766 | -0.82042 | -2.70538 |
| C | 1.05315 | 4.46079 | 1.17933 | N | 1.52328 | 0.29613 | -1.51567 |
| C | 3.27418 | 4.72439 | -0.47542 | | | | |
| H | 2.51932 | 2.99038 | -1.51544 | | | | |
| C | 1.96495 | 5.48642 | 1.39742 | | | | |
| H | 0.17432 | 4.35107 | 1.81489 | | | | |
| C | 3.07826 | 5.62055 | 0.57317 | | | | |
| H | 4.1377 | 4.83129 | -1.13026 | | | | |
| H | 1.80174 | 6.18914 | 2.21283 | | | | |
| H | 3.79143 | 6.42505 | 0.74354 | | | | |
| C | 3.79683 | -1.53202 | -0.13062 | | | | |

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MeC1'(15)

| | | | |
|---|---------|---------|----------|
| C | 3.23332 | 1.37481 | -0.40797 |
| C | 3.25782 | 2.17295 | 0.75078 |
| C | 2.32802 | 2.01746 | 1.76189 |
| C | 1.27332 | 1.13 | 1.52559 |
| C | 1.16023 | 0.36995 | 0.36469 |
| C | 2.22718 | 0.39664 | -0.55353 |

| | | | | | | | |
|----|----------|----------|----------|---|----------|----------|----------|
| H | 2.38009 | 2.60466 | 2.67883 | C | -0.15016 | -5.29393 | -0.05349 |
| H | 0.50803 | 1.02789 | 2.2985 | C | -2.05669 | -4.2138 | -1.07054 |
| C | 4.19136 | 1.97962 | -1.33673 | C | -0.62821 | -6.52866 | -0.46554 |
| C | 4.89773 | 3.11038 | -0.53763 | H | 0.78189 | -5.21658 | 0.50627 |
| O | 4.41165 | 1.77535 | -2.50982 | C | -2.53565 | -5.45528 | -1.47219 |
| O | 5.79594 | 3.82293 | -0.9194 | H | -2.60007 | -3.29859 | -1.309 |
| N | 4.28509 | 3.13064 | 0.69378 | C | -1.82442 | -6.61368 | -1.17557 |
| C | 4.5886 | 4.08275 | 1.72715 | H | -0.06524 | -7.43055 | -0.2306 |
| H | 3.71548 | 4.70988 | 1.95548 | H | -3.4701 | -5.51441 | -2.02747 |
| H | 4.91334 | 3.57984 | 2.64806 | H | -2.19859 | -7.58281 | -1.50122 |
| H | 5.40032 | 4.7168 | 1.35754 | C | -2.98624 | 2.32065 | -0.01385 |
| C | 2.17559 | -0.63765 | -1.5926 | C | -2.86592 | 3.51385 | -0.73808 |
| C | 3.2586 | -1.20471 | -2.29556 | C | -1.95612 | 4.48729 | -0.3635 |
| C | 2.96346 | -2.10523 | -3.32108 | C | -1.16294 | 4.22306 | 0.75474 |
| C | 0.65953 | -2.00109 | -2.776 | C | -1.26345 | 3.03261 | 1.4703 |
| C | 1.66033 | -2.46363 | -3.6158 | C | -2.16012 | 2.04193 | 1.06442 |
| H | 3.79102 | -2.5357 | -3.88544 | H | -1.84635 | 5.4157 | -0.92002 |
| H | -0.37737 | -2.30857 | -2.87537 | H | -0.44109 | 4.97172 | 1.07771 |
| H | 1.41869 | -3.13753 | -4.43282 | H | -0.63139 | 2.87286 | 2.34131 |
| C | 4.69977 | -1.00307 | -1.94104 | C | -4.00677 | 1.49999 | -0.67377 |
| H | 5.23069 | -1.95874 | -2.04053 | C | -4.438 | 2.32816 | -1.91601 |
| H | 5.18354 | -0.27256 | -2.59839 | O | -4.49692 | 0.44416 | -0.3512 |
| H | 4.82511 | -0.65083 | -0.91033 | O | -5.24326 | 2.02486 | -2.76124 |
| N | 0.92964 | -1.16293 | -1.77592 | N | -3.73313 | 3.51866 | -1.83265 |
| Rh | -0.46913 | -0.79209 | -0.34513 | C | -3.78214 | 4.54371 | -2.84227 |
| C | 0.47377 | -2.2897 | 0.93409 | H | -4.10293 | 5.5037 | -2.41627 |
| C | -0.31086 | -2.87208 | 0.13549 | H | -2.8 | 4.66953 | -3.31763 |
| C | 1.42736 | -2.09535 | 1.99134 | H | -4.50846 | 4.22315 | -3.59513 |
| C | 2.7987 | -2.23585 | 1.738 | C | -2.39746 | 0.76604 | 1.78843 |
| C | 1.00186 | -1.72209 | 3.27282 | C | -3.22183 | 0.83967 | 2.9279 |
| C | 3.72408 | -1.98992 | 2.74319 | C | -3.6528 | -0.34601 | 3.50789 |
| H | 3.12259 | -2.52525 | 0.7379 | C | -2.45662 | -1.53632 | 1.83214 |
| C | 1.93311 | -1.48275 | 4.27488 | C | -3.29103 | -1.5525 | 2.93361 |
| H | -0.0658 | -1.60824 | 3.46579 | H | -4.30293 | -0.31489 | 4.38204 |
| C | 3.29479 | -1.6094 | 4.01267 | H | -2.15968 | -2.4707 | 1.37075 |
| H | 4.78769 | -2.09393 | 2.53446 | H | -3.64885 | -2.50267 | 3.32158 |
| H | 1.59402 | -1.19266 | 5.26814 | C | -3.69477 | 2.15816 | 3.46461 |
| H | 4.02275 | -1.41575 | 4.79858 | H | -4.31839 | 2.00924 | 4.35359 |
| C | -0.85989 | -4.1186 | -0.35256 | H | -2.86407 | 2.81981 | 3.73852 |

