Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.


# Supporting Information

# for

# Theoretical study of complexes between fullerenes and concave receptors with interest in photovoltaics

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**Table S1.** Complexation energies for complexes obtained at the B97-D2/def2-TZVP//B97-D2/def2-SVP level in the initial search of the most stable structure for each dimer.

| | cora | suma | porf | sbpc | cora5CN |
|---|---|---|---|---|---|
| $C_{60}$-a | -14.76 | -18.45 | -17.71 | -24.35 | -22.59 |
| $C_{60}$-b | -17.49 | -20.22 | -18.69 | -24.37 | -22.26 |
| $C_{60}$-c | -16.82 | -20.09 | -18.64 | -24.01 | -21.95 |
| $C_{60}$-d | -17.09 | -18.34 | -17.73 | -24.50 | -22.61 |
| $C_{60}$-e | -16.95 | -18.24 | -18.65 | -23.92 | -21.95 |
| $C_{60}$-f | -17.62 | -18.62 | -18.68 | -24.30 | -22.22 |
| $C_{70}$-a | -18.72 | -20.72 | -20.47 | -25.83 | -24.27 |
| $C_{70}$-b | -17.27 | -18.46 | -17.66 | -24.56 | -22.45 |
| $C_{70}$-c | -17.25 | -19.56 | -21.08 | -25.86 | -24.26 |
| $C_{70}$-d | -17.24 | -18.46 | -17.61 | -24.57 | -22.49 |
| $C_{70}$-e | -17.25 | -19.57 | -20.36 | -25.84 | -24.26 |
| $C_{70}$-f | -18.70 | -18.55 | -21.08 | -24.32 | -24.07 |
| $Sc_3N@C_{68}$-a | -18.88 | -19.75 | -21.56 | -26.78 | -26.28 |
| $Sc_3N@C_{68}$-b | -17.68 | -20.23 | -21.24 | -26.27 | -23.61 |
| $Sc_3N@C_{68}$-c | -19.11 | -19.77 | -21.94 | -26.27 | -24.50 |
| $Sc_3N@C_{68}$-d | -18.87 | -19.78 | -21.55 | -26.79 | -26.46 |
| $Sc_3N@C_{68}$-e | -18.97 | -20.22 | -21.24 | -25.66 | -24.49 |
| $Sc_3N@C_{68}$-f | -18.09 | -20.07 | -17.55 | -25.65 | -22.24 |
| $Sc_3N@C_{80}$-a | -16.69 | -19.36 | -21.37 | -26.12 | -26.97 |
| $Sc_3N@C_{80}$-b | -20.44 | -22.96 | -21.81 | -28.50 | -25.28 |
| $Sc_3N@C_{80}$-c | -21.35 | -23.20 | -21.98 | -28.41 | -24.40 |
| $Sc_3N@C_{80}$-d | -18.63 | -19.51 | -21.27 | -26.37 | -27.22 |
| $Sc_3N@C_{80}$-e | -20.75 | -21.90 | -22.32 | -28.59 | -26.34 |
| $Sc_3N@C_{80}$-f | -20.18 | -22.39 | -22.58 | -28.28 | -26.37 |

The values obtained with the B97-D2/def2-TZVP optimised geometry are -14.53, -17.80, -17.09, -17.42, -16.99, -17.90 kcal/mol for cora-$C_{60}$-a to cora-$C_{60}$-f, respectively.

**Table S2.** Number of contacts below 4 Å between non-hydrogen atoms for the dimers studied.

| | $N_{contacts}$< 4 Å | Sum (R) | $R_{average}$ |
|---|---|---|---|
| **cora-$C_{60}$** | 78 | 283.08 | 3.63 |
| **cora-$C_{70}$** | 78 | 282.16 | 3.62 |
| **cora-$Sc_3N@C_{68}$** | 75 | 270.76 | 3.61 |
| **cora-$Sc_3N@C_{80}$** | 80 | 287.70 | 3.60 |
| **suma-$C_{60}$** | 84 | 299.91 | 3.57 |
| **suma-$C_{70}$** | 80 | 286.93 | 3.59 |
| **suma-$Sc_3N@C_{68}$** | 74 | 264.16 | 3.57 |
| **suma-$Sc_3N@C_{80}$** | 84 | 301.58 | 3.59 |
| **porf-$C_{60}$** | 59 | 213.60 | 3.62 |
| **porf-$C_{70}$** | 71 | 254.55 | 3.59 |
| **porf-$Sc_3N@C_{68}$** | 74 | 268.74 | 3.63 |
| **porf-$Sc_3N@C_{80}$** | 74 | 267.66 | 3.62 |
| **sbpc-$C_{60}$** | 109 | 396.39 | 3.64 |
| **sbpc-$C_{70}$** | 100 | 359.14 | 3.59 |
| **sbpc-$Sc_3N@C_{68}$** | 111 | 405.17 | 3.65 |
| **sbpc-$Sc_3N@C_{80}$** | 115 | 416.21 | 3.62 |
| **cora5CN-$C_{60}$** | 92 | 334.49 | 3.64 |
| **cora5CN-$C_{70}$** | 96 | 348.37 | 3.63 |
| **cora5CN-$Sc_3N@C_{68}$** | 103 | 375.57 | 3.65 |
| **cora5CN-$Sc_3N@C_{80}$** | 103 | 375.84 | 3.65 |

**Table S3.** Energy components of the complexation energy obtained with the def2-TZVP basis set. B97-D2/def2-TZVP geometry. The 3-body term is the same for B3LYP and TPSS.

| | B3LYP-D | | | TPSS-D | | | 3body | B97-D2 | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | **B3LYP** | **D** | **BSSE** | **TPSS** | **D** | **BSSE** | | **B97** | **D2** | **BSSE** |
| **cora-$C_{60}$** | 11.99 | -28.49 | 0.96 | 9.16 | -25.13 | 0.80 | 1.29 | 16.21 | -34.11 | 0.97 |
| **cora-$C_{70}$** | 12.29 | -30.38 | 0.90 | 9.54 | -26.82 | 0.78 | 1.41 | 17.00 | -36.11 | 0.94 |
| **cora-$Sc_3N@C_{68}$** | 12.36 | -29.03 | 1.05 | 9.68 | -25.74 | 0.90 | 1.78 | 17.05 | -36.55 | 1.08 |
| **cora-$Sc_3N@C_{80}$** | 12.69 | -31.04 | 1.12 | 9.52 | -27.45 | 0.97 | 1.53 | 17.08 | -38.47 | 1.16 |
| **suma-$C_{60}$** | 14.79 | -32.69 | 0.94 | 10.99 | -28.53 | 0.81 | 1.38 | 20.32 | -41.03 | 0.99 |
| **suma-$C_{70}$** | 14.91 | -33.37 | 0.86 | 11.52 | -29.27 | 0.77 | 1.48 | 20.64 | -41.62 | 0.95 |
| **suma-$Sc_3N@C_{68}$** | 13.43 | -30.32 | 1.16 | 10.31 | -26.70 | 0.99 | 0.81 | 18.74 | -40.04 | 1.22 |
| **suma-$Sc_3N@C_{80}$** | 14.17 | -33.76 | 1.18 | 10.97 | -29.71 | 1.05 | 1.73 | 20.56 | -43.84 | 1.25 |
| **porf-$C_{60}$** | 9.73 | -26.86 | 1.19 | 6.69 | -23.82 | 1.27 | 1.38 | 13.05 | -32.02 | 1.21 |
| **porf-$C_{70}$** | 12.61 | -32.16 | 1.40 | 9.13 | -28.32 | 1.48 | 1.58 | 17.00 | -38.61 | 1.45 |
| **porf-$Sc_3N@C_{68}$** | 11.23 | -30.11 | 1.48 | 8.31 | -26.73 | 1.52 | 0.40 | 15.51 | -38.17 | 1.47 |
| **porf-$Sc_3N@C_{80}$** | 11.85 | -31.37 | 1.61 | 8.23 | -27.81 | 1.71 | 2.00 | 16.22 | -39.32 | 1.67 |
| **sbpc-$C_{60}$** | 16.09 | -39.01 | 1.08 | 12.93 | -34.58 | 0.99 | 2.00 | 21.77 | -47.01 | 1.18 |
| **sbpc-$C_{70}$** | 16.38 | -40.62 | 1.12 | 13.28 | -36.04 | 1.02 | 2.10 | 22.52 | -48.75 | 1.23 |
| **sbpc-$Sc_3N@C_{68}$** | 17.99 | -40.23 | 1.44 | 14.35 | -35.92 | 1.25 | 1.21 | 23.14 | -50.22 | 1.46 |
| **sbpc-$Sc_3N@C_{80}$** | 17.03 | -41.87 | 1.53 | 13.38 | -37.26 | 1.41 | 2.00 | 23.48 | -52.58 | 1.63 |
| **cora5CN-$C_{60}$** | 13.61 | -35.67 | 0.86 | 10.67 | -31.59 | 0.67 | 1.75 | 18.59 | -41.68 | 0.87 |
| **cora5CN-$C_{70}$** | 14.05 | -37.97 | 0.88 | 10.97 | -33.63 | 0.76 | 1.88 | 19.59 | -44.25 | 0.97 |
| **cora5CN-$Sc_3N@C_{68}$** | 13.90 | -38.12 | 1.14 | 10.66 | -33.83 | 0.94 | 1.78 | 19.71 | -46.39 | 1.15 |
| **cora5CN-$Sc_3N@C_{80}$** | 12.34 | -38.96 | 1.08 | 8.96 | -34.54 | 0.95 | 2.20 | 18.14 | -45.86 | 1.16 |

**Table S4.** Electrostatic effect due to the solvent (kcal/mol) upon complexation energies as obtained with the COSMO model at the B3LYP/def2-TZVP level of calculation.

| | | | |
|---|---|---|---|
| **cora-$C_{60}$** | 0.77 | **porf-$C_{60}$** | 0.72 |
| **cora-$C_{70}$** | 0.77 | **porf-$C_{70}$** | 0.78 |
| **cora-$Sc_3N@C_{68}$** | 0.57 | **porf-$Sc_3N@C_{68}$** | 0.62 |
| **cora-$Sc_3N@C_{80}$** | 0.60 | **porf-$Sc_3N@C_{80}$** | 0.67 |
| **suma-$C_{60}$** | 0.83 | **sbpc-$C_{60}$** | 1.13 |
| **suma-$C_{70}$** | 0.84 | **sbpc-$C_{70}$** | 1.09 |
| **suma-$Sc_3N@C_{68}$** | 0.62 | **sbpc-$Sc_3N@C_{68}$** | 0.88 |
| **suma-$Sc_3N@C_{80}$** | 0.72 | **sbpc-$Sc_3N@C_{80}$** | 1.03 |
| **cora5CN-$C_{60}$** | 1.56 | **cora5CN-$Sc_3N@C_{68}$** | 1.77 |
| **cora5CN-$C_{70}$** | 1.48 | **cora5CN-$Sc_3N@C_{80}$** | 1.86 |

**Table S5.** SAPT(DFT) values (kcal/mol) obtained for complexes with $C_{60}$.

| | Electrostatic | Induction | Repulsion | Dispersion |
|---|---|---|---|---|
| **cora** | -16.44 | -0.47 | 38.55 | -27.9 |
| **suma** | -21.65 | -0.75 | 50.13 | -33.5 |
| **porf** | -14.21 | -1.72 | 33.95 | -25.4 |
| **sbpc** | -19.81 | -0.73 | 48.17 | -37.5 |
| **cora5CN** | -16.83 | -1.85 | 40.84 | -32.4 |

SAPT(DFT) calculations have been performed with the PBE functional and the def2-SVP basis set. These calculations need a shift parameter obtained as the sum of the ionization potential and the energy of the highest occupied molecular orbital. Orbital energies and ionization potentials have been obtained by using the PBE functional with the def2-SVP basis set.

**Table S6.** Summary of the 12 most intense transitions in **cora** complexes. $N_{tr}$ is the number of the transition, the transition from the ground state to the $N^{th}$ excited state. The values are ordered by decreasing value of the oscillator strength. q and R are the amount of charge transferred and the transfer distance as commented in the text.

| | $C_{60}$ | | | | | $Sc_3N@C_{68}$ | | | |
|---|---|---|---|---|---|---|---|---|---|
| **ν /nm** | **$f_{osc}$ /$10^{-2}$** | **$N_{tr}$** | **q** | **R /Å** | **ν /nm** | **$f_{osc}$ /$10^{-2}$** | **$N_{tr}$** | **q** | **R /Å** |
| 349.4 | 0.1 | 19 | 0.69 | 4.97 | 430.6 | 13.7 | 9 | 0.44 | 1.16 |
| 348.9 | 0.1 | 20 | 0.65 | 5.05 | 426.9 | 9.4 | 10 | 0.43 | 1.30 |
| 431.4 | 0.1 | 11 | 0.37 | 0.78 | 472.0 | 6.1 | 6 | 0.56 | 0.25 |
| 423.0 | 0.1 | 15 | 0.42 | 0.35 | 472.3 | 5.4 | 5 | 0.58 | 0.17 |
| 345.7 | 0.1 | 22 | 0.50 | 4.03 | 398.2 | 1.4 | 16 | 0.37 | 0.30 |
| 342.7 | 0.1 | 24 | 0.64 | 4.77 | 531.0 | 1.2 | 2 | 0.41 | 0.25 |
| 354.9 | 0.1 | 17 | 0.30 | 2.38 | 373.0 | 1.1 | 22 | 0.35 | 0.16 |
| 430.5 | 0.1 | 12 | 0.38 | 0.67 | 530.0 | 0.8 | 3 | 0.40 | 0.29 |
| 348.6 | 0.1 | 21 | 0.74 | 5.20 | 414.5 | 0.7 | 14 | 0.42 | 0.27 |
| 426.5 | 0.0 | 14 | 0.37 | 0.47 | 413.5 | 0.5 | 15 | 0.46 | 0.13 |
| 344.9 | 0.0 | 23 | 0.72 | 5.28 | 373.9 | 0.3 | 21 | 0.52 | 0.19 |
| 427.1 | 0.0 | 13 | 0.38 | 0.53 | 384.5 | 0.3 | 18 | 0.41 | 0.25 |
| | $C_{70}$ | | | | | $Sc_3N@C_{80}$ | | | |
| **ν /nm** | **$f_{osc}$ /$10^{-2}$** | **$N_{tr}$** | **q** | **R /Å** | **ν /nm** | **$f_{osc}$ /$10^{-2}$** | **$N_{tr}$** | **q** | **R /Å** |
| 458.1 | 5.8 | 8 | 0.34 | 1.13 | 437.1 | 1.5 | 17 | 0.57 | 0.68 |
| 471.4 | 3.6 | 6 | 0.49 | 1.79 | 433.7 | 0.9 | 18 | 0.55 | 0.71 |
| 472.1 | 3.0 | 5 | 0.39 | 0.98 | 512.7 | 0.8 | 1 | 0.63 | 0.39 |
| 461.5 | 2.6 | 7 | 0.45 | 2.76 | 433.1 | 0.8 | 19 | 0.55 | 0.63 |
| 477.4 | 0.5 | 3 | 0.44 | 2.20 | 422.6 | 0.8 | 22 | 0.57 | 0.40 |
| 454.0 | 0.4 | 9 | 0.60 | 3.31 | 452.5 | 0.8 | 13 | 0.65 | 0.98 |
| 479.4 | 0.4 | 2 | 0.44 | 1.53 | 477.8 | 0.6 | 6 | 0.58 | 0.60 |
| 442.2 | 0.1 | 10 | 0.26 | 0.66 | 459.0 | 0.6 | 12 | 0.66 | 0.65 |
| 475.5 | 0.1 | 4 | 0.41 | 1.72 | 467.0 | 0.5 | 10 | 0.63 | 0.50 |
| 417.5 | 0.0 | 14 | 0.50 | 0.91 | 429.2 | 0.5 | 20 | 0.61 | 0.67 |
| 418.5 | 0.0 | 13 | 0.44 | 1.02 | 483.0 | 0.4 | 5 | 0.66 | 1.06 |
| 380.4 | 0.0 | 22 | 0.30 | 0.80 | 501.9 | 0.4 | 2 | 0.60 | 0.32 |

**Table S7.** Summary of the 12 most intense transitions in **suma** complexes. $N_{tr}$ is the number of the transition, the transition from the ground state to the $N^{th}$ excited state. The values are ordered by decreasing value of the oscillator strength. q and R are the amount of charge transferred and the transfer distance as commented in the text.

| | $C_{60}$ | | | | | $Sc_3N@C_{68}$ | | | |
|---|---|---|---|---|---|---|---|---|---|
| **ν /nm** | **$f_{osc}$ /$10^{-2}$** | **$N_{tr}$** | **q** | **R /Å** | **ν /nm** | **$f_{osc}$ /$10^{-2}$** | **$N_{tr}$** | **q** | **R /Å** |
| 414.8 | 2.4 | 17 | 0.84 | 5.11 | 429.7 | 13.2 | 9 | 0.42 | 1.00 |
| 421.1 | 0.2 | 15 | 0.42 | 0.56 | 428.1 | 10.5 | 10 | 0.43 | 1.34 |
| 413.9 | 0.2 | 19 | 0.74 | 4.78 | 471.5 | 5.0 | 6 | 0.58 | 0.27 |
| 485.2 | 0.2 | 7 | 0.41 | 1.21 | 476.0 | 5.0 | 5 | 0.57 | 0.15 |
| 413.9 | 0.1 | 18 | 0.72 | 4.83 | 398.3 | 1.4 | 16 | 0.37 | 0.63 |
| 350.1 | 0.0 | 24 | 0.25 | 1.05 | 532.0 | 1.0 | 2 | 0.40 | 0.20 |
| 434.2 | 0.0 | 12 | 0.41 | 2.85 | 528.3 | 1.0 | 3 | 0.41 | 0.22 |
| 434.2 | 0.0 | 11 | 0.43 | 2.69 | 373.1 | 1.0 | 22 | 0.47 | 2.68 |
| 432.4 | 0.0 | 13 | 0.43 | 3.26 | 413.3 | 0.9 | 15 | 0.46 | 0.35 |
| 431.9 | 0.0 | 14 | 0.43 | 3.20 | 420.5 | 0.6 | 11 | 0.51 | 0.26 |
| 487.7 | 0.0 | 5 | 0.37 | 0.56 | 375.3 | 0.5 | 21 | 0.51 | 4.00 |
| 487.5 | 0.0 | 6 | 0.36 | 0.61 | 415.1 | 0.4 | 14 | 0.43 | 0.41 |
| | $C_{70}$ | | | | | $Sc_3N@C_{80}$ | | | |
| **ν /nm** | **$f_{osc}$ /$10^{-2}$** | **$N_{tr}$** | **q** | **R /Å** | **ν /nm** | **$f_{osc}$ /$10^{-2}$** | **$N_{tr}$** | **q** | **R /Å** |
| 466.4 | 8.8 | 7 | 0.51 | 3.39 | 433.8 | 1.4 | 17 | 0.56 | 0.63 |
| 472.0 | 3.5 | 5 | 0.40 | 0.96 | 450.6 | 1.2 | 13 | 0.66 | 0.85 |
| 471.4 | 2.9 | 6 | 0.44 | 0.76 | 431.8 | 1.0 | 18 | 0.54 | 0.14 |
| 462.2 | 1.3 | 8 | 0.52 | 4.42 | 421.5 | 0.9 | 22 | 0.57 | 0.47 |
| 449.4 | 1.3 | 11 | 0.63 | 0.58 | 429.9 | 0.9 | 19 | 0.56 | 0.63 |
| 450.3 | 0.5 | 10 | 0.48 | 1.48 | 509.5 | 0.9 | 1 | 0.63 | 0.31 |
| 475.1 | 0.3 | 4 | 0.55 | 0.74 | 474.7 | 0.6 | 6 | 0.62 | 0.72 |
| 454.1 | 0.3 | 9 | 0.59 | 1.10 | 422.6 | 0.5 | 21 | 0.59 | 0.76 |
| 423.8 | 0.3 | 14 | 0.60 | 4.13 | 498.3 | 0.5 | 2 | 0.59 | 0.36 |
| 478.6 | 0.2 | 3 | 0.35 | 2.76 | 477.6 | 0.5 | 5 | 0.65 | 1.03 |
| 438.1 | 0.1 | 12 | 0.37 | 2.60 | 496.7 | 0.4 | 3 | 0.58 | 0.24 |
| 419.4 | 0.1 | 15 | 0.43 | 2.43 | 469.7 | 0.4 | 8 | 0.63 | 0.70 |

**Table S8.** Summary of the 12 most intense transitions in **porf** complexes. $N_{tr}$ is the number of the transition, the transition from the ground state to the $N^{th}$ excited state. The values are ordered by decreasing value of the oscillator strength. q and R are the amount of charge transferred and the transfer distance as commented in the text.

