

Supporting Information: Excited-State Proton-Transfer-Induced Trapping Enhances the Fluorescence Emission of Locked GFP Chromophore

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1. Active Orbitals in CASSCF Computations

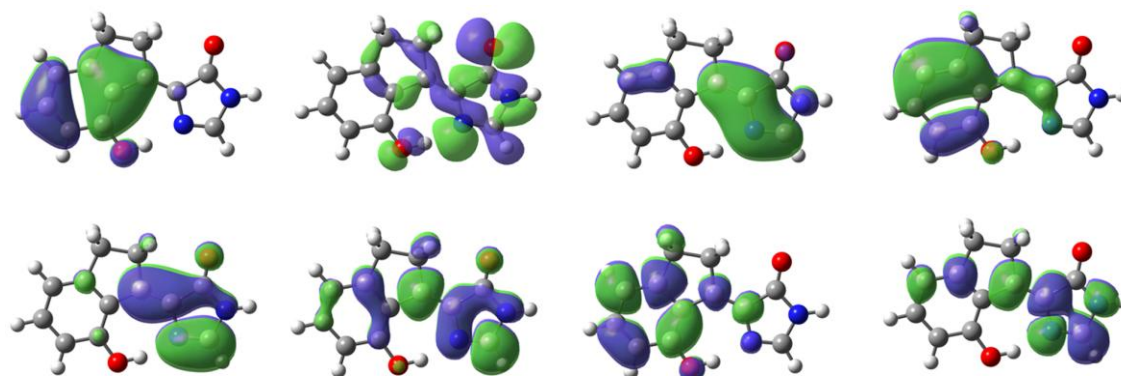


Fig. S1: Molecular orbitals used for the active space of CASSCF and MS-CASPT2 methods.

2. Active Orbitals in OM2/MRCI Computations

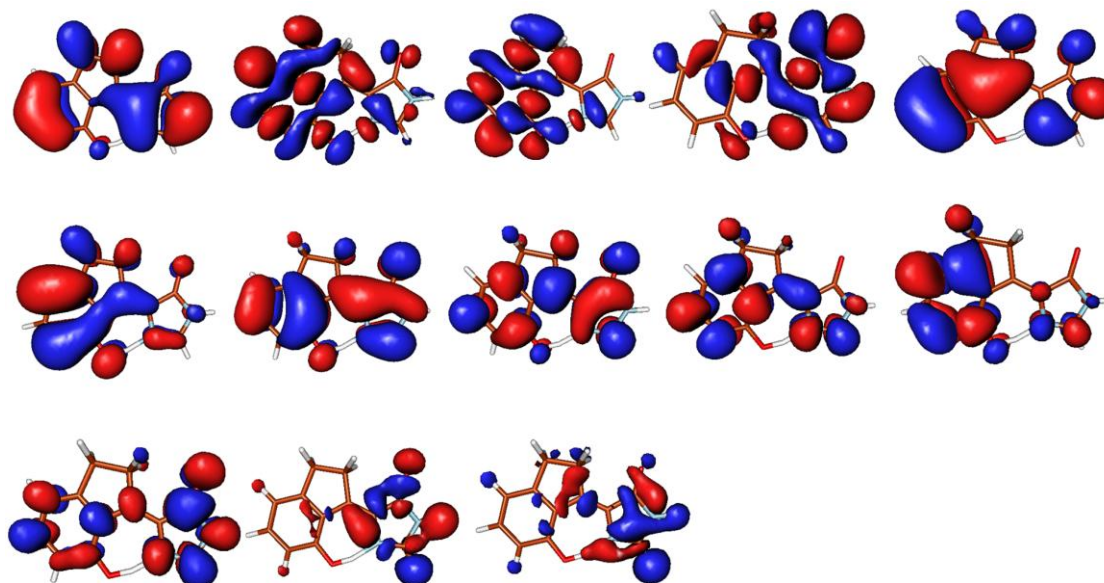


Fig. S2: Molecular orbitals used for the active space of OM2/MRCI method.

3. Spatial Superposition of S_1/S_0 Conical Intersections

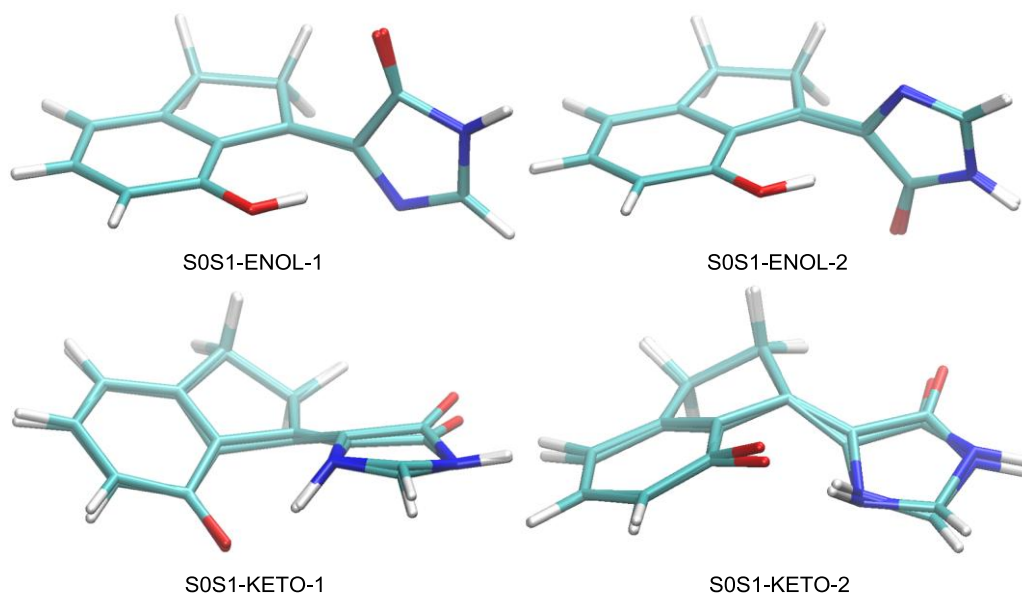


Fig. S3: Spatial superposition of the S_1/S_0 conical intersections optimized by the CASSCF and OM2/MRCI methods.

4. OM2/MRCI and CASSCF Geometry Parameters

Table S1: Key Geometry Parameters of Critical Structures Optimized at the OM2/MRCI and CASSCF Levels, Respectively (^aOM2/MRCI, ^bCASSCF/6-31G*)

| Structures | N1C2 | C2C3 | C3C4 | C4C5 | C5O6 | O6H7 | H7N1 |
|----------------------|-------|-------|-------|-------|-------|-------|-------|
| S0-ENOL ^a | 1.399 | 1.370 | 1.448 | 1.414 | 1.334 | 1.024 | 1.593 |
| S0-ENOL ^b | 1.414 | 1.354 | 1.482 | 1.393 | 1.334 | 0.957 | 1.804 |
| S0-KETO ^b | 1.400 | 1.399 | 1.400 | 1.439 | 1.245 | 1.558 | 1.044 |
| S1-KETO ^a | 1.389 | 1.372 | 1.468 | 1.451 | 1.263 | 1.575 | 1.045 |
| S1-KETO ^b | 1.382 | 1.364 | 1.481 | 1.452 | 1.235 | 1.746 | 1.016 |
| S1-ENOL ^b | 1.395 | 1.395 | 1.401 | 1.439 | 1.299 | 0.985 | 1.665 |
| S0-ENOL ^a | 1.379 | 1.413 | 1.420 | 1.413 | 1.339 | 1.006 | 2.613 |
| S0-ENOL ^b | 1.412 | 1.442 | 1.385 | 1.400 | 1.329 | 0.982 | 2.633 |

| | | | | | | | |
|--------------------------|-------|-------|-------|-------|-------|-------|-------|
| S0-KETO ^b | 1.379 | 1.413 | 1.420 | 1.413 | 1.339 | 1.006 | 2.612 |
| S1-KETO ^a | 1.411 | 1.444 | 1.386 | 1.399 | 1.328 | 0.981 | 2.631 |
| S1-KETO ^b | 1.448 | 1.347 | 1.510 | 1.436 | 1.263 | 1.540 | 1.091 |
| S1-ENOL ^b | 1.441 | 1.313 | 1.494 | 1.429 | 1.276 | 1.720 | 1.041 |
| S0S1-ENOL-1 ^a | 1.443 | 1.352 | 1.508 | 1.437 | 1.263 | 1.543 | 1.091 |
| S0S1-ENOL-1 ^b | 1.407 | 1.329 | 1.496 | 1.442 | 1.240 | 1.748 | 1.034 |

| Structures | C5C4C3C2 | C4C3C2N1 |
|--------------------------|----------|----------|
| S0-ENOL ^a | 0.0 | 0.0 |
| S0-ENOL ^b | -0.3 | 0.0 |
| S0-KETO ^b | -0.3 | -0.1 |
| S1-KETO ^a | 0.0 | 0.0 |
| S1-KETO ^b | -7.0 | 0.2 |
| S1-ENOL ^b | -0.2 | -0.1 |
| S0S1-ENOL-1 ^a | -3.6 | 102.3 |
| S0S1-ENOL-1 ^b | -1.4 | 98.7 |
| S0S1-ENOL-2 ^a | 3.6 | -96.5 |
| S0S1-ENOL-2 ^b | 1.1 | -98.1 |
| S0S1-KETO-1 ^a | -37.8 | 19.5 |
| S0S1-KETO-1 ^b | -36.7 | -0.7 |
| S0S1-KETO-2 ^a | 39.6 | -22.6 |
| S0S1-KETO-2 ^b | 38.9 | -3.5 |

5. Energies of Critical Structures

Table S2: Relative Energies (kcal/mol) of Critical Structures at Different Computational Levels.

| Structures | OM2/MRCI | | CASSCF(10,8) | | MS-CASPT2//CASSCF | |
|-------------|----------------|----------------|----------------|----------------|-------------------|----------------|
| | S ₀ | S ₁ | S ₀ | S ₁ | S ₀ | S ₁ |
| S0-ENOL | 0.0 | 81.7 | 0.0 | 103.9 | 0.0 | 82.1 |
| S0-KETO | — | — | 23.0 | 106.2 | 12.0 | 71.1 |
| S1-ENOL | — | — | 9.9 | 92.3 | 3.5 | 70.0 |
| S1-KETO | 17.4 | 63.2 | 42.7 | 86.9 | 22.9 | 65.3 |
| S0S1-ENOL-1 | 49.5 | 49.5 | 70.9 | 71.0 | 52.1 | 63.5 |
| S0S1-ENOL-2 | 49.5 | 49.5 | 70.8 | 71.1 | 52.1 | 63.7 |
| S0S1-KETO-1 | 75.6 | 75.6 | 88.6 | 91.6 | 68.9 | 74.8 |
| S0S1-KETO-2 | 73.6 | 73.6 | 92.2 | 95.3 | 66.7 | 77.9 |

6. S₀ Relaxed Hydrogen Transfer Minimum Energy Path

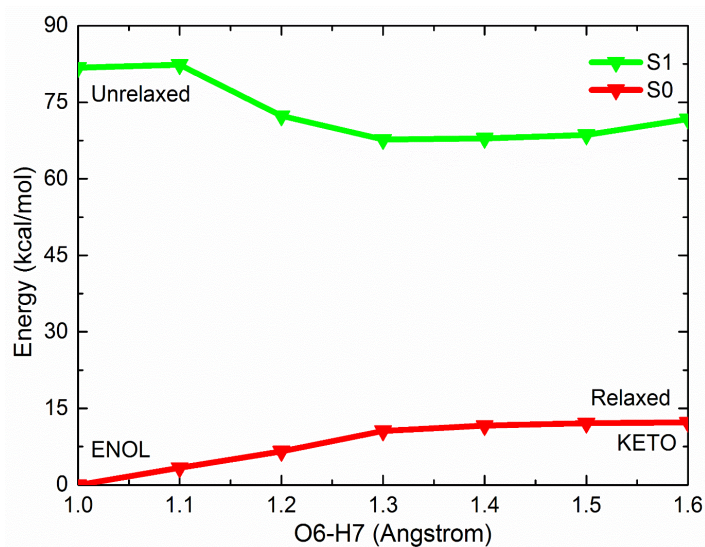


Fig. S4: MS-CASPT2//CASSCF computed S₀ relaxed minimum-energy intramolecular proton transfer path.

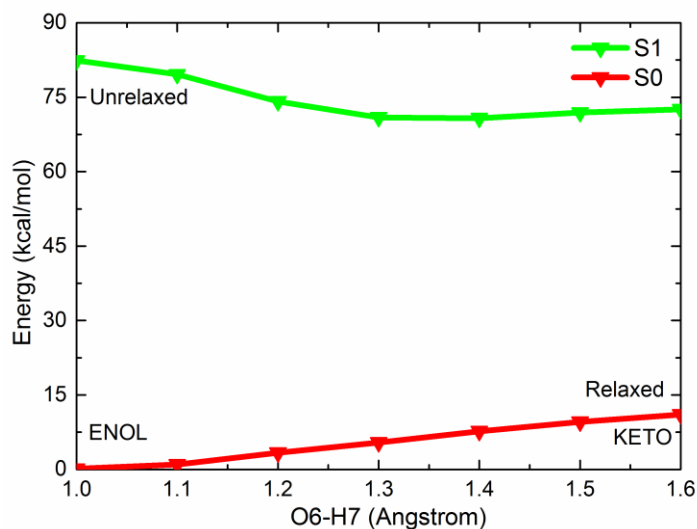


Fig. S5: OM2/MRCI computed S_0 relaxed minimum-energy intramolecular proton transfer path.

7. OM2/MRCI Computed Paths on S_1 Surface Using Different Active Space

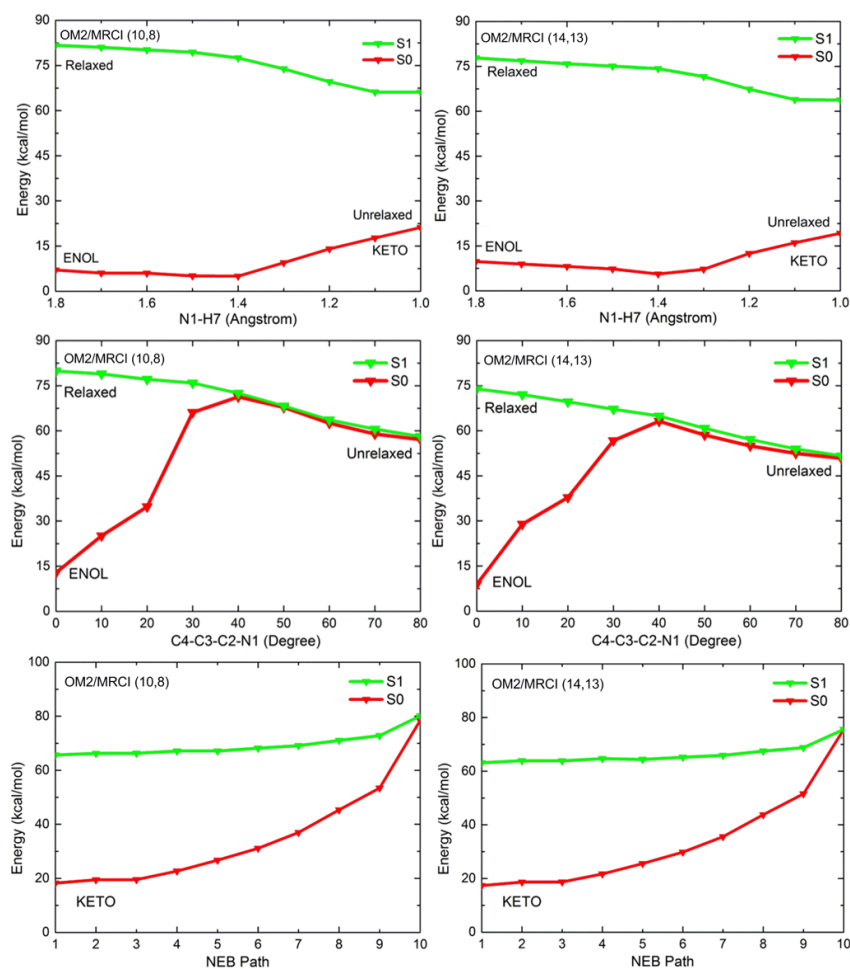


Fig. S6: OM2/MRCI computed important paths on S_1 state using (10,8) (left) and (14,13) (right) active space respectively.

8. Time-Dependent S₁ and S₀ Energies of Two Typical Trajectories

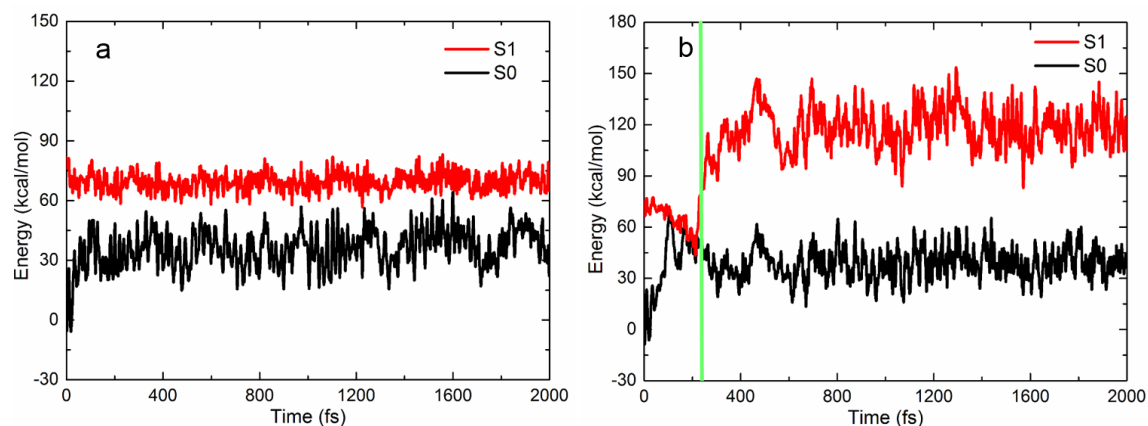


Fig. S7: Time evolution of the S₁ and S₀ energies of the two typical trajectories in the main text: (a) ultrafast excited-state proton transfer, systems remains in the S₁ state for 2 ps; (b) excited state deactivation by hopping to the ground state at 218 fs.

9. Cartesian Coordinates of All Optimized Structures and Paths

In xyz format (unit: Ångstrom)

CASSCF method

S0-ENOL

| | | | |
|---|---------------|---------------|---------------|
| O | 2.2403440000 | 2.3272800000 | -0.0049050000 |
| O | -1.0598100000 | -2.4008480000 | -0.0066730000 |
| H | -0.1528700000 | -2.0940550000 | -0.0028820000 |
| N | 3.1442390000 | 0.2206490000 | 0.0027820000 |
| N | 1.3329520000 | -1.0713490000 | 0.0035910000 |
| C | 2.6097190000 | -1.0536400000 | 0.0052820000 |
| C | 2.1190370000 | 1.1396790000 | -0.0013350000 |
| C | 0.9032430000 | 0.2756250000 | -0.0002800000 |
| C | -0.3789500000 | 0.7091770000 | -0.0017510000 |
| C | -1.6570370000 | -0.0402540000 | -0.0008200000 |
| C | -1.9443490000 | -1.4029090000 | -0.0032160000 |
| C | -3.2896930000 | -1.8099970000 | -0.0027610000 |
| H | -3.4846750000 | -2.8659610000 | -0.0048410000 |
| C | -4.3207830000 | -0.8898950000 | 0.0000030000 |
| H | -5.3387920000 | -1.2367140000 | 0.0001200000 |
| C | -4.0454670000 | 0.4827640000 | 0.0024930000 |
| H | -4.8427640000 | 1.2045020000 | 0.0046440000 |
| C | -2.7258040000 | 0.8854870000 | 0.0019900000 |
| C | -2.2341470000 | 2.3102980000 | 0.0050850000 |
| H | -2.5899480000 | 2.8417070000 | 0.8818250000 |

| | | | |
|---------|---------------|---------------|---------------|
| C | -0.6999200000 | 2.1991800000 | -0.0054640000 |
| H | -0.2635060000 | 2.6718100000 | -0.8755460000 |
| H | -2.6019680000 | 2.8508130000 | -0.8609850000 |
| H | -0.2498970000 | 2.6809890000 | 0.8523100000 |
| H | 4.1077470000 | 0.4653750000 | 0.0027980000 |
| H | 3.2334380000 | -1.9240860000 | 0.0082360000 |
| S1-ENOL | | | |
| O | 2.3097508900 | 2.2975153200 | -0.0075212500 |
| O | -1.0072998300 | -2.3210199800 | -0.0030103500 |
| H | -0.0803210200 | -1.9883290100 | 0.0001356800 |
| N | 3.1340846700 | 0.1424557400 | 0.0025745500 |
| N | 1.2967538200 | -1.0529904200 | 0.0057892500 |
| C | 2.5723112100 | -1.0935917200 | 0.0068055300 |
| C | 2.1214206600 | 1.1041070100 | -0.0024105700 |
| C | 0.9254442400 | 0.2921851600 | 0.0001265600 |
| C | -0.3912430800 | 0.7529020900 | -0.0015569100 |
| C | -1.5918605300 | 0.0300875000 | -0.0006200000 |
| C | -1.8988544900 | -1.3759177300 | -0.0021282700 |
| C | -3.2636090500 | -1.8261066800 | -0.0034795100 |
| H | -3.4107690500 | -2.8886180200 | -0.0053383300 |
| C | -4.3553579900 | -0.9265562300 | -0.0027343300 |
| H | -5.3629091800 | -1.2930451700 | -0.0040746500 |
| C | -4.0733038800 | 0.4424734400 | -0.0000984800 |
| H | -4.8644616000 | 1.1693583000 | 0.0011838200 |
| C | -2.7111743600 | 0.8968759900 | 0.0009332600 |
| C | -2.2553337200 | 2.3291238900 | 0.0090827200 |
| H | -2.6265340700 | 2.8442118500 | 0.8910870300 |
| C | -0.7118871300 | 2.2424959400 | -0.0085286800 |
| H | -0.2906947900 | 2.7228662700 | -0.8830530400 |
| H | -2.6473838500 | 2.8647133900 | -0.8511250400 |
| H | -0.2683674200 | 2.7386221700 | 0.8454292500 |
| H | 4.1034426600 | 0.3620814700 | 0.0016465100 |
| H | 3.1584978900 | -1.9902745900 | 0.0105882600 |
| S0-KETO | | | |
| O | 2.3125728600 | 2.2519168600 | -0.0048904100 |
| O | -0.9801993600 | -2.2645931600 | -0.0035676400 |
| H | 0.4960437700 | -1.7669206700 | 0.0025597200 |
| N | 3.0815693000 | 0.0794262200 | 0.0001161100 |
| N | 1.2472063400 | -1.0416637200 | 0.0034133900 |
| C | 2.5277794200 | -1.1521522200 | 0.0028841300 |
| C | 2.0793377000 | 1.0711132600 | -0.0019004800 |
| C | 0.8675240100 | 0.3058286300 | 0.0004072800 |

| | | | |
|---|---------------|---------------|---------------|
| C | -0.4614041600 | 0.7429434700 | 0.0004066400 |
| C | -1.6605308100 | 0.0203538800 | 0.0009774000 |
| C | -1.8778781200 | -1.4022933400 | -0.0035116500 |
| C | -3.2691669700 | -1.8203885600 | -0.0092407000 |
| H | -3.4457792100 | -2.8799618400 | -0.0140143600 |
| C | -4.2831696600 | -0.9364138100 | -0.0085940200 |
| H | -5.2962295200 | -1.3009797300 | -0.0131612100 |
| C | -4.0646909900 | 0.4862483600 | -0.0014415000 |
| H | -4.9020275000 | 1.1599841700 | 0.0010479900 |
| C | -2.7809986400 | 0.9303771300 | 0.0036683100 |
| C | -2.2850042000 | 2.3565702700 | 0.0173874400 |
| H | -2.6284439300 | 2.8785067400 | 0.9042041100 |
| C | -0.7486163700 | 2.2337457400 | -0.0052699700 |
| H | -0.3075300100 | 2.6912458800 | -0.8824150700 |
| H | -2.6548524400 | 2.9092580700 | -0.8394211600 |
| H | -0.2778002400 | 2.7089543900 | 0.8460980500 |
| H | 4.0539665800 | 0.2880238000 | -0.0003709700 |
| H | 3.0686421600 | -2.0734898000 | 0.0043555800 |