| | | | | | | | |
|---|----------|----------|----------|---|----------|----------|----------|
| H | -4.29309 | 2.69776 | 2.71808 | C | -0.393 | 2.17444 | -0.00634 |
| N | -1.96865 | -0.41148 | 1.27824 | C | 0.404 | 2.03229 | 0.98926 |
| H | -1.73943 | -1.49046 | -1.10965 | C | -1.3665 | 2.99779 | -0.67881 |
| Cl | -1.03642 | 1.00998 | -1.87243 | C | -1.87939 | 4.13181 | -0.02626 |
| | | | | C | -1.85099 | 2.68512 | -1.95692 |
| 88 | | | | C | -2.84033 | 4.92484 | -0.63627 |
| Me^eTS_{Cl⁻D⁻}(1)} | | | | H | -1.52545 | 4.36671 | 0.97741 |
| C | -3.8204 | -1.11088 | 0.56823 | C | -2.81173 | 3.48264 | -2.56509 |
| C | -3.99805 | -1.04943 | 1.96358 | H | -1.47132 | 1.80212 | -2.46857 |
| C | -3.03729 | -0.51911 | 2.8031 | C | -3.31012 | 4.60403 | -1.90847 |
| C | -1.82892 | -0.11875 | 2.2284 | H | -3.23141 | 5.79633 | -0.11379 |
| C | -1.60729 | -0.19228 | 0.8558 | H | -3.17462 | 3.2217 | -3.55872 |
| C | -2.64026 | -0.60826 | -0.01414 | H | -4.06672 | 5.22544 | -2.38415 |
| H | -3.18727 | -0.47121 | 3.88035 | C | 1.12399 | 2.65534 | 2.07635 |
| H | -1.03048 | 0.23434 | 2.88003 | C | 1.7171 | 1.93128 | 3.11841 |
| C | -4.90244 | -1.9668 | 0.06417 | C | 1.21791 | 4.05758 | 2.09335 |
| C | -5.82415 | -2.24387 | 1.28368 | C | 2.37264 | 2.58785 | 4.15217 |
| O | -5.08815 | -2.47513 | -1.0177 | H | 1.66867 | 0.84079 | 3.10787 |
| O | -6.8624 | -2.86095 | 1.28617 | C | 1.87814 | 4.70804 | 3.12529 |
| N | -5.2074 | -1.6446 | 2.35689 | H | 0.77595 | 4.62546 | 1.27467 |
| C | -5.68298 | -1.73675 | 3.71157 | C | 2.45661 | 3.97704 | 4.16104 |
| H | -4.9736 | -2.28976 | 4.34254 | H | 2.82317 | 2.008 | 4.95647 |
| H | -5.84211 | -0.73981 | 4.14355 | H | 1.94638 | 5.79459 | 3.11927 |
| H | -6.63519 | -2.27518 | 3.68504 | H | 2.97425 | 4.48948 | 4.96993 |
| C | -2.32539 | -0.58076 | -1.44983 | C | 3.61001 | -1.66455 | -0.07665 |
| C | -3.21408 | -0.49668 | -2.53639 | C | 3.84119 | -2.55297 | 0.98222 |
| C | -2.66981 | -0.68062 | -3.8114 | C | 4.19609 | -2.08616 | 2.23717 |
| C | -0.48258 | -0.76794 | -2.89065 | C | 4.30634 | -0.70238 | 2.40187 |
| C | -1.31354 | -0.89281 | -3.99849 | C | 4.06661 | 0.18904 | 1.35782 |
| H | -3.34176 | -0.646 | -4.66976 | C | 3.6954 | -0.29533 | 0.09965 |
| H | 0.60498 | -0.82026 | -2.96046 | H | 4.36685 | -2.76431 | 3.0709 |
| H | -0.89345 | -1.08207 | -4.98269 | H | 4.58353 | -0.30797 | 3.37938 |
| C | -4.64459 | -0.07009 | -2.42479 | H | 4.144 | 1.26402 | 1.52286 |
| H | -4.85863 | 0.66971 | -3.20805 | C | 3.18591 | -2.45072 | -1.24003 |
| H | -5.33854 | -0.90856 | -2.54532 | C | 3.15766 | -3.91686 | -0.73131 |
| H | -4.85157 | 0.40291 | -1.45776 | O | 2.95812 | -2.10526 | -2.37677 |
| N | -0.9869 | -0.55977 | -1.67889 | O | 2.8438 | -4.90576 | -1.34459 |
| Rh | 0.13738 | 0.16645 | -0.00504 | N | 3.61918 | -3.86793 | 0.57945 |
| H | 0.93093 | 0.43119 | 1.34621 | C | 3.55203 | -4.99441 | 1.47331 |

| | | | | | | | |
|----|---------|----------|----------|----|----------|----------|----------|
| H | 4.52121 | -5.1742 | 1.95653 | C | 2.04691 | -1.1309 | -3.64039 |
| H | 2.78429 | -4.83089 | 2.24308 | C | 0.4857 | 0.55131 | -3.03404 |
| H | 3.27981 | -5.8687 | 0.87459 | C | 1.42001 | 0.06031 | -3.94366 |
| C | 3.38684 | 0.61077 | -1.03286 | H | 2.70088 | -1.6075 | -4.37135 |
| C | 4.43581 | 1.1372 | -1.80449 | H | -0.17231 | 1.39076 | -3.25615 |
| C | 4.09825 | 1.97927 | -2.85727 | H | 1.59157 | 0.57419 | -4.8851 |
| C | 1.80334 | 1.69631 | -2.29358 | C | 2.35156 | -3.17869 | -2.26778 |
| C | 2.7648 | 2.27097 | -3.10735 | H | 2.06354 | -3.75307 | -3.15889 |
| H | 4.88593 | 2.40072 | -3.48213 | H | 3.44272 | -3.21283 | -2.1823 |
| H | 0.74767 | 1.91386 | -2.45162 | H | 1.93071 | -3.68857 | -1.39502 |
| H | 2.46959 | 2.93005 | -3.9201 | N | 0.3107 | -0.02627 | -1.85378 |
| C | 5.85948 | 0.76377 | -1.52664 | Rh | -1.47696 | 0.19844 | -0.6781 |
| H | 6.54113 | 1.28239 | -2.21075 | Cl | -2.73901 | 1.26225 | -2.60041 |
| H | 6.15636 | 1.00628 | -0.49827 | H | -2.07796 | -1.17035 | -1.22762 |
| H | 6.0113 | -0.31732 | -1.65292 | C | -3.31201 | -0.90394 | -0.30059 |
| N | 2.09492 | 0.87127 | -1.27954 | C | -3.20003 | 0.10648 | 0.47328 |
| Cl | 0.6151 | -2.23001 | 0.34145 | C | -4.0784 | -2.04529 | -0.74806 |

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Me^cTS_{Cl'-D'}(2)

| | | | | | | | |
|---|----------|----------|----------|---|----------|----------|----------|
| C | 1.72466 | -2.14252 | 0.76836 | H | -5.07475 | -2.21898 | 1.15432 |
| C | 1.39118 | -2.4292 | 2.106 | C | -4.74359 | -3.64126 | -2.43411 |
| C | 0.1635 | -2.09257 | 2.63956 | H | -3.2719 | -2.08926 | -2.74224 |
| C | -0.7081 | -1.35523 | 1.83083 | C | -5.64851 | -4.21262 | -1.54389 |
| C | -0.38702 | -0.98036 | 0.52515 | H | -6.47748 | -4.14317 | 0.44582 |
| C | 0.80791 | -1.47118 | -0.06322 | H | -4.65003 | -4.03424 | -3.44491 |
| H | -0.09849 | -2.33847 | 3.66789 | H | -6.25855 | -5.0594 | -1.85361 |
| H | -1.65957 | -1.03458 | 2.25648 | C | -3.80847 | 0.93347 | 1.48396 |
| C | 3.16226 | -2.38201 | 0.65075 | C | -3.04309 | 1.76169 | 2.31464 |
| C | 3.61958 | -2.91412 | 2.03417 | C | -5.20275 | 0.90627 | 1.65089 |
| O | 3.94902 | -2.16509 | -0.24654 | C | -3.65275 | 2.5308 | 3.29747 |
| O | 4.75243 | -3.18245 | 2.36568 | H | -1.96406 | 1.79212 | 2.16826 |
| N | 2.48346 | -2.9809 | 2.80236 | C | -5.80714 | 1.68198 | 2.62935 |
| C | 2.48202 | -3.30458 | 4.20464 | H | -5.80116 | 0.27848 | 0.99107 |
| H | 2.20201 | -2.42955 | 4.81001 | C | -5.03478 | 2.49368 | 3.458 |
| H | 1.78136 | -4.12111 | 4.4202 | H | -3.0456 | 3.16798 | 3.93864 |
| H | 3.49632 | -3.61719 | 4.47031 | H | -6.88944 | 1.65675 | 2.74465 |
| C | 1.04351 | -1.11143 | -1.4709 | H | -5.51221 | 3.10083 | 4.22519 |
| C | 1.84102 | -1.77846 | -2.41306 | C | 2.72731 | 1.45948 | 0.07498 |