| | $C_{60}$ | | | | | $Sc_3N@C_{68}$ | | | |
|---|---|---|---|---|---|---|---|---|---|
| **ν /nm** | **$f_{osc}$ /$10^{-2}$** | **$N_{tr}$** | **q** | **R /Å** | **ν /nm** | **$f_{osc}$ /$10^{-2}$** | **$N_{tr}$** | **q** | **R /Å** |
| 470.6 | 4.2 | 15 | 0.59 | 4.28 | 432.9 | 15.3 | 12 | 0.48 | 2.79 |
| 507.6 | 3.4 | 2 | 0.67 | 3.98 | 476.4 | 10.0 | 7 | 0.57 | 0.20 |
| 456.8 | 0.8 | 18 | 0.66 | 5.24 | 433.4 | 4.6 | 11 | 0.43 | 2.38 |
| 499.2 | 0.5 | 4 | 0.14 | 0.12 | 472.2 | 4.1 | 8 | 0.56 | 0.27 |
| 495.5 | 0.4 | 6 | 0.57 | 3.95 | 416.7 | 2.3 | 19 | 0.47 | 3.89 |
| 489.4 | 0.4 | 10 | 0.50 | 2.90 | 419.4 | 2.1 | 17 | 0.56 | 3.83 |
| 427.1 | 0.3 | 20 | 0.41 | 0.49 | 424.2 | 1.6 | 14 | 0.67 | 5.20 |
| 425.8 | 0.3 | 21 | 0.40 | 0.40 | 398.6 | 1.3 | 22 | 0.36 | 0.40 |
| 497.9 | 0.2 | 5 | 0.14 | 0.09 | 535.9 | 1.3 | 2 | 0.40 | 0.52 |
| 422.7 | 0.1 | 23 | 0.38 | 1.49 | 435.2 | 0.9 | 10 | 0.52 | 0.42 |
| 493.5 | 0.1 | 8 | 0.47 | 3.73 | 528.1 | 0.5 | 3 | 0.42 | 0.10 |
| 425.0 | 0.1 | 22 | 0.38 | 0.68 | 413.7 | 0.5 | 21 | 0.52 | 0.38 |
| | $C_{70}$ | | | | | $Sc_3N@C_{80}$ | | | |
| **ν /nm** | **$f_{osc}$ /$10^{-2}$** | **$N_{tr}$** | **q** | **R /Å** | **ν /nm** | **$f_{osc}$ /$10^{-2}$** | **$N_{tr}$** | **q** | **R /Å** |
| 518.1 | 4.3 | 3 | 0.91 | 4.55 | 432.6 | 1.6 | 21 | 0.58 | 0.25 |
| 470.1 | 3.2 | 12 | 0.54 | 1.80 | 435.7 | 1.3 | 19 | 0.57 | 0.67 |
| 435.1 | 2.6 | 18 | 0.81 | 7.48 | 515.1 | 0.8 | 1 | 0.63 | 0.32 |
| 461.8 | 2.6 | 13 | 0.41 | 0.97 | 423.9 | 0.8 | 24 | 0.55 | 0.38 |
| 471.0 | 2.3 | 11 | 0.36 | 1.85 | 434.5 | 0.6 | 20 | 0.55 | 0.41 |
| 457.7 | 1.9 | 14 | 0.35 | 3.69 | 448.4 | 0.6 | 16 | 0.63 | 0.21 |
| 480.8 | 1.4 | 7 | 0.44 | 2.40 | 499.2 | 0.5 | 5 | 0.57 | 0.22 |
| 474.7 | 1.1 | 10 | 0.57 | 3.61 | 459.0 | 0.5 | 14 | 0.64 | 0.45 |
| 411.3 | 0.7 | 24 | 0.44 | 0.75 | 467.4 | 0.4 | 12 | 0.62 | 0.46 |
| 453.1 | 0.6 | 15 | 0.61 | 3.12 | 478.2 | 0.4 | 8 | 0.57 | 0.63 |
| 478.8 | 0.5 | 8 | 0.43 | 2.88 | 504.8 | 0.4 | 2 | 0.19 | 0.17 |
| 500.5 | 0.5 | 4 | 0.15 | 0.84 | 425.9 | 0.4 | 23 | 0.57 | 0.60 |

**Table S9.** Summary of the 12 most intense transitions in **sbpc** complexes. $N_{tr}$ is the number of the transition, the transition from the ground state to the $N^{th}$ excited state. The values are ordered by decreasing value of the oscillator strength. q and R are the amount of charge transferred and the transfer distance as commented in the text.

| | $C_{60}$ | | | | | $Sc_3N@C_{68}$ | | | |
|---|---|---|---|---|---|---|---|---|---|
| **ν /nm** | **$f_{osc}$ /$10^{-2}$** | **$N_{tr}$** | **q** | **R /Å** | **ν /nm** | **$f_{osc}$ /$10^{-2}$** | **$N_{tr}$** | **q** | **R /Å** |
| 466.3 | 29.6 | 15 | 0.39 | 1.03 | 467.7 | 20.5 | 8 | 0.45 | 0.70 |
| 466.9 | 28.4 | 14 | 0.37 | 1.13 | 467.7 | 19.0 | 7 | 0.47 | 0.70 |
| 520.6 | 0.5 | 2 | 0.95 | 5.03 | 428.5 | 16.3 | 14 | 0.41 | 1.08 |
| 423.9 | 0.4 | 20 | 0.40 | 0.34 | 428.5 | 16.1 | 15 | 0.41 | 1.05 |
| 426.5 | 0.3 | 18 | 0.35 | 0.53 | 467.6 | 4.5 | 9 | 0.77 | 4.95 |
| 425.9 | 0.2 | 19 | 0.34 | 0.36 | 421.6 | 1.5 | 17 | 0.54 | 0.49 |
| 482.4 | 0.1 | 10 | 0.38 | 0.45 | 421.8 | 1.5 | 16 | 0.52 | 0.45 |
| 500.9 | 0.1 | 3 | 0.86 | 5.45 | 399.2 | 1.5 | 21 | 0.38 | 0.36 |
| 481.7 | 0.0 | 11 | 0.43 | 1.59 | 478.8 | 1.4 | 6 | 0.51 | 0.34 |
| 429.5 | 0.0 | 16 | 0.34 | 0.44 | 451.0 | 1.2 | 10 | 0.86 | 5.41 |
| 493.3 | 0.0 | 5 | 0.28 | 0.32 | 450.6 | 1.2 | 11 | 0.86 | 5.39 |
| 352.7 | 0.0 | 23 | 0.23 | 0.17 | 479.5 | 1.0 | 5 | 0.52 | 0.32 |
| | $C_{70}$ | | | | | $Sc_3N@C_{80}$ | | | |
| **ν /nm** | **$f_{osc}$ /$10^{-2}$** | **$N_{tr}$** | **q** | **R /Å** | **ν /nm** | **$f_{osc}$ /$10^{-2}$** | **$N_{tr}$** | **q** | **R /Å** |
| 472.7 | 23.7 | 7 | 0.41 | 0.88 | 467.9 | 15.4 | 11 | 0.49 | 0.77 |
| 455.2 | 14.4 | 13 | 0.45 | 1.31 | 466.3 | 15.4 | 12 | 0.49 | 0.71 |
| 464.5 | 7.4 | 10 | 0.45 | 3.27 | 470.2 | 8.7 | 9 | 0.53 | 0.34 |
| 456.1 | 7.4 | 12 | 0.31 | 1.98 | 469.1 | 8.3 | 10 | 0.51 | 0.46 |
| 459.5 | 5.0 | 11 | 0.37 | 1.68 | 450.2 | 2.6 | 16 | 0.64 | 0.42 |
| 468.0 | 2.5 | 9 | 0.50 | 1.18 | 423.5 | 2.0 | 24 | 0.56 | 0.42 |
| 511.8 | 2.4 | 3 | 0.86 | 5.55 | 435.2 | 1.8 | 20 | 0.56 | 0.52 |
| 421.2 | 2.0 | 18 | 0.73 | 4.62 | 435.9 | 1.6 | 19 | 0.55 | 0.48 |
| 471.8 | 1.7 | 8 | 0.52 | 2.20 | 433.8 | 1.3 | 21 | 0.58 | 0.25 |
| 450.9 | 1.3 | 14 | 0.56 | 5.96 | 463.3 | 1.2 | 13 | 0.61 | 0.26 |
| 476.1 | 0.9 | 6 | 0.51 | 1.46 | 474.0 | 1.1 | 8 | 0.62 | 0.33 |
| 571.3 | 0.7 | 1 | 0.94 | 4.27 | 499.7 | 0.5 | 3 | 0.58 | 0.29 |

**Table S10.** Summary of the 12 most intense transitions in **cora5CN** complexes. $N_{tr}$ is the number of the transition, the transition from the ground state to the $N^{th}$ excited state. The values are ordered by decreasing value of the oscillator strength. q and R are the amount of charge transferred and the transfer distance as commented in the text.

| | $C_{60}$ | | | | | $Sc_3N@C_{68}$ | | | |
|---|---|---|---|---|---|---|---|---|---|
| **ν /nm** | **$f_{osc}$ /$10^{-2}$** | **$N_{tr}$** | **q** | **R /Å** | **ν /nm** | **$f_{osc}$ /$10^{-2}$** | **$N_{tr}$** | **q** | **R /Å** |
| 374.9 | 1.7 | 23 | 0.97 | 5.22 | 428.8 | 8.9 | 15 | 0.42 | 1.14 |
| 378.5 | 0.2 | 21 | 0.95 | 5.22 | 427.0 | 8.4 | 16 | 0.44 | 1.46 |
| 378.3 | 0.2 | 22 | 0.95 | 5.21 | 474.0 | 5.6 | 8 | 0.56 | 1.05 |
| 379.0 | 0.1 | 20 | 0.96 | 5.17 | 464.0 | 2.2 | 11 | 0.76 | 5.20 |
| 429.4 | 0.1 | 12 | 0.37 | 0.60 | 467.8 | 2.2 | 10 | 0.67 | 3.75 |
| 429.6 | 0.1 | 11 | 0.37 | 0.61 | 395.6 | 1.5 | 22 | 0.40 | 0.73 |
| 428.0 | 0.0 | 13 | 0.30 | 0.80 | 522.7 | 1.1 | 5 | 0.45 | 1.24 |
| 379.0 | 0.0 | 19 | 0.96 | 5.18 | 470.2 | 1.0 | 9 | 0.73 | 4.72 |
| 382.2 | 0.0 | 16 | 0.94 | 5.14 | 530.7 | 0.7 | 4 | 0.40 | 0.43 |
| 381.9 | 0.0 | 17 | 0.93 | 5.16 | 569.2 | 0.7 | 3 | 0.96 | 5.52 |
| 381.8 | 0.0 | 18 | 0.91 | 5.15 | 410.0 | 0.4 | 21 | 0.45 | 0.85 |
| 356.4 | 0.0 | 24 | 1.00 | 6.00 | 411.1 | 0.4 | 20 | 0.50 | 0.72 |
| | $C_{70}$ | | | | | $Sc_3N@C_{80}$ | | | |
| **ν /nm** | **$f_{osc}$ /$10^{-2}$** | **$N_{tr}$** | **q** | **R /Å** | **ν /nm** | **$f_{osc}$ /$10^{-2}$** | **$N_{tr}$** | **q** | **R /Å** |
| 463.3 | 5.0 | 7 | 0.31 | 1.26 | 452.1 | 3.6 | 16 | 0.73 | 2.23 |
| 459.3 | 3.8 | 8 | 0.43 | 1.45 | 508.6 | 1.2 | 1 | 0.63 | 0.71 |
| 478.0 | 2.1 | 3 | 0.55 | 2.39 | 454.4 | 1.1 | 15 | 0.79 | 3.16 |
| 470.0 | 2.1 | 5 | 0.50 | 2.56 | 432.6 | 1.0 | 23 | 0.57 | 0.66 |
| 467.5 | 2.0 | 6 | 0.47 | 2.51 | 431.7 | 0.9 | 24 | 0.55 | 0.89 |
| 478.7 | 1.1 | 2 | 0.61 | 2.73 | 464.9 | 0.7 | 12 | 0.79 | 4.35 |
| 429.7 | 0.1 | 11 | 0.62 | 4.13 | 474.6 | 0.5 | 7 | 0.63 | 1.04 |
| 475.6 | 0.1 | 4 | 0.44 | 2.74 | 477.8 | 0.4 | 6 | 0.65 | 1.38 |
| 400.1 | 0.1 | 22 | 0.41 | 0.27 | 483.2 | 0.4 | 4 | 0.70 | 3.82 |
| 454.8 | 0.0 | 9 | 0.59 | 3.15 | 494.9 | 0.3 | 3 | 0.58 | 0.25 |
| 389.2 | 0.0 | 24 | 0.51 | 4.91 | 498.0 | 0.2 | 2 | 0.56 | 0.62 |
| 397.1 | 0.0 | 23 | 0.31 | 1.61 | 440.6 | 0.2 | 22 | 0.64 | 2.00 |

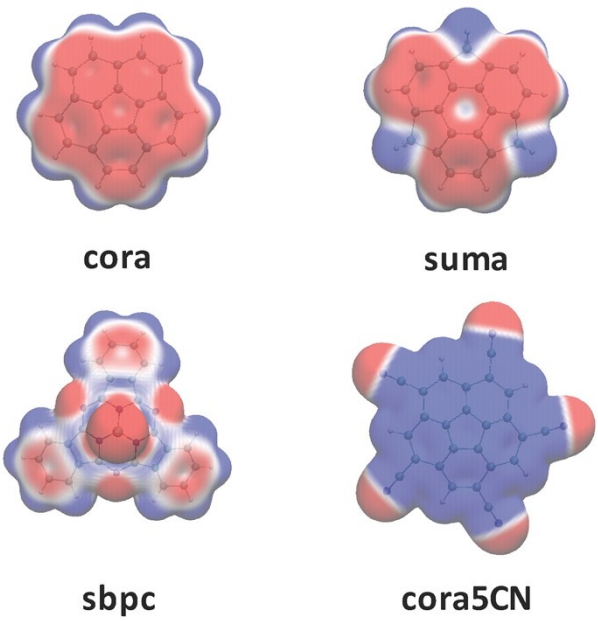


**Figure S1.** Molecular Electrostatic Potentials (MEP) of the bowls employed in this work at the B3LYP-D/def2-TZVP level by the convex face. MEP mapped onto a isodensity surface of 0.002 a.u. Colour scale runs from -0.010 a.u. (red) to 0.010 a.u (blue). White is 0.0.

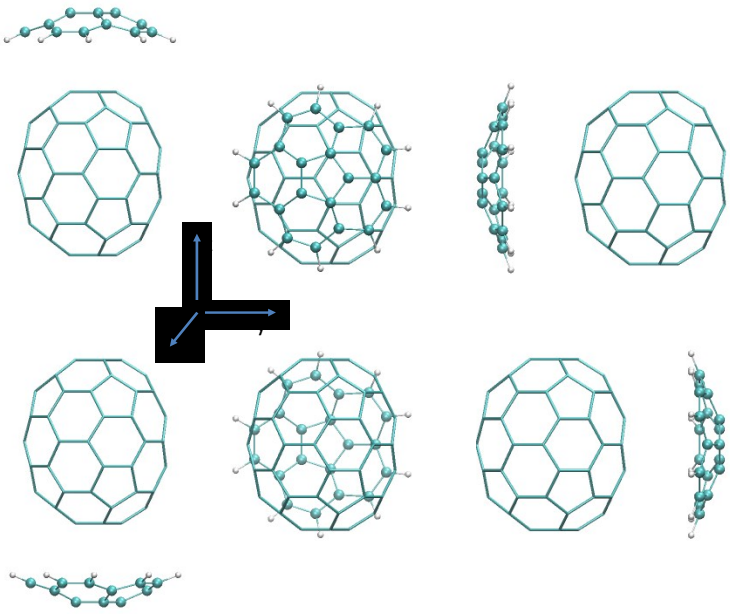

**Figure S2.** Representation of the starting structures employed for searching the minimum energy structures of the dimers. The corannulene-C70 case is shown.

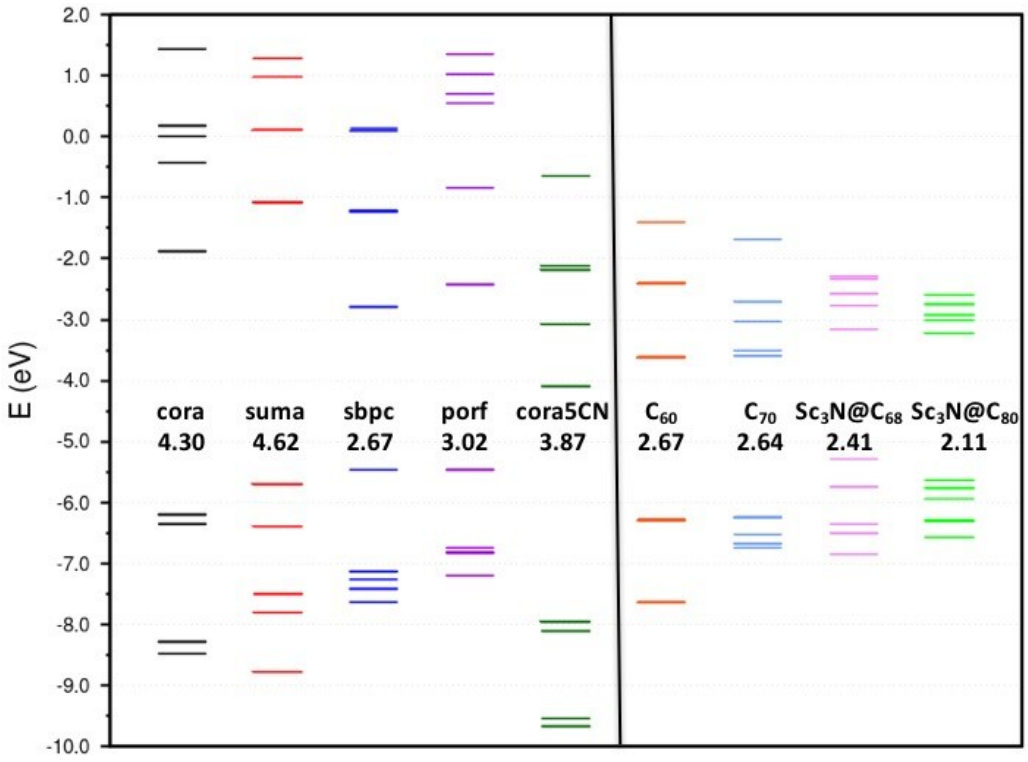


**Figure S3.** Frontier orbital energies of the molecules studied at the B3LYP/def2-TZVP//B97-D2/def2-TZVP level. Numbers correspond to the HOMO-LUMO gap.

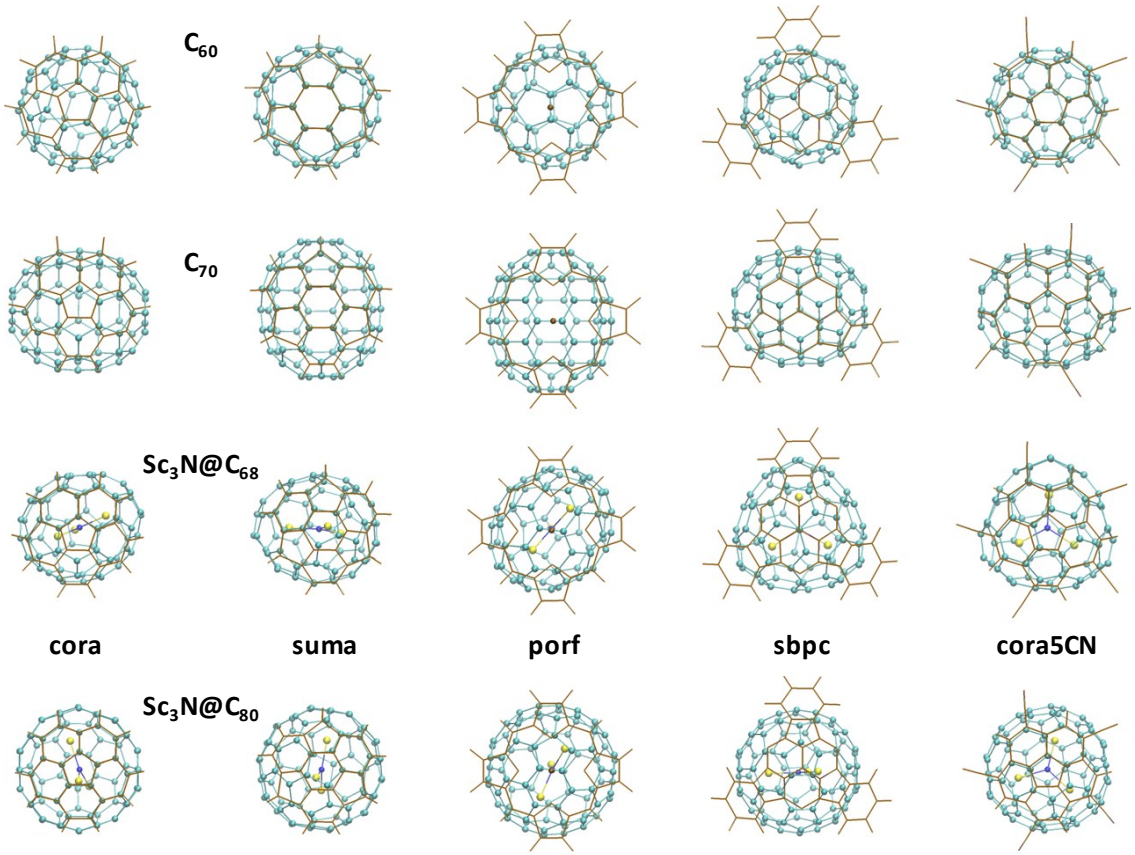


**Figure S4.** Another view of the most stable structures found for the complexes studied at the B3LYP-D/def2-TZVP//B97-D2/def2-TZVP shown in Figure 5. The bowl is shown in ochre, with the complex observed from the bottom of the bowl.