S1-KETO

| | | | |
|---|---------------|---------------|---------------|
| O | 2.2733650000 | 2.2611810000 | -0.0319370000 |
| O | -1.0530030000 | -2.3075500000 | -0.2656350000 |
| H | 0.5939340000 | -1.7959330000 | 0.0086090000 |
| N | 3.1106570000 | 0.1300590000 | 0.0865080000 |
| N | 1.2778730000 | -1.0477410000 | 0.0774380000 |
| C | 2.6091390000 | -1.1466400000 | 0.1150460000 |
| C | 2.1138610000 | 1.0735300000 | 0.0143210000 |
| C | 0.8709610000 | 0.2701970000 | -0.0006480000 |
| C | -0.4068550000 | 0.7425880000 | -0.0675280000 |
| C | -1.6782860000 | -0.0171310000 | -0.0701900000 |
| C | -1.9290240000 | -1.4461150000 | -0.1371500000 |
| C | -3.3168190000 | -1.8093440000 | -0.0630540000 |
| H | -3.5310120000 | -2.8586830000 | -0.1090740000 |
| C | -4.3808810000 | -0.8604910000 | 0.0405110000 |
| H | -5.3929100000 | -1.2211670000 | 0.0840730000 |
| C | -4.1128920000 | 0.4747630000 | 0.0771200000 |
| H | -4.8857650000 | 1.2146640000 | 0.1450590000 |
| C | -2.7209630000 | 0.8775840000 | 0.0193400000 |
| C | -2.2562790000 | 2.3055990000 | 0.0655350000 |
| H | -2.5232270000 | 2.7513860000 | 1.0205590000 |
| C | -0.7318390000 | 2.2261480000 | -0.1277080000 |
| H | -0.4367740000 | 2.6393650000 | -1.0864160000 |
| H | -2.7477330000 | 2.8996500000 | -0.6996060000 |
| H | -0.1901750000 | 2.7856570000 | 0.6222460000 |

| | | | |
|-------------|---------------|---------------|---------------|
| H | 4.0744840000 | 0.3788130000 | 0.1070010000 |
| H | 3.1804860000 | -2.0447480000 | 0.1752990000 |
| S0S1-ENOL-1 | | | |
| O | 1.6548150000 | 0.9639340000 | 1.8868080000 |
| O | -0.8433320000 | -2.0167290000 | 0.7514400000 |
| H | 0.0386630000 | -1.6567100000 | 0.5150200000 |
| N | 2.9874830000 | -0.1994340000 | 0.3433920000 |
| N | 1.5664210000 | -0.5467660000 | -1.3203410000 |
| C | 2.7817140000 | -0.7137420000 | -0.9223110000 |
| C | 1.7966220000 | 0.3810620000 | 0.8110800000 |
| C | 0.8899350000 | 0.0921770000 | -0.2576100000 |
| C | -0.4146730000 | 0.6909170000 | -0.3909420000 |
| C | -1.6226850000 | 0.1206620000 | -0.0267750000 |
| C | -1.8261590000 | -1.1536860000 | 0.5158440000 |
| C | -3.1476880000 | -1.5347400000 | 0.8213890000 |
| H | -3.3042360000 | -2.5065560000 | 1.2378410000 |
| C | -4.1944110000 | -0.6711410000 | 0.5865290000 |
| H | -5.1898280000 | -0.9853720000 | 0.8288830000 |
| C | -3.9963890000 | 0.6263200000 | 0.0312360000 |
| H | -4.8349900000 | 1.2702270000 | -0.1384800000 |
| C | -2.7230670000 | 1.0085100000 | -0.2684690000 |
| C | -2.1960180000 | 2.3055010000 | -0.8645240000 |
| H | -2.4546700000 | 3.1490640000 | -0.2379110000 |
| C | -0.6524810000 | 2.0920290000 | -0.9227110000 |
| H | -0.2522910000 | 2.1629970000 | -1.9276300000 |
| H | -2.6088670000 | 2.4659410000 | -1.8522990000 |
| H | -0.1132840000 | 2.7908970000 | -0.2919860000 |
| H | 3.8371530000 | -0.1919370000 | 0.8599820000 |
| H | 3.5510320000 | -1.1944790000 | -1.4790790000 |
| S0S1-ENOL-2 | | | |
| O | 1.7525850000 | 0.9561010000 | -1.8864920000 |
| O | -0.8012940000 | -1.9942330000 | -0.8020700000 |
| H | 0.0784880000 | -1.6426230000 | -0.5467420000 |
| N | 3.0347280000 | -0.2176280000 | -0.3075170000 |
| N | 1.5679240000 | -0.5406240000 | 1.3215790000 |
| C | 2.7906940000 | -0.7254120000 | 0.9545750000 |
| C | 1.8627240000 | 0.3762090000 | -0.8052090000 |
| C | 0.9285850000 | 0.1050900000 | 0.2423820000 |
| C | -0.3759830000 | 0.7154950000 | 0.3405570000 |
| C | -1.5807030000 | 0.1512830000 | -0.0474850000 |
| C | -1.7810700000 | -1.1228040000 | -0.5902840000 |
| C | -3.0993830000 | -1.4965440000 | -0.9227490000 |

| | | | |
|---|---------------|---------------|---------------|
| H | -3.2529170000 | -2.4688250000 | -1.3392450000 |
| C | -4.1442920000 | -0.6259070000 | -0.7129720000 |
| H | -5.1364710000 | -0.9342150000 | -0.9754400000 |
| C | -3.9493510000 | 0.6727750000 | -0.1571300000 |
| H | -4.7874270000 | 1.3223000000 | -0.0073200000 |
| C | -2.6808610000 | 1.0475250000 | 0.1683390000 |
| C | -2.1577150000 | 2.3433780000 | 0.7710470000 |
| H | -2.5948170000 | 2.5138060000 | 1.7465110000 |
| C | -0.6173880000 | 2.1180070000 | 0.8704610000 |
| H | -0.0561130000 | 2.8159740000 | 0.2591840000 |
| H | -2.3922380000 | 3.1850000000 | 0.1324990000 |
| H | -0.2466430000 | 2.1805060000 | 1.8869910000 |
| H | 3.8972190000 | -0.2228900000 | -0.8023100000 |
| H | 3.5397400000 | -1.2144910000 | 1.5313090000 |

S0S1-KETO-1

| | | | |
|---|---------------|---------------|---------------|
| O | 2.4259700000 | 2.1200210000 | -0.2299080000 |
| O | -0.8927630000 | -1.9167090000 | -1.2214900000 |
| H | 0.4448260000 | -1.6754450000 | -0.1702600000 |
| N | 2.9725340000 | -0.0547310000 | 0.2516140000 |
| N | 0.9003330000 | -0.9929700000 | 0.4704360000 |
| C | 2.2430010000 | -1.1595060000 | 0.7385310000 |
| C | 2.1226820000 | 0.9873370000 | -0.0079350000 |
| C | 0.7662340000 | 0.3698410000 | 0.0220420000 |
| C | -0.3805570000 | 0.9055180000 | -0.3259530000 |
| C | -1.6452960000 | 0.1119800000 | -0.2912560000 |
| C | -1.8118100000 | -1.2694530000 | -0.6179520000 |
| C | -3.0640610000 | -1.8189040000 | -0.2855920000 |
| H | -3.2466950000 | -2.8547900000 | -0.5029660000 |
| C | -4.1316120000 | -0.9873700000 | 0.2023780000 |
| H | -5.0875720000 | -1.4426850000 | 0.3884820000 |
| C | -3.9635790000 | 0.3359970000 | 0.3839600000 |
| H | -4.7787690000 | 0.9617660000 | 0.6991990000 |
| C | -2.6517560000 | 0.9071110000 | 0.1299400000 |
| C | -2.1859970000 | 2.3480870000 | 0.2331560000 |
| H | -2.0502070000 | 2.6389050000 | 1.2712010000 |
| C | -0.8127120000 | 2.3356040000 | -0.5108450000 |
| H | -0.9769690000 | 2.5434040000 | -1.5645450000 |
| H | -2.8920700000 | 3.0432700000 | -0.2082290000 |
| H | -0.0996820000 | 3.0491540000 | -0.1275170000 |
| H | 3.9206400000 | 0.1194010000 | 0.4988630000 |
| H | 2.6914330000 | -2.1306440000 | 0.7742040000 |

S0S1-KETO-2

| | | | |
|---|---------------|---------------|---------------|
| O | 2.4550050000 | 2.1180850000 | 0.1822820000 |
| O | -0.9515280000 | -1.9304970000 | 1.2943360000 |
| H | 0.4509390000 | -1.6584480000 | 0.2863050000 |
| N | 2.9550690000 | -0.0558000000 | -0.3497270000 |
| N | 0.8645270000 | -0.9904770000 | -0.3858180000 |
| C | 2.1819230000 | -1.1652630000 | -0.7715340000 |
| C | 2.1365790000 | 0.9865860000 | -0.0169560000 |
| C | 0.7709410000 | 0.3800590000 | 0.0455880000 |
| C | -0.3751120000 | 0.9250000000 | 0.4408070000 |
| C | -1.6346040000 | 0.1212650000 | 0.3685930000 |
| C | -1.7988890000 | -1.2805130000 | 0.6647410000 |
| C | -3.0333910000 | -1.8293860000 | 0.2183980000 |
| H | -3.2011830000 | -2.8767440000 | 0.3859950000 |
| C | -4.1026070000 | -0.9995150000 | -0.2959600000 |
| H | -5.0387340000 | -1.4682070000 | -0.5385060000 |
| C | -3.9436810000 | 0.3200570000 | -0.4199710000 |
| H | -4.7470050000 | 0.9558180000 | -0.7444460000 |
| C | -2.6271610000 | 0.9021400000 | -0.0881030000 |
| C | -2.1805880000 | 2.3477580000 | -0.1852380000 |
| H | -2.9067030000 | 3.0330620000 | 0.2397180000 |
| C | -0.8193330000 | 2.3592610000 | 0.5786400000 |
| H | -0.1069760000 | 3.0660890000 | 0.1805630000 |
| H | -2.0369760000 | 2.6335260000 | -1.2240630000 |
| H | -0.9970350000 | 2.6028770000 | 1.6219030000 |
| H | 3.8736870000 | 0.1200510000 | -0.6903850000 |
| H | 2.6231720000 | -2.1411560000 | -0.7974580000 |

OM2/MRCI method

S0-ENOL

| | | | |
|---|---------------|---------------|---------------|
| O | 2.3011242216 | 2.3304286723 | 0.0075298008 |
| O | -0.9922940333 | -2.3656091703 | -0.0051425673 |
| H | -0.0339195324 | -2.0054039386 | -0.0044151548 |
| N | 3.1501801208 | 0.1401656127 | 0.0008250630 |
| N | 1.2505781932 | -1.0636970539 | -0.0021420096 |
| C | 2.5647634837 | -1.1233640269 | -0.0027173490 |
| C | 2.1218925413 | 1.1107490196 | 0.0040254156 |
| C | 0.8749205167 | 0.2843512247 | 0.0019597466 |
| C | -0.4080992402 | 0.7644649589 | 0.0037084994 |
| C | -1.6373991597 | -0.0008888104 | 0.0016633925 |
| C | -1.9014432652 | -1.3897769021 | -0.0022557725 |
| C | -3.2495065615 | -1.8284196235 | -0.0032925583 |
| H | -3.4400289808 | -2.9002952341 | -0.0062945948 |
| C | -4.2859391555 | -0.9075294599 | -0.0005149794 |
| H | -5.3236418353 | -1.2654046472 | -0.0013551556 |

| | | | |
|---|---------------|---------------|---------------|
| C | -4.0406097230 | 0.4740456707 | 0.0033443809 |
| H | -4.8676179313 | 1.1860950840 | 0.0054808634 |
| C | -2.7236759162 | 0.9096838813 | 0.0043804491 |
| C | -2.2482196809 | 2.3375618845 | 0.0082474952 |
| H | -2.6193493691 | 2.8552980061 | 0.9140503912 |
| C | -0.7161334398 | 2.2390571922 | 0.0082873615 |
| H | -0.2738462931 | 2.7084532918 | -0.8894278960 |
| H | -2.6189617657 | 2.8599757103 | -0.8950314499 |
| H | -0.2743431143 | 2.7026262344 | 0.9092856122 |
| H | 4.1366441047 | 0.3268821192 | 0.0010694084 |
| H | 3.1514736289 | -2.0487095263 | -0.0056105272 |

S1-KETO

| | | | |
|---|---------------|---------------|---------------|
| O | 2.3363428457 | 2.2994515214 | 0.0065400057 |
| O | -0.9850548275 | -2.2733949312 | -0.0026550979 |
| H | 0.5195352370 | -1.8076736616 | -0.0038097641 |
| N | 3.1394340279 | 0.0990811865 | -0.0009081266 |
| N | 1.2251658789 | -1.0375466120 | -0.0027904539 |
| C | 2.5804666297 | -1.1645094570 | -0.0044148314 |
| C | 2.1323710813 | 1.0816517442 | 0.0029736803 |
| C | 0.8609426487 | 0.3024792160 | 0.0018068454 |
| C | -0.4162476013 | 0.8041573347 | 0.0046492595 |
| C | -1.6603431598 | 0.0250694065 | 0.0033544261 |
| C | -1.9020093778 | -1.4055269956 | -0.0002477157 |
| C | -3.2838110890 | -1.8271951057 | -0.0009014302 |
| H | -3.4862947829 | -2.9009465336 | -0.0036362496 |
| C | -4.3340242704 | -0.9010174353 | 0.0020471351 |
| H | -5.3693342375 | -1.2597816465 | 0.0014842466 |
| C | -4.0793827912 | 0.4672390859 | 0.0057023855 |
| H | -4.8927797245 | 1.1979085339 | 0.0081445305 |
| C | -2.7239409873 | 0.9126923816 | 0.0062671412 |
| C | -2.2768914468 | 2.3456427816 | 0.0099776221 |
| H | -2.6620650450 | 2.8571555826 | 0.9153534473 |
| C | -0.7394462373 | 2.2717239441 | 0.0093258906 |
| H | -0.3146997309 | 2.7530499683 | -0.8920664561 |
| H | -2.6625627544 | 2.8619586599 | -0.8924598156 |
| H | -0.3142479309 | 2.7473785483 | 0.9135199647 |
| H | 4.1268255733 | 0.2870010152 | -0.0013452292 |
| H | 3.1288717853 | -2.0995434826 | -0.0075964749 |

S0S1-ENOL-1

| | | | |
|---|---------------|---------------|--------------|
| O | 1.5426008545 | 0.9152481150 | 1.8884150695 |
| O | -0.8193943854 | -2.0199683224 | 0.7341939366 |
| H | 0.0461079010 | -1.5793194713 | 0.4701270282 |

| | | | |
|---|---------------|---------------|---------------|
| N | 2.9822169344 | -0.2214984059 | 0.3891350123 |
| N | 1.5878539104 | -0.5217811138 | -1.3547120735 |
| C | 2.8137385450 | -0.7363672079 | -0.8919148035 |
| C | 1.7847341007 | 0.4050680987 | 0.7813817210 |
| C | 0.8729386128 | 0.1043329208 | -0.3556070814 |
| C | -0.3930739033 | 0.7198556720 | -0.4744991192 |
| C | -1.6057239761 | 0.1236817677 | -0.0365115109 |
| C | -1.8213329148 | -1.1599222067 | 0.5131267649 |
| C | -3.1366175499 | -1.5580176812 | 0.8347147090 |
| H | -3.3055886413 | -2.5433686065 | 1.2608149970 |
| C | -4.1795580319 | -0.6670184702 | 0.6077735480 |
| H | -5.2006058246 | -0.9756154805 | 0.8677296925 |
| C | -3.9817595497 | 0.6167233418 | 0.0620126863 |
| H | -4.8303693439 | 1.2855516027 | -0.0885674718 |
| C | -2.6940385304 | 1.0076131267 | -0.2596002694 |
| C | -2.1862053605 | 2.2944466637 | -0.8535639138 |
| H | -2.4475660821 | 3.1424935239 | -0.1931176445 |
| C | -0.6611756938 | 2.1161869048 | -0.9601312781 |
| H | -0.2960510828 | 2.2215234243 | -1.9986262684 |
| H | -2.6386428131 | 2.4506273641 | -1.8521394246 |
| H | -0.1168696135 | 2.8313147636 | -0.3152045597 |
| H | 3.8162347888 | -0.2534722415 | 0.9492836797 |
| H | 3.5969165388 | -1.2493717113 | -1.4361363667 |

S0S1-ENOL-2

| | | | |
|---|---------------|---------------|---------------|
| O | 1.6343482786 | 0.9099293824 | -1.8881715233 |
| O | -0.7794109695 | -2.0014424316 | -0.7804192393 |
| H | 0.0834863793 | -1.5674038342 | -0.4975326001 |
| N | 3.0286780239 | -0.2343113909 | -0.3522477235 |
| N | 1.5914118108 | -0.5171540036 | 1.3593768920 |
| C | 2.8258863921 | -0.7436534950 | 0.9260335360 |
| C | 1.8460988699 | 0.4011315685 | -0.7742980019 |
| C | 0.9054144318 | 0.1117578361 | 0.3419236072 |
| C | -0.3576313973 | 0.7385559552 | 0.4294068993 |
| C | -1.5648764936 | 0.1514086989 | -0.0348971488 |
| C | -1.7787364609 | -1.1320946683 | -0.5854464168 |
| C | -3.0895759218 | -1.5199168720 | -0.9363992562 |
| H | -3.2571059741 | -2.5051816103 | -1.3632621471 |
| C | -4.1297546899 | -0.6192352208 | -0.7366279585 |
| H | -5.1470974560 | -0.9198826196 | -1.0194256366 |
| C | -3.9336126372 | 0.6645255058 | -0.1903176459 |
| H | -4.7796785780 | 1.3411051833 | -0.0616199548 |
| C | -2.6503958209 | 1.0453696281 | 0.1600713533 |
| C | -2.1453948364 | 2.3296891642 | 0.7618395811 |

| | | | |
|---|---------------|---------------|---------------|
| H | -2.6195339256 | 2.4928922208 | 1.7491617290 |
| C | -0.6248434367 | 2.1387283793 | 0.9043518798 |
| H | -0.0595860144 | 2.8470145765 | 0.2699794477 |
| H | -2.3840162412 | 3.1778404045 | 0.0929755339 |
| H | -0.2829864628 | 2.2443983583 | 1.9507003390 |
| H | 3.8752351616 | -0.2752385780 | -0.8926494938 |
| H | 3.5916980495 | -1.2615779981 | 1.4899611890 |