| | | | | | | | |
|---|----------|----------|----------|----|----------|----------|----------|
| C | 3.78523 | 0.77797 | 0.7071 | H | 2.9316 | 2.23458 | -3.84524 |
| C | 3.68211 | 0.35176 | 2.02204 | H | 0.54952 | 1.71272 | -3.34588 |
| C | 2.47149 | 0.59546 | 2.67601 | C | 4.39502 | 1.30414 | 0.23541 |
| C | 1.42197 | 1.27774 | 2.06395 | C | 5.54596 | 1.65586 | -0.74705 |
| C | 1.54124 | 1.74332 | 0.75058 | O | 4.61886 | 0.80414 | 1.31989 |
| H | 4.50265 | -0.1623 | 2.52074 | O | 6.73217 | 1.6035 | -0.51938 |
| H | 2.34881 | 0.25191 | 3.70329 | N | 4.93324 | 2.01158 | -1.92203 |
| H | 0.50926 | 1.48237 | 2.62167 | C | 5.6364 | 2.36271 | -3.12758 |
| C | 3.16306 | 1.74976 | -1.29049 | H | 5.45915 | 1.62373 | -3.92137 |
| C | 4.57928 | 1.11933 | -1.40698 | H | 5.32609 | 3.35164 | -3.48898 |
| O | 2.61729 | 2.35829 | -2.18297 | H | 6.70369 | 2.3823 | -2.88713 |
| O | 5.28272 | 1.09068 | -2.38655 | C | 1.22568 | 1.04083 | 1.12695 |
| N | 4.87276 | 0.62403 | -0.1503 | C | 1.736 | 1.40975 | 2.38747 |
| C | 6.10475 | -0.05458 | 0.18365 | C | 1.13363 | 0.85093 | 3.5184 |
| H | 6.6403 | 0.48401 | 0.97642 | C | -0.55365 | -0.09951 | 2.15607 |
| H | 5.90379 | -1.0861 | 0.49841 | C | 0.01368 | 0.0458 | 3.41436 |
| H | 6.71895 | -0.06738 | -0.7214 | H | 1.54521 | 1.09297 | 4.49892 |
| C | 0.52914 | 2.70385 | 0.2308 | H | -1.50894 | -0.60018 | 2.01715 |
| C | 0.88658 | 4.06581 | 0.2417 | H | -0.45128 | -0.41388 | 4.28186 |
| C | -0.09817 | 4.99498 | -0.07784 | C | 2.77015 | 2.47159 | 2.60776 |
| C | -1.63965 | 3.21076 | -0.38777 | H | 2.40879 | 3.15907 | 3.38413 |
| C | -1.37919 | 4.56909 | -0.38333 | H | 3.72762 | 2.0567 | 2.94043 |
| H | 0.14891 | 6.05674 | -0.0709 | H | 2.95885 | 3.06092 | 1.70494 |
| H | -2.61951 | 2.83354 | -0.66653 | N | 0.02453 | 0.38505 | 1.05736 |
| H | -2.17365 | 5.26998 | -0.62524 | Rh | -1.02886 | 0.70557 | -0.73599 |
| C | 2.26664 | 4.53333 | 0.59724 | H | -1.56786 | 2.08724 | 0.02672 |
| H | 2.26917 | 5.61605 | 0.76923 | C | -2.81249 | 1.63194 | 0.36549 |
| H | 2.65445 | 4.04746 | 1.50179 | C | -3.00851 | 0.38477 | 0.17184 |
| H | 2.97605 | 4.33082 | -0.21596 | C | -3.4243 | 2.87538 | 0.80768 |
| N | -0.70829 | 2.28449 | -0.09585 | C | -4.64992 | 2.80687 | 1.4857 |
| | | | | C | -2.84774 | 4.12291 | 0.55652 |
| | | | | C | -5.27744 | 3.96955 | 1.90662 |
| | | | | H | -5.09605 | 1.83041 | 1.67434 |
| C | 3.15191 | 1.57469 | -0.48308 | C | -3.48332 | 5.28384 | 0.97899 |
| C | 3.53667 | 1.89263 | -1.80072 | H | -1.90762 | 4.17549 | 0.00554 |
| C | 2.62036 | 1.98112 | -2.83238 | C | -4.69613 | 5.21169 | 1.65699 |
| C | 1.28761 | 1.68377 | -2.54355 | H | -6.22796 | 3.90717 | 2.43412 |
| C | 0.85221 | 1.33468 | -1.25875 | H | -3.02896 | 6.25157 | 0.77355 |
| C | 1.78348 | 1.3524 | -0.19433 | H | -5.19178 | 6.12249 | 1.98841 |