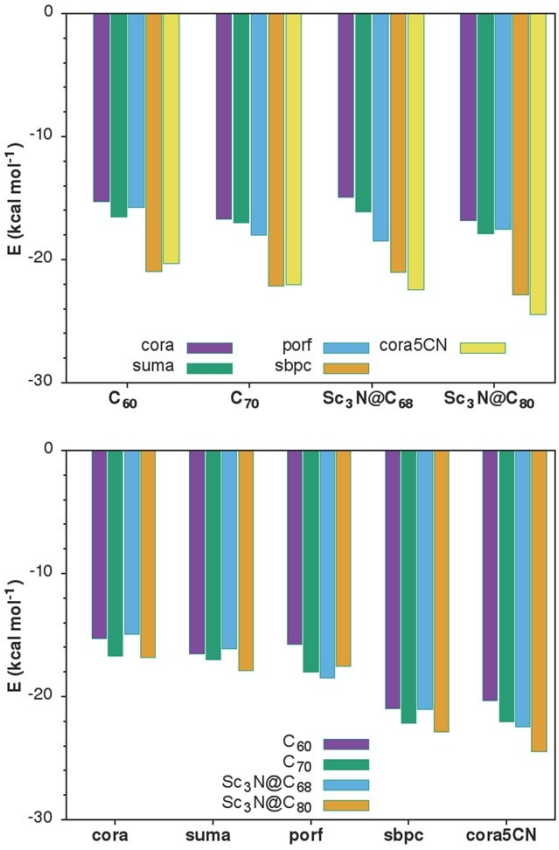


**Figure S5.** Complexation energies of the complexes studied. B3LYP-D/def2-TZVP+ 3-body results.

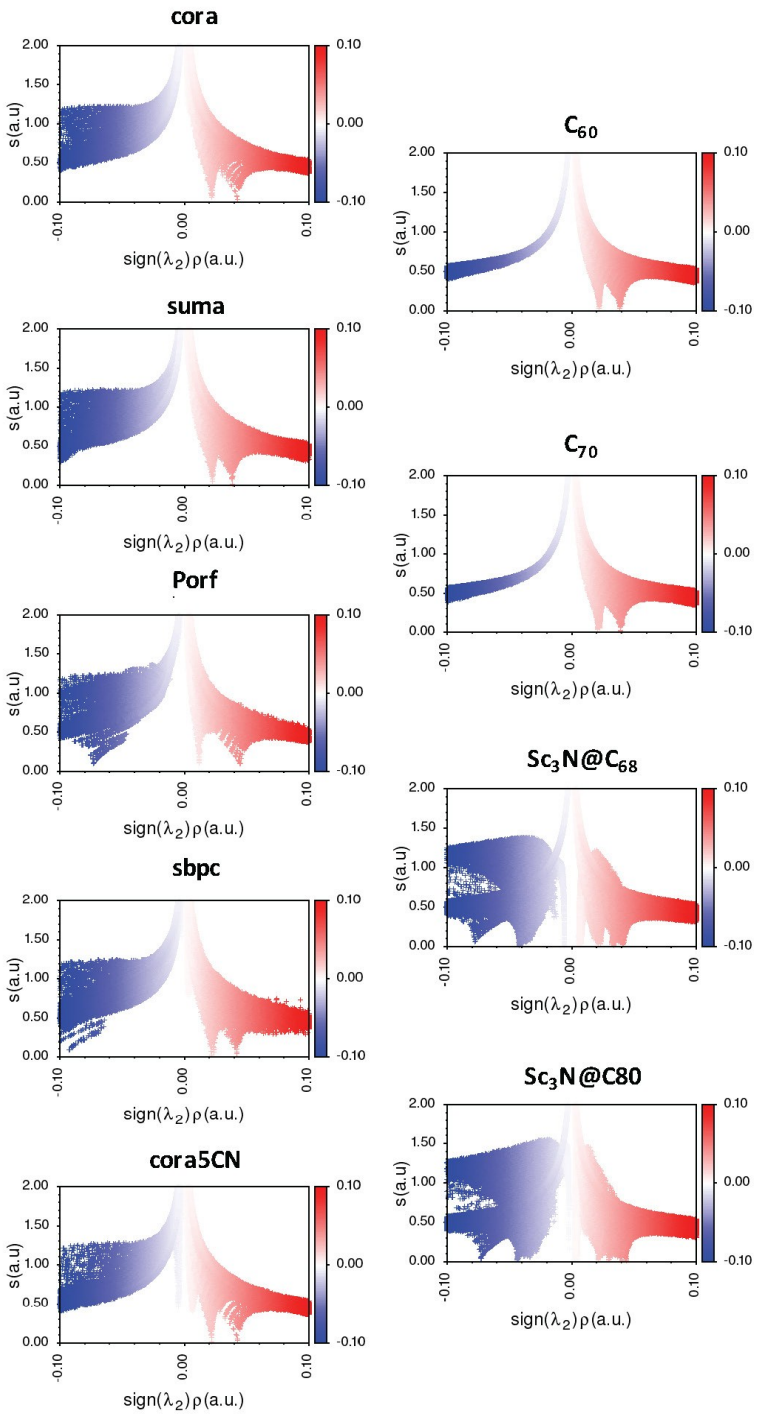


**Figure S6.** Non covalent interaction index for the isolated molecules. The product of the density times the sign of the second eigenvalue of its Hessian is mapped onto an isosurface of reduced density gradient with value 0.5 a.u.; the color scale goes from −0.1 au (blue) to +0.1 au (red).

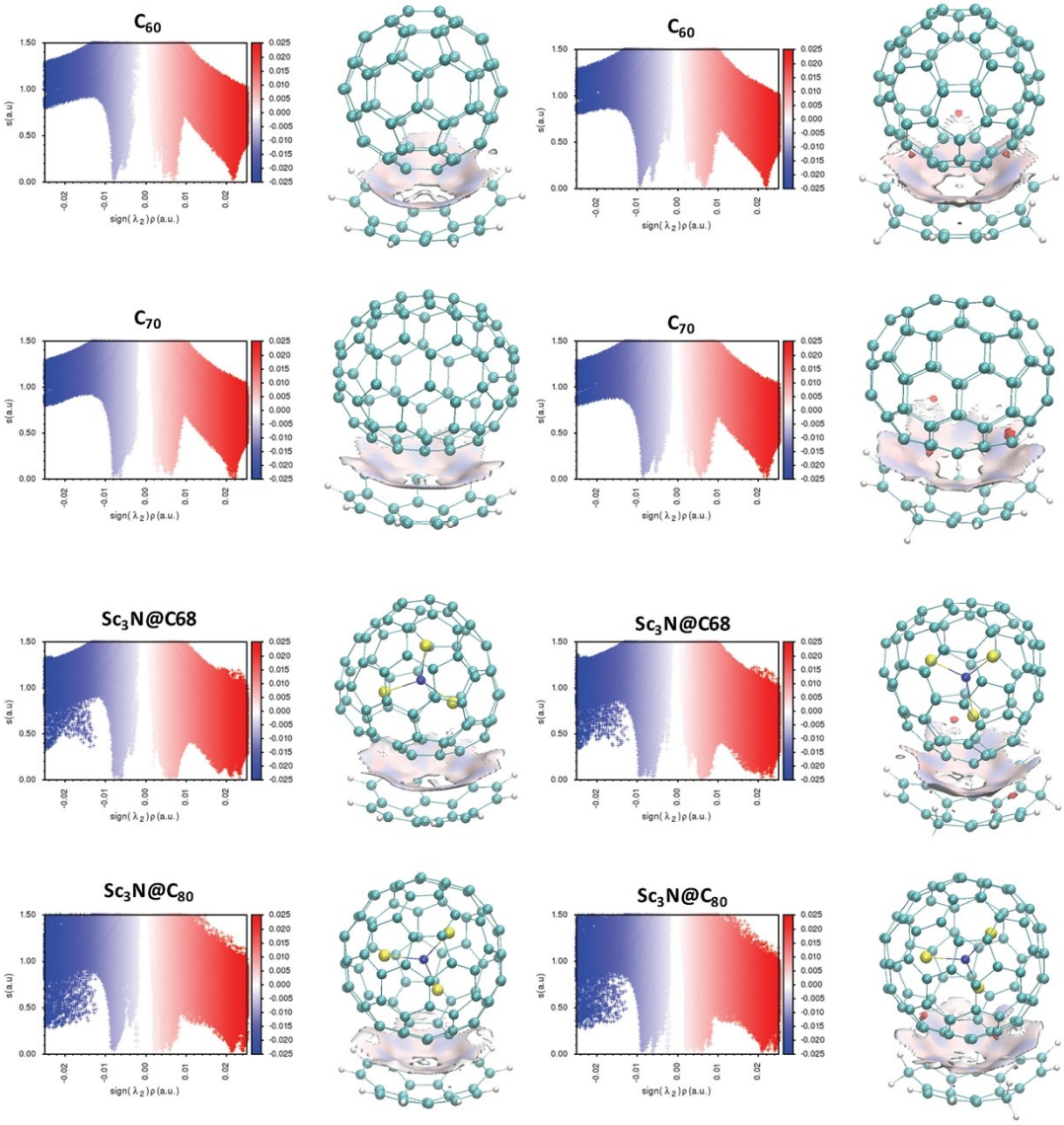


**Figure S7**. NCI plots for the most stable minima found for the dimers formed with cora (left) and suma (right) at the B3LYP-D/def2-TZVP level. Values corresponding to a isosurface of reduced density gradient of 0.5 a.u.; colour scale runs from -0.025 to 0.025.

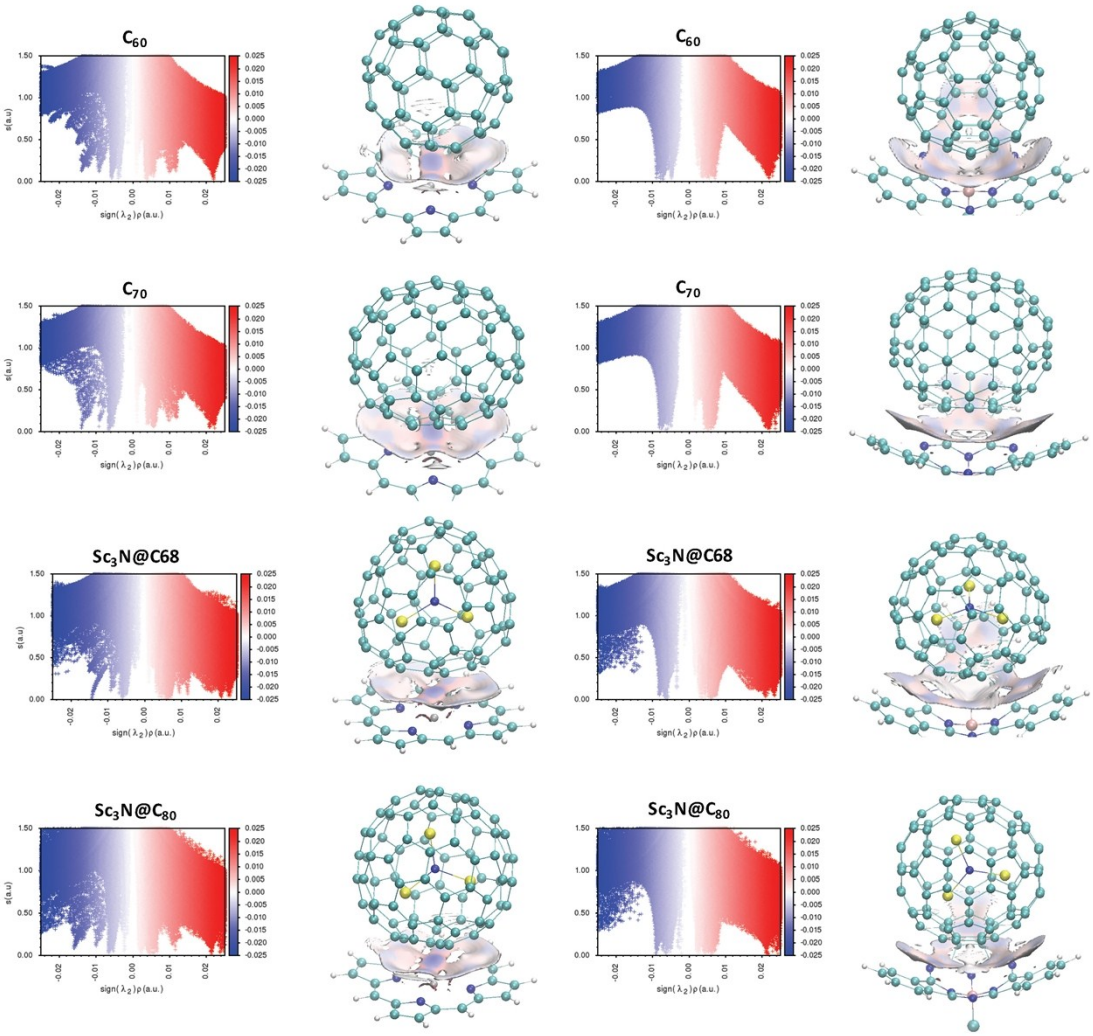


**Figure S8**. NCI plots for the most stable minima found for the dimers formed with porf (left) and sbpc (right) at the B3LYP-D/def2-TZVP level. Values corresponding to a isosurface of reduced density gradient of 0.5 a.u.; colour scale runs from -0.025 to 0.025.

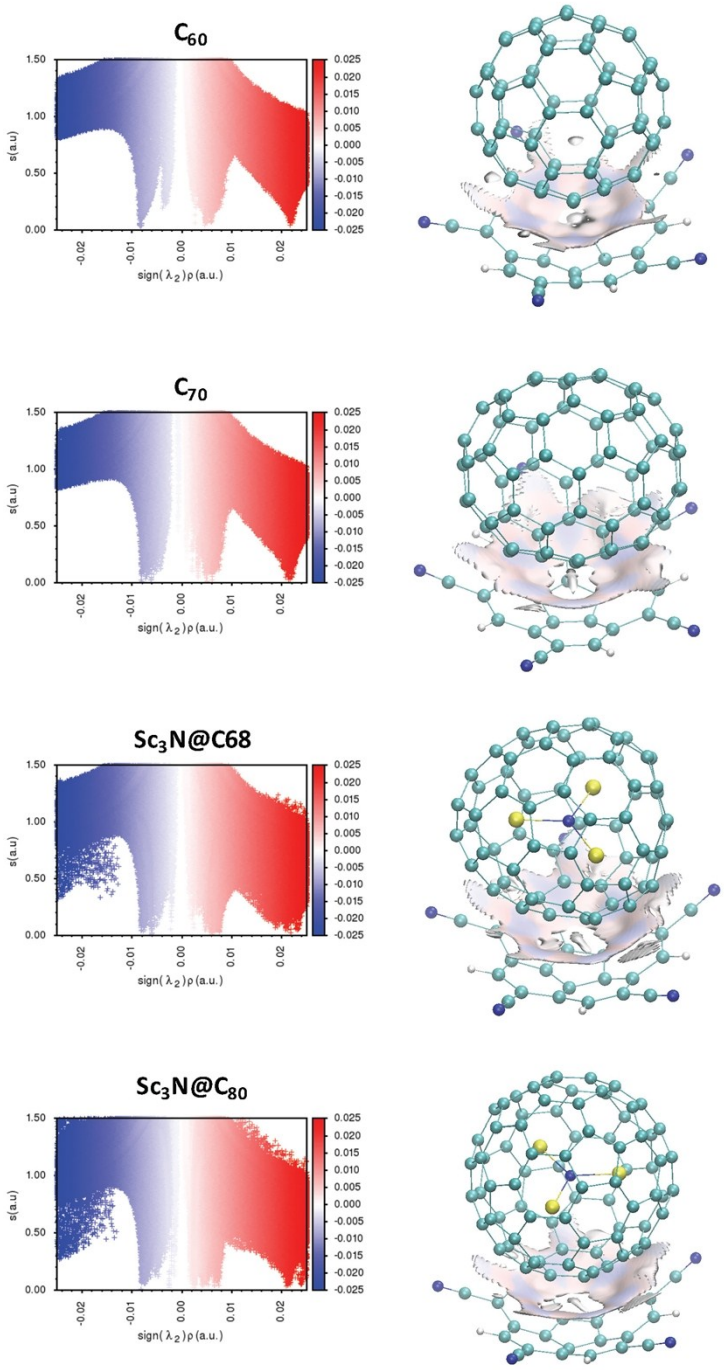


**Figure S9**. NCI plots for the most stable minima found for the dimers formed with cora5CN at the B3LYP-D/def2-TZVP level. Values corresponding to a isosurface of reduced density gradient of 0.5 a.u.; colour scale runs from -0.025 to 0.025.

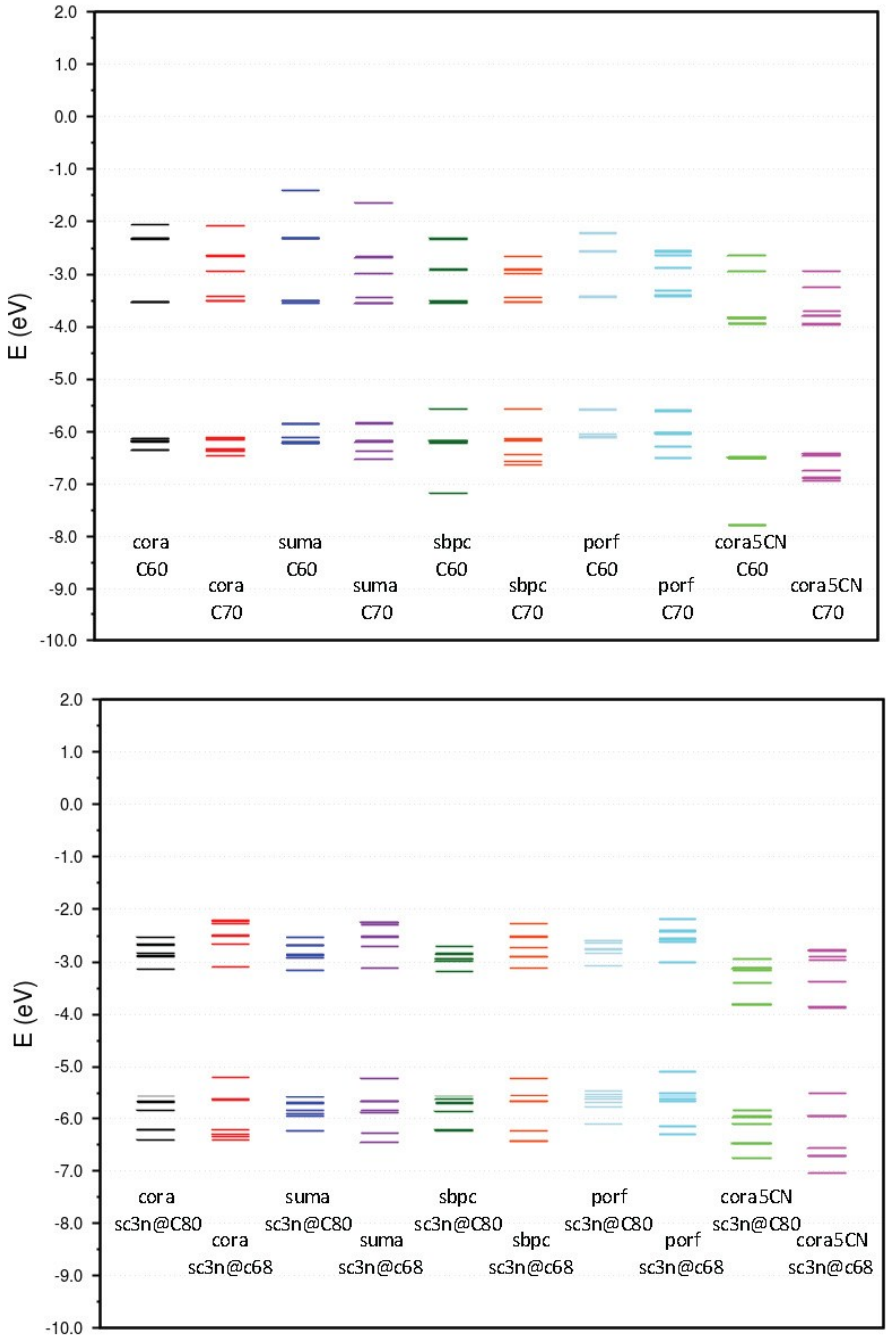


**Figure S10.** Schematic representation of the energy levels of highest occupied and lowest unoccupied molecular orbitals in the dimers studied. B3LYP-D/def2-TZVP//B97-D2/def2-TZVP.