S0S1-KETO-1

| | | | |
|---|---------------|---------------|---------------|
| O | 2.2845276504 | 2.2427937171 | 0.1866297939 |
| O | -0.8636603963 | -1.9802065938 | -1.0957037965 |
| H | 0.3765390430 | -1.6972302724 | -0.2284910164 |
| N | 2.9519546548 | -0.0097845037 | 0.2340577278 |
| N | 0.8734853275 | -1.0367624596 | 0.4842263015 |
| C | 2.2467663812 | -1.2049983937 | 0.5929307921 |
| C | 2.0516857709 | 1.0333970078 | 0.2096909227 |
| C | 0.6838295469 | 0.3604119712 | 0.1543417986 |
| C | -0.3778284443 | 0.9015473207 | -0.4728332318 |
| C | -1.6745461059 | 0.1277170395 | -0.4971973153 |
| C | -1.8199614685 | -1.2934199099 | -0.6394025530 |
| C | -3.0707488365 | -1.8495717565 | -0.1810066136 |
| H | -3.2309222211 | -2.9295687415 | -0.2505390492 |
| C | -4.0971902725 | -1.0050598336 | 0.2667646246 |
| H | -5.0514458153 | -1.4396635668 | 0.5766109694 |
| C | -3.9350054026 | 0.3792825837 | 0.3109426967 |
| H | -4.7886514078 | 1.0315965242 | 0.5018779408 |
| C | -2.6436691205 | 0.9279271313 | 0.0415336199 |
| C | -2.1397684026 | 2.3469775126 | 0.1723357484 |
| H | -2.0054192010 | 2.5967291730 | 1.2428171194 |
| C | -0.7822512677 | 2.3426188026 | -0.5777340094 |
| H | -0.9077817202 | 2.6226683628 | -1.6412050226 |
| H | -2.8558353378 | 3.0641709654 | -0.2810117018 |
| H | -0.0513084729 | 3.0092724838 | -0.0923971635 |
| H | 3.9084502446 | 0.1163339851 | 0.5421007343 |
| H | 2.7343124915 | -2.1829900043 | 0.4402614951 |

S0S1-KETO-2

| | | | |
|---|---------------|---------------|---------------|
| O | 2.2648008663 | 2.2553380973 | -0.1732531028 |
| O | -0.8661909074 | -2.0102855947 | 1.0345484146 |
| H | 0.3683606824 | -1.6988384510 | 0.1635362446 |
| N | 2.9576549953 | 0.0070424728 | -0.1592874843 |
| N | 0.8936890765 | -1.0271711962 | -0.5162578289 |
| C | 2.2711273062 | -1.1854684638 | -0.5645925718 |
| C | 2.0456546453 | 1.0436512591 | -0.1979480574 |
| C | 0.6806682814 | 0.3619944387 | -0.1885234188 |

| | | | |
|---|---------------|---------------|---------------|
| C | -0.3760986671 | 0.8855550707 | 0.4727644345 |
| C | -1.6711008080 | 0.1131426773 | 0.4812505360 |
| C | -1.8263332429 | -1.3095413915 | 0.6072669665 |
| C | -3.0888031306 | -1.8510937202 | 0.1622056377 |
| H | -3.2520255759 | -2.9305535179 | 0.2262131231 |
| C | -4.1071917297 | -0.9998721632 | -0.2705678752 |
| H | -5.0661724833 | -1.4232109444 | -0.5812804774 |
| C | -3.9336802554 | 0.3866020223 | -0.3129046205 |
| H | -4.7843097957 | 1.0441210538 | -0.4980835563 |
| C | -2.6416292536 | 0.9219208772 | -0.0454354798 |
| C | -2.1333932072 | 2.3401739660 | -0.1634842953 |
| H | -2.8512232559 | 3.0596522090 | 0.2841216686 |
| C | -0.7838408819 | 2.3242665465 | 0.5975301245 |
| H | -0.0477595047 | 3.0021212025 | 0.1346070357 |
| H | -1.9868721232 | 2.5909735788 | -1.2329837774 |
| H | -0.9206002736 | 2.5820507500 | 1.6655198921 |
| H | 3.9051851969 | 0.1527209368 | -0.4927955178 |
| H | 2.7604212976 | -2.1596623571 | -0.4324696321 |

CASSCF: S1 N1-H7 bond length (Ångstrom)

1.80

| | | | |
|---|---------------|---------------|---------------|
| O | 2.2759580000 | 2.3199590000 | 0.0037830000 |
| O | -1.0687400000 | -2.3740860000 | 0.0047030000 |
| H | -0.1465680000 | -2.0799940000 | 0.0030380000 |
| N | 3.1584530000 | 0.1946000000 | -0.0024570000 |
| N | 1.3392040000 | -1.0572060000 | -0.0012820000 |
| C | 2.6266740000 | -1.0701510000 | -0.0032440000 |
| C | 2.1273100000 | 1.1213560000 | 0.0009170000 |
| C | 0.9384130000 | 0.2828900000 | 0.0005150000 |
| C | -0.3774210000 | 0.7296150000 | 0.0009610000 |
| C | -1.5892440000 | 0.0053820000 | 0.0007220000 |
| C | -1.9284520000 | -1.3887530000 | 0.0022990000 |
| C | -3.3053770000 | -1.8159970000 | 0.0008920000 |
| H | -3.4648870000 | -2.8767890000 | 0.0014940000 |
| C | -4.3840060000 | -0.9061600000 | -0.0006350000 |
| H | -5.3968350000 | -1.2577520000 | -0.0018230000 |
| C | -4.0766580000 | 0.4535010000 | -0.0020780000 |
| H | -4.8498900000 | 1.1993280000 | -0.0031280000 |
| C | -2.7015400000 | 0.8823780000 | -0.0009510000 |
| C | -2.2400430000 | 2.3107150000 | 0.0000050000 |
| H | -2.6246680000 | 2.8345760000 | 0.8710780000 |
| C | -0.6985000000 | 2.2206420000 | 0.0015710000 |
| H | -0.2662620000 | 2.7110130000 | -0.8614340000 |
| H | -2.6229100000 | 2.8353360000 | -0.8713130000 |

| | | | |
|---|---------------|---------------|---------------|
| H | -0.2681690000 | 2.7097570000 | 0.8662710000 |
| H | 4.1202950000 | 0.4426230000 | -0.0044410000 |
| H | 3.2342030000 | -1.9511550000 | -0.0057590000 |

1.72

| | | | |
|---|---------------|---------------|---------------|
| O | 2.2953000000 | 2.3069480000 | 0.0103660000 |
| O | -1.0356030000 | -2.3459770000 | -0.0015430000 |
| H | -0.1112940000 | -2.0305840000 | -0.0036510000 |
| N | 3.1486600000 | 0.1680100000 | 0.0013430000 |
| N | 1.3123840000 | -1.0565670000 | -0.0048620000 |
| C | 2.6000250000 | -1.0886800000 | -0.0047060000 |
| C | 2.1300710000 | 1.1102550000 | 0.0044040000 |
| C | 0.9316070000 | 0.2897370000 | -0.0013550000 |
| C | -0.3804750000 | 0.7465240000 | -0.0018450000 |
| C | -1.5899680000 | 0.0180570000 | -0.0027780000 |
| C | -1.9117030000 | -1.3792830000 | 0.0002300000 |
| C | -3.2842450000 | -1.8187860000 | 0.0015180000 |
| H | -3.4360640000 | -2.8807280000 | 0.0020180000 |
| C | -4.3702190000 | -0.9163120000 | 0.0048160000 |
| H | -5.3800990000 | -1.2764540000 | 0.0071460000 |
| C | -4.0765940000 | 0.4456740000 | 0.0017230000 |
| H | -4.8575440000 | 1.1834030000 | 0.0024220000 |
| C | -2.7043940000 | 0.8871520000 | -0.0002750000 |
| C | -2.2488710000 | 2.3182470000 | -0.0039030000 |
| H | -2.6376150000 | 2.8446810000 | 0.8636930000 |
| C | -0.7056370000 | 2.2354020000 | 0.0009140000 |
| H | -0.2740840000 | 2.7296760000 | -0.8604900000 |
| H | -2.6319900000 | 2.8370290000 | -0.8786370000 |
| H | -0.2797010000 | 2.7247690000 | 0.8678850000 |
| H | 4.1140470000 | 0.4019760000 | 0.0025910000 |
| H | 3.1943470000 | -1.9785420000 | -0.0073190000 |

1.65

| | | | |
|---|---------------|---------------|---------------|
| O | 2.3150510000 | 2.2935710000 | -0.0010500000 |
| O | -1.0038590000 | -2.3169060000 | -0.0023230000 |
| H | -0.0758040000 | -1.9792280000 | -0.0030970000 |
| N | 3.1388740000 | 0.1413000000 | 0.0008520000 |
| N | 1.2867670000 | -1.0554740000 | -0.0042180000 |
| C | 2.5743210000 | -1.1071090000 | -0.0008120000 |
| C | 2.1326290000 | 1.0989170000 | -0.0013720000 |
| C | 0.9253220000 | 0.2967210000 | -0.0050090000 |
| C | -0.3833030000 | 0.7630790000 | -0.0034650000 |
| C | -1.5910950000 | 0.0303890000 | -0.0037580000 |
| C | -1.8952600000 | -1.3698230000 | -0.0024670000 |

| | | | |
|---|---------------|---------------|---------------|
| C | -3.2637050000 | -1.8211840000 | 0.0000840000 |
| H | -3.4080390000 | -2.8841920000 | 0.0003010000 |
| C | -4.3568370000 | -0.9259760000 | 0.0030040000 |
| H | -5.3635840000 | -1.2950180000 | 0.0057560000 |
| C | -4.0767030000 | 0.4377560000 | 0.0028180000 |
| H | -4.8646360000 | 1.1679820000 | 0.0053360000 |
| C | -2.7068140000 | 0.8910740000 | 0.0000000000 |
| C | -2.2576520000 | 2.3250040000 | -0.0021650000 |
| H | -2.6491490000 | 2.8491290000 | 0.8655260000 |
| C | -0.7127030000 | 2.2497110000 | 0.0024360000 |
| H | -0.2834110000 | 2.7488450000 | -0.8574400000 |
| H | -2.6431220000 | 2.8422080000 | -0.8767980000 |
| H | -0.2897360000 | 2.7387440000 | 0.8714900000 |
| H | 4.1074610000 | 0.3617510000 | 0.0029780000 |
| H | 3.1553250000 | -2.0056430000 | 0.0030940000 |

1.57

| | | | |
|---|---------------|---------------|---------------|
| O | 2.3366990000 | 2.2800500000 | -0.0024310000 |
| O | -0.9740970000 | -2.2886470000 | -0.0007610000 |
| H | -0.0366450000 | -1.9305740000 | 0.0012080000 |
| N | 3.1293430000 | 0.1141670000 | -0.0003480000 |
| N | 1.2618540000 | -1.0527430000 | -0.0009940000 |
| C | 2.5490370000 | -1.1252920000 | 0.0011390000 |
| C | 2.1358550000 | 1.0876930000 | -0.0019320000 |
| C | 0.9199640000 | 0.3050220000 | -0.0023620000 |
| C | -0.3857520000 | 0.7803480000 | -0.0015680000 |
| C | -1.5925850000 | 0.0421950000 | 0.0003010000 |
| C | -1.8789970000 | -1.3611480000 | -0.0010200000 |
| C | -3.2437560000 | -1.8232540000 | -0.0008240000 |
| H | -3.3811790000 | -2.8871800000 | -0.0067090000 |
| C | -4.3437580000 | -0.9348920000 | 0.0019270000 |
| H | -5.3473920000 | -1.3125830000 | 0.0009620000 |
| C | -4.0769580000 | 0.4297480000 | 0.0033840000 |
| H | -4.8713200000 | 1.1529250000 | 0.0038550000 |
| C | -2.7087670000 | 0.8942660000 | 0.0020300000 |
| C | -2.2667730000 | 2.3312160000 | 0.0004430000 |
| H | -2.6583580000 | 2.8513000000 | 0.8705550000 |
| C | -0.7202480000 | 2.2644690000 | -0.0001970000 |
| H | -0.2967120000 | 2.7624200000 | -0.8640440000 |
| H | -2.6581990000 | 2.8479670000 | -0.8717420000 |
| H | -0.2977180000 | 2.7600270000 | 0.8656310000 |
| H | 4.1009590000 | 0.3208770000 | 0.0008050000 |
| H | 3.1158440000 | -2.0327490000 | 0.0023910000 |

1.49

| | | | |
|---|---------------|---------------|---------------|
| O | 2.3611450000 | 2.2670430000 | -0.0009500000 |
| O | -0.9480450000 | -2.2622520000 | 0.0006020000 |
| H | 0.0063330000 | -1.8832370000 | 0.0001070000 |
| N | 3.1206880000 | 0.0876120000 | -0.0021950000 |
| N | 1.2385590000 | -1.0480720000 | -0.0002640000 |
| C | 2.5250360000 | -1.1425740000 | -0.0016790000 |
| C | 2.1402690000 | 1.0774360000 | -0.0016170000 |
| C | 0.9159870000 | 0.3145920000 | -0.0002040000 |
| C | -0.3875070000 | 0.7977310000 | 0.0009150000 |
| C | -1.5948830000 | 0.0525240000 | 0.0014990000 |
| C | -1.8637540000 | -1.3542750000 | 0.0005370000 |
| C | -3.2254780000 | -1.8251100000 | 0.0005720000 |
| H | -3.3570710000 | -2.8898150000 | 0.0003380000 |
| C | -4.3317020000 | -0.9424080000 | -0.0005320000 |
| H | -5.3324430000 | -1.3281550000 | -0.0001180000 |
| C | -4.0775000000 | 0.4219700000 | 0.0003130000 |
| H | -4.8775290000 | 1.1388150000 | 0.0009060000 |
| C | -2.7098890000 | 0.8962000000 | 0.0000720000 |
| C | -2.2760040000 | 2.3363250000 | -0.0007440000 |
| H | -2.6730540000 | 2.8536830000 | 0.8685020000 |
| C | -0.7282600000 | 2.2787410000 | 0.0023850000 |
| H | -0.3068750000 | 2.7802200000 | -0.8608050000 |
| H | -2.6688670000 | 2.8504660000 | -0.8738090000 |
| H | -0.3107660000 | 2.7768900000 | 0.8694500000 |
| H | 4.0952150000 | 0.2803930000 | -0.0015950000 |
| H | 3.0767330000 | -2.0591160000 | -0.0019840000 |

1.41

| | | | |
|---|---------------|---------------|---------------|
| O | 2.3878570000 | 2.2548460000 | 0.0134640000 |
| O | -0.9290710000 | -2.2372470000 | 0.0153720000 |
| H | 0.0554080000 | -1.8351530000 | 0.0023550000 |
| N | 3.1139170000 | 0.0615240000 | -0.0060470000 |
| N | 1.2201010000 | -1.0409320000 | -0.0116520000 |
| C | 2.5058810000 | -1.1594230000 | -0.0135590000 |
| C | 2.1455260000 | 1.0676250000 | 0.0031220000 |
| C | 0.9155790000 | 0.3254010000 | -0.0012820000 |
| C | -0.3877110000 | 0.8157630000 | -0.0019550000 |
| C | -1.6008360000 | 0.0602880000 | -0.0049110000 |
| C | -1.8512970000 | -1.3502040000 | 0.0044730000 |
| C | -3.2110060000 | -1.8267890000 | 0.0053190000 |
| H | -3.3391270000 | -2.8918960000 | 0.0144640000 |
| C | -4.3217720000 | -0.9472780000 | 0.0036610000 |
| H | -5.3197980000 | -1.3405650000 | 0.0072030000 |

| | | | |
|---|---------------|---------------|---------------|
| C | -4.0796140000 | 0.4145010000 | -0.0038920000 |
| H | -4.8837630000 | 1.1265410000 | -0.0067930000 |
| C | -2.7096660000 | 0.8955840000 | -0.0065050000 |
| C | -2.2848940000 | 2.3391580000 | -0.0100020000 |
| H | -2.6972450000 | 2.8596900000 | 0.8500860000 |
| C | -0.7363540000 | 2.2922590000 | 0.0114970000 |
| H | -0.3078170000 | 2.8093410000 | -0.8390340000 |
| H | -2.6714080000 | 2.8430890000 | -0.8919630000 |
| H | -0.3353090000 | 2.7825280000 | 0.8914660000 |
| H | 4.0908110000 | 0.2418870000 | -0.0049550000 |
| H | 3.0419460000 | -2.0849090000 | -0.0202300000 |

1.33

| | | | |
|---|---------------|---------------|---------------|
| O | 2.4162530000 | 2.2460060000 | 0.0072640000 |
| O | -0.9218610000 | -2.2248680000 | 0.0037740000 |
| H | 0.1224100000 | -1.7959680000 | 0.0022040000 |
| N | 3.1114700000 | 0.0409430000 | 0.0003450000 |
| N | 1.2103540000 | -1.0292250000 | 0.0014820000 |
| C | 2.4951060000 | -1.1722460000 | -0.0009450000 |
| C | 2.1532630000 | 1.0617200000 | 0.0044900000 |
| C | 0.9183670000 | 0.3380170000 | 0.0039580000 |
| C | -0.3873670000 | 0.8316270000 | 0.0039190000 |
| C | -1.6102920000 | 0.0625030000 | 0.0016210000 |
| C | -1.8450240000 | -1.3561740000 | 0.0021240000 |
| C | -3.2060460000 | -1.8295550000 | 0.0005630000 |
| H | -3.3369840000 | -2.8944070000 | 0.0012280000 |
| C | -4.3180760000 | -0.9475390000 | -0.0042990000 |
| H | -5.3147270000 | -1.3453120000 | -0.0075870000 |
| C | -4.0841230000 | 0.4101850000 | -0.0056440000 |
| H | -4.8901790000 | 1.1198940000 | -0.0092510000 |
| C | -2.7094610000 | 0.8930620000 | -0.0000010000 |
| C | -2.2931920000 | 2.3396380000 | 0.0085180000 |
| H | -2.6865540000 | 2.8379580000 | 0.8906660000 |
| C | -0.7445010000 | 2.3031750000 | -0.0078890000 |
| H | -0.3447020000 | 2.7995810000 | -0.8855350000 |
| H | -2.7065960000 | 2.8595450000 | -0.8513870000 |
| H | -0.3227170000 | 2.8218700000 | 0.8455300000 |
| H | 4.0902270000 | 0.2113920000 | -0.0002390000 |
| H | 3.0152920000 | -2.1061960000 | -0.0052070000 |

1.25

| | | | |
|---|---------------|---------------|---------------|
| O | 2.4290870000 | 2.2442330000 | -0.0045890000 |
| O | -0.9320220000 | -2.2306640000 | 0.0008010000 |
| H | 0.2160890000 | -1.7703440000 | 0.0025130000 |

| | | | |
|---|---------------|---------------|---------------|
| N | 3.1130680000 | 0.0348350000 | 0.0036200000 |
| N | 1.2164290000 | -1.0171630000 | 0.0041400000 |
| C | 2.5011660000 | -1.1768130000 | 0.0066700000 |
| C | 2.1568200000 | 1.0614630000 | -0.0015740000 |
| C | 0.9212100000 | 0.3456360000 | -0.0013100000 |
| C | -0.3901250000 | 0.8348140000 | -0.0034790000 |
| C | -1.6232960000 | 0.0547230000 | 0.0007100000 |
| C | -1.8497080000 | -1.3731920000 | -0.0038780000 |
| C | -3.2165220000 | -1.8311560000 | -0.0083300000 |
| H | -3.3592930000 | -2.8945490000 | -0.0122450000 |
| C | -4.3259180000 | -0.9387040000 | -0.0047670000 |
| H | -5.3237600000 | -1.3345360000 | -0.0066320000 |
| C | -4.0922250000 | 0.4132610000 | 0.0023620000 |
| H | -4.8954620000 | 1.1261290000 | 0.0050750000 |
| C | -2.7105900000 | 0.8885960000 | 0.0030640000 |
| C | -2.2970700000 | 2.3357060000 | 0.0091660000 |
| H | -2.6915800000 | 2.8360450000 | 0.8894270000 |
| C | -0.7496890000 | 2.3032390000 | -0.0082510000 |
| H | -0.3505370000 | 2.8050880000 | -0.8831580000 |
| H | -2.7119980000 | 2.8518130000 | -0.8525280000 |
| H | -0.3281340000 | 2.8180170000 | 0.8481540000 |
| H | 4.0921850000 | 0.2040920000 | 0.0047070000 |
| H | 3.0122130000 | -2.1149400000 | 0.0100360000 |

1.17

| | | | |
|---|---------------|---------------|---------------|
| O | 2.4072370000 | 2.2533950000 | -0.0042340000 |
| O | -0.9743210000 | -2.2625640000 | -0.0051960000 |
| H | 0.3545260000 | -1.7724390000 | -0.0018170000 |
| N | 3.1221950000 | 0.0560280000 | 0.0047370000 |
| N | 1.2492220000 | -1.0132630000 | -0.0009710000 |
| C | 2.5378990000 | -1.1655450000 | 0.0037380000 |
| C | 2.1495350000 | 1.0691310000 | -0.0012780000 |
| C | 0.9203230000 | 0.3380330000 | -0.0029300000 |
| C | -0.3959540000 | 0.8124550000 | -0.0022670000 |
| C | -1.6410060000 | 0.0305040000 | 0.0026450000 |
| C | -1.8760640000 | -1.4019390000 | -0.0037490000 |
| C | -3.2541900000 | -1.8271190000 | -0.0041660000 |
| H | -3.4190950000 | -2.8874040000 | -0.0087220000 |
| C | -4.3549060000 | -0.9137750000 | -0.0017400000 |
| H | -5.3577910000 | -1.2980420000 | -0.0012980000 |
| C | -4.1072660000 | 0.4288020000 | 0.0060570000 |
| H | -4.8977130000 | 1.1556140000 | 0.0095320000 |
| C | -2.7131450000 | 0.8797390000 | 0.0030230000 |
| C | -2.2917840000 | 2.3233870000 | 0.0011560000 |

| | | | |
|---|---------------|---------------|---------------|
| H | -2.6933730000 | 2.8355810000 | 0.8714870000 |
| C | -0.7474660000 | 2.2824440000 | -0.0010470000 |
| H | -0.3341550000 | 2.7886900000 | -0.8665980000 |
| H | -2.6947890000 | 2.8322420000 | -0.8705830000 |
| H | -0.3323210000 | 2.7873310000 | 0.8645500000 |
| H | 4.0983750000 | 0.2430220000 | 0.0029440000 |
| H | 3.0563640000 | -2.0986790000 | 0.0064330000 |

OM2/MRCI: S1 N1-H7 bond length (Ångstrom)