88

Me^cTS_{Cl⁻D⁻}(3)}

| | | | | | | | |
|---|----------|----------|----------|--|----------|----------|----------|
| C | -3.88922 | -0.74863 | 0.11567 | H | 1.27406 | -4.75684 | -1.51301 |
| C | -3.48995 | -2.01371 | 0.57085 | H | 0.16305 | -5.10334 | -0.17986 |
| C | -5.15405 | -0.60515 | -0.47878 | N | -1.0419 | -1.38094 | -1.67877 |
| C | -4.3476 | -3.09952 | 0.46321 | Cl | -1.99912 | 1.60448 | -2.72629 |
| H | -2.48903 | -2.15602 | 0.97992 | | | | |
| C | -5.99759 | -1.70176 | -0.60081 | 88 | | | |
| H | -5.44977 | 0.37443 | -0.85476 | Me^eTS_{Cl^e-D^e}(4)} | | | |
| C | -5.60104 | -2.95022 | -0.12511 | C | 2.81609 | -0.91586 | -1.36178 |
| H | -4.0203 | -4.07329 | 0.82459 | C | 3.14044 | -2.18749 | -0.84715 |
| H | -6.9738 | -1.5798 | -1.06804 | C | 2.16562 | -3.05373 | -0.39043 |
| H | -6.26774 | -3.80606 | -0.21785 | C | 0.84267 | -2.5956 | -0.38999 |
| C | 1.41723 | -2.40405 | 0.52237 | C | 0.47816 | -1.3338 | -0.86519 |
| C | 2.71977 | -2.15783 | 0.98873 | C | 1.47023 | -0.50384 | -1.42112 |
| C | 3.74173 | -1.81108 | 0.1232 | H | 2.42106 | -4.0319 | 0.01344 |
| C | 3.4011 | -1.61571 | -1.21682 | H | 0.07341 | -3.24629 | 0.03023 |
| C | 2.09524 | -1.77319 | -1.67932 | C | 4.08078 | -0.20301 | -1.50996 |
| C | 1.08092 | -2.18341 | -0.81028 | C | 5.18713 | -1.22347 | -1.12747 |
| H | 4.75709 | -1.64927 | 0.47743 | O | 4.32834 | 0.95674 | -1.77707 |
| H | 4.17908 | -1.31891 | -1.92049 | O | 6.37783 | -1.00828 | -1.09832 |
| H | 1.85335 | -1.57651 | -2.723 | N | 4.5326 | -2.38318 | -0.79625 |
| C | 0.62526 | -2.8416 | 1.66777 | C | 5.17247 | -3.50634 | -0.15591 |
| C | 1.57997 | -2.71596 | 2.89189 | H | 4.82699 | -3.59348 | 0.88292 |
| O | -0.51497 | -3.24669 | 1.73832 | H | 4.96904 | -4.43654 | -0.70125 |
| O | 1.30069 | -2.89858 | 4.05314 | H | 6.24854 | -3.3096 | -0.15519 |
| N | 2.79728 | -2.32803 | 2.3757 | C | 0.99273 | 0.7905 | -1.93132 |
| C | 3.94528 | -1.98282 | 3.18181 | C | 1.4986 | 1.49805 | -3.03771 |
| H | 4.76472 | -2.69762 | 3.03092 | C | 0.90945 | 2.72865 | -3.32946 |
| H | 4.29196 | -0.97356 | 2.9253 | C | -0.69227 | 2.37858 | -1.61564 |
| H | 3.62961 | -2.01861 | 4.22888 | C | -0.16552 | 3.2034 | -2.59619 |
| C | -0.27285 | -2.44036 | -1.36257 | H | 1.28732 | 3.29735 | -4.17973 |
| C | -0.64247 | -3.76243 | -1.65641 | H | -1.59555 | 2.64932 | -1.06771 |
| C | -1.84001 | -3.96098 | -2.33699 | H | -0.63625 | 4.15733 | -2.82094 |
| C | -2.18057 | -1.60372 | -2.35739 | C | 2.5151 | 0.95605 | -3.99397 |
| C | -2.60891 | -2.87184 | -2.71191 | H | 2.21071 | 1.19753 | -5.02028 |
| H | -2.15246 | -4.97618 | -2.58261 | H | 3.5087 | 1.38452 | -3.82188 |
| H | -2.75384 | -0.71671 | -2.61984 | H | 2.60462 | -0.1332 | -3.92247 |
| H | -3.54579 | -2.99027 | -3.25072 | N | -0.13119 | 1.2138 | -1.30081 |
| C | 0.21871 | -4.92379 | -1.26233 | Rh | -1.34445 | -0.44312 | -0.59332 |
| H | -0.11053 | -5.83943 | -1.76719 | C | -3.55325 | -0.86704 | -0.25075 |

| | | | | | | | |
|---|----------|----------|----------|----|----------|----------|----------|
| C | -3.33219 | 0.38224 | -0.12868 | H | 5.79637 | 2.17201 | 1.64645 |
| C | -4.5913 | -1.88697 | -0.30035 | H | 6.35636 | 0.48901 | 1.38697 |
| C | -5.9078 | -1.52066 | 0.01232 | C | -0.31872 | 0.40814 | 2.34595 |
| C | -4.3148 | -3.21033 | -0.65344 | C | -0.45113 | 0.49726 | 3.7432 |
| C | -6.92043 | -2.46705 | -0.02314 | C | -1.30738 | -0.39623 | 4.3756 |
| H | -6.11955 | -0.48475 | 0.2771 | C | -1.80788 | -1.34856 | 2.25498 |
| C | -5.33448 | -4.15398 | -0.69009 | C | -1.96935 | -1.3556 | 3.62747 |
| H | -3.29424 | -3.48703 | -0.92499 | H | -1.42562 | -0.35292 | 5.45805 |
| C | -6.63788 | -3.78717 | -0.37216 | H | -2.33419 | -2.07543 | 1.64309 |
| H | -7.94024 | -2.17419 | 0.22149 | H | -2.6144 | -2.09792 | 4.08992 |
| H | -5.10842 | -5.1803 | -0.97413 | C | 0.34282 | 1.48546 | 4.54358 |
| H | -7.43624 | -4.52658 | -0.40209 | H | -0.02137 | 1.52594 | 5.57661 |
| C | -3.66304 | 1.75676 | 0.06502 | H | 1.40542 | 1.20694 | 4.5785 |
| C | -3.30901 | 2.411 | 1.25868 | H | 0.29223 | 2.49694 | 4.12246 |
| C | -4.26151 | 2.49908 | -0.9667 | N | -1.03123 | -0.46332 | 1.60439 |
| C | -3.56063 | 3.76785 | 1.41536 | H | -2.44316 | -1.67558 | -0.40915 |
| H | -2.82851 | 1.83577 | 2.05324 | Cl | -1.7985 | -0.69637 | -2.89983 |
| C | -4.50283 | 3.85734 | -0.79986 | | | | |
| H | -4.51082 | 1.99314 | -1.89895 | | | | |
| C | -4.15589 | 4.49755 | 0.38764 | | | | |
| H | -3.28944 | 4.26158 | 2.34784 | | | | |
| H | -4.96772 | 4.4211 | -1.6073 | | | | |
| H | -4.34814 | 5.56163 | 0.5127 | | | | |
| C | 2.03165 | 0.70499 | 1.68397 | | | | |
| C | 3.12277 | 1.45465 | 1.21808 | | | | |
| C | 2.94462 | 2.74007 | 0.73272 | | | | |
| C | 1.65115 | 3.26661 | 0.77773 | | | | |
| C | 0.56636 | 2.54487 | 1.27813 | | | | |
| C | 0.74316 | 1.23247 | 1.71265 | | | | |
| H | 3.77428 | 3.31347 | 0.3254 | | | | |
| H | 1.48393 | 4.27612 | 0.40475 | | | | |
| H | -0.42983 | 2.98951 | 1.29416 | | | | |
| C | 2.54373 | -0.59021 | 2.13048 | | | | |
| C | 4.0728 | -0.52636 | 1.86263 | | | | |
| O | 1.97953 | -1.53194 | 2.63753 | | | | |
| O | 4.88602 | -1.39339 | 2.08219 | | | | |
| N | 4.31413 | 0.72573 | 1.32923 | | | | |
| C | 5.63864 | 1.25098 | 1.07017 | | | | |
| H | 5.77614 | 1.44368 | -0.00094 | | | | |