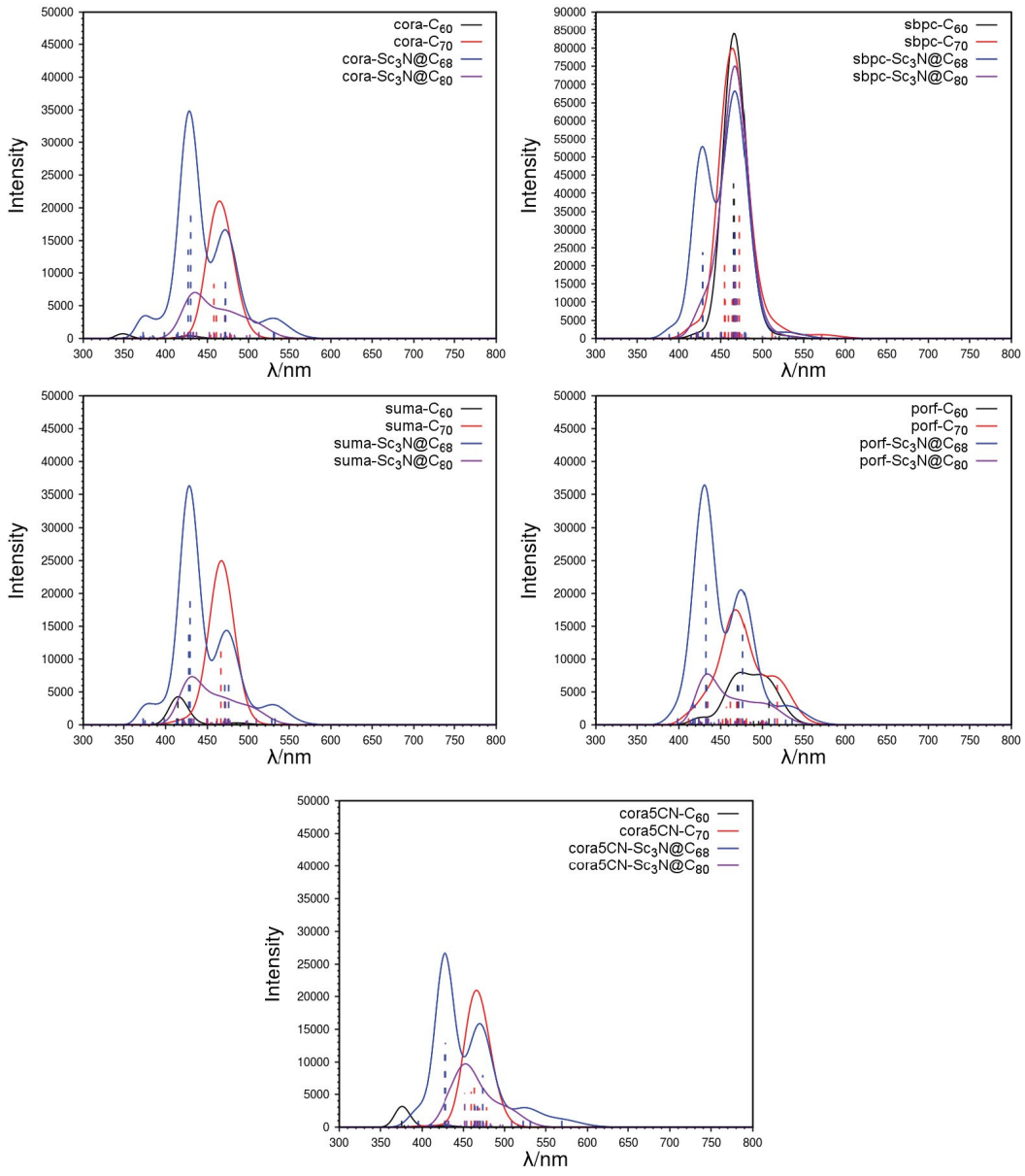


**Figure S11.** Predicted absorption spectra of the dimers studied as obtained at the CAM-B3LYP/TZVP level.

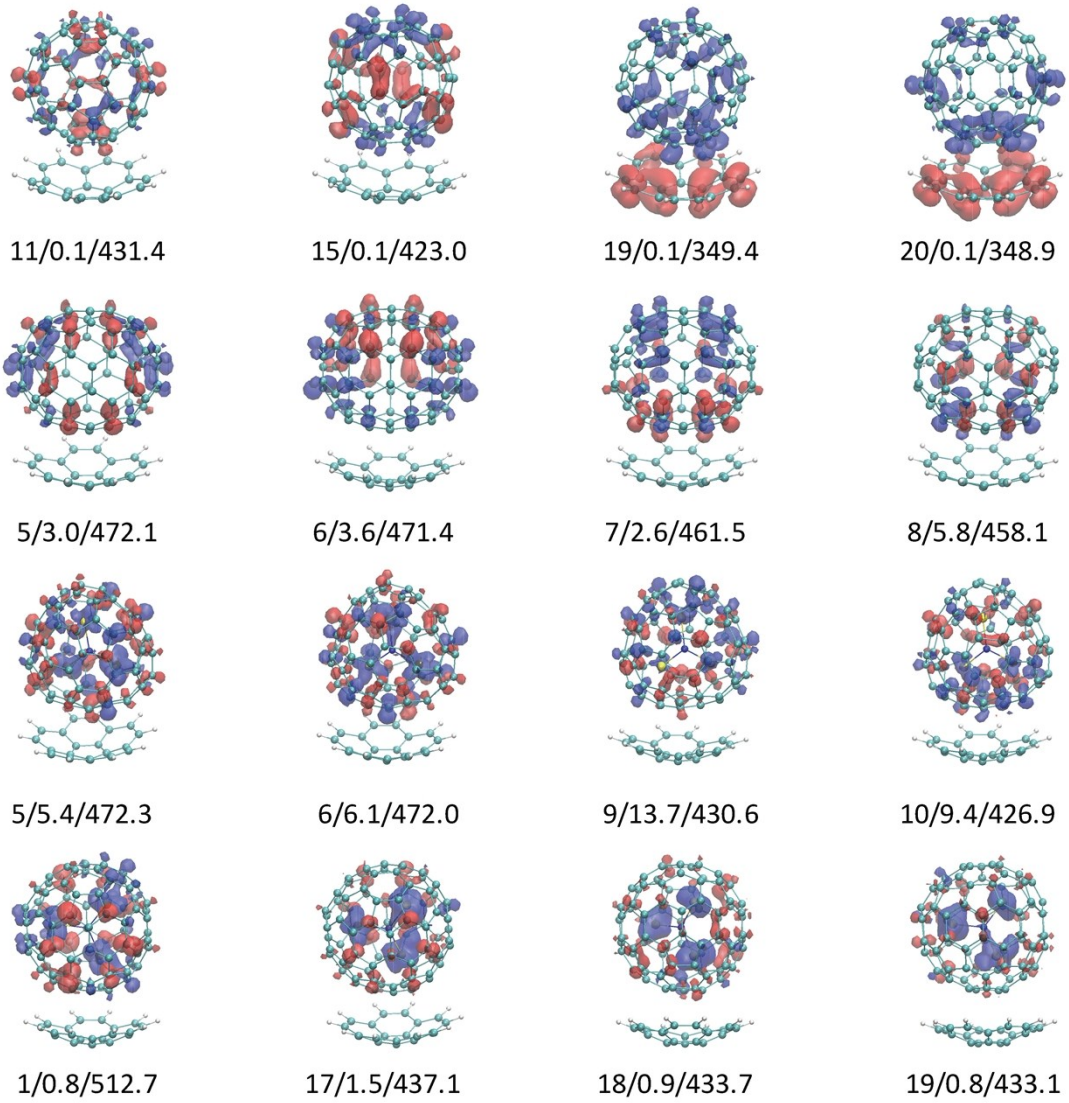


**Figure S12.** Density difference upon transition for the four most intense transitions in cora complexes. The numbers are the number of the transition/ oscillator strength * 100/ wavenumber (nm). Surfaces correspond to +0.001 a.u. (blue) and -0.001 a.u. (red).

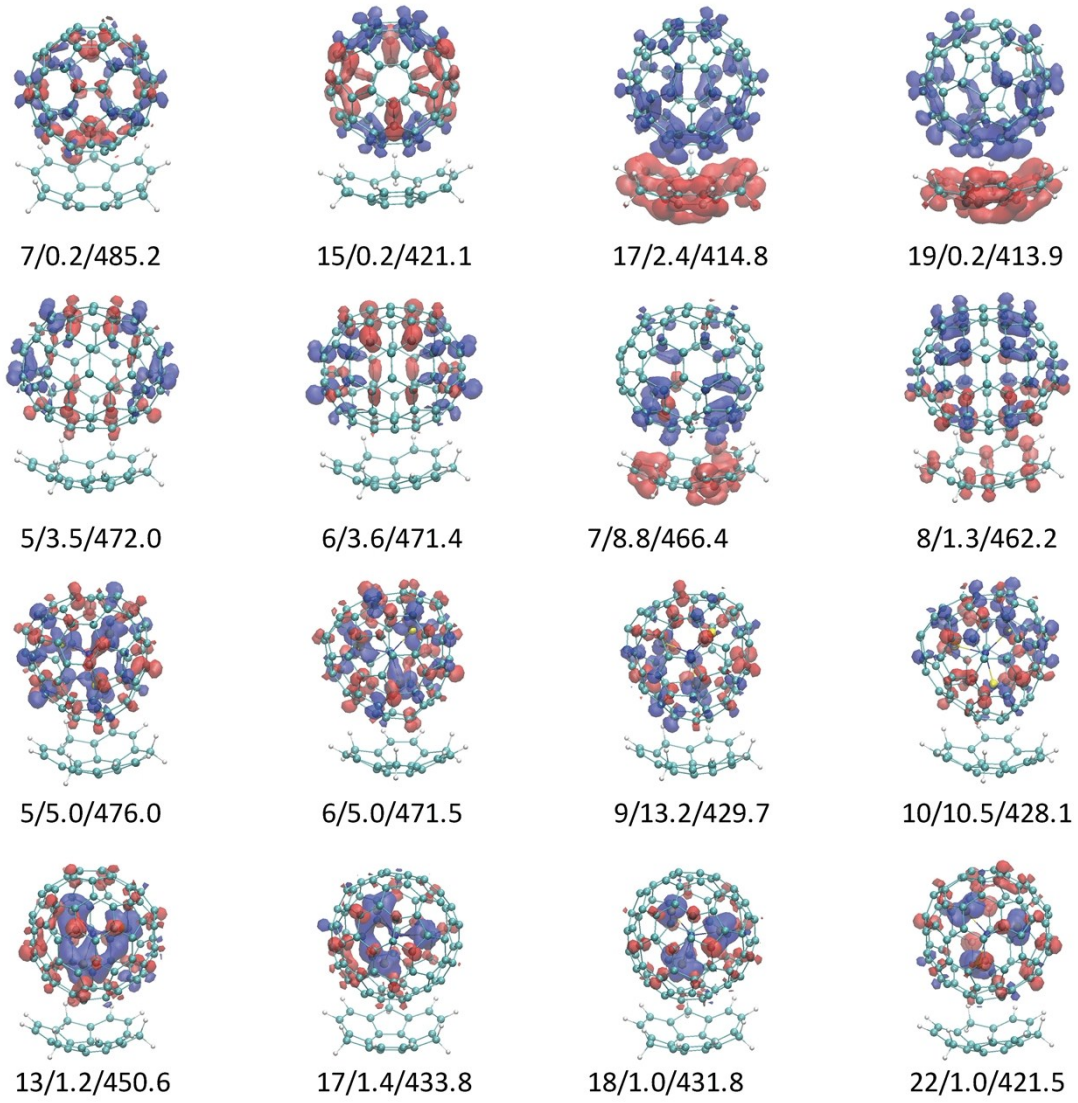


**Figure S13.** Density difference upon transition for the four most intense transitions in suma complexes. The numbers are the number of the transition/ oscillator strength * 100/ wavenumber (nm). Surfaces correspond to +0.001 a.u. (blue) and -0.001 a.u. (red).

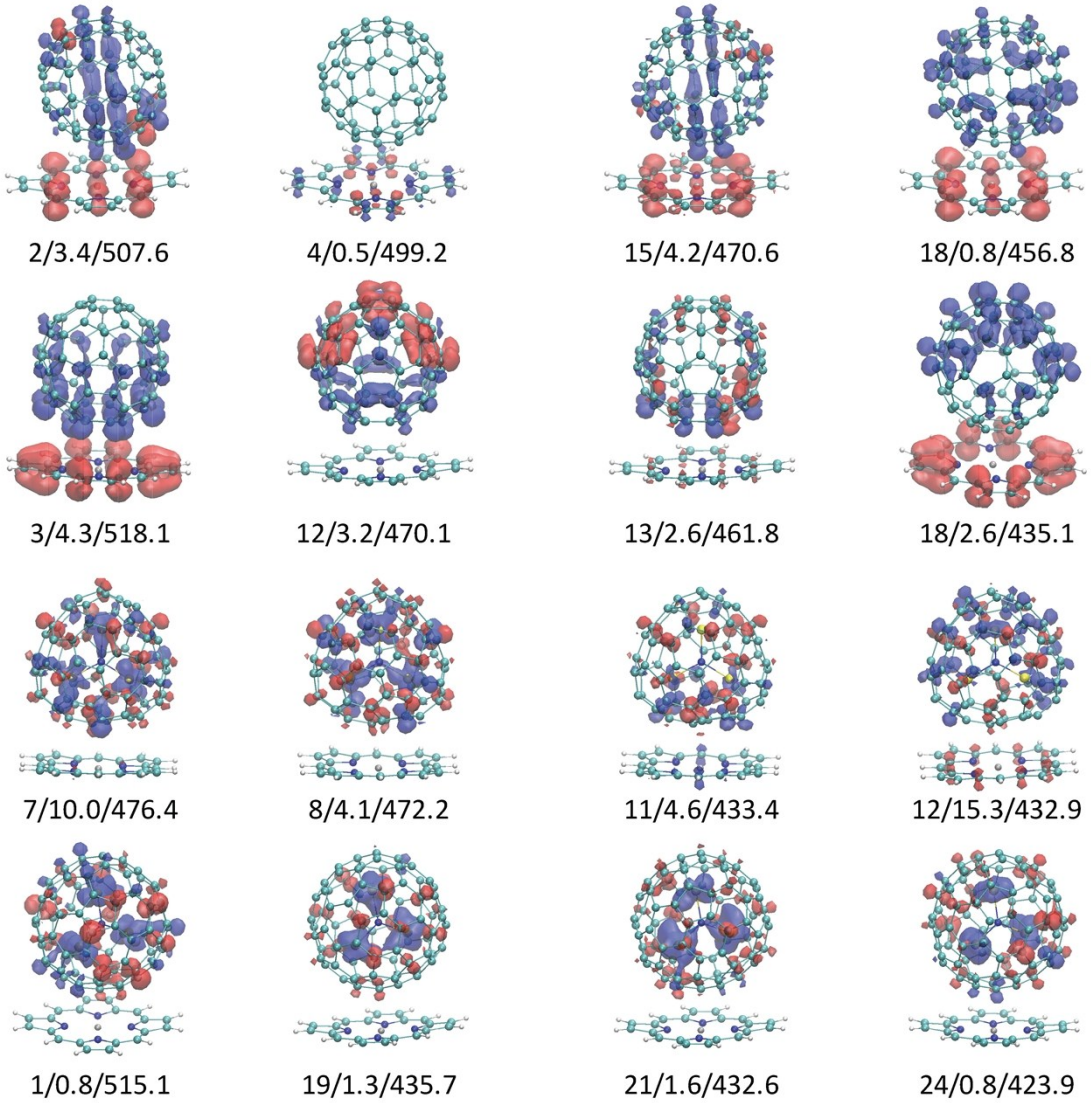


**Figure S14.** Density difference upon transition for the four most intense transitions in porf complexes. The numbers are the number of the transition/ oscillator strength * 100/ wavenumber (nm). Surfaces correspond to +0.001 a.u. (blue) and -0.001 a.u. (red).

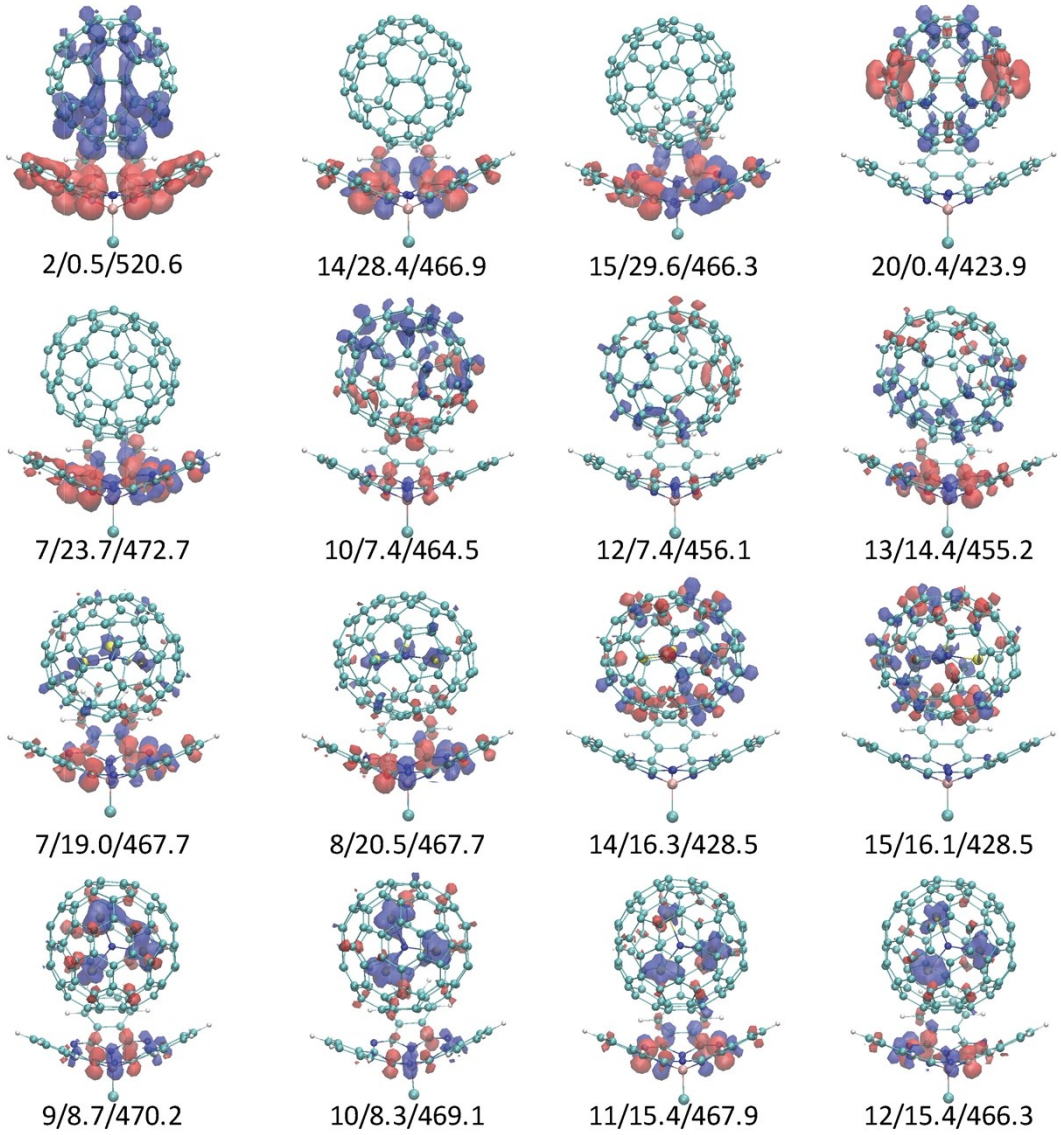


**Figure S15.** Density difference upon transition for the four most intense transitions in sbpc complexes. The numbers are the number of the transition/ oscillator strength * 100/ wavenumber (nm). Surfaces correspond to +0.001 a.u. (blue) and -0.001 a.u. (red).