1.8

| | | | |
|---|---------------|---------------|---------------|
| O | 2.2745523000 | 2.3586787000 | 0.0075502000 |
| O | -1.0765739000 | -2.4201386000 | -0.0052918000 |
| H | -0.1265548000 | -2.1084668000 | -0.0046840000 |
| N | 3.1944929000 | 0.1931559000 | 0.0011185000 |
| N | 1.3213048000 | -1.0407286000 | -0.0017944000 |
| C | 2.6726992000 | -1.0818598000 | -0.0025084000 |
| C | 2.1138599000 | 1.1274816000 | 0.0038749000 |
| C | 0.9285352000 | 0.2474208000 | 0.0019949000 |
| C | -0.4439925000 | 0.7232922000 | 0.0037930000 |
| C | -1.6307506000 | -0.0140518000 | 0.0014779000 |
| C | -1.9507225000 | -1.4182514000 | -0.0024248000 |
| C | -3.3014988000 | -1.8277650000 | -0.0033247000 |
| H | -3.5187794000 | -2.8936453000 | -0.0062463000 |
| C | -4.3218836000 | -0.8874369000 | -0.0004957000 |
| H | -5.3645401000 | -1.2257370000 | -0.0012141000 |
| C | -4.0494314000 | 0.4952267000 | 0.0033830000 |
| H | -4.8695328000 | 1.2154185000 | 0.0056264000 |
| C | -2.7395143000 | 0.9160938000 | 0.0042986000 |
| C | -2.2393348000 | 2.3315204000 | 0.0082287000 |
| H | -2.6001587000 | 2.8552947000 | 0.9128975000 |
| C | -0.7104280000 | 2.1936503000 | 0.0081555000 |
| H | -0.2498415000 | 2.6525001000 | -0.8885345000 |
| H | -2.5997330000 | 2.8601602000 | -0.8937730000 |
| H | -0.2503725000 | 2.6469026000 | 0.9079937000 |
| H | 4.1729589000 | 0.4286687000 | 0.0011207000 |
| H | 3.2617818000 | -1.9966417000 | -0.0055638000 |

1.7

| | | | |
|---|---------------|---------------|---------------|
| O | 2.3190043000 | 2.3393502000 | 0.0075568000 |
| O | -1.0299825000 | -2.3889819000 | -0.0051973000 |
| H | -0.0685810000 | -2.0757877000 | -0.0046046000 |
| N | 3.1775158000 | 0.1463757000 | 0.0008883000 |
| N | 1.2700840000 | -1.0296243000 | -0.0019631000 |

| | | | |
|---|---------------|---------------|---------------|
| C | 2.6182617000 | -1.1128516000 | -0.0027038000 |
| C | 2.1277249000 | 1.1131633000 | 0.0039543000 |
| C | 0.9170055000 | 0.2702423000 | 0.0019302000 |
| C | -0.4471382000 | 0.7626607000 | 0.0037493000 |
| C | -1.6236101000 | 0.0105534000 | 0.0016373000 |
| C | -1.9153463000 | -1.4022909000 | -0.0023183000 |
| C | -3.2620053000 | -1.8324223000 | -0.0033015000 |
| H | -3.4552556000 | -2.9034441000 | -0.0062954000 |
| C | -4.2966197000 | -0.9088723000 | -0.0005150000 |
| H | -5.3345959000 | -1.2646145000 | -0.0013573000 |
| C | -4.0465695000 | 0.4804018000 | 0.0033744000 |
| H | -4.8806944000 | 1.1857749000 | 0.0054896000 |
| C | -2.7437344000 | 0.9258128000 | 0.0044027000 |
| C | -2.2578202000 | 2.3481271000 | 0.0082873000 |
| H | -2.6238157000 | 2.8696522000 | 0.9139258000 |
| C | -0.7253372000 | 2.2298858000 | 0.0082909000 |
| H | -0.2676088000 | 2.6979734000 | -0.8859020000 |
| H | -2.6234243000 | 2.8743242000 | -0.8948043000 |
| H | -0.2680890000 | 2.6922359000 | 0.9056695000 |
| H | 4.1616635000 | 0.3485865000 | 0.0011022000 |
| H | 3.1755099000 | -2.0454886000 | -0.0056379000 |

1.6

| | | | |
|---|---------------|---------------|---------------|
| O | 2.3131734000 | 2.3273632000 | 0.0075158000 |
| O | -0.9928816000 | -2.3555792000 | -0.0051580000 |
| H | -0.0232725000 | -2.0051431000 | -0.0043903000 |
| N | 3.1634995000 | 0.1295048000 | 0.0008232000 |
| N | 1.2514510000 | -1.0394920000 | -0.0021116000 |
| C | 2.5997468000 | -1.1292891000 | -0.0026379000 |
| C | 2.1198750000 | 1.1014494000 | 0.0038716000 |
| C | 0.9061578000 | 0.2637373000 | 0.0019293000 |
| C | -0.4514409000 | 0.7671192000 | 0.0039107000 |
| C | -1.6287947000 | 0.0176658000 | 0.0016773000 |
| C | -1.9037096000 | -1.4002206000 | -0.0023575000 |
| C | -3.2498378000 | -1.8365757000 | -0.0033614000 |
| H | -3.4460916000 | -2.9070526000 | -0.0062580000 |
| C | -4.2864013000 | -0.9148740000 | -0.0005398000 |
| H | -5.3231293000 | -1.2726843000 | -0.0013830000 |
| C | -4.0474099000 | 0.4771754000 | 0.0034250000 |
| H | -4.8857057000 | 1.1779149000 | 0.0054364000 |
| C | -2.7475331000 | 0.9301817000 | 0.0043920000 |
| C | -2.2598267000 | 2.3516374000 | 0.0082689000 |
| H | -2.6254810000 | 2.8733201000 | 0.9133172000 |
| C | -0.7268822000 | 2.2342765000 | 0.0083158000 |

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|---|---------------|---------------|---------------|
| H | -0.2687613000 | 2.7008373000 | -0.8866338000 |
| H | -2.6252369000 | 2.8780604000 | -0.8942479000 |
| H | -0.2692005000 | 2.6950372000 | 0.9064869000 |
| H | 4.1482723000 | 0.3294524000 | 0.0010370000 |
| H | 3.1559623000 | -2.0630805000 | -0.0056699000 |

1.5

| | | | |
|---|---------------|---------------|---------------|
| O | 2.3478196000 | 2.3104657000 | 0.0069803000 |
| O | -0.9592389000 | -2.3213929000 | -0.0050567000 |
| H | 0.0309499000 | -1.9503970000 | -0.0030324000 |
| N | 3.1488885000 | 0.0961751000 | 0.0004527000 |
| N | 1.2187399000 | -1.0353986000 | -0.0011890000 |
| C | 2.5628526000 | -1.1539084000 | -0.0019589000 |
| C | 2.1277251000 | 1.0899490000 | 0.0033072000 |
| C | 0.8947670000 | 0.2781450000 | 0.0028034000 |
| C | -0.4541913000 | 0.7917700000 | 0.0036298000 |
| C | -1.6296294000 | 0.0346377000 | 0.0003430000 |
| C | -1.8839273000 | -1.3896744000 | -0.0023319000 |
| C | -3.2280556000 | -1.8413380000 | -0.0031354000 |
| H | -3.4061793000 | -2.9145570000 | -0.0064048000 |
| C | -4.2748471000 | -0.9323433000 | -0.0012820000 |
| H | -5.3076582000 | -1.3025382000 | -0.0029519000 |
| C | -4.0492720000 | 0.4643114000 | 0.0042813000 |
| H | -4.8994904000 | 1.1506222000 | 0.0058420000 |
| C | -2.7540104000 | 0.9367508000 | 0.0038344000 |
| C | -2.2683086000 | 2.3604941000 | 0.0089355000 |
| H | -2.6354848000 | 2.8846763000 | 0.9144579000 |
| C | -0.7350809000 | 2.2579124000 | 0.0081865000 |
| H | -0.2780632000 | 2.7266565000 | -0.8864291000 |
| H | -2.6341375000 | 2.8899812000 | -0.8940543000 |
| H | -0.2798258000 | 2.7222980000 | 0.9062624000 |
| H | 4.1376605000 | 0.2744773000 | -0.0000092000 |
| H | 3.1045270000 | -2.0970293000 | -0.0058216000 |

1.4

| | | | |
|---|---------------|---------------|---------------|
| O | 2.3973607000 | 2.2918948000 | -0.0053821000 |
| O | -0.9371670000 | -2.2915276000 | 0.0021902000 |
| H | 0.0981968000 | -1.8981911000 | 0.0023975000 |
| N | 3.1415411000 | 0.0619825000 | -0.0053108000 |
| N | 1.1920254000 | -1.0261825000 | 0.0029406000 |
| C | 2.5278960000 | -1.1771313000 | -0.0018057000 |
| C | 2.1466001000 | 1.0785398000 | -0.0033661000 |
| C | 0.8885572000 | 0.3017982000 | 0.0008223000 |
| C | -0.4415925000 | 0.8194692000 | 0.0045896000 |

| | | | |
|---|---------------|---------------|---------------|
| C | -1.6252625000 | 0.0499951000 | 0.0055220000 |
| C | -1.8668872000 | -1.3823815000 | 0.0012068000 |
| C | -3.2146494000 | -1.8446509000 | -0.0035704000 |
| H | -3.3850301000 | -2.9201167000 | -0.0037871000 |
| C | -4.2692535000 | -0.9455389000 | -0.0051693000 |
| H | -5.2984167000 | -1.3222299000 | -0.0110005000 |
| C | -4.0465563000 | 0.4514158000 | -0.0018594000 |
| H | -4.8990076000 | 1.1365042000 | -0.0044066000 |
| C | -2.7478449000 | 0.9328603000 | 0.0047716000 |
| C | -2.2801815000 | 2.3623230000 | 0.0116050000 |
| H | -2.6611406000 | 2.8745510000 | 0.9189550000 |
| C | -0.7454488000 | 2.2834763000 | 0.0126133000 |
| H | -0.3007278000 | 2.7659083000 | -0.8809599000 |
| H | -2.6581128000 | 2.8856285000 | -0.8905411000 |
| H | -0.3046090000 | 2.7555870000 | 0.9141360000 |
| H | 4.1338996000 | 0.2166665000 | -0.0061578000 |
| H | 3.0523465000 | -2.1299061000 | -0.0027747000 |

1.3

| | | | |
|---|---------------|---------------|---------------|
| O | 2.4132109000 | 2.2815458000 | 0.0072613000 |
| O | -0.9496510000 | -2.2740906000 | -0.0049887000 |
| H | 0.2044595000 | -1.8714823000 | -0.0039184000 |
| N | 3.1385100000 | 0.0510224000 | 0.0003571000 |
| N | 1.1901975000 | -1.0290803000 | -0.0020296000 |
| C | 2.5233318000 | -1.1889625000 | -0.0027908000 |
| C | 2.1566656000 | 1.0710090000 | 0.0038771000 |
| C | 0.8810802000 | 0.3150897000 | 0.0023438000 |
| C | -0.4121720000 | 0.8311109000 | 0.0040563000 |
| C | -1.6283417000 | 0.0519803000 | 0.0017524000 |
| C | -1.8689568000 | -1.3821137000 | -0.0026604000 |
| C | -3.2332014000 | -1.8455988000 | -0.0033279000 |
| H | -3.4029841000 | -2.9230292000 | -0.0065058000 |
| C | -4.2892429000 | -0.9426046000 | -0.0006922000 |
| H | -5.3177673000 | -1.3149540000 | -0.0013282000 |
| C | -4.0534709000 | 0.4405110000 | 0.0030765000 |
| H | -4.8903964000 | 1.1463455000 | 0.0052112000 |
| C | -2.7257625000 | 0.9192472000 | 0.0045885000 |
| C | -2.2861544000 | 2.3555032000 | 0.0083948000 |
| H | -2.6739855000 | 2.8645627000 | 0.9146140000 |
| C | -0.7471483000 | 2.2925002000 | 0.0085430000 |
| H | -0.3212789000 | 2.7784292000 | -0.8913890000 |
| H | -2.6736901000 | 2.8688986000 | -0.8955277000 |
| H | -0.3215177000 | 2.7723622000 | 0.9119276000 |
| H | 4.1317152000 | 0.2016066000 | 0.0005603000 |

| | | | |
|-----|---------------|---------------|---------------|
| H | 3.0530926000 | -2.1390661000 | -0.0057469000 |
| 1.2 | | | |
| O | 2.3943150000 | 2.2821689000 | 0.0073621000 |
| O | -0.9646826000 | -2.2765397000 | -0.0049173000 |
| H | 0.3241440000 | -1.8481796000 | -0.0040884000 |
| N | 3.1385980000 | 0.0586662000 | 0.0005643000 |
| N | 1.1997951000 | -1.0332728000 | -0.0020594000 |
| C | 2.5400241000 | -1.1906059000 | -0.0028983000 |
| C | 2.1540818000 | 1.0685397000 | 0.0038899000 |
| C | 0.8760916000 | 0.3125331000 | 0.0019837000 |
| C | -0.4070854000 | 0.8218537000 | 0.0039905000 |
| C | -1.6401784000 | 0.0364235000 | 0.0017827000 |
| C | -1.8806952000 | -1.3960636000 | -0.0022606000 |
| C | -3.2565585000 | -1.8413542000 | -0.0032150000 |
| H | -3.4405903000 | -2.9177436000 | -0.0063810000 |
| C | -4.3117753000 | -0.9277116000 | -0.0005774000 |
| H | -5.3432225000 | -1.2934768000 | -0.0015514000 |
| C | -4.0644877000 | 0.4439642000 | 0.0033442000 |
| H | -4.8842083000 | 1.1692572000 | 0.0054565000 |
| C | -2.7191705000 | 0.9083907000 | 0.0041706000 |
| C | -2.2834491000 | 2.3453410000 | 0.0083137000 |
| H | -2.6743644000 | 2.8524208000 | 0.9147354000 |
| C | -0.7441827000 | 2.2833463000 | 0.0083812000 |
| H | -0.3217792000 | 2.7696121000 | -0.8933709000 |
| H | -2.6741515000 | 2.8570368000 | -0.8957251000 |
| H | -0.3220989000 | 2.7638332000 | 0.9137863000 |
| H | 4.1310121000 | 0.2193652000 | 0.0007908000 |
| H | 3.0711600000 | -2.1370627000 | -0.0058492000 |
| 1.1 | | | |
| O | 2.3255471000 | 2.2848926000 | 0.0073903000 |
| O | -0.9883483000 | -2.2849046000 | -0.0048886000 |
| H | 0.4632867000 | -1.8515937000 | -0.0041480000 |
| N | 3.1342271000 | 0.0833812000 | 0.0007026000 |
| N | 1.2177326000 | -1.0542097000 | -0.0021270000 |
| C | 2.5701953000 | -1.1813832000 | -0.0029018000 |
| C | 2.1264085000 | 1.0656014000 | 0.0038819000 |
| C | 0.8582094000 | 0.2855423000 | 0.0019582000 |
| C | -0.4172097000 | 0.7935834000 | 0.0038048000 |
| C | -1.6611991000 | 0.0175779000 | 0.0017745000 |
| C | -1.9039496000 | -1.4129843000 | -0.0022886000 |
| C | -3.2860586000 | -1.8353192000 | -0.0033181000 |
| H | -3.4904676000 | -2.9083936000 | -0.0063021000 |

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|-----|---------------|---------------|---------------|
| C | -4.3326191000 | -0.9069709000 | -0.0005653000 |
| H | -5.3669695000 | -1.2667325000 | -0.0013514000 |
| C | -4.0760498000 | 0.4606221000 | 0.0032948000 |
| H | -4.8943890000 | 1.1856144000 | 0.0054956000 |
| C | -2.7218048000 | 0.9083142000 | 0.0044103000 |
| C | -2.2681344000 | 2.3404745000 | 0.0082670000 |
| H | -2.6496625000 | 2.8542156000 | 0.9131477000 |
| C | -0.7317086000 | 2.2614795000 | 0.0084044000 |
| H | -0.3013153000 | 2.7404529000 | -0.8919971000 |
| H | -2.6492109000 | 2.8589178000 | -0.8940909000 |
| H | -0.3018641000 | 2.7346230000 | 0.9119800000 |
| H | 4.1228609000 | 0.2739740000 | 0.0009155000 |
| H | 3.1190348000 | -2.1160332000 | -0.0057909000 |
| 1.0 | | | |
| O | 2.3188790000 | 2.2779711000 | 0.0073918000 |
| O | -0.9992951000 | -2.2849287000 | -0.0048862000 |
| H | 0.5584391000 | -1.8117482000 | -0.0040707000 |
| N | 3.1355902000 | 0.0817994000 | 0.0006694000 |
| N | 1.2221968000 | -1.0606344000 | -0.0020952000 |
| C | 2.5810426000 | -1.1830366000 | -0.0029123000 |
| C | 2.1235825000 | 1.0595833000 | 0.0038690000 |
| C | 0.8528163000 | 0.2788375000 | 0.0019049000 |
| C | -0.4211913000 | 0.7857128000 | 0.0037256000 |
| C | -1.6685885000 | 0.0132621000 | 0.0018209000 |
| C | -1.9145266000 | -1.4160665000 | -0.0022821000 |
| C | -3.2963231000 | -1.8323781000 | -0.0032907000 |
| H | -3.5031064000 | -2.9050186000 | -0.0062957000 |
| C | -4.3428350000 | -0.9015871000 | -0.0006524000 |
| H | -5.3774852000 | -1.2596470000 | -0.0012769000 |
| C | -4.0832753000 | 0.4664290000 | 0.0032749000 |
| H | -4.8982779000 | 1.1935044000 | 0.0055568000 |
| C | -2.7264866000 | 0.9084311000 | 0.0045547000 |
| C | -2.2698286000 | 2.3377843000 | 0.0083295000 |
| H | -2.6515666000 | 2.8523850000 | 0.9132298000 |
| C | -0.7336114000 | 2.2563814000 | 0.0084837000 |
| H | -0.3040349000 | 2.7334567000 | -0.8930378000 |
| H | -2.6509175000 | 2.8571905000 | -0.8941821000 |
| H | -0.3050192000 | 2.7276591000 | 0.9127126000 |
| H | 4.1231839000 | 0.2744121000 | 0.0009233000 |
| H | 3.1271804000 | -2.1190124000 | -0.0058071000 |

CASSCF: S0 O6-H7 bond length (Ångstrom)

1.00

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|---|---------------|---------------|---------------|
| O | 2.2682323700 | 2.3197847300 | -0.1720110900 |
| O | -1.0375350700 | -2.3898169200 | -0.3637756400 |
| H | -0.1099860400 | -2.0859202900 | -0.1462908600 |
| N | 3.1189529200 | 0.2186393900 | 0.1728184100 |
| N | 1.3008208700 | -1.0429228400 | 0.1834730900 |
| C | 2.5607603100 | -1.0284527200 | 0.2732246600 |
| C | 2.1111085200 | 1.1465247000 | -0.0247627200 |
| C | 0.8876724400 | 0.2967006800 | -0.0000545900 |
| C | -0.3698706700 | 0.7270417200 | -0.1074991900 |
| C | -1.6501154600 | -0.0355757000 | -0.0635570300 |
| C | -1.9365381900 | -1.4126929500 | -0.1738776500 |
| C | -3.2792036100 | -1.8128617200 | -0.1318902800 |
| H | -3.4896187600 | -2.8617088700 | -0.2259050500 |
| C | -4.3088676800 | -0.8869763500 | 0.0211642800 |
| H | -5.3269908000 | -1.2322416700 | 0.0491454100 |
| C | -4.0321220300 | 0.4825393700 | 0.1350275400 |
| H | -4.8276005900 | 1.1970188600 | 0.2489951700 |
| C | -2.7087525300 | 0.8911184000 | 0.0849527800 |
| C | -2.1911882400 | 2.3051339300 | 0.1844132000 |
| H | -2.2460993000 | 2.6603507100 | 1.2094586300 |
| C | -0.7283647400 | 2.1927505400 | -0.2723495000 |
| H | -0.6412470600 | 2.4392227800 | -1.3269570600 |
| H | -2.7589822000 | 2.9976194600 | -0.4262298600 |
| H | -0.0516992000 | 2.8432280600 | 0.2583664000 |
| H | 4.0867415800 | 0.4463447300 | 0.2003263400 |
| H | 3.1708131700 | -1.8992080000 | 0.4135216200 |

1.10

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|---|---------------|---------------|---------------|
| O | 2.2422115100 | 2.3221459400 | -0.0064140500 |
| O | -1.0387690800 | -2.4205646900 | -0.0172214800 |
| H | -0.0062103700 | -2.0415456600 | -0.0042733300 |
| N | 3.1210812100 | 0.2017183800 | 0.0049038800 |
| N | 1.3098313200 | -1.0628128100 | 0.0062449200 |
| C | 2.5729700200 | -1.0521143500 | 0.0084538300 |
| C | 2.1003499400 | 1.1389711300 | -0.0009575200 |
| C | 0.8820307800 | 0.2850499900 | 0.0008797700 |
| C | -0.3753317900 | 0.7211806300 | -0.0022581500 |
| C | -1.6596462000 | -0.0407568200 | -0.0019765800 |
| C | -1.9363415500 | -1.4295373100 | -0.0097971000 |
| C | -3.2833775800 | -1.8244079900 | -0.0113202700 |
| H | -3.4910710200 | -2.8779591400 | -0.0179344200 |
| C | -4.3191949600 | -0.8921428300 | -0.0045190900 |
| H | -5.3377971300 | -1.2376476500 | -0.0058383100 |

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|---|---------------|---------------|---------------|
| C | -4.0499517600 | 0.4859368200 | 0.0043654300 |
| H | -4.8511107300 | 1.2032983800 | 0.0102226200 |
| C | -2.7272046500 | 0.8946014500 | 0.0052604200 |
| C | -2.2346616100 | 2.3200898600 | 0.0172564100 |
| H | -2.5756282900 | 2.8448433200 | 0.9034559500 |
| C | -0.7012293700 | 2.2060475800 | -0.0089714900 |
| H | -0.2690832600 | 2.6679907000 | -0.8874295200 |
| H | -2.6050907900 | 2.8726480200 | -0.8395422200 |
| H | -0.2343979300 | 2.6891497000 | 0.8391672000 |
| H | 4.0890579600 | 0.4312052500 | 0.0055481800 |
| H | 3.1888853300 | -1.9297478700 | 0.0124219200 |