88

Me^eTS_{Cl⁻-D⁺}(5)

| | | | |
|---|----------|----------|----------|
| C | -4.18041 | -0.45717 | 0.33025 |
| C | -4.44048 | 0.19519 | 1.55145 |
| C | -3.50012 | 0.99692 | 2.16692 |
| C | -2.23371 | 1.07433 | 1.58213 |
| C | -1.93356 | 0.42155 | 0.38845 |
| C | -2.93851 | -0.2856 | -0.31164 |
| H | -3.71036 | 1.50148 | 3.10861 |
| H | -1.45886 | 1.64175 | 2.09462 |
| C | -5.27784 | -1.41833 | 0.15038 |
| C | -6.29307 | -1.11569 | 1.28702 |
| O | -5.42142 | -2.34223 | -0.61679 |
| O | -7.36822 | -1.63771 | 1.46023 |
| N | -5.70748 | -0.1369 | 2.05507 |
| C | -6.27531 | 0.37851 | 3.27236 |
| H | -5.65016 | 0.12458 | 4.13955 |
| H | -6.39054 | 1.46933 | 3.22293 |
| H | -7.25985 | -0.08377 | 3.39236 |
| C | -2.54216 | -0.87404 | -1.59855 |

| | | | | | | | |
|----|----------|----------|----------|----|---------|----------|----------|
| C | -3.36177 | -1.2265 | -2.68421 | C | 3.49407 | -2.27147 | 1.39248 |
| C | -2.76005 | -1.9464 | -3.7219 | C | 4.14614 | -1.49492 | 2.33581 |
| C | -0.63789 | -1.71586 | -2.68043 | C | 4.51736 | -0.2018 | 1.9619 |
| C | -1.41321 | -2.25883 | -3.69934 | C | 4.23614 | 0.3061 | 0.69662 |
| H | -3.38082 | -2.25481 | -4.56394 | C | 3.56749 | -0.48013 | -0.24682 |
| H | 0.44482 | -1.8375 | -2.64487 | H | 4.34904 | -1.86589 | 3.33876 |
| H | -0.94953 | -2.85512 | -4.48042 | H | 5.00445 | 0.44092 | 2.69426 |
| C | -4.78048 | -0.78243 | -2.8633 | H | 4.50291 | 1.33361 | 0.44808 |
| H | -4.91458 | -0.41717 | -3.89028 | C | 2.53633 | -2.8387 | -0.6369 |
| H | -5.49068 | -1.59941 | -2.69623 | C | 2.36801 | -3.99434 | 0.38394 |
| H | -5.04875 | 0.03236 | -2.18201 | O | 2.22063 | -2.90683 | -1.80367 |
| N | -1.19294 | -1.01071 | -1.70116 | O | 1.82559 | -5.05616 | 0.2103 |
| Rh | -0.11143 | 0.27189 | -0.37068 | N | 3.01825 | -3.57335 | 1.53727 |
| H | -0.44274 | 1.51504 | -1.30616 | C | 2.88767 | -4.25057 | 2.80062 |
| C | 0.32916 | 2.34415 | -0.05336 | H | 3.86888 | -4.42143 | 3.26217 |
| C | 0.81426 | 1.63756 | 0.89846 | H | 2.25859 | -3.66319 | 3.48605 |
| C | -0.00288 | 3.66815 | -0.53298 | H | 2.40669 | -5.21418 | 2.60815 |
| C | 0.2338 | 4.7533 | 0.32833 | C | 3.22611 | 0.04772 | -1.58952 |
| C | -0.53892 | 3.92534 | -1.79985 | C | 4.24193 | 0.25041 | -2.54022 |
| C | -0.04822 | 6.04932 | -0.07512 | C | 3.86478 | 0.73698 | -3.78722 |
| H | 0.6281 | 4.56025 | 1.32557 | C | 1.60362 | 0.76461 | -3.05111 |
| C | -0.82055 | 5.22524 | -2.20005 | C | 2.52948 | 1.00312 | -4.05309 |
| H | -0.7387 | 3.09297 | -2.47588 | H | 4.62493 | 0.89513 | -4.55272 |
| C | -0.57366 | 6.29249 | -1.34268 | H | 0.54266 | 0.95042 | -3.22167 |
| H | 0.13672 | 6.87658 | 0.60813 | H | 2.20582 | 1.38113 | -5.01987 |
| H | -1.23828 | 5.40387 | -3.18944 | C | 5.6733 | -0.08003 | -2.24156 |
| H | -0.79563 | 7.3106 | -1.65713 | H | 6.2807 | -0.02804 | -3.15285 |
| C | 1.51128 | 1.61458 | 2.1609 | H | 6.11192 | 0.60902 | -1.50791 |
| C | 1.29813 | 0.59974 | 3.10345 | H | 5.7727 | -1.09024 | -1.82411 |
| C | 2.4027 | 2.65766 | 2.47021 | N | 1.93129 | 0.2942 | -1.84149 |
| C | 1.94845 | 0.64486 | 4.33134 | Cl | 0.17539 | -1.8068 | 0.93669 |
| H | 0.6369 | -0.2275 | 2.8475 | | | | |
| C | 3.05618 | 2.68781 | 3.69345 | | | | |
| H | 2.58635 | 3.4341 | 1.72656 | | | | |
| C | 2.82618 | 1.68227 | 4.63194 | | | | |
| H | 1.7716 | -0.14649 | 5.05871 | | | | |
| H | 3.74454 | 3.50112 | 3.91908 | | | | |
| H | 3.33269 | 1.70993 | 5.59568 | | | | |
| C | 3.22271 | -1.77648 | 0.10762 | | | | |

88

Me^eTS_{Cl⁺-D⁺}(6)

| | | | |
|---|----------|----------|----------|
| C | -3.72278 | -0.64982 | -1.05313 |
| C | -4.07675 | 0.54522 | -1.70509 |
| C | -3.12383 | 1.44806 | -2.13821 |
| C | -1.79389 | 1.20691 | -1.77817 |
| C | -1.42542 | 0.07598 | -1.0525 |