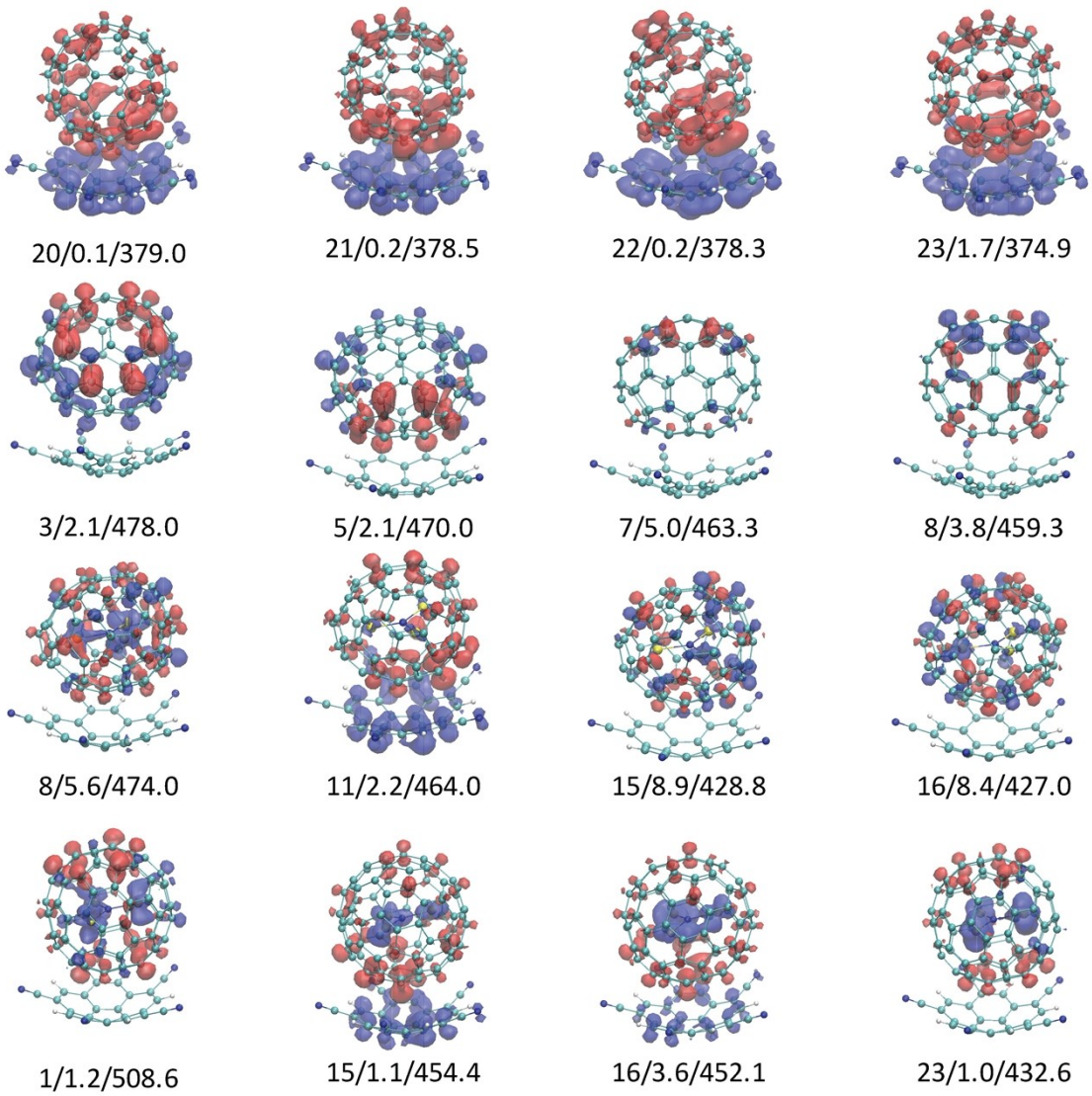


**Figure S16.** Density difference upon transition for the four most intense transitions in cora5CN complexes. The numbers are the number of the transition/ oscillator strength * 100/ wavenumber (nm). Surfaces correspond to +0.001 a.u. (blue) and -0.001 a.u. (red).

Cartesian coordinates in Å of the molecules studied and their most stable dimers at the B97-D2/def2-TZVP level.

----------cora----------
30

| | | | |
|---|---|---|---|
| C | -0.975354 | 0.708579 | 0.830891 |
| C | -0.975354 | -0.708579 | 0.830891 |
| C | 0.372686 | -1.146675 | 0.830803 |
| C | 1.205856 | 0.000000 | 0.830732 |
| C | 0.372686 | 1.146675 | 0.830803 |
| C | -2.009581 | 1.460003 | 0.284351 |
| C | -2.009581 | -1.460003 | 0.284351 |
| C | 0.767565 | -2.362410 | 0.284201 |
| C | 2.483972 | -0.000000 | 0.283891 |
| C | 0.767565 | 2.362410 | 0.284201 |
| C | 2.164328 | 2.432962 | -0.086266 |
| C | 2.982527 | 1.306699 | -0.086507 |
| C | 2.982527 | -1.306699 | -0.086507 |
| C | 2.164328 | -2.432962 | -0.086266 |
| C | -1.644991 | -2.810107 | -0.086026 |
| C | -0.321092 | -3.240343 | -0.086056 |
| C | -3.180873 | -0.696021 | -0.086492 |
| C | -3.180874 | 0.696021 | -0.086492 |
| C | -1.644991 | 2.810108 | -0.086026 |
| C | -0.321092 | 3.240343 | -0.086056 |
| H | 2.568532 | 3.368418 | -0.470944 |
| H | 3.996877 | 1.402202 | -0.471676 |
| H | 3.996877 | -1.402202 | -0.471676 |
| H | 2.568532 | -3.368418 | -0.470944 |
| H | -2.409634 | -3.483622 | -0.470975 |
| H | -0.098443 | -4.234812 | -0.470585 |
| H | -4.057459 | -1.215067 | -0.472037 |
| H | -4.057459 | 1.215067 | -0.472037 |
| H | -2.409634 | 3.483622 | -0.470975 |
| H | -0.098443 | 4.234812 | -0.470585 |

----------suma----------
33

| | | | |
|---|---|---|---|
| C | -3.305259 | 0.716304 | -0.250402 |
| C | -3.305259 | -0.716304 | -0.250402 |
| C | 3.295909 | -0.000000 | 0.018488 |
| C | 2.361699 | -1.211557 | 0.280929 |
| C | 1.216661 | -0.716177 | 0.918337 |
| C | 1.216661 | 0.716177 | 0.918337 |
| C | 2.361699 | 1.211557 | 0.280929 |
| C | 1.032128 | -3.220549 | -0.251246 |
| C | 2.272930 | -2.504186 | -0.250761 |
| C | -2.229953 | -1.439096 | 0.281146 |
| C | -1.228068 | -0.695551 | 0.918626 |
| C | 0.012140 | -1.411914 | 0.918299 |
| C | -0.131637 | -2.651061 | 0.280539 |
| C | -1.648063 | -2.853814 | 0.017931 |
| C | -1.648063 | 2.853814 | 0.017930 |
| C | -0.131637 | 2.651061 | 0.280539 |
| C | 0.012140 | 1.411914 | 0.918299 |
| C | -1.228068 | 0.695551 | 0.918626 |
| C | -2.229953 | 1.439096 | 0.281146 |
| C | 2.272930 | 2.504186 | -0.250761 |
| C | 1.032128 | 3.220549 | -0.251246 |
| H | -4.101238 | 1.220969 | -0.796456 |
| H | -4.101238 | -1.220969 | -0.796456 |
| H | 3.679171 | -0.000000 | -1.009680 |
| H | 0.993293 | -4.162096 | -0.797534 |
| H | 3.107918 | -2.941627 | -0.796582 |
| H | -1.839731 | -3.185161 | -1.010415 |
| H | -1.839731 | 3.185161 | -1.010415 |
| H | -2.084941 | 3.610394 | 0.688414 |
| H | 3.107918 | 2.941626 | -0.796582 |
| H | 0.993293 | 4.162096 | -0.797534 |
| H | -2.084941 | -3.610394 | 0.688414 |
| H | 4.169168 | -0.000000 | 0.689536 |

----------porf----------
37

| | | | |
|---|---|---|---|
| C | 4.258041 | 0.683636 | -0.000000 |
| C | 4.258041 | -0.683637 | -0.000000 |
| C | 2.874519 | -1.104163 | 0.000000 |
| C | 2.874519 | 1.104163 | 0.000000 |
| C | -0.683636 | 4.258041 | -0.000000 |
| C | 0.683637 | 4.258041 | -0.000000 |
| C | 1.104163 | 2.874519 | 0.000000 |
| C | -1.104163 | 2.874519 | 0.000000 |
| C | 2.430311 | 2.430311 | 0.000000 |
| C | -4.258041 | -0.683637 | -0.000000 |
| C | -4.258041 | 0.683636 | -0.000000 |
| C | -2.874519 | 1.104163 | 0.000000 |
| C | -2.874519 | -1.104163 | 0.000000 |
| C | -2.430311 | 2.430311 | 0.000000 |
| C | 0.683636 | -4.258041 | -0.000000 |
| C | -0.683636 | -4.258041 | -0.000000 |
| C | -1.104163 | -2.874519 | 0.000000 |
| C | 1.104163 | -2.874519 | 0.000000 |
| C | 2.430311 | -2.430311 | 0.000000 |
| C | -2.430311 | -2.430311 | 0.000000 |
| H | 5.110291 | 1.354123 | -0.000000 |
| H | 5.110291 | -1.354123 | -0.000000 |
| H | -1.354123 | 5.110291 | -0.000000 |
| H | 1.354123 | 5.110291 | -0.000000 |
| H | 3.199525 | 3.199524 | 0.000000 |
| H | -5.110291 | -1.354123 | -0.000000 |
| H | -5.110291 | 1.354123 | -0.000000 |
| H | -3.199524 | 3.199524 | 0.000000 |
| H | 1.354123 | -5.110291 | -0.000000 |
| H | -1.354123 | -5.110291 | -0.000000 |
| H | 3.199524 | -3.199524 | 0.000000 |
| H | -3.199524 | -3.199524 | -0.000000 |
| N | 2.058691 | -0.000000 | 0.000000 |
| N | 0.000000 | 2.058691 | 0.000000 |

N -2.058691 -0.000000 0.000000
N -0.000000 -2.058691 0.000000
Zn 0.000000 0.000000 0.000000
----------sbpc----------
44

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C -3.266029 0.717143 0.223390
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C -5.404814 0.705032 -0.858368
C -5.404814 -0.705033 -0.858368
C -4.333304 -1.427770 -0.333126
C -1.986923 -1.147014 0.767098
C -1.986923 1.147014 0.767097
H -4.321193 2.514511 -0.349660
H -6.254495 1.236107 -1.281424
H -6.254495 -1.236108 -1.281423
H -4.321193 -2.514511 -0.349660
C 2.253956 -2.471144 0.221069
C 1.011939 -3.188622 0.223549
C 0.929953 -4.469834 -0.329259
C 2.091437 -5.037655 -0.853647
C 3.312359 -4.332248 -0.856251
C 3.402720 -3.041438 -0.334608
C 1.986871 -1.147658 0.763376
C 0.000388 -2.295030 0.766786
H -0.017127 -5.002976 -0.342927
H 2.056329 -6.040419 -1.273420
H 4.197180 -4.803540 -1.278088
H 4.337961 -2.487910 -0.352773
C 1.011940 3.188623 0.223549
C 2.253956 2.471144 0.221069
C 3.402720 3.041438 -0.334608
C 3.312359 4.332247 -0.856252
C 2.091437 5.037655 -0.853647
C 0.929953 4.469835 -0.329259
C 0.000388 2.295031 0.766787
C 1.986871 1.147658 0.763376
H 4.337961 2.487910 -0.352774
H 4.197180 4.803539 -1.278089
H 2.056330 6.040418 -1.273420
H -0.017126 5.002977 -0.342927
N 0.685806 1.187177 1.197261
N -1.370181 0.000000 1.199290
N 0.685806 -1.187177 1.197260
N -1.334680 2.311913 0.628543
N -1.334680 -2.311913 0.628543
N 2.668826 0.000000 0.623257
B 0.001296 0.000000 1.801844
Cl 0.003391 -0.000001 3.680575
----------cora5CN----------
35

C -0.080266 -1.201368 0.950301
C 1.117836 -0.447794 0.950153
C 0.771330 0.924573 0.950740
C -0.641037 1.019256 0.951138
C -1.167233 -0.294794 0.950887
C -0.158607 -2.478819 0.418584
C 2.308535 -0.916879 0.418086
C 1.585276 1.912235 0.419009
C -1.328686 2.098791 0.419464
C -2.406101 -0.615024 0.418617
C -3.223835 0.540941 0.062699
C -2.698128 1.842012 0.060788
C -0.482014 3.233793 0.063642
C 0.917849 3.135328 0.060887
C 3.265366 0.095960 0.059762
C 2.926183 1.457659 0.062698
C 2.290421 -2.332785 0.062300
C 1.100126 -3.076117 0.060074
C -1.510804 -2.899300 0.062961
C -2.585342 -1.996778 0.060212
H -3.322258 2.652371 -0.308393
H 1.495769 3.979119 -0.308650
H 4.246544 -0.192662 -0.309807
H 1.128275 -4.098567 -0.309288
H -3.548976 -2.339548 -0.309253
C -1.101999 4.432727 -0.404245
N -1.645825 5.389528 -0.779852
C -4.555570 0.321390 -0.405350
N -5.633441 0.099092 -0.780946
C -1.714091 -4.234198 -0.403333
N -1.836448 -5.328503 -0.777271
C 3.496899 -2.938652 -0.404680
N 4.499399 -3.393724 -0.779134
C 3.874770 2.418351 -0.404249
N 4.616084 3.232389 -0.778558
----------c60----------
60

C -0.998749 0.725818 -3.328693
C -0.998749 -0.725818 -3.328693
C -1.960649 -1.424615 -2.592169
C -2.960192 -0.699083 -1.829480
C -2.960192 0.699083 -1.829480
C -1.960649 1.424615 -2.592169
C 0.381993 1.174548 -3.328877
C 1.235589 0.000000 -3.329682
C 0.381993 -1.174548 -3.328878
C 0.749345 -2.305663 -2.592971
C -1.579139 -2.598731 -1.828863
C -3.196340 -1.424946 -0.594475
C -3.423301 -0.725888 0.595039
C -3.423301 0.725888 0.595039
C -3.196341 1.424946 -0.594475
C -2.343334 2.599712 -0.594605
C -1.579139 2.598732 -1.828863
C -0.249582 3.031413 -1.829400
C 0.749345 2.305663 -2.592971
C 2.424524 0.000000 -2.593267
C 2.805724 1.174571 -1.829762
C 1.983894 2.305910 -1.829669
C 1.748789 3.032369 -0.594968

| | | | |
|---|---|---|---|
| C | 0.367689 | 3.480152 | -0.594567 |
| C | -0.367690 | 3.480152 | 0.594567 |
| C | -1.748788 | 3.032369 | 0.594968 |
| C | -1.983894 | 2.305910 | 1.829669 |
| C | -2.805725 | 1.174572 | 1.829762 |
| C | -2.343334 | -2.599711 | -0.594605 |
| C | -0.381993 | -1.174549 | 3.328877 |
| C | -0.749344 | -2.305663 | 2.592970 |
| C | 0.249582 | -3.031413 | 1.829400 |
| C | 1.579138 | -2.598732 | 1.828863 |
| C | 1.960649 | -1.424615 | 2.592169 |
| C | 0.998749 | 0.725818 | 3.328693 |
| C | -0.381994 | 1.174549 | 3.328877 |
| C | -1.235589 | 0.000000 | 3.329682 |
| C | -2.424525 | 0.000000 | 2.593268 |
| C | -2.805725 | -1.174572 | 1.829762 |
| C | -1.983894 | -2.305910 | 1.829669 |
| C | -0.367689 | -3.480152 | 0.594567 |
| C | 0.367689 | -3.480152 | -0.594567 |
| C | 1.748789 | -3.032369 | -0.594968 |
| C | 2.343335 | -2.599712 | 0.594605 |
| C | 3.196341 | -1.424946 | 0.594474 |
| C | 2.960192 | -0.699083 | 1.829480 |
| C | 2.960192 | 0.699083 | 1.829480 |
| C | 1.960649 | 1.424615 | 2.592169 |
| C | -0.749345 | 2.305663 | 2.592970 |
| C | 0.249582 | 3.031412 | 1.829400 |
| C | 1.579138 | 2.598732 | 1.828863 |
| C | 2.343334 | 2.599712 | 0.594605 |
| C | 3.196341 | 1.424946 | 0.594474 |
| C | 3.423300 | 0.725887 | -0.595039 |
| C | 3.423300 | -0.725888 | -0.595039 |
| C | 2.805725 | -1.174571 | -1.829762 |
| C | 1.983895 | -2.305910 | -1.829670 |
| C | -1.748788 | -3.032369 | 0.594968 |
| C | -0.249582 | -3.031413 | -1.829400 |
| C | 0.998749 | -0.725818 | 3.328693 |

----------c70----------

70

| | | | |
|---|---|---|---|
| C | 0.746978 | 2.298772 | 3.218361 |
| C | 1.966851 | 2.290187 | 2.440723 |
| C | 0.381347 | 1.173360 | 3.965992 |
| C | 2.785729 | 1.163339 | 2.441041 |
| C | 3.394286 | 0.718494 | 1.208192 |
| C | 3.253798 | 1.455099 | -0.000000 |
| C | 3.394286 | 0.718494 | -1.208192 |
| C | -1.955272 | 1.420628 | 3.217958 |
| C | -1.569778 | 2.578201 | 2.440421 |
| C | -0.998135 | 0.725142 | 3.966047 |
| C | -0.245186 | 3.009113 | 2.440794 |
| C | 0.365669 | 3.450471 | 1.207910 |
| C | -0.378958 | 3.544878 | -0.000000 |
| C | 0.365670 | 3.450472 | -1.207911 |
| C | 2.390398 | 2.645285 | -0.000000 |
| C | 1.732616 | 3.006795 | 1.207973 |
| C | 1.732616 | 3.006795 | -1.207974 |
| C | -1.955272 | -1.420628 | 3.217958 |
| C | -2.937639 | -0.696475 | 2.440874 |
| C | -0.998135 | -0.725142 | 3.966046 |
| C | -2.937639 | 0.696474 | 2.440874 |
| C | -3.168876 | 1.414274 | 1.208046 |
| C | -3.487411 | 0.735072 | -0.000000 |
| C | -3.168876 | 1.414274 | -1.208046 |
| C | -1.777506 | 3.091117 | -0.000000 |
| C | -2.324455 | 2.577290 | 1.208136 |
| C | -2.324455 | 2.577290 | -1.208137 |
| C | 0.746979 | -2.298773 | 3.218361 |
| C | -0.245186 | -3.009113 | 2.440794 |
| C | 0.381347 | -1.173360 | 3.965992 |
| C | -1.569778 | -2.578201 | 2.440421 |
| C | -2.324455 | -2.577290 | 1.208136 |
| C | -1.777506 | -3.091117 | -0.000000 |
| C | -2.324455 | -2.577290 | -1.208136 |
| C | -3.487412 | -0.735072 | -0.000000 |
| C | -3.168876 | -1.414274 | 1.208046 |
| C | -3.168876 | -1.414274 | -1.208046 |
| C | 2.417308 | 0.000000 | 3.218866 |
| C | 2.785730 | -1.163339 | 2.441041 |
| C | 1.234098 | -0.000000 | 3.966792 |
| C | 1.966851 | -2.290187 | 2.440724 |
| C | 1.732616 | -3.006795 | 1.207974 |
| C | 2.390398 | -2.645285 | -0.000000 |
| C | 1.732616 | -3.006795 | -1.207974 |
| C | -0.378958 | -3.544878 | -0.000000 |
| C | 0.365669 | -3.450471 | 1.207911 |
| C | 0.365670 | -3.450471 | -1.207911 |
| C | 3.253798 | -1.455099 | -0.000000 |
| C | 3.394286 | -0.718494 | 1.208192 |
| C | 3.394286 | -0.718494 | -1.208192 |
| C | 0.746979 | -2.298772 | -3.218360 |
| C | 1.966851 | -2.290187 | -2.440723 |
| C | 2.785729 | -1.163339 | -2.441041 |
| C | 0.381347 | -1.173360 | -3.965992 |
| C | -1.955272 | -1.420628 | -3.217957 |
| C | -1.569778 | -2.578201 | -2.440420 |
| C | -0.245186 | -3.009113 | -2.440794 |
| C | -0.998135 | -0.725142 | -3.966046 |
| C | -1.955272 | 1.420628 | -3.217957 |
| C | -2.937639 | 0.696474 | -2.440874 |
| C | -2.937639 | -0.696475 | -2.440874 |
| C | -0.998135 | 0.725142 | -3.966046 |
| C | 0.746978 | 2.298772 | -3.218360 |
| C | -0.245186 | 3.009113 | -2.440794 |
| C | -1.569778 | 2.578201 | -2.440421 |
| C | 0.381347 | 1.173360 | -3.965992 |
| C | 2.417308 | 0.000000 | -3.218866 |
| C | 2.785729 | 1.163339 | -2.441041 |
| C | 1.966851 | 2.290187 | -2.440723 |
| C | 1.234098 | -0.000000 | -3.966792 |