1.20

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|---|---------------|---------------|---------------|
| O | 2.2836339200 | 2.2807656500 | -0.0030269900 |
| O | -0.9545610500 | -2.3296159000 | -0.0086567500 |
| H | 0.1591095100 | -1.8827425700 | -0.0021607900 |
| N | 3.0834681600 | 0.1253663800 | 0.0021676600 |
| N | 1.2407676800 | -1.0585195900 | 0.0025590800 |
| C | 2.5050623900 | -1.1065606800 | 0.0035264600 |
| C | 2.0885659300 | 1.1039479100 | -0.0005669600 |
| C | 0.8578003000 | 0.3020686700 | 0.0003189000 |
| C | -0.4149798300 | 0.7450541500 | -0.0006996700 |
| C | -1.6447775500 | -0.0000408000 | -0.0003701900 |
| C | -1.8796097600 | -1.4042606600 | -0.0057495800 |
| C | -3.2301450100 | -1.8242262800 | -0.0088883100 |
| H | -3.4146269000 | -2.8821265300 | -0.0138383000 |
| C | -4.2807565100 | -0.9163637100 | -0.0059428300 |
| H | -5.2913596700 | -1.2852650100 | -0.0086585600 |
| C | -4.0492080900 | 0.4746084400 | 0.0009844900 |
| H | -4.8711472000 | 1.1679720900 | 0.0043920400 |
| C | -2.7441859600 | 0.9140701500 | 0.0038068900 |
| C | -2.2616554800 | 2.3433185000 | 0.0158085300 |
| H | -2.6075584400 | 2.8671254400 | 0.9006336900 |
| C | -0.7267087000 | 2.2326383800 | -0.0053646700 |
| H | -0.2872576000 | 2.6909659600 | -0.8820096300 |
| H | -2.6317218000 | 2.8933091500 | -0.8427702100 |
| H | -0.2588608300 | 2.7080630500 | 0.8466477000 |
| H | 4.0582272500 | 0.3250232200 | 0.0026094500 |
| H | 3.0828052200 | -2.0089354000 | 0.0049755500 |

1.30

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|---|---------------|---------------|---------------|
| O | 2.3319466200 | 2.2478957700 | -0.0028683200 |
| O | -0.9120633600 | -2.2558217800 | -0.0055146200 |
| H | 0.2953725200 | -1.7740823200 | -0.0004444100 |

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|---|---------------|---------------|---------------|
| N | 3.0660351200 | 0.0632828400 | 0.0009930700 |
| N | 1.2043619100 | -1.0450423700 | 0.0020782500 |
| C | 2.4724566800 | -1.1488837800 | 0.0023335400 |
| C | 2.0887225900 | 1.0756881100 | -0.0008706700 |
| C | 0.8544945700 | 0.3176627600 | 0.0002383400 |
| C | -0.4403621300 | 0.7686456600 | -0.0000341500 |
| C | -1.6444977700 | 0.0273694700 | 0.0004632400 |
| C | -1.8423276100 | -1.3836261800 | -0.0041913200 |
| C | -3.2067487000 | -1.8253060000 | -0.0084402300 |
| H | -3.3712035100 | -2.8866302300 | -0.0131076700 |
| C | -4.2572441600 | -0.9398474700 | -0.0069232000 |
| H | -5.2632297500 | -1.3219785200 | -0.0104684200 |
| C | -4.0501311100 | 0.4679529500 | -0.0003116700 |
| H | -4.8880588500 | 1.1416765900 | 0.0023175600 |
| C | -2.7631161200 | 0.9257129900 | 0.0035953900 |
| C | -2.2856478700 | 2.3585250300 | 0.0159781700 |
| H | -2.6354592000 | 2.8790477900 | 0.9011355900 |
| C | -0.7477285700 | 2.2556891400 | -0.0048377700 |
| H | -0.3108650000 | 2.7172037900 | -0.8817467600 |
| H | -2.6597023600 | 2.9061723900 | -0.8422787800 |
| H | -0.2833319300 | 2.7338305500 | 0.8482496900 |
| H | 4.0448366300 | 0.2427987800 | 0.0011195700 |
| H | 3.0138113900 | -2.0722959300 | 0.0032625900 |

1.40

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|---|---------------|---------------|---------------|
| O | 2.3376391600 | 2.2430363700 | -0.0033526800 |
| O | -0.9268415900 | -2.2474370500 | -0.0044749400 |
| H | 0.3831301700 | -1.7535253300 | 0.0005709600 |
| N | 3.0671259300 | 0.0548114100 | 0.0005910500 |
| N | 1.2124040100 | -1.0413994600 | 0.0022953500 |
| C | 2.4837358300 | -1.1557495500 | 0.0022547000 |
| C | 2.0850116600 | 1.0702149200 | -0.0011840100 |
| C | 0.8580819300 | 0.3174291100 | 0.0002493400 |
| C | -0.4500708900 | 0.7659952600 | 0.0002161000 |
| C | -1.6492751200 | 0.0293217900 | 0.0008235300 |
| C | -1.8445636200 | -1.3876224600 | -0.0036965000 |
| C | -3.2212694400 | -1.8265755000 | -0.0085616000 |
| H | -3.3850497200 | -2.8881031300 | -0.0132524700 |
| C | -4.2633490300 | -0.9430837200 | -0.0075174200 |
| H | -5.2705047500 | -1.3224803700 | -0.0114706700 |
| C | -4.0554276500 | 0.4736728800 | -0.0008192300 |
| H | -4.8962503300 | 1.1437286500 | 0.0016027900 |
| C | -2.7745697300 | 0.9303065400 | 0.0035816900 |
| C | -2.2904244000 | 2.3617410600 | 0.0163680500 |

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|---|---------------|---------------|---------------|
| H | -2.6379229600 | 2.8828892900 | 0.9019881300 |
| C | -0.7521414200 | 2.2539882200 | -0.0048587400 |
| H | -0.3144970500 | 2.7149603100 | -0.8818566700 |
| H | -2.6626850700 | 2.9110522100 | -0.8415216500 |
| H | -0.2866275500 | 2.7317537700 | 0.8480225600 |
| H | 4.0452279900 | 0.2384880100 | 0.0005100300 |
| H | 3.0194336200 | -2.0817732000 | 0.0032193200 |

1.50

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|---|---------------|---------------|---------------|
| O | 2.3245063600 | 2.2468289500 | -0.0039108300 |
| O | -0.9561309600 | -2.2573899700 | -0.0039107400 |
| H | 0.4593929500 | -1.7611404600 | 0.0014300800 |
| N | 3.0724256600 | 0.0646516300 | 0.0003429500 |
| N | 1.2334150200 | -1.0434882800 | 0.0026051200 |
| C | 2.5079790600 | -1.1505144600 | 0.0023771300 |
| C | 2.0768542100 | 1.0712861300 | -0.0014816600 |
| C | 0.8611936300 | 0.3097512100 | 0.0002674800 |
| C | -0.4569874100 | 0.7526455700 | 0.0003540400 |
| C | -1.6550015700 | 0.0240163000 | 0.0010184500 |
| C | -1.8600586300 | -1.3981207900 | -0.0034719200 |
| C | -3.2466899100 | -1.8264480700 | -0.0087728100 |
| H | -3.4165146400 | -2.8870936900 | -0.0135132600 |
| C | -4.2795866700 | -0.9374689000 | -0.0079825400 |
| H | -5.2898463300 | -1.3086855300 | -0.0122214600 |
| C | -4.0614433500 | 0.4824913000 | -0.0011335900 |
| H | -4.8992043700 | 1.1563722600 | 0.0012020500 |
| C | -2.7807820400 | 0.9315310500 | 0.0036074300 |
| C | -2.2880172200 | 2.3599563400 | 0.0167032300 |
| H | -2.6321899400 | 2.8826889800 | 0.9026741600 |
| C | -0.7507365400 | 2.2428776200 | -0.0048845400 |
| H | -0.3105534300 | 2.7016407100 | -0.8817716200 |
| H | -2.6572929900 | 2.9116749300 | -0.8409136600 |
| H | -0.2822864100 | 2.7185328800 | 0.8475479800 |
| H | 4.0479922900 | 0.2615742000 | 0.0000795900 |
| H | 3.0498832600 | -2.0725298600 | 0.0034859500 |

1.60

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|---|---------------|---------------|---------------|
| O | 2.3022123700 | 2.2549181700 | -0.0037723700 |
| O | -0.9952943700 | -2.2716779000 | -0.0036374100 |
| H | 0.5257488000 | -1.7752945200 | 0.0019568800 |
| N | 3.0843263400 | 0.0876513300 | 0.0001268100 |
| N | 1.2584739200 | -1.0431365000 | 0.0025995200 |
| C | 2.5406579200 | -1.1475273500 | 0.0022036300 |
| C | 2.0753874200 | 1.0722912500 | -0.0014656400 |

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|---|---------------|---------------|---------------|
| C | 0.8688120800 | 0.2997925700 | 0.0003174000 |
| C | -0.4637105400 | 0.7349510700 | 0.0005711000 |
| C | -1.6635856600 | 0.0164458100 | 0.0011464600 |
| C | -1.8870938400 | -1.4076718800 | -0.0033547400 |
| C | -3.2819256600 | -1.8198798500 | -0.0087579800 |
| H | -3.4625097400 | -2.8787770000 | -0.0134590500 |
| C | -4.2916294500 | -0.9321349400 | -0.0080738100 |
| H | -5.3063229700 | -1.2921863800 | -0.0123122600 |
| C | -4.0673142700 | 0.4905265300 | -0.0013202800 |
| H | -4.9023238600 | 1.1671423800 | 0.0008252300 |
| C | -2.7826666300 | 0.9302080200 | 0.0035317500 |
| C | -2.2823463400 | 2.3546807500 | 0.0164952000 |
| H | -2.6251653300 | 2.8785274100 | 0.9024164600 |
| C | -0.7466229300 | 2.2269664600 | -0.0046332800 |
| H | -0.3030915700 | 2.6838889100 | -0.8807622800 |
| H | -2.6496948100 | 2.9075300500 | -0.8413059600 |
| H | -0.2753345600 | 2.7003005800 | 0.8474526300 |
| H | 4.0550545300 | 0.3039754300 | -0.0002808500 |
| H | 3.0862791500 | -2.0658703800 | 0.0032198500 |

OM2/MRCI: S1 C4-C3-C2-N1 (degree)

| | | | |
|---|---------------|---------------|---------------|
| O | | | |
| O | 2.3194894000 | 2.3396345000 | 0.0075568000 |
| O | -1.0298386000 | -2.3888582000 | -0.0052065000 |
| H | -0.0687789000 | -2.0742840000 | -0.0045943000 |
| N | 3.1772151000 | 0.1467217000 | 0.0008837000 |
| N | 1.2713451000 | -1.0298827000 | -0.0020428000 |
| C | 2.6193836000 | -1.1129603000 | -0.0026959000 |
| C | 2.1265621000 | 1.1133238000 | 0.0039921000 |
| C | 0.9167932000 | 0.2699312000 | 0.0020110000 |
| C | -0.4472383000 | 0.7622669000 | 0.0036878000 |
| C | -1.6245412000 | 0.0106345000 | 0.0016911000 |
| C | -1.9153869000 | -1.4021066000 | -0.0023032000 |
| C | -3.2619130000 | -1.8320982000 | -0.0032971000 |
| H | -3.4566267000 | -2.9028886000 | -0.0062935000 |
| C | -4.2963006000 | -0.9088090000 | -0.0005228000 |
| H | -5.3345951000 | -1.2638871000 | -0.0013506000 |
| C | -4.0470852000 | 0.4802796000 | 0.0033696000 |
| H | -4.8808241000 | 1.1855218000 | 0.0054874000 |
| C | -2.7443549000 | 0.9256318000 | 0.0044495000 |
| C | -2.2577373000 | 2.3480919000 | 0.0082926000 |
| H | -2.6233324000 | 2.8695725000 | 0.9130261000 |
| C | -0.7254933000 | 2.2296626000 | 0.0081855000 |
| H | -0.2676734000 | 2.6968605000 | -0.8862286000 |

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|---|---------------|---------------|---------------|
| H | -2.6229290000 | 2.8742534000 | -0.8939053000 |
| H | -0.2681449000 | 2.6910892000 | 0.9060083000 |
| H | 4.1609683000 | 0.3490146000 | 0.0011010000 |
| H | 3.1775786000 | -2.0459737000 | -0.0056441000 |

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| | | | |
|---|---------------|---------------|---------------|
| O | -0.8112796000 | 1.8032852000 | 1.2598570000 |
| O | 4.6415255000 | 0.5832426000 | 0.8450159000 |
| H | 3.7957458000 | 0.4054240000 | 1.4288553000 |
| N | 0.1849201000 | -0.1172439000 | 2.1904645000 |
| N | 2.3337335000 | 0.4067699000 | 1.8975770000 |
| C | 1.4717706000 | -0.5501142000 | 2.2999711000 |
| C | 0.1842117000 | 1.0793264000 | 1.3344789000 |
| C | 1.6654554000 | 1.5081005000 | 1.4775342000 |
| C | 2.1375103000 | 2.4653431000 | 0.5106689000 |
| C | 3.2940776000 | 2.2705355000 | -0.2949182000 |
| C | 4.4103014000 | 1.3962054000 | -0.1748589000 |
| C | 5.4186365000 | 1.4485110000 | -1.1722844000 |
| H | 6.2715085000 | 0.7801085000 | -1.0795245000 |
| C | 5.3198680000 | 2.3458222000 | -2.2225647000 |
| H | 6.1202511000 | 2.3843991000 | -2.9699463000 |
| C | 4.2326310000 | 3.2382598000 | -2.3314475000 |
| H | 4.1932057000 | 3.9413844000 | -3.1626011000 |
| C | 3.2396173000 | 3.2009633000 | -1.3769006000 |
| C | 2.0130427000 | 4.0665225000 | -1.2578427000 |
| H | 1.3430336000 | 3.9323005000 | -2.1267367000 |
| C | 1.3128983000 | 3.6024403000 | 0.0374729000 |
| H | 1.3328678000 | 4.4053469000 | 0.8087052000 |
| H | 2.3331113000 | 5.1260481000 | -1.1894570000 |
| H | 0.2621077000 | 3.2983126000 | -0.1067460000 |
| H | -0.6101377000 | -0.7188091000 | 2.3138704000 |
| H | 1.7821876000 | -1.5315008000 | 2.6723970000 |

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|---|---------------|---------------|---------------|
| O | 2.0209796000 | 2.2912327000 | 0.4657366000 |
| O | -0.9533590000 | -2.3285689000 | -0.1797897000 |
| H | -0.0239357000 | -1.9854914000 | -0.4018329000 |
| N | 2.9540719000 | 0.1277802000 | 0.5788902000 |
| N | 1.3074440000 | -1.0007175000 | -0.4382841000 |
| C | 2.4891831000 | -1.0958826000 | 0.2015937000 |
| C | 1.8312253000 | 1.0740815000 | 0.4919813000 |
| C | 0.8923146000 | 0.2842614000 | -0.4894237000 |
| C | -0.4486937000 | 0.7878071000 | -0.4949696000 |
| C | -1.5769923000 | 0.0394686000 | -0.0361512000 |

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|----|---------------|---------------|---------------|
| C | -1.8084573000 | -1.3494446000 | 0.1216172000 |
| C | -3.0844113000 | -1.7862607000 | 0.5573614000 |
| H | -3.2495965000 | -2.8550471000 | 0.6754553000 |
| C | -4.0873961000 | -0.8611247000 | 0.8088197000 |
| H | -5.0672558000 | -1.2190052000 | 1.1476115000 |
| C | -3.8826085000 | 0.5175528000 | 0.6141339000 |
| H | -4.6975247000 | 1.2210671000 | 0.7928154000 |
| C | -2.6418380000 | 0.9590606000 | 0.1984072000 |
| C | -2.1905915000 | 2.3635254000 | -0.0942340000 |
| H | -2.1659643000 | 2.9591838000 | 0.8385365000 |
| C | -0.7726337000 | 2.2241251000 | -0.6814445000 |
| H | -0.7629783000 | 2.4584840000 | -1.7688670000 |
| H | -2.8860076000 | 2.8394266000 | -0.8143662000 |
| H | -0.0258107000 | 2.8668349000 | -0.1863997000 |
| H | 3.7295762000 | 0.2380554000 | 1.2138328000 |
| H | 2.9932039000 | -2.0487162000 | 0.3916928000 |
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| O | 1.7351882000 | 2.0384878000 | 0.8607435000 |
| O | -0.8331622000 | -2.2357576000 | -0.0274205000 |
| H | -0.0332263000 | -1.9523662000 | -0.5437600000 |
| N | 2.8794079000 | 0.0061518000 | 0.5408854000 |
| N | 1.5096036000 | -0.8900970000 | -1.0034706000 |
| C | 2.6080564000 | -1.0734652000 | -0.2430486000 |
| C | 1.6860448000 | 0.8492208000 | 0.5516873000 |
| C | 0.9594704000 | 0.3113108000 | -0.7838557000 |
| C | -0.3569874000 | 0.8314891000 | -0.7096988000 |
| C | -1.5149005000 | 0.1083512000 | -0.2705929000 |
| C | -1.7597155000 | -1.2568701000 | -0.0082184000 |
| C | -3.0633965000 | -1.6819967000 | 0.3231024000 |
| H | -3.2289627000 | -2.7342410000 | 0.5425957000 |
| C | -4.0965832000 | -0.7535289000 | 0.3761714000 |
| H | -5.1065204000 | -1.0959448000 | 0.6340472000 |
| C | -3.8821065000 | 0.6040986000 | 0.0924843000 |
| H | -4.7116200000 | 1.3123440000 | 0.1156667000 |
| C | -2.5962450000 | 1.0296172000 | -0.2043043000 |
| C | -2.1331871000 | 2.4280584000 | -0.5095661000 |
| H | -2.2196205000 | 3.0480765000 | 0.4037387000 |
| C | -0.6648061000 | 2.2710017000 | -0.9392351000 |
| H | -0.5202287000 | 2.5260364000 | -2.0094393000 |
| H | -2.7526498000 | 2.8742237000 | -1.3129768000 |
| H | 0.0248223000 | 2.8872272000 | -0.3321668000 |
| H | 3.5360908000 | -0.0398322000 | 1.3087140000 |
| H | 3.1836144000 | -2.0035641000 | -0.2514432000 |

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|---|---------------|---------------|---------------|
| O | 1.8282628000 | 1.6435957000 | 1.2151665000 |
| O | -0.7335696000 | -1.9899433000 | 0.8344810000 |
| H | 0.1330972000 | -1.6252131000 | 0.5111257000 |
| N | 2.9667797000 | -0.1919771000 | 0.2798443000 |
| N | 1.4447328000 | -0.7758660000 | -1.2704930000 |
| C | 2.6251415000 | -1.0790990000 | -0.7065893000 |
| C | 1.7862547000 | 0.5813188000 | 0.5895511000 |
| C | 0.9258370000 | 0.3367564000 | -0.7125192000 |
| C | -0.3597518000 | 0.8508281000 | -0.4505417000 |
| C | -1.5257627000 | 0.1626614000 | 0.0181106000 |
| C | -1.7309756000 | -1.1441137000 | 0.5074275000 |
| C | -3.0419027000 | -1.6208386000 | 0.7138005000 |
| H | -3.1855558000 | -2.6338592000 | 1.0818137000 |
| C | -4.1181615000 | -0.7763407000 | 0.4631757000 |
| H | -5.1392201000 | -1.1439350000 | 0.6279486000 |
| C | -3.9384761000 | 0.5357769000 | -0.0007230000 |
| H | -4.7976740000 | 1.1801077000 | -0.1926068000 |
| C | -2.6490669000 | 1.0078988000 | -0.1943198000 |
| C | -2.2269275000 | 2.3581844000 | -0.7065795000 |
| H | -2.5662731000 | 3.1546870000 | -0.0191793000 |
| C | -0.6976800000 | 2.2701544000 | -0.7811721000 |
| H | -0.3038561000 | 2.5585447000 | -1.7717206000 |
| H | -2.6634703000 | 2.5279450000 | -1.7114217000 |
| H | -0.2099555000 | 2.8944826000 | -0.0074984000 |
| H | 3.6954251000 | -0.3773557000 | 0.9575210000 |
| H | 3.2115142000 | -1.9554520000 | -0.9862285000 |

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|---|---------------|---------------|---------------|
| O | 1.8255497000 | 1.5261143000 | 1.3834280000 |
| O | -0.7237620000 | -1.9656257000 | 0.8490026000 |
| H | 0.1414656000 | -1.5924055000 | 0.5291914000 |
| N | 2.9659014000 | -0.2322661000 | 0.2991590000 |
| N | 1.4473160000 | -0.7107156000 | -1.2905053000 |
| C | 2.6208920000 | -1.0557254000 | -0.7509995000 |
| C | 1.8080918000 | 0.5376918000 | 0.6380915000 |
| C | 0.9436030000 | 0.3639452000 | -0.6262152000 |
| C | -0.3565369000 | 0.8689505000 | -0.4223251000 |
| C | -1.5257620000 | 0.1825421000 | 0.0361183000 |
| C | -1.7240427000 | -1.1262052000 | 0.5262625000 |
| C | -3.0343838000 | -1.6112062000 | 0.7266409000 |
| H | -3.1719561000 | -2.6233199000 | 1.0995095000 |
| C | -4.1131154000 | -0.7738807000 | 0.4672760000 |