| | | | | | | | |
|----|----------|----------|----------|---|----------|----------|----------|
| C | -2.37238 | -0.93783 | -0.79041 | H | -4.96296 | 2.63754 | 2.23777 |
| H | -3.39734 | 2.35314 | -2.67805 | H | -5.48827 | 0.61116 | 3.57792 |
| H | -1.03852 | 1.95044 | -2.03019 | C | 0.55735 | 3.28704 | 0.40224 |
| C | -4.96866 | -1.22178 | -0.53508 | C | 0.13067 | 4.28281 | 1.29811 |
| C | -6.1034 | -0.30609 | -1.07533 | C | 1.36594 | 3.64953 | -0.67883 |
| O | -5.17528 | -2.14724 | 0.2176 | C | 0.50291 | 5.60411 | 1.10559 |
| O | -7.29191 | -0.44399 | -0.9075 | H | -0.49168 | 3.99834 | 2.14699 |
| N | -5.47157 | 0.69378 | -1.77836 | C | 1.7364 | 4.97416 | -0.86638 |
| C | -6.1551 | 1.80446 | -2.38551 | H | 1.72415 | 2.89463 | -1.3772 |
| H | -5.85787 | 2.75343 | -1.9179 | C | 1.30684 | 5.95502 | 0.02151 |
| H | -5.94507 | 1.85798 | -3.46185 | H | 0.16661 | 6.36583 | 1.80736 |
| H | -7.22753 | 1.64829 | -2.23383 | H | 2.37624 | 5.22721 | -1.70973 |
| C | -1.83968 | -2.17573 | -0.20595 | H | 1.60187 | 6.99283 | -0.12477 |
| C | -2.31608 | -3.48256 | -0.41461 | C | 4.03615 | -0.46842 | -0.65122 |
| C | -1.63237 | -4.51616 | 0.22953 | C | 4.365 | -0.92731 | -1.93473 |
| C | -0.03024 | -2.97147 | 1.04963 | C | 4.6355 | -2.26184 | -2.17641 |
| C | -0.50457 | -4.27328 | 0.99517 | C | 4.50942 | -3.14262 | -1.10176 |
| H | -1.98966 | -5.53706 | 0.09198 | C | 4.11828 | -2.71004 | 0.16283 |
| H | 0.9055 | -2.70912 | 1.54227 | C | 3.85965 | -1.35736 | 0.39985 |
| H | 0.03081 | -5.07828 | 1.49207 | H | 4.89445 | -2.62257 | -3.16939 |
| C | -3.42691 | -3.84519 | -1.34835 | H | 4.69616 | -4.20276 | -1.26524 |
| H | -3.19983 | -4.80066 | -1.83708 | H | 3.98254 | -3.43241 | 0.96783 |
| H | -4.38056 | -3.94769 | -0.81746 | C | 3.82859 | 0.97496 | -0.74487 |
| H | -3.5673 | -3.09186 | -2.13188 | C | 3.91776 | 1.28748 | -2.26394 |
| N | -0.6797 | -1.96947 | 0.46639 | O | 3.65738 | 1.81661 | 0.10618 |
| Rh | 0.25149 | -0.10031 | -0.02568 | O | 3.66935 | 2.34135 | -2.80433 |
| Cl | 1.17907 | -1.38887 | -1.90123 | N | 4.33201 | 0.11831 | -2.86547 |
| H | 0.93837 | 1.21411 | -0.63128 | C | 4.32782 | -0.07887 | -4.29399 |
| C | -0.71362 | 1.18503 | 1.28914 | H | 5.288 | -0.48309 | -4.63825 |
| C | 0.09014 | 1.93909 | 0.63504 | H | 3.5159 | -0.76242 | -4.579 |
| C | -1.95976 | 1.04153 | 2.00066 | H | 4.16017 | 0.89714 | -4.75857 |
| C | -2.2688 | -0.09776 | 2.75563 | C | 3.36802 | -0.89568 | 1.7207 |
| C | -2.94457 | 2.02836 | 1.828 | C | 4.22243 | -0.95279 | 2.83456 |
| C | -3.52572 | -0.24242 | 3.32767 | C | 3.70753 | -0.54047 | 4.06003 |
| H | -1.5194 | -0.88121 | 2.86771 | C | 1.64179 | -0.05825 | 2.98182 |
| C | -4.20356 | 1.87218 | 2.39131 | C | 2.3981 | -0.09521 | 4.14339 |
| H | -2.7101 | 2.89958 | 1.21554 | H | 4.34528 | -0.56114 | 4.94417 |
| C | -4.49798 | 0.73787 | 3.14447 | H | 0.61794 | 0.31352 | 3.00152 |
| H | -3.75668 | -1.13594 | 3.90473 | H | 1.96835 | 0.23566 | 5.08581 |

| | | | |
|---|---------|----------|---------|
| C | 5.64868 | -1.39899 | 2.71083 |
| H | 6.20608 | -1.16822 | 3.6264 |
| H | 5.73259 | -2.47923 | 2.53357 |
| H | 6.1523 | -0.90221 | 1.87174 |
| N | 2.10192 | -0.44478 | 1.78705 |

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P-TS_{C2-D}(1)

| | | | |
|----|----------|----------|----------|
| C | 1.097 | -0.27199 | 1.28931 |
| C | 0.77785 | 0.40305 | 2.49754 |
| C | 1.04034 | -0.20741 | 3.71884 |
| C | 1.45965 | -1.54053 | 3.72414 |
| C | 1.58888 | -2.27771 | 2.54671 |
| C | 1.39375 | -1.66969 | 1.30026 |
| H | 0.84792 | 0.30708 | 4.65906 |
| H | 1.63486 | -2.03467 | 4.67855 |
| H | 1.81749 | -3.33496 | 2.62641 |
| C | -0.35031 | 1.93199 | 1.03722 |
| O | -1.0132 | 2.93052 | 0.86365 |
| N | 0.17345 | 1.62855 | 2.32023 |
| C | -0.17905 | 2.46127 | 3.45352 |
| H | 0.71267 | 2.70662 | 4.04359 |
| H | -0.62649 | 3.37806 | 3.06457 |
| H | -0.90898 | 1.94517 | 4.09484 |
| C | 1.44474 | -2.29899 | -0.02749 |
| C | 2.0366 | -3.54288 | -0.34356 |
| C | 1.99378 | -3.95685 | -1.67257 |
| C | 0.8966 | -1.94325 | -2.28532 |
| C | 1.42343 | -3.16782 | -2.66047 |
| H | 2.44735 | -4.91342 | -1.93431 |
| H | 0.47213 | -1.233 | -2.99852 |
| H | 1.40407 | -3.4819 | -3.70113 |
| C | 2.7495 | -4.41005 | 0.64934 |
| H | 3.46744 | -3.83123 | 1.24571 |
| H | 2.06299 | -4.91128 | 1.34565 |
| H | 3.30751 | -5.19743 | 0.1287 |
| N | 0.90473 | -1.53501 | -1.01866 |
| Rh | 0.16797 | 0.49769 | -0.30916 |
| Cl | -0.36812 | 1.20329 | -2.6875 |