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| | | | |
|---|---|---|---|
| C | -0.000270 | -0.000309 | 3.477189 |

| | | | |
|---|---|---|---|
| C | -0.998894 | 1.001515 | 3.262567 |
| C | -2.312226 | 0.650170 | 2.797677 |
| C | -2.651649 | -0.718703 | 2.487505 |
| C | -1.654487 | -1.714535 | 2.726732 |
| C | -0.368231 | -1.365848 | 3.263055 |
| C | 0.593615 | -2.326806 | 2.797442 |
| C | 1.949443 | -1.937607 | 2.486425 |
| C | 2.312180 | -0.576222 | 2.727469 |
| C | 1.366594 | 0.363349 | 3.263343 |
| C | 1.718211 | 1.676322 | 2.796989 |
| C | 0.702514 | 2.655319 | 2.485955 |
| C | -0.657784 | 2.289637 | 2.726526 |
| C | -1.725546 | 2.710678 | 1.844016 |
| C | -2.774190 | 1.739241 | 1.959538 |
| C | -1.485211 | -2.849055 | 1.843861 |
| C | -0.118812 | -3.270477 | 1.958869 |
| C | 3.208822 | 0.138220 | 1.843455 |
| C | 2.891176 | 1.532470 | 1.958149 |
| C | 3.105989 | 2.415604 | 0.871593 |
| C | 2.222000 | 3.546577 | 0.704466 |
| C | 0.956969 | 3.594232 | 1.418196 |
| C | -0.094683 | 3.857431 | 0.432507 |
| C | -1.454177 | 3.366473 | 0.595136 |
| C | -2.189240 | 2.942400 | -0.594954 |
| C | -3.293432 | 2.009667 | -0.433262 |
| C | -3.644125 | 1.482347 | 0.871377 |
| C | -4.181907 | 0.151699 | 0.704634 |
| C | -3.591566 | -0.967465 | 1.419388 |
| C | -3.293428 | -2.009665 | 0.433257 |
| C | -2.189240 | -2.942401 | 0.594954 |
| C | -1.454177 | -3.366476 | -0.595137 |
| C | -0.094683 | -3.857439 | -0.432512 |
| C | 0.538634 | -3.897095 | 0.871971 |
| C | 1.960114 | -3.697615 | 0.704582 |
| C | 2.635836 | -2.627698 | 1.419004 |
| C | 3.388960 | -1.847949 | 0.432641 |
| C | 3.641633 | -0.424627 | 0.594695 |
| C | 3.641633 | 0.424628 | -0.594695 |
| C | 3.388963 | 1.847952 | -0.432644 |
| C | 2.635838 | 2.627705 | -1.419005 |
| C | 1.960118 | 3.697623 | -0.704576 |
| C | 0.538636 | 3.897100 | -0.871974 |
| C | -0.118812 | 3.270482 | -1.958872 |
| C | -1.485210 | 2.849054 | -1.843860 |
| C | -1.654481 | 1.714532 | -2.726726 |
| C | -2.651650 | 0.718705 | -2.487504 |
| C | -3.591570 | 0.967461 | -1.419388 |
| C | -4.181911 | -0.151699 | -0.704625 |
| C | -3.644132 | -1.482348 | -0.871381 |
| C | -2.774195 | -1.739243 | -1.959542 |
| C | -1.725543 | -2.710673 | -1.844012 |
| C | -0.657783 | -2.289631 | -2.726519 |
| C | 0.702513 | -2.655321 | -2.485954 |
| C | 0.956974 | -3.594236 | -1.418199 |
| C | 2.222003 | -3.546581 | -0.704460 |
| C | 3.105990 | -2.415606 | -0.871596 |
| C | 2.891182 | -1.532473 | -1.958153 |
| C | 3.208814 | -0.138220 | -1.843450 |
| C | 2.312172 | 0.576220 | -2.727460 |
| C | 1.949446 | 1.937610 | -2.486425 |
| C | 0.593617 | 2.326808 | -2.797440 |
| C | -0.368226 | 1.365848 | -3.263052 |
| C | -2.312229 | -0.650170 | -2.797677 |
| C | -0.998897 | -1.001512 | -3.262565 |
| C | 1.718214 | -1.676325 | -2.796991 |
| C | 1.366591 | -0.363352 | -3.263337 |
| C | -0.000270 | 0.000308 | -3.477187 |
| N | 0.001018 | 0.000001 | -0.000007 |
| Sc | 0.985882 | -1.701794 | -0.000543 |
| Sc | -1.965313 | -0.000009 | -0.000002 |
| Sc | 0.985877 | 1.701795 | 0.000524 |

----------sc3nc80----------

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| | | | |
|---|---|---|---|
| C | -2.365884 | -0.292930 | 3.355891 |
| C | -3.201904 | 0.524876 | 2.520279 |
| C | -2.666049 | 1.861969 | 2.524460 |
| C | -1.308583 | 0.530912 | 3.875425 |
| C | -1.490004 | 1.857283 | 3.364705 |
| C | 0.000153 | 0.000454 | 4.091237 |
| C | 0.195328 | -1.398342 | 3.875817 |
| C | -2.135044 | -1.665517 | 3.053625 |
| C | -0.862709 | -2.218735 | 3.363872 |
| C | -2.833561 | -2.226564 | 1.925960 |
| C | -3.831536 | -0.001068 | 1.361443 |
| C | -3.651527 | -1.397158 | 1.092920 |
| C | -4.001670 | 0.853698 | 0.234792 |
| C | -2.789630 | 2.726364 | 1.386695 |
| C | -3.480630 | 2.198098 | 0.240826 |
| C | -1.716927 | 3.665819 | 1.126925 |
| C | -0.374845 | 2.683187 | 3.054180 |
| C | -0.512039 | 3.569283 | 1.926114 |
| C | 1.114099 | 0.868752 | 3.875328 |
| C | 0.929674 | 2.196948 | 3.356287 |
| C | 2.352390 | 0.362802 | 3.363159 |
| C | 1.437952 | -1.901885 | 3.356712 |
| C | 2.511376 | -1.016033 | 3.054051 |
| C | -0.279409 | -3.238217 | 2.523518 |
| C | 1.146318 | -3.034341 | 2.520072 |
| C | -2.314089 | -3.316152 | 1.125236 |
| C | -0.965352 | -3.776133 | 1.384906 |
| C | -3.604871 | -1.921923 | -0.244382 |
| C | -2.813117 | -3.136551 | -0.245593 |
| C | -3.929792 | 0.349750 | -1.107667 |
| C | -3.694525 | -1.032854 | -1.373941 |
| C | -3.074637 | 2.519686 | -1.118638 |
| C | -3.346368 | 1.362583 | -1.938794 |
| C | -1.309899 | 4.003064 | -0.245709 |
| C | -1.964322 | 3.393284 | -1.392446 |
| C | 0.615527 | 3.861241 | 1.091912 |
| C | 0.137349 | 4.081610 | -0.245285 |
| C | 2.055666 | 2.511767 | 2.519526 |
| C | 2.944505 | 1.377784 | 2.522174 |
| C | 1.915060 | 3.319335 | 1.360617 |

| | | | |
|---|---|---|---|
| C | 3.757861 | 1.053076 | 1.386567 |
| C | 3.348031 | -1.340114 | 1.926289 |
| C | 4.037007 | -0.346183 | 1.127938 |
| C | 1.915250 | -3.315949 | 1.361155 |
| C | 3.033992 | -2.461254 | 1.091771 |
| C | -0.163499 | -4.114279 | 0.239370 |
| C | 1.260729 | -3.891588 | 0.234013 |
| C | -1.959359 | -3.403107 | -1.393202 |
| C | -0.646317 | -3.928193 | -1.120636 |
| C | -2.940155 | -1.370782 | -2.528039 |
| C | -2.058047 | -2.518406 | -2.519732 |
| C | -2.517571 | 1.020560 | -3.051738 |
| C | -2.361411 | -0.363897 | -3.367126 |
| C | -1.150702 | 3.040395 | -2.520637 |
| C | -1.436608 | 1.897346 | -3.353048 |
| C | 0.953082 | 3.716344 | -1.375432 |
| C | 0.283196 | 3.231889 | -2.529044 |
| C | 2.741340 | 3.040530 | 0.234085 |
| C | 3.642948 | 1.914897 | 0.240368 |
| C | 2.268586 | 3.229919 | -1.108708 |
| C | 3.717513 | 1.403061 | -1.118685 |
| C | 2.853387 | 2.217607 | -1.939976 |
| C | 4.121372 | -0.866554 | -0.244930 |
| C | 3.464795 | -2.158889 | -0.245341 |
| C | 3.918081 | 0.004950 | -1.391034 |
| C | 1.661095 | -3.577610 | -1.108764 |
| C | 0.492494 | -3.582504 | -1.941228 |
| C | 2.741446 | -2.683098 | -1.375784 |
| C | -0.925549 | -2.193195 | -3.353495 |
| C | -1.113614 | -0.868465 | -3.869553 |
| C | 0.374703 | -2.690943 | -3.053026 |
| C | -0.195284 | 1.398240 | -3.870411 |
| C | 0.865825 | 2.226553 | -3.367822 |
| C | 2.142011 | 1.668851 | -3.051600 |
| C | 0.000078 | -0.000328 | -4.088564 |
| C | 3.208924 | -0.524164 | -2.520752 |
| C | 2.658004 | -1.861476 | -2.529648 |
| C | 1.495411 | -1.863652 | -3.368031 |
| C | 2.362037 | 0.294619 | -3.352859 |
| C | 1.308269 | -0.530407 | -3.869583 |
| N | -0.001192 | -0.000968 | 0.046702 |
| Sc | -1.008000 | -1.736265 | 0.013725 |
| Sc | -0.992280 | 1.744979 | 0.048051 |
| Sc | 2.005648 | -0.017696 | 0.062189 |

----------cora-c60----------
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| | | | |
|---|---|---|---|
| C | -4.772972 | -0.789886 | 0.786595 |
| C | -4.765824 | -1.044727 | -0.604702 |
| C | -4.747494 | 0.200300 | -1.277679 |
| C | -4.744391 | 1.225296 | -0.301335 |
| C | -4.760043 | 0.613476 | 0.974277 |
| C | -4.263688 | -1.681907 | 1.720637 |
| C | -4.249763 | -2.209754 | -1.156130 |
| C | -4.213894 | 0.364992 | -2.548666 |
| C | -4.200944 | 2.482789 | -0.528703 |
| C | -4.235956 | 1.218508 | 2.108477 |
| C | -3.861695 | 2.605332 | 1.928715 |
| C | -3.844313 | 3.206868 | 0.673484 |
| C | -3.833408 | 2.734206 | -1.905838 |
| C | -3.839215 | 1.726216 | -2.867090 |
| C | -3.883532 | -2.097299 | -2.551919 |
| C | -3.865421 | -0.871973 | -3.214112 |
| C | -3.912748 | -3.231786 | -0.187430 |
| C | -3.920108 | -2.980963 | 1.181961 |
| C | -3.913009 | -1.081317 | 2.990145 |
| C | -3.899570 | 0.298786 | 3.174440 |
| H | -3.482838 | 3.171073 | 2.778290 |
| H | -3.452172 | 4.219225 | 0.591247 |
| H | -3.439772 | 3.710722 | -2.183913 |
| H | -3.451711 | 1.956653 | -3.858233 |
| H | -3.512707 | -2.974494 | -3.079967 |
| H | -3.479052 | -0.841784 | -4.231697 |
| H | -3.542995 | -4.195371 | -0.534072 |
| H | -3.554851 | -3.757929 | 1.851569 |
| H | -3.548955 | -1.713564 | 3.798253 |
| H | -3.524785 | 0.689732 | 4.118876 |
| C | 0.875099 | 1.080121 | -3.153574 |
| C | 0.888870 | -0.362030 | -3.323284 |
| C | -0.042813 | -1.153444 | -2.644866 |
| C | -1.020822 | -0.534103 | -1.771863 |
| C | -1.033976 | 0.851425 | -1.608861 |
| C | -0.070211 | 1.674988 | -2.312380 |
| C | 2.250594 | 1.543246 | -3.139295 |
| C | 3.114703 | 0.387478 | -3.299615 |
| C | 2.273259 | -0.790120 | -3.412918 |
| C | 2.672964 | -1.994761 | -2.825362 |
| C | 0.370299 | -2.404939 | -2.035842 |
| C | -1.213696 | -1.398972 | -0.626581 |
| C | -1.410816 | -0.847033 | 0.639015 |
| C | -1.425089 | 0.589686 | 0.807948 |
| C | -1.240277 | 1.423273 | -0.294809 |
| C | -0.405181 | 2.603409 | -0.181924 |
| C | 0.320509 | 2.759133 | -1.429504 |
| C | 1.645669 | 3.206536 | -1.417386 |
| C | 2.628846 | 2.586882 | -2.287933 |
| C | 4.325157 | 0.317342 | -2.602726 |
| C | 4.717507 | 1.399756 | -1.718756 |
| C | 3.884776 | 2.512753 | -1.563947 |
| C | 3.678046 | 3.086849 | -0.246445 |
| C | 2.294285 | 3.516178 | -0.155940 |
| C | 1.593469 | 3.366611 | 1.045737 |
| C | 0.217566 | 2.904875 | 1.032846 |
| C | 0.024792 | 2.036901 | 2.181430 |
| C | -0.779390 | 0.900235 | 2.067579 |
| C | -0.355368 | -2.556608 | -0.788018 |
| C | 1.705208 | -1.575474 | 3.218594 |
| C | 1.326427 | -2.618330 | 2.366254 |
| C | 2.309450 | -3.237088 | 1.495551 |
| C | 3.634765 | -2.790254 | 1.508199 |
| C | 4.027504 | -1.708090 | 2.392197 |
| C | 3.066369 | 0.330397 | 3.400215 |
| C | 1.682480 | 0.758781 | 3.492449 |
| C | 0.841601 | -0.419186 | 3.378754 |
| C | -0.366432 | -0.348748 | 2.679010 |
| C | -0.757062 | -1.429398 | 1.793892 |
| C | 0.069382 | -2.545974 | 1.642918 |
| C | 1.660187 | -3.547302 | 0.234121 |
| C | 2.361011 | -3.398729 | -0.967579 |
| C | 3.736328 | -2.934933 | -0.953781 |
| C | 4.361666 | -2.636774 | 0.260844 |
| C | 5.203049 | -1.459071 | 0.373929 |
| C | 4.996437 | -0.885190 | 1.691314 |
| C | 4.982706 | 0.503578 | 1.854357 |
| C | 3.999807 | 1.122792 | 2.724722 |
| C | 1.282234 | 1.962895 | 2.903778 |
| C | 2.251267 | 2.784491 | 2.201713 |
| C | 3.584996 | 2.372736 | 2.114374 |
| C | 4.311357 | 2.526178 | 0.867161 |
| C | 5.175260 | 1.370786 | 0.706309 |
| C | 5.374663 | 0.818161 | -0.562447 |
| C | 5.389021 | -0.623545 | -0.731925 |
| C | 4.740326 | -0.933251 | -1.993100 |
| C | 3.929410 | -2.067395 | -2.101984 |
| C | 0.275596 | -3.120532 | 0.325070 |
| C | 1.703838 | -2.817102 | -2.123698 |
| C | 3.080210 | -1.111517 | 3.230591 |

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| | | | |
|---|---|---|---|
| C | -1.099102 | 0.665538 | 5.034558 |
| C | -0.790614 | -0.713586 | 5.110856 |
| C | 0.618633 | -0.847217 | 5.113037 |
| C | 1.180841 | 0.449231 | 5.037459 |
| C | 0.119450 | 1.383826 | 4.985444 |
| C | -2.282236 | 1.145683 | 4.489359 |
| C | -1.642278 | -1.704807 | 4.642339 |
| C | 1.270976 | -1.981067 | 4.648234 |
| C | 2.434324 | 0.698056 | 4.495169 |
| C | 0.238388 | 2.627440 | 4.380069 |
| C | 1.589374 | 2.979688 | 3.997195 |
| C | 2.634931 | 2.062538 | 4.055075 |
| C | 3.209341 | -0.490469 | 4.210152 |
| C | 2.654658 | -1.765718 | 4.280375 |
| C | -0.990906 | -2.964280 | 4.351463 |
| C | 0.395521 | -3.095796 | 4.354620 |
| C | -2.959013 | -1.233060 | 4.269048 |
| C | -3.264647 | 0.123510 | 4.199253 |

| | | | |
|---|---|---|---|
| C | -2.221125 | 2.523883 | 4.050354 |
| C | -1.021420 | 3.227569 | 3.994942 |
| H | 1.782703 | 3.956216 | 3.556286 |
| H | 3.603315 | 2.356937 | 3.654500 |
| H | 4.222353 | -0.388868 | 3.824697 |
| H | 3.256556 | -2.609642 | 3.947509 |
| H | -1.589504 | -3.812154 | 4.021733 |
| H | 0.825894 | -4.041171 | 4.027607 |
| H | -3.707891 | -1.948525 | 3.933284 |
| H | -4.239396 | 0.413127 | 3.810509 |
| H | -3.116059 | 2.997350 | 3.650671 |
| H | -1.027089 | 4.223909 | 3.555873 |
| C | 2.980039 | -2.711219 | -1.282087 |
| C | 2.190824 | -2.744322 | -0.069286 |
| C | 3.833457 | -1.631547 | -1.537606 |
| C | 2.282028 | -1.701082 | 0.848256 |
| C | 1.087593 | -1.199527 | 1.484773 |
| C | -0.178423 | -1.803641 | 1.271367 |
| C | -1.311226 | -0.973689 | 1.475952 |
| C | 3.096508 | -1.588538 | -3.889906 |
| C | 2.210227 | -2.699073 | -3.618379 |
| C | 3.892417 | -1.057914 | -2.868102 |
| C | 2.152906 | -3.250061 | -2.339988 |
| C | 0.876396 | -3.630425 | -1.778710 |
| C | -0.325899 | -3.539339 | -2.533549 |
| C | -1.530003 | -3.402929 | -1.788672 |
| C | -0.278059 | -2.904784 | 0.305462 |
| C | 0.899664 | -3.317400 | -0.376234 |
| C | -1.506362 | -3.090855 | -0.386177 |
| C | 3.360401 | 1.229632 | -3.622172 |
| C | 2.532464 | 0.675440 | -4.671882 |
| C | 4.026753 | 0.380071 | -2.731298 |
| C | 2.402636 | -0.705654 | -4.802664 |
| C | 1.111560 | -1.279287 | -5.105219 |
| C | -0.023945 | -0.463414 | -5.364265 |
| C | -1.293695 | -1.053588 | -5.115519 |
| C | -0.264905 | -2.957717 | -3.882015 |
| C | 0.992549 | -2.510539 | -4.373270 |
| C | -1.412866 | -2.284865 | -4.384115 |
| C | 3.406330 | 1.847325 | -0.849470 |
| C | 2.711584 | 2.717640 | -1.773669 |
| C | 4.051376 | 0.695696 | -1.316334 |
| C | 2.688890 | 2.414037 | -3.133362 |
| C | 1.470894 | 2.596773 | -3.889057 |
| C | 0.308689 | 3.167817 | -3.300868 |
| C | -0.934554 | 2.823657 | -3.899563 |
| C | 0.112590 | 0.993359 | -5.226467 |
| C | 1.374589 | 1.523609 | -4.840397 |
| C | -1.031351 | 1.750316 | -4.850388 |
| C | 3.169526 | -0.587255 | 0.594930 |
| C | 2.495672 | 0.602796 | 1.063323 |
| C | 3.930760 | -0.547195 | -0.578721 |
| C | 2.615344 | 1.797825 | 0.360455 |
| C | 1.457583 | 2.645755 | 0.189560 |
| C | 0.213278 | 2.336790 | 0.803027 |
| C | -0.946821 | 2.872169 | 0.180239 |
| C | 0.332616 | 3.489281 | -1.866714 |
| C | 1.517253 | 3.214543 | -1.129168 |
| C | -0.888471 | 3.440082 | -1.139010 |
| C | 0.091656 | 1.077253 | 1.547831 |
| C | 1.220159 | 0.220990 | 1.619033 |
| C | -1.177796 | 0.446573 | 1.610655 |
| C | -3.001251 | 2.450032 | -0.876769 |
| C | -2.243425 | 2.254155 | 0.340159 |
| C | -2.355324 | 1.059351 | 1.044258 |
| C | -3.845967 | 1.438792 | -1.349815 |
| C | -3.047799 | 1.831466 | -3.649606 |
| C | -2.171679 | 2.870993 | -3.154165 |
| C | -2.148727 | 3.174350 | -1.794540 |
| C | -3.869359 | 1.123061 | -2.765010 |
| C | -3.311227 | -0.984928 | -3.916906 |
| C | -2.457039 | -0.248434 | -4.822683 |
| C | -2.327922 | 1.132335 | -4.691881 |
| C | -4.003391 | -0.314954 | -2.901412 |
| C | -3.429223 | -2.107716 | -1.309190 |
| C | -2.708379 | -2.792329 | -2.360624 |
| C | -2.650575 | -2.241585 | -3.639210 |
| C | -4.063727 | -0.887727 | -1.570909 |
| C | -3.235583 | 0.015557 | 0.569090 |
| C | -2.573082 | -1.243989 | 0.828371 |
| C | -2.670240 | -2.286117 | -0.089659 |
| C | -3.964892 | 0.195977 | -0.611729 |