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| H | -5.1317405000 | -1.1490782000 | 0.6304720000 |
| C | -3.9423471000 | 0.5362268000 | -0.0085510000 |
| H | -4.8083526000 | 1.1690624000 | -0.2097235000 |
| C | -2.6560499000 | 1.0141708000 | -0.2015101000 |
| C | -2.2385960000 | 2.3575797000 | -0.7350074000 |
| H | -2.5759803000 | 3.1577377000 | -0.0514008000 |
| C | -0.7099062000 | 2.2701650000 | -0.8179331000 |
| H | -0.3279139000 | 2.5041590000 | -1.8260562000 |
| H | -2.6815509000 | 2.5156764000 | -1.7384983000 |
| H | -0.2177210000 | 2.9348841000 | -0.0834498000 |
| H | 3.6999206000 | -0.4480275000 | 0.9600299000 |
| H | 3.2157421000 | -1.9015016000 | -1.0946321000 |
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| O | 1.8003997000 | 1.4078525000 | 1.5313468000 |
| O | -0.7259650000 | -1.9523329000 | 0.8483934000 |
| H | 0.1390815000 | -1.5664875000 | 0.5394479000 |
| N | 2.9663011000 | -0.2579009000 | 0.3161544000 |
| N | 1.4590266000 | -0.6512484000 | -1.3053460000 |
| C | 2.6329298000 | -1.0166402000 | -0.7947318000 |
| C | 1.8251933000 | 0.4997104000 | 0.6836863000 |
| C | 0.9486205000 | 0.3644136000 | -0.5399802000 |
| C | -0.3569300000 | 0.8702293000 | -0.4017921000 |
| C | -1.5343274000 | 0.1917447000 | 0.0417348000 |
| C | -1.7284011000 | -1.1162480000 | 0.5378968000 |
| C | -3.0382060000 | -1.6003946000 | 0.7439662000 |
| H | -3.1747076000 | -2.6086646000 | 1.1253737000 |
| C | -4.1162499000 | -0.7646941000 | 0.4792219000 |
| H | -5.1329595000 | -1.1406976000 | 0.6494491000 |
| C | -3.9503876000 | 0.5414674000 | -0.0106513000 |
| H | -4.8186181000 | 1.1691356000 | -0.2134394000 |
| C | -2.6651392000 | 1.0172224000 | -0.2140783000 |
| C | -2.2413166000 | 2.3510336000 | -0.7644378000 |
| H | -2.5731292000 | 3.1576594000 | -0.0862570000 |
| C | -0.7128828000 | 2.2566892000 | -0.8498909000 |
| H | -0.3359309000 | 2.4399142000 | -1.8698930000 |
| H | -2.6865734000 | 2.5037048000 | -1.7672519000 |
| H | -0.2142958000 | 2.9547575000 | -0.1521515000 |
| H | 3.7117950000 | -0.4833243000 | 0.9576385000 |
| H | 3.2514375000 | -1.8179534000 | -1.1960347000 |
| 70 | | | |
| O | 1.7454843000 | 1.2587725000 | 1.6757674000 |
| O | -0.7175537000 | -1.9346159000 | 0.8361716000 |

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|----|---------------|---------------|---------------|
| H | 0.1460840000 | -1.5224572000 | 0.5509689000 |
| N | 2.9597936000 | -0.2827035000 | 0.3359365000 |
| N | 1.4706935000 | -0.6035871000 | -1.3196345000 |
| C | 2.6490852000 | -0.9729895000 | -0.8344669000 |
| C | 1.8270532000 | 0.4591080000 | 0.7238455000 |
| C | 0.9422914000 | 0.3445256000 | -0.4698564000 |
| C | -0.3606179000 | 0.8654596000 | -0.4039877000 |
| C | -1.5434090000 | 0.1956556000 | 0.0324673000 |
| C | -1.7282635000 | -1.1075970000 | 0.5438106000 |
| C | -3.0384605000 | -1.5888159000 | 0.7656190000 |
| H | -3.1746991000 | -2.5973237000 | 1.1443495000 |
| C | -4.1169228000 | -0.7547109000 | 0.5005004000 |
| H | -5.1341664000 | -1.1261771000 | 0.6808913000 |
| C | -3.9565468000 | 0.5483101000 | -0.0037681000 |
| H | -4.8258262000 | 1.1719589000 | -0.2121759000 |
| C | -2.6741115000 | 1.0202506000 | -0.2222613000 |
| C | -2.2431458000 | 2.3464947000 | -0.7877096000 |
| H | -2.5591009000 | 3.1653031000 | -0.1159123000 |
| C | -0.7152310000 | 2.2418176000 | -0.8883344000 |
| H | -0.3439564000 | 2.3916557000 | -1.9159362000 |
| H | -2.6966286000 | 2.4924984000 | -1.7862785000 |
| H | -0.2082482000 | 2.9589923000 | -0.2196588000 |
| H | 3.7243092000 | -0.4994489000 | 0.9570533000 |
| H | 3.3008589000 | -1.7214291000 | -1.2790270000 |
| 80 | | | |
| O | 1.6833084000 | 1.1341905000 | 1.7709163000 |
| O | -0.7279999000 | -1.9305405000 | 0.8269379000 |
| H | 0.1367014000 | -1.4978727000 | 0.5701160000 |
| N | 2.9509965000 | -0.3033207000 | 0.3566077000 |
| N | 1.5008452000 | -0.5524980000 | -1.3444783000 |
| C | 2.6817416000 | -0.9163909000 | -0.8687794000 |
| C | 1.8247716000 | 0.4337342000 | 0.7473795000 |
| C | 0.9267101000 | 0.3011611000 | -0.4196858000 |
| C | -0.3651819000 | 0.8451568000 | -0.4129824000 |
| C | -1.5569525000 | 0.1893899000 | 0.0151122000 |
| C | -1.7407255000 | -1.1072157000 | 0.5425294000 |
| C | -3.0504178000 | -1.5792679000 | 0.7850017000 |
| H | -3.1873980000 | -2.5796489000 | 1.1843092000 |
| C | -4.1240153000 | -0.7400968000 | 0.5208276000 |
| H | -5.1401955000 | -1.1045559000 | 0.7198652000 |
| C | -3.9633312000 | 0.5581200000 | 0.0016736000 |
| H | -4.8343328000 | 1.1831878000 | -0.1910822000 |
| C | -2.6821367000 | 1.0193067000 | -0.2433416000 |

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|---|---------------|---------------|---------------|
| C | -2.2344678000 | 2.3371922000 | -0.8155860000 |
| H | -2.5423222000 | 3.1572008000 | -0.1426534000 |
| C | -0.7065047000 | 2.2215335000 | -0.9097652000 |
| H | -0.3387442000 | 2.3452829000 | -1.9412079000 |
| H | -2.6852850000 | 2.4867853000 | -1.8151583000 |
| H | -0.1941273000 | 2.9462435000 | -0.2529750000 |
| H | 3.7358103000 | -0.4915178000 | 0.9606073000 |
| H | 3.3620183000 | -1.6066117000 | -1.3558141000 |

CASSCF: S1 C4-C3-C2-N1 (degree)

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|----|---------------|---------------|---------------|
| 0 | | | |
| O | 1.7794720100 | 0.6706662300 | 1.9508065800 |
| O | -0.7446958900 | -1.9738441100 | 0.5841802000 |
| H | 0.0954368800 | -1.5231165500 | 0.4660780300 |
| N | 2.9208914700 | -0.4322362300 | 0.2483074600 |
| N | 1.4758956300 | -0.3426891600 | -1.4131063200 |
| C | 2.6326780200 | -0.7480148800 | -1.0502250500 |
| C | 1.8435301000 | 0.2588053700 | 0.8022744300 |
| C | 0.9553005300 | 0.3171533700 | -0.3004217800 |
| C | -0.3935272700 | 0.8590951400 | -0.2987054500 |
| C | -1.5779614600 | 0.1674358600 | -0.0947208400 |
| C | -1.7383470100 | -1.1801868500 | 0.2917785100 |
| C | -3.0503596100 | -1.6994804600 | 0.3589680600 |
| H | -3.1778326500 | -2.7269384700 | 0.6405575600 |
| C | -4.1273828900 | -0.8896869100 | 0.0673459700 |
| H | -5.1154483500 | -1.3087314500 | 0.1269885400 |
| C | -3.9811084300 | 0.4755722400 | -0.3152349900 |
| H | -4.8501314500 | 1.0641876100 | -0.5440450200 |
| C | -2.7204466400 | 0.9923448600 | -0.3865882100 |
| C | -2.2490377400 | 2.3718200000 | -0.7839876600 |
| H | -2.5752863900 | 3.1114003200 | -0.0608694300 |
| C | -0.7122940900 | 2.2424905300 | -0.8067367100 |
| H | -0.2879620100 | 2.3465445800 | -1.8019155200 |
| H | -2.6513231300 | 2.6633747500 | -1.7473750100 |
| H | -0.2076634400 | 2.9698668400 | -0.1790873600 |
| H | 3.7662457900 | -0.6116013300 | 0.7392527600 |
| H | 3.3042509600 | -1.3155731800 | -1.6622765000 |
| 10 | | | |
| O | -0.8049617200 | 1.9131192400 | 1.5685776800 |
| O | 4.4751922400 | 0.2155744800 | 0.3425971700 |
| H | 3.6953251400 | 0.0716444800 | 0.9259929400 |
| N | 0.2160455000 | 0.1143689600 | 2.5911247100 |
| N | 2.2155103700 | 0.1485942300 | 1.6929331800 |

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|----|---------------|---------------|---------------|
| C | 1.4497868500 | -0.4485336600 | 2.5210265800 |
| C | 0.1617125100 | 1.2043855900 | 1.7201571600 |
| C | 1.4823943100 | 1.1955779400 | 1.1322182600 |
| C | 1.9933186900 | 2.1244594300 | 0.2248558000 |
| C | 3.2182541500 | 2.1259300900 | -0.4559887700 |
| C | 4.3650660600 | 1.2576086100 | -0.4258810400 |
| C | 5.4951196800 | 1.5099854400 | -1.2770048400 |
| H | 6.3061755900 | 0.8115696500 | -1.2058436700 |
| C | 5.5445052200 | 2.6162130800 | -2.1574253200 |
| H | 6.4010939700 | 2.7771068600 | -2.7818843800 |
| C | 4.4481511600 | 3.4829703300 | -2.1798302600 |
| H | 4.4363437500 | 4.3419650000 | -2.8250152200 |
| C | 3.3145230700 | 3.2315204100 | -1.3349230100 |
| C | 2.0814829800 | 4.0840280400 | -1.2251743000 |
| H | 1.6294430900 | 4.2543288000 | -2.1977770200 |
| C | 1.1553527200 | 3.2969776500 | -0.2703799200 |
| H | 0.8046133800 | 3.9058130400 | 0.5526975500 |
| H | 2.3372044200 | 5.0621617900 | -0.8248124000 |
| H | 0.2665350800 | 2.9415388000 | -0.7781226600 |
| H | -0.5412720800 | -0.1675387000 | 3.1698208700 |
| H | 1.7258855600 | -1.3003857900 | 3.1091006100 |
| 20 | | | |
| O | -0.8256013100 | 1.8678774100 | 1.5050672000 |
| O | 4.4784099900 | 0.2267882800 | 0.3542433100 |
| H | 3.7059541500 | 0.0957330000 | 0.9512184800 |
| N | 0.2029167500 | 0.0948344400 | 2.5639512400 |
| N | 2.2323631800 | 0.1773734100 | 1.7368452400 |
| C | 1.4541214400 | -0.4352967400 | 2.5416399100 |
| C | 0.1479206000 | 1.1730880800 | 1.6780395700 |
| C | 1.4835831300 | 1.1840262400 | 1.1217794200 |
| C | 2.0151049700 | 2.1483167700 | 0.2627143000 |
| C | 3.2180647500 | 2.1284008900 | -0.4569318900 |
| C | 4.3635150000 | 1.2584865500 | -0.4277833300 |
| C | 5.4877835900 | 1.5020869600 | -1.2891193900 |
| H | 6.2978756900 | 0.8024449800 | -1.2190290300 |
| C | 5.5339773000 | 2.6038078100 | -2.1755618900 |
| H | 6.3873684800 | 2.7599696800 | -2.8056179400 |
| C | 4.4398128400 | 3.4736079800 | -2.1949419700 |
| H | 4.4260329700 | 4.3294001400 | -2.8443157800 |
| C | 3.3125125600 | 3.2312431800 | -1.3388275400 |
| C | 2.0884296200 | 4.0941373600 | -1.2118890900 |
| H | 1.6253611900 | 4.2621388500 | -2.1798247500 |
| C | 1.1734174500 | 3.3168198800 | -0.2384714900 |

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| H | 0.8142749800 | 3.9293468900 | 0.5771711300 |
| H | 2.3534119700 | 5.0727972800 | -0.8191410200 |
| H | 0.2885500200 | 2.9494775900 | -0.7470422100 |
| H | -0.5652120000 | -0.1999454300 | 3.1222207900 |
| H | 1.7328523800 | -1.2759776700 | 3.1446464100 |

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|---|---------------|---------------|---------------|
| O | 2.2576320400 | 2.1174799900 | 0.6597982000 |
| O | -0.9574937000 | -2.2336558000 | 0.3108687500 |
| H | -0.0874499600 | -1.9402944400 | -0.0087067900 |
| N | 3.1246210700 | 0.0128743600 | 0.1840488400 |
| N | 1.3268969200 | -1.0382304700 | -0.4810205800 |
| C | 2.6021453300 | -1.1512780200 | -0.2398290800 |
| C | 2.1045193400 | 0.9708354300 | 0.2747599200 |
| C | 0.9851770400 | 0.2438980200 | -0.2067687000 |
| C | -0.4179233800 | 0.7536672300 | -0.2663380100 |
| C | -1.5961189800 | 0.0934746400 | -0.0390903200 |
| C | -1.8704748700 | -1.3053052400 | 0.2859678200 |
| C | -3.1787612800 | -1.6761125100 | 0.5444190000 |
| H | -3.3663406300 | -2.7016540200 | 0.8001461700 |
| C | -4.2285380500 | -0.7642915400 | 0.4264988500 |
| H | -5.2309773300 | -1.1028755700 | 0.6113894400 |
| C | -4.0062600900 | 0.5875088700 | 0.0348755800 |
| H | -4.8409534600 | 1.2570874000 | -0.0664543400 |
| C | -2.7256511900 | 1.0039962700 | -0.1916056700 |
| C | -2.2005876800 | 2.3710502000 | -0.5625710000 |
| H | -2.4040816500 | 3.0836966000 | 0.2302831700 |
| C | -0.6798406400 | 2.1628548200 | -0.7328699000 |
| H | -0.3602108300 | 2.2568629000 | -1.7695424900 |
| H | -2.6724133900 | 2.7508872000 | -1.4620990400 |
| H | -0.0814672700 | 2.8656153700 | -0.1659300300 |
| H | 4.0652041900 | 0.1839895000 | 0.4583645100 |
| H | 3.1681141600 | -2.0531326800 | -0.3402210200 |

40

| | | | |
|---|---------------|---------------|---------------|
| O | 2.1118706700 | 1.8866113100 | 1.1195796900 |
| O | -0.8662429800 | -2.1538641900 | 0.4028815200 |
| H | -0.0411369600 | -1.8660734200 | -0.0034038300 |
| N | 3.0647927700 | -0.0733385000 | 0.2922666100 |
| N | 1.3602505600 | -0.9308778900 | -0.7915848300 |
| C | 2.5942036200 | -1.1124803700 | -0.4281010100 |
| C | 2.0327107400 | 0.8538786600 | 0.4762984700 |
| C | 0.9926504600 | 0.2877469300 | -0.3046799600 |
| C | -0.4089329400 | 0.8039251300 | -0.2925393200 |

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|----|---------------|---------------|---------------|
| C | -1.5769279000 | 0.1365159600 | -0.0154432400 |
| C | -1.8092592900 | -1.2462514700 | 0.3475844500 |
| C | -3.1073811900 | -1.6428638400 | 0.6179528400 |
| H | -3.2722413800 | -2.6645896900 | 0.9030820900 |
| C | -4.1748504100 | -0.7604665700 | 0.4766094000 |
| H | -5.1687384800 | -1.1186897400 | 0.6718661900 |
| C | -3.9896179600 | 0.5814895600 | 0.0456322400 |
| H | -4.8404639900 | 1.2257364700 | -0.0806993700 |
| C | -2.7179800400 | 1.0193248600 | -0.1887560400 |
| C | -2.2227206900 | 2.3781840300 | -0.6238198800 |
| H | -2.4002801800 | 3.1128269100 | 0.1549945700 |
| C | -0.7074677600 | 2.1738463800 | -0.8396994400 |
| H | -0.4205015500 | 2.2082627600 | -1.8901616100 |
| H | -2.7339150900 | 2.7251020700 | -1.5148736200 |
| H | -0.0985280100 | 2.9118716400 | -0.3289268400 |
| H | 3.9601303800 | 0.0035870300 | 0.7183144400 |
| H | 3.1693433100 | -1.9904655200 | -0.6360002000 |
| 50 | | | |
| O | 2.0600992000 | 1.0311471200 | 1.7678500000 |
| O | -0.6054004500 | -1.6280807300 | 1.2225203200 |
| H | 0.2146325200 | -1.1534243200 | 1.1142806400 |
| N | 2.8558840800 | -0.4987572700 | 0.2087991800 |
| N | 1.2206268600 | -0.4919391800 | -1.2714860100 |
| C | 2.3244230000 | -1.0347170600 | -0.9332337000 |
| C | 1.9647503600 | 0.4492309200 | 0.7004268300 |
| C | 1.0009070000 | 0.5411316800 | -0.3529505300 |
| C | -0.3520483100 | 1.0504559900 | -0.1013453600 |
| C | -1.5175028200 | 0.3376338800 | 0.1940869600 |
| C | -1.6209911700 | -0.9645881900 | 0.7221758000 |
| C | -2.8811934300 | -1.5873180900 | 0.7303155600 |
| H | -2.9530094900 | -2.5889011700 | 1.1086412400 |
| C | -3.9926047700 | -0.9017665500 | 0.2790171700 |
| H | -4.9470732200 | -1.3953593100 | 0.3001926600 |
| C | -3.9134895500 | 0.4286856800 | -0.2141037800 |
| H | -4.7979023000 | 0.9232289900 | -0.5710152900 |
| C | -2.6934510900 | 1.0445942500 | -0.2326277000 |
| C | -2.2974697800 | 2.4064431000 | -0.7400628800 |
| H | -2.5794131800 | 3.1728867500 | -0.0248879400 |
| C | -0.7669373400 | 2.2964605800 | -0.8546022100 |
| H | -0.4267249500 | 2.1773108200 | -1.8825377400 |
| H | -2.7791597600 | 2.6466315000 | -1.6803868100 |
| H | -0.2344719300 | 3.1525803300 | -0.4553281500 |
| H | 3.6728840500 | -0.7967823300 | 0.6902295600 |

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|----|---------------|---------------|---------------|
| H | 2.7734013700 | -1.8678391900 | -1.4355936200 |
| 60 | | | |
| O | 1.7963624500 | 0.4245497100 | 1.9066720800 |
| O | -0.6561746000 | -1.9424364900 | 0.4404967200 |
| H | 0.1616007600 | -1.4513769100 | 0.4980862500 |
| N | 2.8285177300 | -0.5920543300 | 0.0862111900 |
| N | 1.3847860900 | -0.1845312500 | -1.5279251600 |
| C | 2.4678508600 | -0.7835317200 | -1.2207171700 |
| C | 1.8435328200 | 0.1671754900 | 0.7122141900 |
| C | 1.0047358600 | 0.5233233400 | -0.3804241200 |
| C | -0.3748990900 | 0.9692087800 | -0.2124334600 |
| C | -1.5379457000 | 0.2046210800 | -0.1607545700 |
| C | -1.6484674200 | -1.1838853900 | 0.0570870000 |
| C | -2.9052669300 | -1.7941151800 | -0.1399360800 |
| H | -2.9844821000 | -2.8543989000 | 0.0036845400 |
| C | -3.9955286200 | -1.0261913300 | -0.4902565300 |
| H | -4.9438468300 | -1.5124133700 | -0.6299115700 |
| C | -3.9087611500 | 0.3825457400 | -0.6795342600 |
| H | -4.7801738700 | 0.9397210800 | -0.9695305600 |
| C | -2.6986696300 | 0.9867464300 | -0.4972134100 |
| C | -2.2911557000 | 2.4276296500 | -0.6725710500 |
| H | -2.6534697300 | 3.0264826100 | 0.1568291900 |
| C | -0.7535438300 | 2.3569486000 | -0.6750096700 |
| H | -0.3224421400 | 2.4944402600 | -1.6648979600 |
| H | -2.6968134700 | 2.8539931100 | -1.5822543200 |
| H | -0.2786694800 | 3.0887247200 | -0.0309207400 |
| H | 3.6058518000 | -0.9892160800 | 0.5615417800 |
| H | 3.0234016500 | -1.4203745000 | -1.8793153500 |
| 70 | | | |
| O | 1.7798208000 | 0.5275763200 | 1.9492220300 |
| O | -0.6764071400 | -1.9398512100 | 0.5016167000 |
| H | 0.1526978900 | -1.4591394300 | 0.4608774200 |
| N | 2.8606256000 | -0.5333138700 | 0.1802368700 |
| N | 1.4285290800 | -0.2531184500 | -1.4690805400 |
| C | 2.5402719600 | -0.7790790000 | -1.1271541300 |
| C | 1.8344078000 | 0.2044050700 | 0.7696683900 |
| C | 0.9838007000 | 0.4392806700 | -0.3378926400 |
| C | -0.3832130600 | 0.9337737000 | -0.2584779600 |
| C | -1.5521636900 | 0.1991113400 | -0.1251761600 |
| C | -1.6768914000 | -1.1752843900 | 0.1703637300 |
| C | -2.9642368500 | -1.7571757500 | 0.1026596800 |
| H | -3.0607293400 | -2.8050121400 | 0.3116926400 |