| | | | |
|---|----------|----------|----------|
| C | 2.29575 | 0.67261 | 0.3028 |
| C | 1.82286 | 1.80245 | -0.1356 |
| C | 3.50865 | -0.07745 | -0.03416 |
| C | 3.89769 | -0.17957 | -1.37443 |
| C | 4.2904 | -0.67281 | 0.96068 |
| C | 5.04698 | -0.8822 | -1.71434 |
| H | 3.27163 | 0.28542 | -2.13753 |
| C | 5.44734 | -1.36291 | 0.61639 |
| H | 3.98408 | -0.58587 | 2.00312 |
| C | 5.82035 | -1.47766 | -0.72064 |
| H | 5.33905 | -0.96669 | -2.75969 |
| H | 6.06059 | -1.81397 | 1.39529 |
| H | 6.72066 | -2.02874 | -0.98846 |
| C | 2.09243 | 3.16202 | -0.46724 |
| C | 3.29849 | 3.73007 | -0.00915 |
| C | 1.20667 | 3.94278 | -1.22645 |
| C | 3.61385 | 5.04175 | -0.3205 |
| H | 3.97652 | 3.11812 | 0.58591 |
| C | 1.53515 | 5.2565 | -1.52943 |
| H | 0.28306 | 3.49154 | -1.58338 |
| C | 2.73161 | 5.8099 | -1.08063 |
| H | 4.55062 | 5.47071 | 0.03206 |
| H | 0.84803 | 5.85602 | -2.12399 |
| H | 2.97892 | 6.84284 | -1.32125 |
| P | -2.12434 | -0.25718 | -0.12533 |
| C | -2.70446 | -0.41257 | 1.60833 |
| C | -1.97677 | -1.19118 | 2.51792 |
| C | -3.79375 | 0.32898 | 2.07987 |
| C | -2.35683 | -1.26008 | 3.85406 |
| H | -1.0951 | -1.74337 | 2.18887 |
| C | -4.16352 | 0.26694 | 3.41957 |
| H | -4.35832 | 0.96269 | 1.39792 |
| C | -3.45249 | -0.53294 | 4.30852 |
| H | -1.78024 | -1.87686 | 4.54233 |
| H | -5.01528 | 0.84925 | 3.76742 |
| H | -3.74644 | -0.58245 | 5.35587 |
| C | -2.30545 | -1.90206 | -0.90907 |
| C | -2.29274 | -1.93205 | -2.31056 |
| C | -2.32847 | -3.10343 | -0.19959 |

| | | | | | | | |
|---|----------|----------|----------|----|----------|----------|----------|
| C | -2.31384 | -3.14681 | -2.98353 | C | -3.98085 | -2.35644 | 0.48643 |
| H | -2.23888 | -0.99603 | -2.87007 | C | -3.583 | -3.37434 | 1.35154 |
| C | -2.32567 | -4.31862 | -0.88078 | C | -1.31197 | -2.84044 | 0.92688 |
| H | -2.36014 | -3.09925 | 0.88894 | C | -2.2417 | -3.65804 | 1.55238 |
| C | -2.32056 | -4.34333 | -2.2707 | H | -4.35038 | -3.94762 | 1.87318 |
| H | -2.31014 | -3.15793 | -4.07254 | H | -0.24351 | -2.99195 | 1.07267 |
| H | -2.34224 | -5.25025 | -0.31691 | H | -1.91529 | -4.46603 | 2.20324 |
| H | -2.32512 | -5.29519 | -2.79977 | C | -5.44694 | -2.06177 | 0.36013 |
| C | -3.44621 | 0.72166 | -0.92149 | H | -5.63877 | -0.98525 | 0.27348 |
| C | -3.26111 | 2.07899 | -1.19129 | H | -5.90508 | -2.55489 | -0.50884 |
| C | -4.67905 | 0.1202 | -1.20234 | H | -5.97575 | -2.42554 | 1.25014 |
| C | -4.30257 | 2.82158 | -1.74107 | N | -1.65864 | -1.83011 | 0.1365 |
| H | -2.31037 | 2.55396 | -0.96217 | Rh | -0.24311 | -0.05141 | -0.80983 |
| C | -5.71278 | 0.86672 | -1.75367 | Cl | -0.12703 | -1.52373 | -2.7555 |
| H | -4.83021 | -0.93812 | -0.98674 | C | -1.69554 | 1.22068 | 0.35781 |
| C | -5.52259 | 2.21959 | -2.02583 | C | -0.48065 | 1.63593 | 0.46153 |
| H | -4.15101 | 3.8784 | -1.95342 | C | -2.87476 | 1.13552 | 1.21904 |
| H | -6.66786 | 0.39131 | -1.97191 | C | -2.76067 | 0.5359 | 2.4776 |
| H | -6.33098 | 2.80457 | -2.46246 | C | -4.10911 | 1.65915 | 0.8196 |

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P-TS_{C2-D}(2)

| | | | | | | | |
|---|----------|----------|----------|---|----------|----------|----------|
| C | -2.16091 | 0.38106 | -1.31911 | H | -1.80046 | 0.11312 | 2.77601 |
| C | -2.19812 | 1.3238 | -2.36137 | C | -5.20449 | 1.59397 | 1.67107 |
| C | -3.34862 | 1.46219 | -3.13597 | H | -4.19695 | 2.11963 | -0.16397 |
| C | -4.39475 | 0.5643 | -2.93725 | C | -5.0869 | 0.98257 | 2.91813 |
| C | -4.31431 | -0.45534 | -1.98989 | H | -3.7676 | -0.02681 | 4.29179 |
| C | -3.19579 | -0.56064 | -1.15996 | H | -6.15747 | 2.01771 | 1.35811 |
| H | -3.40512 | 2.19938 | -3.93476 | H | -5.95048 | 0.92291 | 3.57864 |
| H | -5.27821 | 0.63183 | -3.56976 | C | 0.35887 | 2.70956 | 0.94731 |
| H | -5.11472 | -1.18736 | -1.94252 | C | 0.39825 | 3.90761 | 0.21714 |
| C | 0.16884 | 1.43636 | -2.07625 | C | 1.11401 | 2.61277 | 2.12288 |
| O | 1.25839 | 1.83546 | -2.41559 | C | 1.16441 | 4.97783 | 0.65723 |
| N | -1.00728 | 1.99736 | -2.59439 | H | -0.18083 | 3.97589 | -0.70392 |
| C | -0.91775 | 3.04871 | -3.58967 | C | 1.87618 | 3.68806 | 2.56055 |
| H | -1.66464 | 3.82659 | -3.38618 | H | 1.10002 | 1.69167 | 2.7034 |
| H | 0.08539 | 3.47663 | -3.53616 | C | 1.90675 | 4.87235 | 1.83037 |
| H | -1.07729 | 2.64933 | -4.60095 | H | 1.1818 | 5.90038 | 0.07894 |
| C | -2.9647 | -1.62084 | -0.1606 | H | 2.46309 | 3.59168 | 3.47281 |
| | | | | H | 2.51211 | 5.71035 | 2.17204 |
| | | | | P | 2.06661 | -0.63912 | -0.04477 |