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| | | | |
|---|---|---|---|
| C | 5.155396 | -1.385806 | 0.621240 |
| C | 5.142520 | -1.488633 | -0.790584 |
| C | 5.189041 | -0.178022 | -1.324537 |
| C | 5.239573 | 0.734421 | -0.243200 |
| C | 5.213478 | -0.012038 | 0.959478 |
| C | 4.591349 | -2.344928 | 1.451843 |
| C | 4.566280 | -2.558237 | -1.463578 |
| C | 4.654072 | 0.150620 | -2.563171 |
| C | 4.770475 | 2.038258 | -0.333424 |
| C | 4.709838 | 0.494127 | 2.150056 |
| C | 4.417409 | 1.911403 | 2.121212 |
| C | 4.449532 | 2.646892 | 0.940145 |
| C | 4.416460 | 2.457054 | -1.672395 |
| C | 4.353868 | 1.556524 | -2.732447 |
| C | 4.195706 | -2.275316 | -2.833116 |
| C | 4.233661 | -0.984839 | -3.355143 |
| C | 4.177980 | -3.661711 | -0.610911 |
| C | 4.189572 | -3.560068 | 0.777307 |
| C | 4.248163 | -1.864953 | 2.774022 |
| C | 4.304336 | -0.514021 | 3.106306 |
| H | 4.062747 | 2.403154 | 3.025310 |
| H | 4.118202 | 3.683363 | 0.968794 |
| H | 4.080251 | 3.478658 | -1.842117 |
| H | 3.970118 | 1.908863 | -3.688492 |
| H | 3.770950 | -3.068260 | -3.446875 |
| H | 3.837622 | -0.819910 | -4.355945 |
| H | 3.760036 | -4.561600 | -1.058961 |
| H | 3.782242 | -4.385135 | 1.359230 |
| H | 3.836099 | -2.559544 | 3.504300 |

| | | | |
|---|---|---|---|
| H | 3.931436 | -0.206725 | 4.081822 |
| C | -1.992699 | 0.027159 | 3.529742 |
| C | -3.091770 | 0.913924 | 3.302533 |
| C | -4.328692 | 0.431839 | 2.751624 |
| C | -4.489043 | -0.952730 | 2.372574 |
| C | -3.393603 | -1.834168 | 2.629102 |
| C | -2.185234 | -1.361608 | 3.245722 |
| C | -1.094928 | -2.183264 | 2.795779 |
| C | 0.219010 | -1.623371 | 2.573665 |
| C | 0.404786 | -0.241158 | 2.885387 |
| C | -0.670139 | 0.557329 | 3.408728 |
| C | -0.454673 | 1.921503 | 3.011408 |
| C | -1.562548 | 2.787726 | 2.682502 |
| C | -2.880796 | 2.256387 | 2.835803 |
| C | -3.945853 | 2.588380 | 1.913343 |
| C | -4.875378 | 1.495197 | 1.932593 |
| C | -3.047883 | -2.901752 | 1.714226 |
| C | -1.648030 | -3.166288 | 1.885645 |
| C | 1.249277 | 0.610048 | 2.077813 |
| C | 0.766574 | 1.950127 | 2.229589 |
| C | 0.925811 | 2.897334 | 1.188716 |
| C | -0.075360 | 3.924787 | 1.017818 |
| C | -1.369593 | 3.794559 | 1.665004 |
| C | -2.396053 | 3.978024 | 0.635422 |
| C | -3.693562 | 3.325455 | 0.705812 |
| C | -4.315178 | 2.871219 | -0.537154 |
| C | -5.310268 | 1.811884 | -0.469146 |
| C | -5.661074 | 1.188969 | 0.793869 |
| C | -6.026050 | -0.188375 | 0.547665 |
| C | -5.341624 | -1.262928 | 1.248659 |
| C | -4.872322 | -2.218039 | 0.241148 |
| C | -3.673859 | -3.021068 | 0.426431 |
| C | -2.836213 | -3.304027 | -0.737622 |
| C | -1.438010 | -3.640805 | -0.520917 |
| C | -0.867978 | -3.664773 | 0.813153 |
| C | 0.526674 | -3.290420 | 0.730597 |
| C | 1.033309 | -2.179216 | 1.519898 |
| C | 1.729829 | -1.272628 | 0.605323 |
| C | 1.801976 | 0.156923 | 0.833205 |
| C | 1.756429 | 1.048349 | -0.318189 |
| C | 1.331868 | 2.422490 | -0.118200 |
| C | 0.547453 | 3.154420 | -1.113653 |
| C | -0.283942 | 4.108648 | -0.396124 |
| C | -1.709106 | 4.148180 | -0.631125 |
| C | -2.233506 | 3.496342 | -1.774234 |
| C | -3.543911 | 2.912940 | -1.748748 |
| C | -3.534479 | 1.806687 | -2.682011 |
| C | -4.417031 | 0.692815 | -2.532895 |
| C | -5.430524 | 0.784310 | -1.507436 |
| C | -5.918346 | -0.426534 | -0.869670 |
| C | -5.218538 | -1.676723 | -1.058817 |
| C | -4.271272 | -1.782196 | -2.106673 |
| C | -3.122127 | -2.630698 | -1.974497 |
| C | -2.070648 | -2.050088 | -2.782941 |
| C | -0.689528 | -2.262918 | -2.483351 |
| C | -0.378647 | -3.208954 | -1.436691 |
| C | 0.831604 | -3.041369 | -0.654589 |
| C | 1.577977 | -1.808807 | -0.729558 |
| C | 1.314796 | -0.914500 | -1.790930 |
| C | 1.458042 | 0.497456 | -1.606693 |
| C | 0.534069 | 1.141033 | -2.515998 |
| C | 0.001202 | 2.438358 | -2.244179 |
| C | -1.374948 | 2.681632 | -2.610933 |
| C | -2.191794 | 1.635192 | -3.162805 |
| C | -3.902852 | -0.612023 | -2.877961 |
| C | -2.535742 | -0.787698 | -3.286710 |
| C | 0.216090 | -1.160354 | -2.702376 |
| C | -0.264312 | 0.121786 | -3.140570 |
| C | -1.653786 | 0.332365 | -3.408435 |
| N | -1.827949 | 0.181257 | 0.052052 |
| Sc | -0.654423 | -1.397616 | 0.065634 |
| Sc | -3.779044 | -0.039952 | -0.032039 |
| Sc | -1.050316 | 1.980422 | 0.169516 |

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| | | | |
|---|---|---|---|
| C | -0.509953 | 0.351748 | 5.725108 |
| C | -0.496345 | -1.064769 | 5.678864 |
| C | 0.850000 | -1.485010 | 5.539150 |
| C | 1.668247 | -0.328583 | 5.500631 |
| C | 0.828170 | 0.806743 | 5.617908 |
| C | -1.597846 | 1.108690 | 5.306995 |
| C | -1.570196 | -1.812096 | 5.209851 |
| C | 1.205815 | -2.679270 | 4.923714 |
| C | 2.892294 | -0.294158 | 4.843512 |
| C | 1.161220 | 2.047006 | 5.087392 |
| C | 2.519097 | 2.147786 | 4.595152 |
| C | 3.343249 | 1.032337 | 4.477537 |
| C | 3.367204 | -1.582468 | 4.384533 |
| C | 2.564180 | -2.718819 | 4.423412 |
| C | -1.227469 | -3.146723 | 4.765110 |
| C | 0.094899 | -3.560018 | 4.629299 |
| C | -2.778300 | -1.049585 | 4.974141 |
| C | -2.791835 | 0.341592 | 5.020262 |
| C | -1.280529 | 2.477196 | 4.955216 |
| C | 0.033721 | 2.924070 | 4.850711 |
| H | 2.873538 | 3.098174 | 4.199276 |
| H | 4.312508 | 1.152795 | 3.996597 |
| H | 4.339113 | -1.650844 | 3.898220 |
| H | 2.936898 | -3.633111 | 3.963685 |
| H | -2.017331 | -3.815979 | 4.426500 |
| H | 0.290604 | -4.537301 | 4.189912 |
| H | -3.679906 | -1.565969 | 4.647492 |
| H | -3.703096 | 0.860920 | 4.727326 |
| H | -2.082708 | 3.152610 | 4.661655 |
| H | 0.210962 | 3.931836 | 4.478244 |
| C | 3.194605 | -2.293064 | -1.487377 |
| C | 2.267935 | -3.059042 | -0.697557 |
| C | 2.145187 | -2.423740 | 0.590523 |
| C | 3.644867 | -1.180022 | -0.695577 |
| C | 2.999365 | -1.257109 | 0.582211 |
| C | 3.930531 | 0.084652 | -1.297984 |
| C | 3.859401 | 0.175496 | -2.722757 |
| C | 3.034961 | -2.164101 | -2.897863 |

| | | | |
|---|---|---|---|
| C | 3.417835 | -0.938616 | -3.509685 |
| C | 1.960031 | -2.897657 | -3.519398 |
| C | 1.158769 | -3.719441 | -1.290542 |
| C | 1.034667 | -3.643192 | -2.717586 |
| C | -0.048788 | -3.819285 | -0.541592 |
| C | 0.925076 | -2.472021 | 1.343265 |
| C | -0.169512 | -3.192417 | 0.751817 |
| C | 0.589347 | -1.333450 | 2.172907 |
| C | 2.622735 | -0.081060 | 1.285669 |
| C | 1.409392 | -0.146236 | 2.059698 |
| C | 3.646377 | 1.262478 | -0.540174 |
| C | 2.992639 | 1.180817 | 0.738956 |
| C | 3.205793 | 2.465457 | -1.185699 |
| C | 3.409814 | 1.380555 | -3.367030 |
| C | 3.035668 | 2.520021 | -2.596631 |
| C | 2.689945 | -0.427744 | -4.650241 |
| C | 2.684890 | 1.010659 | -4.552788 |
| C | 1.280932 | -2.459135 | -4.723383 |
| C | 1.602834 | -1.146094 | -5.250369 |
| C | -0.243619 | -3.628408 | -3.376367 |
| C | -0.111110 | -2.931267 | -4.642611 |
| C | -1.334888 | -3.779307 | -1.181583 |
| C | -1.457688 | -3.643810 | -2.597886 |
| C | -1.546913 | -2.753466 | 0.901835 |
| C | -2.255804 | -3.114233 | -0.303075 |
| C | -0.801311 | -0.891506 | 2.333901 |
| C | -1.886625 | -1.579034 | 1.657710 |
| C | 0.566440 | 1.002900 | 2.171906 |
| C | -0.789778 | 0.554615 | 2.302887 |
| C | 2.145505 | 2.334491 | 0.882778 |
| C | 2.276390 | 3.137890 | -0.306487 |
| C | 0.907576 | 2.257266 | 1.570344 |
| C | 1.185838 | 3.925602 | -0.804901 |
| C | 1.957410 | 3.337806 | -3.094039 |
| C | 1.071553 | 4.103369 | -2.239586 |
| C | 1.571558 | 1.766433 | -5.006276 |
| C | 1.235426 | 2.950681 | -4.269934 |
| C | 0.507153 | -0.361585 | -5.756164 |
| C | 0.499821 | 1.076636 | -5.643110 |
| C | -1.214179 | -2.087270 | -5.079408 |
| C | -0.871825 | -0.819011 | -5.670382 |
| C | -2.561364 | -2.907903 | -3.105511 |
| C | -2.424511 | -2.113167 | -4.307827 |
| C | -3.313979 | -2.301535 | -0.815423 |
| C | -3.487688 | -2.247313 | -2.232807 |
| C | -2.968274 | -0.789802 | 1.141818 |
| C | -3.686265 | -1.155582 | -0.054373 |
| C | -1.864803 | 1.349759 | 1.767779 |
| C | -2.975375 | 0.654893 | 1.224227 |
| C | -0.171751 | 3.071368 | 1.125383 |
| C | -0.041525 | 3.888839 | -0.055081 |
| C | -1.533836 | 2.623965 | 1.215524 |
| C | -1.342997 | 3.940340 | -0.704804 |
| C | -2.252595 | 3.140570 | 0.085139 |
| C | -0.240718 | 4.171567 | -2.904153 |
| C | -0.119017 | 3.417142 | -4.139774 |
| C | -1.472690 | 4.044089 | -2.136391 |
| C | -0.861916 | 1.509395 | -5.498011 |
| C | -1.706351 | 0.347964 | -5.497299 |
| C | -1.200868 | 2.657699 | -4.717864 |
| C | -3.269657 | -0.953309 | -4.154431 |
| C | -3.919928 | -1.037282 | -2.877633 |
| C | -2.901095 | 0.303941 | -4.713969 |
| C | -4.132705 | 0.048942 | -0.696193 |
| C | -3.701402 | 1.166609 | 0.097330 |
| C | -3.313275 | 2.395415 | -0.518762 |
| C | -4.207098 | 0.140443 | -2.120509 |
| C | -2.548865 | 3.293414 | -2.721368 |
| C | -2.432398 | 2.642335 | -4.010474 |
| C | -3.282374 | 1.487448 | -4.009280 |
| C | -3.472239 | 2.514159 | -1.930046 |
| C | -3.917920 | 1.404801 | -2.722547 |
| N | -0.087175 | 0.119120 | -1.713613 |
| Sc | 0.061914 | -1.038188 | -3.342166 |
| Sc | -0.244108 | -0.696854 | 0.112851 |
| Sc | -0.097579 | 2.112422 | -1.897510 |

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| | | | |
|---|---|---|---|
| C | -3.103490 | -3.771562 | 0.716209 |
| C | -3.103481 | -3.771571 | -0.716220 |
| C | 3.545568 | -3.512951 | 0.000003 |
| C | 2.634426 | -3.844056 | -1.219040 |
| C | 1.520040 | -4.517179 | -0.713002 |
| C | 1.520037 | -4.517155 | 0.713014 |
| C | 2.634422 | -3.844031 | 1.219047 |
| C | 1.288269 | -3.474883 | -3.260176 |
| C | 2.525527 | -3.387588 | -2.543496 |
| C | -1.967335 | -4.161377 | -1.444819 |
| C | -0.911822 | -4.685291 | -0.694410 |
| C | 0.320260 | -4.601259 | -1.407411 |
| C | 0.138252 | -4.019470 | -2.664354 |
| C | -1.398393 | -3.860694 | -2.862671 |
| C | -1.398400 | -3.860663 | 2.862674 |
| C | 0.138245 | -4.019447 | 2.664353 |
| C | 0.320252 | -4.601234 | 1.407409 |
| C | -0.911829 | -4.685263 | 0.694411 |
| C | -1.967328 | -4.161316 | 1.444810 |
| C | 2.525528 | -3.387590 | 2.543515 |
| C | 1.288270 | -3.474898 | 3.260196 |
| H | -3.961789 | -3.325509 | 1.215693 |
| H | -3.961732 | -3.325428 | -1.215707 |
| H | 3.844813 | -2.457658 | -0.000006 |
| H | 1.234315 | -2.976252 | -4.226364 |
| H | 3.334493 | -2.827962 | -3.009861 |
| H | -1.655877 | -2.846818 | -3.192639 |
| H | -1.655853 | -2.846762 | 3.192593 |
| H | -1.790241 | -4.556601 | 3.619866 |
| H | 3.334501 | -2.827989 | 3.009897 |
| H | 1.234340 | -2.976360 | 4.226434 |
| H | -1.790215 | -4.556668 | -3.619845 |
| H | 4.469239 | -4.111338 | 0.000009 |
| C | -3.317436 | 3.463555 | 0.725950 |
| C | -3.317438 | 3.463558 | -0.725943 |

| | | | |
|---|---|---|---|
| C | -2.469823 | 4.328509 | -1.425506 |
| C | -1.588612 | 5.224610 | -0.699269 |
| C | -1.588610 | 5.224608 | 0.699277 |
| C | -2.469820 | 4.328505 | 1.425513 |
| C | -3.488721 | 2.093939 | 1.174799 |
| C | -3.593527 | 1.247190 | 0.000000 |
| C | -3.488724 | 2.093943 | -1.174796 |
| C | -2.803650 | 1.638352 | -2.305968 |
| C | -1.759532 | 3.855755 | -2.600220 |
| C | -0.334327 | 5.306304 | -1.425125 |
| C | 0.874014 | 5.385085 | -0.725790 |
| C | 0.874015 | 5.385083 | 0.725794 |
| C | -0.334323 | 5.306301 | 1.425131 |
| C | -0.439471 | 4.460037 | 2.599898 |
| C | -1.759525 | 3.855746 | 2.600222 |
| C | -1.923136 | 2.535588 | 3.032499 |
| C | -2.803646 | 1.638343 | 2.305969 |
| C | -3.009082 | -0.023394 | -0.000001 |
| C | -2.296101 | -0.492818 | 1.173005 |
| C | -2.199115 | 0.318782 | 2.306547 |
| C | -0.943222 | 0.400990 | 3.032732 |
| C | -0.773343 | 1.770772 | 3.481576 |
| C | 0.498337 | 2.353721 | 3.482319 |
| C | 0.667650 | 3.722928 | 3.031663 |
| C | 1.922692 | 3.805025 | 2.306022 |
| C | 2.023512 | 4.620638 | 1.174531 |
| C | -0.439476 | 4.460043 | -2.599894 |
| C | 3.212110 | 2.030398 | -1.174945 |
| C | 2.528408 | 2.486059 | -2.306891 |
| C | 1.648180 | 1.589050 | -3.033646 |
| C | 1.483716 | 0.269253 | -2.599919 |
| C | 2.190907 | -0.200770 | -1.423404 |
| C | 3.042548 | 0.660521 | 0.726426 |
| C | 3.212117 | 2.030394 | 1.174937 |
| C | 3.316553 | 2.877199 | -0.000004 |
| C | 2.733835 | 4.148285 | -0.000001 |
| C | 2.023510 | 4.620641 | -1.174531 |
| C | 1.922687 | 3.805032 | -2.306025 |
| C | 0.498330 | 2.353730 | -3.482320 |
| C | -0.773350 | 1.770781 | -3.481587 |
| C | -0.943229 | 0.401000 | -3.032737 |
| C | 0.163420 | -0.332140 | -2.596215 |
| C | 0.058690 | -1.174791 | -1.420671 |
| C | 1.308240 | -1.093177 | -0.697365 |
| C | 1.308244 | -1.093179 | 0.697349 |
| C | 2.190915 | -0.200777 | 1.423393 |
| C | 2.528415 | 2.486052 | 2.306884 |
| C | 1.648184 | 1.589043 | 3.033633 |
| C | 1.483723 | 0.269245 | 2.599908 |
| C | 0.163427 | -0.332148 | 2.596205 |
| C | 0.058696 | -1.174790 | 1.420657 |
| C | -1.146325 | -1.253412 | 0.723139 |
| C | -1.146330 | -1.253410 | -0.723151 |
| C | -2.296107 | -0.492815 | -1.173013 |
| C | -2.199121 | 0.318790 | -2.306551 |
| C | 0.667643 | 3.722937 | -3.031665 |
| C | -1.923142 | 2.535598 | -3.032498 |
| C | 3.042540 | 0.660526 | -0.726436 |