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|----|---------------|---------------|---------------|
| C | -4.0540158300 | -0.9771385700 | -0.2140958500 |
| H | -5.0225164200 | -1.4414816900 | -0.2556404000 |
| C | -3.9472321400 | 0.4171882900 | -0.4976229200 |
| H | -4.8247653200 | 0.9794682700 | -0.7575477900 |
| C | -2.7131415200 | 0.9932261200 | -0.4395129500 |
| C | -2.2781343800 | 2.4106510400 | -0.7223653400 |
| H | -2.6136438800 | 3.0744929800 | 0.0674812100 |
| C | -0.7406668300 | 2.3135936400 | -0.7528108400 |
| H | -0.3252140900 | 2.4198868400 | -1.7523850900 |
| H | -2.6939618100 | 2.7782591400 | -1.6529602300 |
| H | -0.2423201700 | 3.0510341700 | -0.1331986100 |
| H | 3.6630979500 | -0.8487632700 | 0.6744012600 |
| H | 3.1502675400 | -1.3912893000 | -1.7603451500 |
| 80 | | | |
| O | 1.7794720100 | 0.6706662300 | 1.9508065800 |
| O | -0.7446958900 | -1.9738441100 | 0.5841802000 |
| H | 0.0954368800 | -1.5231165500 | 0.4660780300 |
| N | 2.9208914700 | -0.4322362300 | 0.2483074600 |
| N | 1.4758956300 | -0.3426891600 | -1.4131063200 |
| C | 2.6326780200 | -0.7480148800 | -1.0502250500 |
| C | 1.8435301000 | 0.2588053700 | 0.8022744300 |
| C | 0.9553005300 | 0.3171533700 | -0.3004217800 |
| C | -0.3935272700 | 0.8590951400 | -0.2987054500 |
| C | -1.5779614600 | 0.1674358600 | -0.0947208400 |
| C | -1.7383470100 | -1.1801868500 | 0.2917785100 |
| C | -3.0503596100 | -1.6994804600 | 0.3589680600 |
| H | -3.1778326500 | -2.7269384700 | 0.6405575600 |
| C | -4.1273828900 | -0.8896869100 | 0.0673459700 |
| H | -5.1154483500 | -1.3087314500 | 0.1269885400 |
| C | -3.9811084300 | 0.4755722400 | -0.3152349900 |
| H | -4.8501314500 | 1.0641876100 | -0.5440450200 |
| C | -2.7204466400 | 0.9923448600 | -0.3865882100 |
| C | -2.2490377400 | 2.3718200000 | -0.7839876600 |
| H | -2.5752863900 | 3.1114003200 | -0.0608694300 |
| C | -0.7122940900 | 2.2424905300 | -0.8067367100 |
| H | -0.2879620100 | 2.3465445800 | -1.8019155200 |
| H | -2.6513231300 | 2.6633747500 | -1.7473750100 |
| H | -0.2076634400 | 2.9698668400 | -0.1790873600 |
| H | 3.7662457900 | -0.6116013300 | 0.7392527600 |
| H | 3.3042509600 | -1.3155731800 | -1.6622765000 |

CASSCF: S1 NEB path S1-KETO_S0S1-KETO-1

coord_1

| | | | |
|---|---------------|---------------|---------------|
| O | 2.2733656000 | 2.2611816000 | -0.0319370000 |
| O | -1.0530033000 | -2.3075506000 | -0.2656351000 |
| H | 0.5939342000 | -1.7959335000 | 0.0086090000 |
| N | 3.1106579000 | 0.1300590000 | 0.0865080000 |
| N | 1.2778734000 | -1.0477413000 | 0.0774380000 |
| C | 2.6091397000 | -1.1466403000 | 0.1150460000 |
| C | 2.1138616000 | 1.0735303000 | 0.0143210000 |
| C | 0.8709612000 | 0.2701971000 | -0.0006480000 |
| C | -0.4068551000 | 0.7425882000 | -0.0675280000 |
| C | -1.6782865000 | -0.0171310000 | -0.0701900000 |
| C | -1.9290245000 | -1.4461154000 | -0.1371500000 |
| C | -3.3168199000 | -1.8093445000 | -0.0630540000 |
| H | -3.5310130000 | -2.8586838000 | -0.1090740000 |
| C | -4.3808822000 | -0.8604912000 | 0.0405110000 |
| H | -5.3929115000 | -1.2211673000 | 0.0840730000 |
| C | -4.1128932000 | 0.4747631000 | 0.0771200000 |
| H | -4.8857664000 | 1.2146643000 | 0.1450590000 |
| C | -2.7209638000 | 0.8775842000 | 0.0193400000 |
| C | -2.2562796000 | 2.3055996000 | 0.0655350000 |
| H | -2.5232277000 | 2.7513868000 | 1.0205593000 |
| C | -0.7318392000 | 2.2261486000 | -0.1277080000 |
| H | -0.4367741000 | 2.6393657000 | -1.0864163000 |
| H | -2.7477338000 | 2.8996508000 | -0.6996062000 |
| H | -0.1901751000 | 2.7856578000 | 0.6222462000 |
| H | 4.0744851000 | 0.3788131000 | 0.1070010000 |
| H | 3.1804869000 | -2.0447486000 | 0.1752990000 |

coord_2

| | | | |
|---|---------------|---------------|---------------|
| O | 2.3011163000 | 2.2474228000 | -0.0701535000 |
| O | -1.0293119000 | -2.2679411000 | -0.3732095000 |
| H | 0.5595515000 | -1.7761491000 | -0.0022400000 |
| N | 3.1004432000 | 0.1075211000 | 0.1006119000 |
| N | 1.2349762000 | -1.0370447000 | 0.1283550000 |
| C | 2.5794125000 | -1.1674105000 | 0.1904012000 |
| C | 2.1253747000 | 1.0598296000 | 0.0036192000 |
| C | 0.8632156000 | 0.2785398000 | 0.0010028000 |
| C | -0.4070395000 | 0.7698471000 | -0.0991133000 |
| C | -1.6718114000 | 0.0076713000 | -0.0948428000 |
| C | -1.9003419000 | -1.4266300000 | -0.1928912000 |
| C | -3.2901711000 | -1.8126274000 | -0.0845851000 |
| H | -3.4894626000 | -2.8638744000 | -0.1499288000 |
| C | -4.3558180000 | -0.8718081000 | 0.0612276000 |
| H | -5.3614426000 | -1.2494154000 | 0.1213159000 |
| C | -4.1022422000 | 0.4490969000 | 0.1114702000 |

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|---|---------------|---------------|---------------|
| H | -4.8859584000 | 1.1855794000 | 0.2072357000 |
| C | -2.7189137000 | 0.8826877000 | 0.0298282000 |
| C | -2.2611552000 | 2.3158502000 | 0.0846866000 |
| H | -2.4878307000 | 2.7416364000 | 1.0585875000 |
| C | -0.7417781000 | 2.2476803000 | -0.1710104000 |
| H | -0.4973742000 | 2.6433149000 | -1.1509101000 |
| H | -2.7836236000 | 2.9219001000 | -0.6491896000 |
| H | -0.1738187000 | 2.8259578000 | 0.5440496000 |
| H | 4.0687667000 | 0.3311763000 | 0.1430025000 |
| H | 3.1355539000 | -2.0671684000 | 0.2523993000 |

coord_3

| | | | |
|---|---------------|---------------|---------------|
| O | 2.3263146000 | 2.2315631000 | -0.1051149000 |
| O | -1.0055181000 | -2.2302223000 | -0.4820315000 |
| H | 0.5274924000 | -1.7586184000 | -0.0147958000 |
| N | 3.0892625000 | 0.0823602000 | 0.1160967000 |
| N | 1.1988078000 | -1.0289498000 | 0.1777790000 |
| C | 2.5429808000 | -1.1784939000 | 0.2660414000 |
| C | 2.1328646000 | 1.0490041000 | -0.0054780000 |
| C | 0.8546048000 | 0.2901584000 | 0.0016885000 |
| C | -0.4059325000 | 0.7934610000 | -0.1306644000 |
| C | -1.6648052000 | 0.0268007000 | -0.1195987000 |
| C | -1.8800188000 | -1.4066297000 | -0.2469447000 |
| C | -3.2609629000 | -1.8149574000 | -0.1056824000 |
| H | -3.4499557000 | -2.8672945000 | -0.1898988000 |
| C | -4.3298125000 | -0.8900009000 | 0.0820103000 |
| H | -5.3294995000 | -1.2768171000 | 0.1593587000 |
| C | -4.0899044000 | 0.4346934000 | 0.1465655000 |
| H | -4.8823730000 | 1.1566521000 | 0.2697929000 |
| C | -2.7165330000 | 0.8887345000 | 0.0407435000 |
| C | -2.2625103000 | 2.3245822000 | 0.1030768000 |
| H | -2.4476842000 | 2.7315704000 | 1.0935710000 |
| C | -0.7521985000 | 2.2669082000 | -0.2151360000 |
| H | -0.5581855000 | 2.6431836000 | -1.2139844000 |
| H | -2.8150561000 | 2.9422064000 | -0.5979795000 |
| H | -0.1587612000 | 2.8639115000 | 0.4629583000 |
| H | 4.0599684000 | 0.2886032000 | 0.1814139000 |
| H | 3.0877321000 | -2.0867665000 | 0.3259316000 |

coord_4

| | | | |
|---|---------------|---------------|---------------|
| O | 2.3462770000 | 2.2129468000 | -0.1363522000 |
| O | -1.0292993000 | -2.2131797000 | -0.6106462000 |
| H | 0.5245061000 | -1.7335210000 | -0.0193598000 |
| N | 3.0808250000 | 0.0616501000 | 0.1350235000 |

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|---|---------------|---------------|---------------|
| N | 1.1762685000 | -1.0186260000 | 0.2404181000 |
| C | 2.5156533000 | -1.1806903000 | 0.3576568000 |
| C | 2.1415910000 | 1.0378866000 | -0.0144377000 |
| C | 0.8509529000 | 0.2987463000 | -0.0024576000 |
| C | -0.3922546000 | 0.8138375000 | -0.1649238000 |
| C | -1.6500962000 | 0.0494395000 | -0.1367240000 |
| C | -1.8763262000 | -1.3788355000 | -0.3023249000 |
| C | -3.2403248000 | -1.8128226000 | -0.1246415000 |
| H | -3.4163715000 | -2.8701790000 | -0.2278251000 |
| C | -4.3090551000 | -0.9095688000 | 0.1026386000 |
| H | -5.2991399000 | -1.3024099000 | 0.1983791000 |
| C | -4.0734269000 | 0.4157268000 | 0.1800742000 |
| H | -4.8692991000 | 1.1192823000 | 0.3323077000 |
| C | -2.7102969000 | 0.8949286000 | 0.0487244000 |
| C | -2.2626023000 | 2.3329016000 | 0.1209957000 |
| H | -2.4032825000 | 2.7207855000 | 1.1274343000 |
| C | -0.7624191000 | 2.2833092000 | -0.2624371000 |
| H | -0.6208020000 | 2.6416102000 | -1.2765882000 |
| H | -2.8425848000 | 2.9625715000 | -0.5454554000 |
| H | -0.1479652000 | 2.8985025000 | 0.3766655000 |
| H | 4.0453944000 | 0.2596710000 | 0.2223533000 |
| H | 3.0343953000 | -2.1083204000 | 0.3812210000 |

coord_5

| | | | |
|---|---------------|---------------|---------------|
| O | 2.3660037000 | 2.1963432000 | -0.1644136000 |
| O | -1.0143734000 | -2.1725722000 | -0.7203911000 |
| H | 0.5042292000 | -1.7180119000 | -0.0344824000 |
| N | 3.0671621000 | 0.0392559000 | 0.1514710000 |
| N | 1.1379440000 | -1.0109038000 | 0.2879278000 |
| C | 2.4775210000 | -1.1827151000 | 0.4385236000 |
| C | 2.1447671000 | 1.0277907000 | -0.0207528000 |
| C | 0.8414222000 | 0.3090048000 | -0.0029909000 |
| C | -0.3907367000 | 0.8315278000 | -0.1964880000 |
| C | -1.6452890000 | 0.0643334000 | -0.1596499000 |
| C | -1.8613826000 | -1.3614661000 | -0.3548808000 |
| C | -3.2128991000 | -1.8150953000 | -0.1451793000 |
| H | -3.3823387000 | -2.8715299000 | -0.2658567000 |
| C | -4.2805150000 | -0.9258559000 | 0.1232998000 |
| H | -5.2651743000 | -1.3281657000 | 0.2367454000 |
| C | -4.0568398000 | 0.4028138000 | 0.2146847000 |
| H | -4.8594847000 | 1.0927629000 | 0.3948286000 |
| C | -2.7046812000 | 0.9008124000 | 0.0594290000 |
| C | -2.2579042000 | 2.3399399000 | 0.1380050000 |
| H | -2.3544385000 | 2.7102698000 | 1.1560879000 |

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|---|---------------|---------------|---------------|
| C | -0.7729836000 | 2.2972168000 | -0.3070931000 |
| H | -0.6813748000 | 2.6332523000 | -1.3348954000 |
| H | -2.8642193000 | 2.9798434000 | -0.4935350000 |
| H | -0.1365903000 | 2.9304265000 | 0.2916315000 |
| H | 4.0309470000 | 0.2274814000 | 0.2636509000 |
| H | 2.9815457000 | -2.1211163000 | 0.4440427000 |

coord_6

| | | | |
|---|---------------|---------------|---------------|
| O | 2.3830909000 | 2.1793549000 | -0.1894143000 |
| O | -0.9995727000 | -2.1286682000 | -0.8252299000 |
| H | 0.4884389000 | -1.7039727000 | -0.0522639000 |
| N | 3.0516779000 | 0.0174112000 | 0.1694737000 |
| N | 1.0980912000 | -1.0032690000 | 0.3312785000 |
| C | 2.4372637000 | -1.1817315000 | 0.5150854000 |
| C | 2.1453278000 | 1.0176236000 | -0.0255768000 |
| C | 0.8308707000 | 0.3190843000 | -0.0028857000 |
| C | -0.3902735000 | 0.8474523000 | -0.2278095000 |
| C | -1.6416489000 | 0.0777141000 | -0.1825385000 |
| C | -1.8477485000 | -1.3444065000 | -0.4072035000 |
| C | -3.1860557000 | -1.8170465000 | -0.1664914000 |
| H | -3.3510335000 | -2.8719304000 | -0.3036890000 |
| C | -4.2509097000 | -0.9414528000 | 0.1438591000 |
| H | -5.2301599000 | -1.3527708000 | 0.2751345000 |
| C | -4.0385069000 | 0.3903464000 | 0.2494910000 |
| H | -4.8466635000 | 1.0666143000 | 0.4576708000 |
| C | -2.6980732000 | 0.9060602000 | 0.0705933000 |
| C | -2.2503246000 | 2.3458648000 | 0.1545422000 |
| H | -2.3010613000 | 2.6993571000 | 1.1817187000 |
| C | -0.7835492000 | 2.3089623000 | -0.3518456000 |
| H | -0.7421303000 | 2.6207976000 | -1.3908231000 |
| H | -2.8809404000 | 2.9957178000 | -0.4411061000 |
| H | -0.1267734000 | 2.9597414000 | 0.2046586000 |
| H | 4.0139547000 | 0.1992053000 | 0.3061724000 |
| H | 2.9270264000 | -2.1304164000 | 0.5069182000 |

coord_7

| | | | |
|---|---------------|---------------|---------------|
| O | 2.3975635000 | 2.1621975000 | -0.2115209000 |
| O | -0.9847371000 | -2.0823854000 | -0.9243897000 |
| H | 0.4766879000 | -1.6910947000 | -0.0714280000 |
| N | 3.0340639000 | -0.0035019000 | 0.1901527000 |
| N | 1.0577077000 | -0.9954446000 | 0.3687963000 |
| C | 2.3951179000 | -1.1784635000 | 0.5849093000 |
| C | 2.1431626000 | 1.0075034000 | -0.0288027000 |
| C | 0.8193394000 | 0.3292394000 | -0.0018951000 |

| | | | |
|---|---------------|---------------|---------------|
| C | -0.3909371000 | 0.8614736000 | -0.2588011000 |
| C | -1.6392421000 | 0.0894647000 | -0.2055278000 |
| C | -1.8353153000 | -1.3277128000 | -0.4595590000 |
| C | -3.1599485000 | -1.8184066000 | -0.1888225000 |
| H | -3.3223955000 | -2.8712868000 | -0.3416781000 |
| C | -4.2203904000 | -0.9562399000 | 0.1642348000 |
| H | -5.1942006000 | -1.3762288000 | 0.3134557000 |
| C | -4.0186275000 | 0.3784891000 | 0.2846655000 |
| H | -4.8310037000 | 1.0408901000 | 0.5209744000 |
| C | -2.6905218000 | 0.9104737000 | 0.0823653000 |
| C | -2.2397909000 | 2.3506088000 | 0.1706703000 |
| H | -2.2430550000 | 2.6879141000 | 1.2043280000 |
| C | -0.7940794000 | 2.3184655000 | -0.3966541000 |
| H | -0.8030802000 | 2.6041792000 | -1.4442750000 |
| H | -2.8926400000 | 3.0103700000 | -0.3880034000 |
| H | -0.1184643000 | 2.9863821000 | 0.1156498000 |
| H | 3.9944281000 | 0.1747028000 | 0.3498061000 |
| H | 2.8706752000 | -2.1359462000 | 0.5710682000 |

coord_8

| | | | |
|---|---------------|---------------|---------------|
| O | 2.4094654000 | 2.1448620000 | -0.2310631000 |
| O | -0.9698976000 | -2.0338602000 | -1.0190488000 |
| H | 0.4681927000 | -1.6789435000 | -0.0907449000 |
| N | 3.0136965000 | -0.0228252000 | 0.2145888000 |
| N | 1.0167455000 | -0.9870226000 | 0.3993517000 |
| C | 2.3511609000 | -1.1737479000 | 0.6472438000 |
| C | 2.1382334000 | 0.9975459000 | -0.0303208000 |
| C | 0.8062699000 | 0.3399408000 | 0.0002815000 |
| C | -0.3927360000 | 0.8734465000 | -0.2897482000 |
| C | -1.6381559000 | 0.0996593000 | -0.2290496000 |
| C | -1.8236206000 | -1.3113858000 | -0.5130595000 |
| C | -3.1346860000 | -1.8189395000 | -0.2124781000 |
| H | -3.2960734000 | -2.8692840000 | -0.3807417000 |
| C | -4.1884334000 | -0.9704713000 | 0.1845603000 |
| H | -5.1568199000 | -1.3987987000 | 0.3520931000 |
| C | -3.9968510000 | 0.3673207000 | 0.3209094000 |
| H | -4.8123280000 | 1.0153143000 | 0.5857744000 |
| C | -2.6819230000 | 0.9138282000 | 0.0951697000 |
| C | -2.2259141000 | 2.3540514000 | 0.1866818000 |
| H | -2.1792317000 | 2.6756114000 | 1.2240832000 |
| C | -0.8046704000 | 2.3255790000 | -0.4421393000 |
| H | -0.8650675000 | 2.5828076000 | -1.4957939000 |
| H | -2.8990257000 | 3.0240964000 | -0.3332859000 |
| H | -0.1115126000 | 3.0104706000 | 0.0231371000 |

| | | | |
|---|--------------|---------------|--------------|
| H | 3.9720194000 | 0.1537648000 | 0.3951484000 |
| H | 2.8114800000 | -2.1373772000 | 0.6381696000 |

coord_9

| | | | |
|---|---------------|---------------|---------------|
| O | 2.4190766000 | 2.1315386000 | -0.2481036000 |
| O | -0.9239383000 | -1.9696280000 | -1.0992011000 |
| H | 0.4458834000 | -1.6788282000 | -0.1282024000 |
| N | 2.9914014000 | -0.0399883000 | 0.2251043000 |
| N | 0.9515894000 | -0.9864036000 | 0.4299776000 |
| C | 2.2937811000 | -1.1667943000 | 0.6878506000 |
| C | 2.1306766000 | 0.9923093000 | -0.0285504000 |
| C | 0.7888720000 | 0.3501843000 | 0.0119370000 |
| C | -0.4015629000 | 0.8900495000 | -0.3147491000 |
| C | -1.6361511000 | 0.1068960000 | -0.2622578000 |
| C | -1.8020658000 | -1.2986856000 | -0.5613343000 |
| C | -3.1045377000 | -1.8209485000 | -0.2317500000 |
| H | -3.2696863000 | -2.8637760000 | -0.4225022000 |
| C | -4.1547832000 | -0.9839932000 | 0.2058909000 |
| H | -5.1214506000 | -1.4187701000 | 0.3887165000 |
| C | -3.9773002000 | 0.3594350000 | 0.3604318000 |
| H | -4.7978526000 | 0.9947139000 | 0.6488499000 |
| C | -2.6734296000 | 0.9117135000 | 0.1161696000 |
| C | -2.2046598000 | 2.3521440000 | 0.2022783000 |
| H | -2.1113032000 | 2.6636255000 | 1.2391918000 |
| C | -0.8097039000 | 2.3303181000 | -0.4874858000 |
| H | -0.9256018000 | 2.5551071000 | -1.5443238000 |
| H | -2.8974881000 | 3.0316871000 | -0.2793846000 |
| H | -0.1030418000 | 3.0319610000 | -0.0696796000 |
| H | 3.9477817000 | 0.1329448000 | 0.4393807000 |
| H | 2.7558112000 | -2.1311691000 | 0.7214648000 |

coord_10

| | | | |
|---|---------------|---------------|---------------|
| O | 2.4241029000 | 2.1176258000 | -0.2610846000 |
| O | -0.8994729000 | -1.9298034000 | -1.1986811000 |
| H | 0.4447953000 | -1.6780605000 | -0.1561706000 |
| N | 2.9736100000 | -0.0520309000 | 0.2395196000 |
| N | 0.9026854000 | -0.9889336000 | 0.4749668000 |
| C | 2.2464807000 | -1.1525731000 | 0.7394455000 |
| C | 2.1222706000 | 0.9870150000 | -0.0269475000 |
| C | 0.7662746000 | 0.3690876000 | 0.0135970000 |
| C | -0.3819265000 | 0.9013636000 | -0.3350799000 |
| C | -1.6469422000 | 0.1087258000 | -0.2865069000 |
| C | -1.8153678000 | -1.2760371000 | -0.5976844000 |
| C | -3.0669091000 | -1.8210102000 | -0.2549053000 |

| | | | |
|---|---------------|---------------|---------------|
| H | -3.2510744000 | -2.8589347000 | -0.4609305000 |
| C | -4.1320392000 | -0.9837519000 | 0.2285409000 |
| H | -5.0876051000 | -1.4364528000 | 0.4228259000 |
| C | -3.9624541000 | 0.3412040000 | 0.3958758000 |
| H | -4.7760000000 | 0.9708690000 | 0.7075541000 |
| C | -2.6512346000 | 0.9088230000 | 0.1305419000 |
| C | -2.1842760000 | 2.3504345000 | 0.2174007000 |
| H | -2.0437634000 | 2.6514720000 | 1.2518866000 |
| C | -0.8142807000 | 2.3296871000 | -0.5324780000 |
| H | -0.9832334000 | 2.5267373000 | -1.5874806000 |
| H | -2.8918983000 | 3.0415891000 | -0.2277781000 |
| H | -0.0992115000 | 3.0467963000 | -0.1597647000 |
| H | 3.9224538000 | 0.1250797000 | 0.4817912000 |
| H | 2.6953325000 | -2.1232788000 | 0.7812652000 |