| | | | | | | | |
|-------------------------------|----------|----------|----------|----|----------|----------|----------|
| C | 3.11364 | -1.69259 | -1.11413 | C | -4.57102 | 0.87989 | -2.68694 |
| C | 2.57474 | -2.8913 | -1.59828 | C | -4.531 | -0.2282 | -1.84929 |
| C | 4.4221 | -1.34494 | -1.45623 | C | -3.31882 | -0.61337 | -1.24648 |
| C | 3.34328 | -3.73467 | -2.38978 | H | -3.48775 | 2.49151 | -3.63193 |
| H | 1.54344 | -3.15449 | -1.36483 | H | -5.51624 | 1.15968 | -3.14869 |
| C | 5.18309 | -2.18568 | -2.2635 | H | -5.45037 | -0.78009 | -1.69293 |
| H | 4.85337 | -0.41374 | -1.0911 | C | 0.08672 | 1.5346 | -1.80169 |
| C | 4.64785 | -3.38242 | -2.726 | O | 1.24097 | 1.77673 | -2.10194 |
| H | 2.91407 | -4.66411 | -2.76002 | N | -1.00252 | 1.90187 | -2.59017 |
| H | 6.20138 | -1.90288 | -2.52607 | C | -0.78037 | 2.65449 | -3.80937 |
| H | 5.24601 | -4.04029 | -3.35499 | H | -1.11389 | 2.07224 | -4.67845 |
| C | 1.85906 | -1.66438 | 1.47431 | H | -1.32087 | 3.61063 | -3.78567 |
| C | 0.99881 | -1.1779 | 2.46581 | H | 0.29154 | 2.84513 | -3.89891 |
| C | 2.50233 | -2.88576 | 1.68668 | C | -3.04898 | -1.75673 | -0.36253 |
| C | 0.78382 | -1.88823 | 3.63979 | C | -3.98774 | -2.67247 | 0.15856 |
| H | 0.46368 | -0.24325 | 2.28883 | C | -3.51907 | -3.6885 | 0.98762 |
| C | 2.27445 | -3.60847 | 2.85671 | C | -1.30797 | -2.87012 | 0.75429 |
| H | 3.18109 | -3.27917 | 0.93075 | C | -2.17249 | -3.80755 | 1.29098 |
| C | 1.41705 | -3.11385 | 3.83391 | H | -4.23636 | -4.3998 | 1.3978 |
| H | 0.10613 | -1.49417 | 4.39641 | H | -0.24043 | -2.9008 | 0.96161 |
| H | 2.77544 | -4.56415 | 3.00409 | H | -1.79301 | -4.60019 | 1.93049 |
| H | 1.24222 | -3.68135 | 4.74662 | C | -5.45903 | -2.60564 | -0.11713 |
| C | 3.25363 | 0.62989 | 0.55832 | H | -5.88878 | -1.64034 | 0.18115 |
| C | 3.41501 | 1.80641 | -0.18009 | H | -5.68695 | -2.75783 | -1.18029 |
| C | 4.0451 | 0.4216 | 1.69344 | H | -5.98378 | -3.38827 | 0.4432 |
| C | 4.34992 | 2.75765 | 0.21562 | N | -1.73058 | -1.88125 | -0.03273 |
| H | 2.80032 | 1.97319 | -1.06363 | Rh | -0.44761 | -0.29301 | -0.73087 |
| C | 4.97315 | 1.37944 | 2.08858 | Cl | 0.0066 | -1.74259 | -2.70697 |
| H | 3.94297 | -0.49446 | 2.27416 | C | -1.07734 | 1.06955 | 0.62259 |
| C | 5.12616 | 2.54992 | 1.35097 | C | -0.34954 | 1.92652 | -0.0375 |
| H | 4.4599 | 3.6735 | -0.36332 | C | -2.08524 | 0.98598 | 1.65149 |
| H | 5.58314 | 1.20533 | 2.97401 | C | -2.07199 | -0.03617 | 2.61049 |
| H | 5.85343 | 3.29884 | 1.66215 | C | -3.14502 | 1.90687 | 1.65272 |
| | | | | C | -3.08791 | -0.132 | 3.55099 |
| | | | | H | -1.26036 | -0.76257 | 2.59382 |
| | | | | C | -4.16094 | 1.80406 | 2.59289 |
| | | | | H | -3.16301 | 2.68578 | 0.89009 |
| | | | | C | -4.13575 | 0.78613 | 3.54408 |
| | | | | H | -3.06607 | -0.93231 | 4.28908 |
| 89 | | | | | | | |
| P-TS_{C2-D(3)} | | | | | | | |
| C | -2.19082 | 0.16291 | -1.51687 | | | | |
| C | -2.22886 | 1.26467 | -2.36452 | | | | |
| C | -3.43236 | 1.63756 | -2.95818 | | | | |

| | | | | | | | |
|---|----------|----------|----------|---|---------|----------|----------|
| H | -4.98225 | 2.51868 | 2.57983 | C | 2.89897 | -4.07511 | 2.51002 |
| H | -4.93675 | 0.7044 | 4.27702 | H | 3.00134 | -1.94129 | 2.76264 |
| C | 0.26542 | 3.20727 | 0.34079 | C | 2.07251 | -4.85807 | 0.38785 |
| C | 0.14885 | 3.56593 | 1.69521 | H | 1.47729 | -3.33201 | -1.01972 |
| C | 0.86911 | 4.11825 | -0.53422 | C | 2.56968 | -5.12648 | 1.66159 |
| C | 0.60004 | 4.79504 | 2.15077 | H | 3.29888 | -4.27787 | 3.50276 |
| H | -0.27865 | 2.85295 | 2.39902 | H | 1.81751 | -5.67592 | -0.28425 |
| C | 1.33002 | 5.34386 | -0.06934 | H | 2.70444 | -6.15592 | 1.99044 |
| H | 1.00987 | 3.85718 | -1.57961 | | | | |
| C | 1.19679 | 5.69277 | 1.27072 | | | | |
| H | 0.50337 | 5.04087 | 3.20769 | | | | |
| H | 1.80071 | 6.03359 | -0.76831 | | | | |
| H | 1.56396 | 6.65343 | 1.62853 | | | | |
| P | 1.92049 | -0.80061 | 0.1275 | | | | |
| C | 2.36112 | 0.37549 | 1.46225 | | | | |
| C | 3.165 | 1.48884 | 1.19839 | | | | |
| C | 1.75117 | 0.26961 | 2.71869 | | | | |
| C | 3.39614 | 2.44203 | 2.18553 | | | | |
| H | 3.60087 | 1.61754 | 0.20772 | | | | |
| C | 1.99272 | 1.21536 | 3.70885 | | | | |
| H | 1.08872 | -0.57201 | 2.93157 | | | | |
| C | 2.82491 | 2.30079 | 3.44529 | | | | |
| H | 4.01284 | 3.31051 | 1.95851 | | | | |
| H | 1.52518 | 1.10597 | 4.68665 | | | | |
| H | 3.00752 | 3.04882 | 4.21574 | | | | |
| C | 3.36911 | -0.70714 | -1.00565 | | | | |
| C | 4.65797 | -0.8906 | -0.48645 | | | | |
| C | 3.20557 | -0.51205 | -2.37692 | | | | |
| C | 5.7659 | -0.85809 | -1.32194 | | | | |
| H | 4.79704 | -1.05746 | 0.58275 | | | | |
| C | 4.32057 | -0.48734 | -3.21248 | | | | |
| H | 2.20753 | -0.39957 | -2.79317 | | | | |
| C | 5.59654 | -0.65463 | -2.69044 | | | | |
| H | 6.76267 | -0.99716 | -0.90553 | | | | |
| H | 4.18205 | -0.33879 | -4.28215 | | | | |
| H | 6.46443 | -0.63407 | -3.34842 | | | | |
| C | 2.21517 | -2.48022 | 0.82415 | | | | |
| C | 2.72708 | -2.75684 | 2.09363 | | | | |
| C | 1.89437 | -3.54522 | -0.03072 | | | | |