OM2/MRCI: S1 NEB path S1-KETO_S0S1-KETO-1

coord_1

| | | | |
|---|---------------|---------------|---------------|
| O | 2.3363435000 | 2.2994522000 | 0.0065400000 |
| O | -0.9850551000 | -2.2733956000 | -0.0026551000 |
| H | 0.5195354000 | -1.8076742000 | -0.0038098000 |
| N | 3.1394349000 | 0.0990812000 | -0.0009081000 |
| N | 1.2251662000 | -1.0375469000 | -0.0027905000 |
| C | 2.5804674000 | -1.1645098000 | -0.0044148000 |
| C | 2.1323717000 | 1.0816520000 | 0.0029737000 |
| C | 0.8609429000 | 0.3024793000 | 0.0018068000 |
| C | -0.4162477000 | 0.8041576000 | 0.0046493000 |
| C | -1.6603436000 | 0.0250694000 | 0.0033544000 |
| C | -1.9020099000 | -1.4055274000 | -0.0002477000 |
| C | -3.2838120000 | -1.8271956000 | -0.0009014000 |
| H | -3.4862958000 | -2.9009473000 | -0.0036363000 |
| C | -4.3340255000 | -0.9010177000 | 0.0020471000 |
| H | -5.3693357000 | -1.2597820000 | 0.0014842000 |
| C | -4.0793839000 | 0.4672392000 | 0.0057024000 |
| H | -4.8927811000 | 1.1979089000 | 0.0081445000 |
| C | -2.7239417000 | 0.9126926000 | 0.0062671000 |
| C | -2.2768921000 | 2.3456434000 | 0.0099776000 |
| H | -2.6620658000 | 2.8571564000 | 0.9153537000 |
| C | -0.7394464000 | 2.2717246000 | 0.0093259000 |
| H | -0.3146998000 | 2.7530507000 | -0.8920667000 |
| H | -2.6625635000 | 2.8619595000 | -0.8924601000 |
| H | -0.3142480000 | 2.7473793000 | 0.9135202000 |
| H | 4.1268267000 | 0.2870011000 | -0.0013452000 |
| H | 3.1288727000 | -2.0995441000 | -0.0075965000 |

coord_2

| | | | |
|---|---------------|---------------|---------------|
| O | 2.3327761000 | 2.2978148000 | 0.0259911000 |
| O | -0.9670895000 | -2.2539850000 | -0.1306341000 |
| H | 0.4937150000 | -1.8029615000 | -0.0283049000 |
| N | 3.1191329000 | 0.0951516000 | 0.0267820000 |
| N | 1.2017666000 | -1.0368664000 | 0.0542513000 |
| C | 2.5455438000 | -1.1783302000 | 0.0596967000 |
| C | 2.1252591000 | 1.0786210000 | 0.0243557000 |
| C | 0.8496798000 | 0.3133985000 | 0.0176481000 |
| C | -0.4172129000 | 0.8153095000 | -0.0512439000 |
| C | -1.6599880000 | 0.0338557000 | -0.0532411000 |
| C | -1.8833252000 | -1.3929019000 | -0.0703092000 |
| C | -3.2630348000 | -1.8308259000 | -0.0224025000 |
| H | -3.4555386000 | -2.9053200000 | -0.0301805000 |
| C | -4.3105159000 | -0.9087499000 | 0.0345026000 |
| H | -5.3387604000 | -1.2780601000 | 0.0711498000 |
| C | -4.0712510000 | 0.4633873000 | 0.0435297000 |
| H | -4.8852943000 | 1.1822318000 | 0.0628170000 |
| C | -2.7149414000 | 0.9122304000 | 0.0109656000 |
| C | -2.2708392000 | 2.3457332000 | 0.0290260000 |
| H | -2.5941415000 | 2.8379908000 | 0.9660678000 |
| C | -0.7447727000 | 2.2700134000 | -0.0544926000 |
| H | -0.3737676000 | 2.7447290000 | -0.9873042000 |
| H | -2.6914672000 | 2.8914226000 | -0.8293405000 |
| H | -0.2745208000 | 2.7841567000 | 0.8078410000 |
| H | 4.1088921000 | 0.2687021000 | 0.0585752000 |
| H | 3.0865093000 | -2.1102406000 | 0.0425688000 |

coord_3

| | | | |
|---|---------------|---------------|---------------|
| O | 2.3335672000 | 2.2999810000 | 0.0453381000 |
| O | -0.9538276000 | -2.2543169000 | -0.2729638000 |
| H | 0.4659747000 | -1.7992182000 | -0.0492856000 |
| N | 3.1072360000 | 0.0843383000 | 0.0596550000 |
| N | 1.1779914000 | -1.0370427000 | 0.1137250000 |
| C | 2.5262852000 | -1.1824048000 | 0.1259495000 |
| C | 2.1231618000 | 1.0805877000 | 0.0464887000 |
| C | 0.8448052000 | 0.3140838000 | 0.0298828000 |
| C | -0.4159471000 | 0.8241806000 | -0.1023283000 |
| C | -1.6559639000 | 0.0394957000 | -0.1005625000 |
| C | -1.8661938000 | -1.3932985000 | -0.1451504000 |
| C | -3.2396710000 | -1.8325663000 | -0.0302138000 |
| H | -3.4241752000 | -2.9111541000 | -0.0593350000 |
| C | -4.2932331000 | -0.9184997000 | 0.0670283000 |
| H | -5.3178935000 | -1.2942566000 | 0.1350832000 |

| | | | |
|---|---------------|---------------|---------------|
| C | -4.0643564000 | 0.4580189000 | 0.0765040000 |
| H | -4.8876091000 | 1.1741708000 | 0.1305656000 |
| C | -2.7163737000 | 0.9158413000 | 0.0087226000 |
| C | -2.2706214000 | 2.3535379000 | 0.0455889000 |
| H | -2.5336538000 | 2.8173487000 | 1.0230569000 |
| C | -0.7464239000 | 2.2853967000 | -0.1227354000 |
| H | -0.4334199000 | 2.7350507000 | -1.0861174000 |
| H | -2.7401103000 | 2.9342573000 | -0.7737868000 |
| H | -0.2222785000 | 2.8185346000 | 0.7033460000 |
| H | 4.0966667000 | 0.2519640000 | 0.1174261000 |
| H | 3.0528774000 | -2.1275234000 | 0.0924334000 |

coord_4

| | | | |
|---|---------------|---------------|---------------|
| O | 2.3277454000 | 2.2955723000 | 0.0624873000 |
| O | -0.9366990000 | -2.2261102000 | -0.4025450000 |
| H | 0.4466859000 | -1.7911254000 | -0.0773087000 |
| N | 3.0866523000 | 0.0716749000 | 0.0845869000 |
| N | 1.1461781000 | -1.0317977000 | 0.1809230000 |
| C | 2.4937031000 | -1.1879785000 | 0.1939006000 |
| C | 2.1139103000 | 1.0772936000 | 0.0683418000 |
| C | 0.8299130000 | 0.3220439000 | 0.0466886000 |
| C | -0.4136680000 | 0.8326230000 | -0.1668816000 |
| C | -1.6543709000 | 0.0490855000 | -0.1580595000 |
| C | -1.8528877000 | -1.3814167000 | -0.2134211000 |
| C | -3.2190800000 | -1.8356619000 | -0.0540548000 |
| H | -3.3942827000 | -2.9163354000 | -0.0838075000 |
| C | -4.2653342000 | -0.9271178000 | 0.0983618000 |
| H | -5.2843878000 | -1.3134200000 | 0.2044465000 |
| C | -4.0502040000 | 0.4517184000 | 0.1163396000 |
| H | -4.8782031000 | 1.1588854000 | 0.1823692000 |
| C | -2.7096895000 | 0.9183320000 | 0.0145710000 |
| C | -2.2613502000 | 2.3531635000 | 0.0689283000 |
| H | -2.4608563000 | 2.7967442000 | 1.0718071000 |
| C | -0.7484765000 | 2.2881393000 | -0.1825115000 |
| H | -0.4958964000 | 2.7223670000 | -1.1784417000 |
| H | -2.7627924000 | 2.9598061000 | -0.7071813000 |
| H | -0.1913724000 | 2.8538227000 | 0.5965065000 |
| H | 4.0732351000 | 0.2335270000 | 0.1759500000 |
| H | 3.0083413000 | -2.1373285000 | 0.1363194000 |

coord_5

| | | | |
|---|---------------|---------------|---------------|
| O | 2.3268227000 | 2.2890368000 | 0.0798412000 |
| O | -0.9320551000 | -2.2059239000 | -0.5431077000 |
| H | 0.4358308000 | -1.7773652000 | -0.0958055000 |

| | | | |
|---|---------------|---------------|---------------|
| N | 3.0738443000 | 0.0633030000 | 0.1163584000 |
| N | 1.1147910000 | -1.0330720000 | 0.2345627000 |
| C | 2.4681726000 | -1.1920368000 | 0.2677573000 |
| C | 2.1117300000 | 1.0715420000 | 0.0904771000 |
| C | 0.8148957000 | 0.3223493000 | 0.0583804000 |
| C | -0.4123194000 | 0.8470740000 | -0.2094859000 |
| C | -1.6513844000 | 0.0577077000 | -0.2023757000 |
| C | -1.8442823000 | -1.3749387000 | -0.2834388000 |
| C | -3.1959713000 | -1.8390455000 | -0.0630007000 |
| H | -3.3667206000 | -2.9173427000 | -0.1107288000 |
| C | -4.2445004000 | -0.9400897000 | 0.1280971000 |
| H | -5.2573854000 | -1.3300862000 | 0.2643311000 |
| C | -4.0367303000 | 0.4420547000 | 0.1468506000 |
| H | -4.8704289000 | 1.1444699000 | 0.2524761000 |
| C | -2.7065585000 | 0.9271428000 | 0.0122382000 |
| C | -2.2540557000 | 2.3626725000 | 0.0823568000 |
| H | -2.3937670000 | 2.7634678000 | 1.1146562000 |
| C | -0.7504651000 | 2.3046908000 | -0.2506025000 |
| H | -0.5618168000 | 2.7100655000 | -1.2663085000 |
| H | -2.8015495000 | 2.9942875000 | -0.6410881000 |
| H | -0.1509452000 | 2.8789151000 | 0.4852069000 |
| H | 4.0583758000 | 0.2165823000 | 0.2315413000 |
| H | 2.9732867000 | -2.1489541000 | 0.1791258000 |

coord_6

| | | | |
|---|---------------|---------------|---------------|
| O | 2.3190417000 | 2.2819662000 | 0.0987217000 |
| O | -0.9136732000 | -2.1612700000 | -0.6527373000 |
| H | 0.4198267000 | -1.7651794000 | -0.1274512000 |
| N | 3.0468945000 | 0.0487342000 | 0.1384620000 |
| N | 1.0741337000 | -1.0272527000 | 0.2850284000 |
| C | 2.4282195000 | -1.1965129000 | 0.3322928000 |
| C | 2.0968234000 | 1.0677915000 | 0.1144119000 |
| C | 0.7946277000 | 0.3324682000 | 0.0769058000 |
| C | -0.4107048000 | 0.8534269000 | -0.2632572000 |
| C | -1.6502661000 | 0.0728798000 | -0.2571740000 |
| C | -1.8355444000 | -1.3559697000 | -0.3526080000 |
| C | -3.1708533000 | -1.8415470000 | -0.0820930000 |
| H | -3.3386205000 | -2.9206003000 | -0.1374769000 |
| C | -4.2132470000 | -0.9519095000 | 0.1576739000 |
| H | -5.2165533000 | -1.3519264000 | 0.3284280000 |
| C | -4.0140346000 | 0.4375334000 | 0.1827230000 |
| H | -4.8509501000 | 1.1227317000 | 0.3094646000 |
| C | -2.7001833000 | 0.9281412000 | 0.0152549000 |
| C | -2.2364877000 | 2.3578800000 | 0.1041542000 |

| | | | |
|---|---------------|---------------|---------------|
| H | -2.3081304000 | 2.7307552000 | 1.1497126000 |
| C | -0.7543607000 | 2.3085491000 | -0.3110507000 |
| H | -0.6323794000 | 2.6975693000 | -1.3490363000 |
| H | -2.8135818000 | 3.0155732000 | -0.5735142000 |
| H | -0.1254375000 | 2.9115110000 | 0.3756762000 |
| H | 4.0287876000 | 0.1966549000 | 0.2885314000 |
| H | 2.9234670000 | -2.1554911000 | 0.2272724000 |

coord_7

| | | | |
|---|---------------|---------------|---------------|
| O | 2.3126703000 | 2.2720940000 | 0.1178396000 |
| O | -0.9009649000 | -2.1163937000 | -0.7683719000 |
| H | 0.4098190000 | -1.7468922000 | -0.1516134000 |
| N | 3.0226224000 | 0.0333131000 | 0.1655785000 |
| N | 1.0317475000 | -1.0217375000 | 0.3285716000 |
| C | 2.3882532000 | -1.1982693000 | 0.3960623000 |
| C | 2.0827242000 | 1.0608058000 | 0.1379139000 |
| C | 0.7711633000 | 0.3390976000 | 0.0939913000 |
| C | -0.4083945000 | 0.8646055000 | -0.3128281000 |
| C | -1.6490938000 | 0.0876492000 | -0.3120862000 |
| C | -1.8303438000 | -1.3383144000 | -0.4239160000 |
| C | -3.1471545000 | -1.8433526000 | -0.1017392000 |
| H | -3.3102618000 | -2.9208852000 | -0.1643269000 |
| C | -4.1812682000 | -0.9637397000 | 0.1877909000 |
| H | -5.1741329000 | -1.3725717000 | 0.3944204000 |
| C | -3.9906440000 | 0.4255490000 | 0.2178110000 |
| H | -4.8319252000 | 1.1016408000 | 0.3680116000 |
| C | -2.6919016000 | 0.9341408000 | 0.0197245000 |
| C | -2.2183556000 | 2.3558277000 | 0.1220250000 |
| H | -2.2249967000 | 2.6962820000 | 1.1807342000 |
| C | -0.7573369000 | 2.3162461000 | -0.3764200000 |
| H | -0.7055798000 | 2.6819316000 | -1.4266939000 |
| H | -2.8261960000 | 3.0335359000 | -0.4981482000 |
| H | -0.1002488000 | 2.9403467000 | 0.2587782000 |
| H | 4.0007228000 | 0.1765258000 | 0.3471020000 |
| H | 2.8758897000 | -2.1609284000 | 0.2781037000 |

coord_8

| | | | |
|---|---------------|---------------|---------------|
| O | 2.3049989000 | 2.2615980000 | 0.1378800000 |
| O | -0.8870204000 | -2.0637709000 | -0.8720519000 |
| H | 0.4017212000 | -1.7263574000 | -0.1772638000 |
| N | 2.9976313000 | 0.0186057000 | 0.1867330000 |
| N | 0.9827694000 | -1.0185163000 | 0.3727296000 |
| C | 2.3394227000 | -1.2001180000 | 0.4550881000 |
| C | 2.0686628000 | 1.0528636000 | 0.1590286000 |

| | | | |
|---|---------------|---------------|---------------|
| C | 0.7441878000 | 0.3474633000 | 0.1135591000 |
| C | -0.4038369000 | 0.8773875000 | -0.3663180000 |
| C | -1.6491849000 | 0.1042351000 | -0.3712614000 |
| C | -1.8273734000 | -1.3178588000 | -0.4942079000 |
| C | -3.1232680000 | -1.8439794000 | -0.1268675000 |
| H | -3.2823303000 | -2.9196835000 | -0.1890962000 |
| C | -4.1473122000 | -0.9775998000 | 0.2178310000 |
| H | -5.1277763000 | -1.3934102000 | 0.4621395000 |
| C | -3.9651264000 | 0.4162831000 | 0.2539353000 |
| H | -4.8122480000 | 1.0788774000 | 0.4175490000 |
| C | -2.6774160000 | 0.9366203000 | 0.0316601000 |
| C | -2.1888382000 | 2.3520357000 | 0.1414699000 |
| H | -2.1445964000 | 2.6638349000 | 1.2002395000 |
| C | -0.7640339000 | 2.3237051000 | -0.4395109000 |
| H | -0.7754268000 | 2.6633395000 | -1.4934864000 |
| H | -2.8290019000 | 3.0422149000 | -0.4177063000 |
| H | -0.0862634000 | 2.9652884000 | 0.1400567000 |
| H | 3.9704245000 | 0.1573797000 | 0.4066507000 |
| H | 2.8280483000 | -2.1639312000 | 0.3295352000 |

coord_9

| | | | |
|---|---------------|---------------|---------------|
| O | 2.2996893000 | 2.2530027000 | 0.1570593000 |
| O | -0.8767027000 | -2.0220631000 | -0.9869594000 |
| H | 0.3907719000 | -1.7071594000 | -0.1964604000 |
| N | 2.9760528000 | 0.0029346000 | 0.2171424000 |
| N | 0.9401983000 | -1.0153636000 | 0.4118729000 |
| C | 2.2996669000 | -1.2007110000 | 0.5159041000 |
| C | 2.0551373000 | 1.0467788000 | 0.1813952000 |
| C | 0.7202365000 | 0.3548712000 | 0.1283473000 |
| C | -0.3995897000 | 0.8878338000 | -0.4160496000 |
| C | -1.6510738000 | 0.1187823000 | -0.4234120000 |
| C | -1.8212990000 | -1.3045566000 | -0.5654524000 |
| C | -3.0981864000 | -1.8431613000 | -0.1495471000 |
| H | -3.2530334000 | -2.9201654000 | -0.2153246000 |
| C | -4.1154288000 | -0.9920973000 | 0.2473677000 |
| H | -5.0859886000 | -1.4130695000 | 0.5292742000 |
| C | -3.9442794000 | 0.4081073000 | 0.2891391000 |
| H | -4.7959007000 | 1.0591000000 | 0.4750960000 |
| C | -2.6639969000 | 0.9387920000 | 0.0355794000 |
| C | -2.1666176000 | 2.3537447000 | 0.1594354000 |
| H | -2.0668988000 | 2.6320865000 | 1.2276891000 |
| C | -0.7716897000 | 2.3337716000 | -0.5032648000 |
| H | -0.8443968000 | 2.6463757000 | -1.5676193000 |
| H | -2.8422824000 | 3.0598655000 | -0.3417000000 |

| | | | |
|----------|---------------|---------------|---------------|
| H | -0.0633524000 | 2.9920200000 | 0.0219907000 |
| H | 3.9432207000 | 0.1379216000 | 0.4654890000 |
| H | 2.7825572000 | -2.1711342000 | 0.3813228000 |
| coord_10 | | | |
| O | 2.2907376000 | 2.2482137000 | 0.1786084000 |
| O | -0.8633832000 | -1.9733307000 | -1.0939090000 |
| H | 0.3802422000 | -1.6911364000 | -0.2313595000 |
| N | 2.9578252000 | -0.0045443000 | 0.2221477000 |
| N | 0.8801066000 | -1.0311922000 | 0.4798010000 |
| C | 2.2537613000 | -1.1998040000 | 0.5830714000 |
| C | 2.0577085000 | 1.0388567000 | 0.2018791000 |
| C | 0.6894921000 | 0.3662155000 | 0.1514591000 |
| C | -0.3744706000 | 0.9079541000 | -0.4712747000 |
| C | -1.6714517000 | 0.1344336000 | -0.4910443000 |
| C | -1.8177460000 | -1.2865884000 | -0.6335002000 |
| C | -3.0668711000 | -1.8427189000 | -0.1705668000 |
| H | -3.2275623000 | -2.9226394000 | -0.2400970000 |
| C | -4.0913705000 | -0.9982305000 | 0.2816753000 |
| H | -5.0445152000 | -1.4327949000 | 0.5949778000 |
| C | -3.9286962000 | 0.3860496000 | 0.3260185000 |
| H | -4.7814438000 | 1.0384484000 | 0.5206445000 |
| C | -2.6382899000 | 0.9345547000 | 0.0519086000 |
| C | -2.1335577000 | 2.3534150000 | 0.1815672000 |
| H | -1.9949922000 | 2.6025198000 | 1.2516621000 |
| C | -0.7789661000 | 2.3491784000 | -0.5737748000 |
| H | -0.9085637000 | 2.6298688000 | -1.6365891000 |
| H | -2.8512158000 | 3.0710328000 | -0.2685820000 |
| H | -0.0459891000 | 3.0153860000 | -0.0908988000 |
| H | 3.9155399000 | 0.1211787000 | 0.5265439000 |
| H | 2.7404853000 | -2.1778191000 | 0.4279465000 |