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| | | | |
|---|---|---|---|
| C | -3.378339 | 0.667436 | 3.896671 |
| C | -3.377573 | -0.764920 | 3.878644 |
| C | 3.291415 | -0.048597 | 4.127086 |
| C | 2.351993 | -1.269887 | 4.352096 |
| C | 1.187684 | -0.773260 | 4.943623 |
| C | 1.186873 | 0.653428 | 4.960788 |
| C | 2.350727 | 1.165800 | 4.381988 |
| C | 1.033115 | -3.295667 | 3.828681 |
| C | 2.275906 | -2.582203 | 3.857497 |
| C | -2.266569 | -1.497895 | 4.326464 |
| C | -1.249483 | -0.755298 | 4.930918 |
| C | -0.014111 | -1.467703 | 4.923132 |
| C | -0.152961 | -2.711413 | 4.301645 |
| C | -1.675243 | -2.908233 | 4.035635 |
| C | -1.678323 | 2.808067 | 4.107940 |
| C | -0.155729 | 2.605956 | 4.368135 |
| C | -0.015500 | 1.346923 | 4.957753 |
| C | -1.250081 | 0.633343 | 4.947890 |
| C | -2.267944 | 1.389962 | 4.362500 |
| C | 2.273228 | 2.489938 | 3.920234 |
| C | 1.029749 | 3.202802 | 3.909625 |
| H | -4.209541 | 1.171789 | 3.407683 |
| H | -4.208022 | -1.257472 | 3.376536 |
| H | 3.702869 | -0.035724 | 3.111152 |
| H | 1.017355 | -4.250331 | 3.305437 |
| H | 3.125203 | -3.039277 | 3.353055 |
| H | -1.867425 | -3.217159 | 3.000677 |
| H | -1.872123 | 3.143608 | 3.081701 |
| H | -2.113203 | 3.562857 | 4.780660 |
| H | 3.121999 | 2.960556 | 3.427478 |
| H | 1.013330 | 4.170463 | 3.410830 |
| H | -2.109833 | -3.680996 | 4.687819 |
| H | 4.146538 | -0.056794 | 4.820048 |
| C | 3.231508 | -2.288425 | -1.233989 |
| C | 2.462546 | -2.294858 | -0.008468 |
| C | 3.979072 | -1.159684 | -1.591829 |
| C | 2.464676 | -1.175193 | 0.817132 |
| C | 1.238484 | -0.735916 | 1.438183 |
| C | 0.032411 | -1.470540 | 1.302709 |
| C | -1.169739 | -0.733577 | 1.456502 |
| C | 3.212512 | -1.376734 | -3.924778 |
| C | 2.436608 | -2.538247 | -3.547973 |
| C | 3.969035 | -0.693994 | -2.965079 |
| C | 2.445941 | -2.986040 | -2.228617 |
| C | 1.217155 | -3.434601 | -1.614090 |
| C | 0.003743 | -3.517828 | -2.351298 |
| C | -1.198831 | -3.432005 | -1.596664 |
| C | 0.025090 | -2.651792 | 0.428598 |
| C | 1.227481 | -3.008685 | -0.241271 |
| C | -1.187613 | -3.005418 | -0.224262 |
| C | 3.215983 | 1.464940 | -3.889445 |
| C | 2.430665 | 0.753709 | -4.874798 |
| C | 3.970773 | 0.756722 | -2.946978 |

| | | | |
|---|---|---|---|
| C | 2.428974 | -0.639262 | -4.892039 |
| C | 1.193896 | -1.352702 | -5.123351 |
| C | -0.015504 | -0.668226 | -5.424624 |
| C | -1.222001 | -1.349980 | -5.105705 |
| C | -0.005947 | -3.045419 | -3.743585 |
| C | 1.198751 | -2.526088 | -4.293200 |
| C | -1.217365 | -2.523350 | -4.275465 |
| C | 3.237376 | 2.309679 | -1.176865 |
| C | 2.453265 | 3.033456 | -2.153914 |
| C | 3.982033 | 1.188175 | -1.562551 |
| C | 2.442857 | 2.618464 | -3.483827 |
| C | 1.204980 | 2.627852 | -4.228940 |
| C | 0.001612 | 3.136459 | -3.666563 |
| C | -1.210943 | 2.630434 | -4.211093 |
| C | -0.013693 | 0.801704 | -5.406265 |
| C | 1.197292 | 1.475686 | -5.088160 |
| C | -1.218469 | 1.478353 | -5.070388 |
| C | 3.243338 | -0.010229 | 0.460136 |
| C | 2.467574 | 1.147447 | 0.845751 |
| C | 3.986616 | 0.003579 | -0.725789 |
| C | 2.468300 | 2.287383 | 0.048333 |
| C | 1.234864 | 3.009644 | -0.166526 |
| C | 0.031486 | 2.638923 | 0.494027 |
| C | -1.180403 | 3.011935 | -0.149491 |
| C | 0.012357 | 3.574637 | -2.263035 |
| C | 1.225616 | 3.469743 | -1.528168 |
| C | -1.190529 | 3.472696 | -1.510740 |
| C | 0.035920 | 1.436508 | 1.338433 |
| C | 1.240234 | 0.695967 | 1.455821 |
| C | -1.167990 | 0.698821 | 1.473964 |
| C | -3.199774 | 2.317404 | -1.129832 |
| C | -2.412699 | 2.292876 | 0.084042 |
| C | -2.403007 | 1.152615 | 0.881501 |
| C | -3.951664 | 1.197184 | -1.504409 |
| C | -3.219434 | 1.472316 | -3.842257 |
| C | -2.437979 | 2.623898 | -3.448155 |
| C | -2.428137 | 3.039045 | -2.118195 |
| C | -3.961651 | 0.765693 | -2.888534 |
| C | -3.222890 | -1.369612 | -3.877661 |
| C | -2.451884 | -0.633763 | -4.856378 |
| C | -2.450169 | 0.759215 | -4.839081 |
| C | -3.963483 | -0.685149 | -2.906714 |
| C | -3.205156 | -2.281766 | -1.187019 |
| C | -2.435448 | -2.980654 | -2.192920 |
| C | -2.444352 | -2.532735 | -3.512365 |
| C | -3.954503 | -1.150989 | -1.533786 |
| C | -3.185982 | -0.003123 | 0.506981 |
| C | -2.405860 | -1.169660 | 0.853151 |
| C | -2.418112 | -2.289396 | 0.027251 |
| C | -3.945795 | 0.012379 | -0.667405 |

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| | | | |
|---|---|---|---|
| C | -2.836683 | 4.354701 | -0.130989 |
| C | -2.431294 | 4.429433 | -1.502166 |
| C | 3.737878 | 4.079001 | 1.041159 |
| C | 3.201772 | 4.480652 | -0.361620 |
| C | 1.994657 | 5.156353 | -0.155300 |
| C | 1.591462 | 5.075232 | 1.213148 |
| C | 2.515150 | 4.341161 | 1.964948 |
| C | 2.478905 | 4.208832 | -2.706535 |
| C | 3.463640 | 4.068507 | -1.676151 |
| C | -1.143294 | 4.861061 | -1.856242 |
| C | -0.348071 | 5.346472 | -0.813637 |
| C | 1.037965 | 5.288865 | -1.154136 |
| C | 1.217006 | 4.758981 | -2.435533 |
| C | -0.197662 | 4.619946 | -3.067075 |
| C | -1.810361 | 4.304653 | 2.401572 |
| C | -0.283444 | 4.461025 | 2.653310 |
| C | 0.242950 | 5.130314 | 1.544109 |
| C | -0.740313 | 5.270421 | 0.517230 |
| C | -1.958331 | 4.705250 | 0.906168 |
| C | 2.036522 | 3.780049 | 3.157448 |
| C | 0.647179 | 3.842712 | 3.501316 |
| H | -3.792618 | 3.879810 | 0.082979 |
| H | -3.103610 | 4.005851 | -2.246296 |
| H | 4.045203 | 3.026597 | 1.068191 |
| H | 2.690026 | 3.742743 | -3.667703 |
| H | 4.365001 | 3.507135 | -1.917155 |
| H | -0.347595 | 3.620684 | -3.494767 |
| H | -2.140270 | 3.272234 | 2.571573 |
| H | -2.407950 | 4.948121 | 3.064994 |
| H | 2.679429 | 3.163679 | 3.783631 |
| H | 0.318429 | 3.268525 | 4.365851 |
| H | -0.365152 | 5.347141 | -3.876025 |
| H | 4.611496 | 4.680649 | 1.335639 |
| C | 0.293116 | -1.777245 | 3.369985 |
| C | -0.897590 | -0.986918 | 3.297402 |
| C | -2.178130 | -1.598022 | 3.068466 |
| C | -2.301593 | -3.022861 | 2.863492 |
| C | -1.108600 | -3.804746 | 2.960076 |
| C | 0.158734 | -3.197667 | 3.262349 |
| C | 1.196756 | -3.995111 | 2.669095 |
| C | 2.386883 | -3.385398 | 2.122115 |
| C | 2.522272 | -1.969824 | 2.258678 |
| C | 1.514866 | -1.186059 | 2.918621 |
| C | 1.532954 | 0.137796 | 2.359843 |
| C | 0.315069 | 0.889859 | 2.190040 |
| C | -0.894629 | 0.306179 | 2.672363 |
| C | -2.149239 | 0.473520 | 1.969524 |
| C | -2.964771 | -0.664118 | 2.287513 |
| C | -0.870694 | -4.940284 | 2.093547 |
| C | 0.550394 | -5.100072 | 1.989904 |
| C | 3.116512 | -1.158501 | 1.216278 |
| C | 2.563548 | 0.159002 | 1.341884 |
| C | 2.425583 | 0.994768 | 0.207637 |
| C | 1.328973 | 1.929533 | 0.157607 |
| C | 0.212735 | 1.786723 | 1.067951 |
| C | -1.009137 | 1.800839 | 0.269890 |
| C | -2.207489 | 1.087778 | 0.672800 |
| C | -3.034511 | 0.471788 | -0.360663 |
| C | -3.904102 | -0.632948 | 0.013360 |
| C | -3.940461 | -1.135830 | 1.374537 |
| C | -4.236223 | -2.551168 | 1.340439 |

| | | | |
|---|---|---|---|
| C | -3.338583 | -3.501659 | 1.978435 |
| C | -3.006181 | -4.527055 | 0.984123 |
| C | -1.734844 | -5.232937 | 0.984025 |
| C | -1.134092 | -5.588931 | -0.300432 |
| C | 0.301550 | -5.815438 | -0.354383 |
| C | 1.130706 | -5.659857 | 0.825459 |
| C | 2.442904 | -5.216987 | 0.415135 |
| C | 3.010225 | -4.001937 | 0.974188 |
| C | 3.438452 | -3.160870 | -0.146643 |
| C | 3.442001 | -1.707661 | -0.070982 |
| C | 3.091631 | -0.945022 | -1.267816 |
| C | 2.603588 | 0.415758 | -1.108590 |
| C | 1.569453 | 0.987779 | -1.977122 |
| C | 0.825244 | 1.951870 | -1.188255 |
| C | -0.613152 | 1.884921 | -1.120123 |
| C | -1.305125 | 1.083678 | -2.059839 |
| C | -2.532567 | 0.431297 | -1.706797 |
| C | -2.624226 | -0.766199 | -2.515203 |
| C | -3.363631 | -1.909618 | -2.080738 |
| C | -4.148795 | -1.770823 | -0.876505 |
| C | -4.396334 | -2.932308 | -0.040667 |
| C | -3.650489 | -4.149665 | -0.257799 |
| C | -2.936986 | -4.312901 | -1.470376 |
| C | -1.720412 | -5.070737 | -1.505042 |
| C | -0.905471 | -4.518224 | -2.567132 |
| C | 0.520102 | -4.617041 | -2.547425 |
| C | 1.114507 | -5.429406 | -1.511316 |
| C | 2.445440 | -5.108803 | -1.021561 |
| C | 3.063991 | -3.849224 | -1.367892 |
| C | 2.513830 | -3.085491 | -2.426718 |
| C | 2.578899 | -1.652025 | -2.408574 |
| C | 1.433843 | -1.166010 | -3.149298 |
| C | 0.865231 | 0.120600 | -2.891262 |
| C | -0.572364 | 0.237227 | -2.979417 |
| C | -1.398702 | -0.908525 | -3.249900 |
| C | -2.827908 | -3.210385 | -2.404668 |
| C | -1.563988 | -3.346417 | -3.074708 |
| C | 1.270332 | -3.489445 | -3.052111 |
| C | 0.608373 | -2.291756 | -3.490471 |
| C | -0.819279 | -2.195258 | -3.482990 |
| N | -0.267327 | -1.992738 | -0.064599 |
| Sc | 1.012335 | -3.474710 | -0.189219 |
| Sc | -2.164795 | -2.325756 | 0.307426 |
| Sc | 0.353372 | -0.139111 | -0.308883 |

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| | | | |
|---|---|---|---|
| C | -2.699766 | 1.174693 | 4.712662 |
| C | -3.086539 | -0.204223 | 4.660982 |
| C | 3.487890 | -1.290935 | 4.336159 |
| C | 2.285813 | -2.230156 | 4.643027 |
| C | 1.358724 | -1.473167 | 5.366021 |
| C | 1.744709 | -0.099530 | 5.418160 |
| C | 2.944263 | 0.111660 | 4.732802 |
| C | 0.429950 | -3.800618 | 4.199597 |
| C | 1.816471 | -3.444085 | 4.120307 |
| C | -2.197070 | -1.221920 | 5.034147 |
| C | -0.978250 | -0.804243 | 5.578894 |
| C | 0.016064 | -1.820077 | 5.444637 |
| C | -0.504615 | -2.951288 | 4.808330 |
| C | -2.040122 | -2.731273 | 4.694183 |
| C | -0.489202 | 2.777434 | 4.867514 |
| C | 0.935259 | 2.166560 | 5.001348 |
| C | 0.777150 | 0.889503 | 5.546757 |
| C | -0.603075 | 0.532099 | 5.626169 |
| C | -1.416687 | 1.556191 | 5.132700 |
| C | 3.188664 | 1.427291 | 4.308351 |
| C | 2.191758 | 2.447165 | 4.442226 |
| H | -3.384779 | 1.901358 | 4.279839 |
| H | -4.041320 | -0.438480 | 4.193641 |
| H | 3.764171 | -1.327158 | 3.274851 |
| H | 0.108662 | -4.685464 | 3.652544 |
| H | 2.461849 | -4.079149 | 3.515814 |
| H | -2.415702 | -2.967363 | 3.691850 |
| H | -0.652115 | 3.194628 | 3.866144 |
| H | -0.660835 | 3.591895 | 5.587595 |
| H | 4.082312 | 1.674198 | 3.738343 |
| H | 2.391427 | 3.405818 | 3.967160 |
| H | -2.594811 | -3.366018 | 5.402362 |
| H | 4.385727 | -1.565359 | 4.910563 |
| C | 3.433745 | -1.884134 | -1.524303 |
| C | 2.591341 | -2.704890 | -0.696526 |
| C | 2.411545 | -2.033667 | 0.564392 |
| C | 3.774157 | -0.700773 | -0.782616 |
| C | 3.144766 | -0.789673 | 0.502021 |
| C | 3.928959 | 0.560215 | -1.437416 |
| C | 3.840127 | 0.584747 | -2.862960 |
| C | 3.255977 | -1.829559 | -2.936747 |
| C | 3.509667 | -0.598291 | -3.600552 |
| C | 2.256893 | -2.691368 | -3.517997 |
| C | 1.552414 | -3.496417 | -1.252674 |
| C | 1.414230 | -3.490362 | -2.679416 |
| C | 0.363557 | -3.686000 | -0.493049 |
| C | 1.202639 | -2.170012 | 1.321970 |
| C | 0.185207 | -3.020023 | 0.772109 |
| C | 0.756409 | -1.039549 | 2.105367 |
| C | 2.650149 | 0.369794 | 1.155985 |
| C | 1.451865 | 0.215897 | 1.937536 |
| C | 3.527433 | 1.733162 | -0.726698 |
| C | 2.890647 | 1.639016 | 0.558623 |
| C | 2.966397 | 2.856608 | -1.416983 |
| C | 3.270500 | 1.710652 | -3.552237 |
| C | 2.787247 | 2.837590 | -2.827221 |
| C | 2.732374 | -0.210867 | -4.755482 |
| C | 2.582884 | 1.221121 | -4.716446 |
| C | 1.533025 | -2.373799 | -4.732704 |
| C | 1.718898 | -1.058350 | -5.313487 |
| C | 0.140152 | -3.633575 | -3.329096 |
| C | 0.196730 | -2.978851 | -4.621734 |
| C | -0.921949 | -3.801262 | -1.123543 |
| C | -1.063696 | -3.740080 | -2.542502 |
| C | -1.227815 | -2.718310 | 0.918349 |
| C | -1.900636 | -3.196274 | -0.266105 |
| C | -0.669553 | -0.736604 | 2.272432 |

| | | | |
|---|---|---|---|
| C | -1.682292 | -1.555612 | 1.630113 |
| C | 0.499956 | 1.277553 | 2.014594 |
| C | -0.802865 | 0.701580 | 2.173915 |
| C | 1.931550 | 2.705095 | 0.661228 |
| C | 1.976406 | 3.468076 | -0.559517 |
| C | 0.711412 | 2.535047 | 1.362676 |
| C | 0.812903 | 4.126627 | -1.079419 |
| C | 1.630063 | 3.522545 | -3.348104 |
| C | 0.676612 | 4.233657 | -2.519418 |
| C | 1.396838 | 1.840033 | -5.190592 |
| C | 0.945545 | 3.011510 | -4.497910 |
| C | 0.549115 | -0.409949 | -5.841587 |
| C | 0.397411 | 1.022936 | -5.791509 |
| C | -0.985770 | -2.267941 | -5.082273 |
| C | -0.775116 | -0.998006 | -5.724493 |
| C | -2.237227 | -3.140129 | -3.070666 |
| C | -2.185695 | -2.385849 | -4.304322 |
| C | -3.037827 | -2.518651 | -0.802659 |
| C | -3.221932 | -2.541097 | -2.218725 |
| C | -2.836413 | -0.900027 | 1.086964 |
| C | -3.519493 | -1.384724 | -0.087187 |
| C | -1.952675 | 1.361989 | 1.615110 |
| C | -2.989867 | 0.537672 | 1.110540 |
| C | -0.445153 | 3.217608 | 0.893775 |
| C | -0.402101 | 3.994082 | -0.320237 |
| C | -1.754621 | 2.639104 | 1.012186 |
| C | -1.702415 | 3.881058 | -0.960963 |
| C | -2.525258 | 3.032008 | -0.132507 |
| C | -0.637760 | 4.130047 | -3.172308 |
| C | -0.447552 | 3.342593 | -4.374965 |
| C | -1.845295 | 3.906187 | -2.392478 |
| C | -1.000379 | 1.322210 | -5.653181 |
| C | -1.722244 | 0.083520 | -5.594902 |
| C | -1.450352 | 2.459508 | -4.916277 |
| C | -3.141620 | -1.311913 | -4.191192 |
| C | -3.774759 | -1.408248 | -2.907664 |
| C | -2.905080 | -0.048537 | -4.804936 |
| C | -4.088959 | -0.259829 | -0.771740 |
| C | -3.769088 | 0.926619 | -0.027808 |
| C | -3.508665 | 2.161993 | -0.696025 |
| C | -4.178971 | -0.236126 | -2.197511 |
| C | -2.846949 | 3.036531 | -2.938437 |
| C | -2.670574 | 2.349192 | -4.199682 |
| C | -3.399781 | 1.116796 | -4.144730 |
| C | -3.682673 | 2.204044 | -2.108805 |
| C | -4.019145 | 1.024173 | -2.851991 |
| N | -0.058345 | 0.174252 | -1.816082 |
| Sc | 0.195299 | -1.043306 | -3.389030 |
| Sc | -0.177596 | -0.584145 | 0.044438 |
| Sc | -0.232861 | 2.152154 | -2.079682 |

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|---|---|---|---|
| C | 4.009897 | -3.680711 | 0.696247 |
| C | 4.014143 | -3.681620 | -0.670417 |
| C | 2.638078 | -3.813584 | -1.093696 |
| C | 2.631197 | -3.812212 | 1.111160 |
| C | -0.932070 | -3.769837 | 4.253866 |
| C | 0.434429 | -3.761643 | 4.257123 |
| C | 0.857383 | -3.866318 | 2.878133 |
| C | -1.347259 | -3.877749 | 2.872679 |
| C | 2.182185 | -3.809451 | 2.435612 |
| C | -4.479644 | -3.709735 | -0.697020 |
| C | -4.483917 | -3.709182 | 0.669685 |
| C | -3.106836 | -3.828067 | 1.093671 |
| C | -3.099931 | -3.828982 | -1.112292 |
| C | -2.669181 | -3.832276 | 2.421676 |
| C | 0.461160 | -3.765691 | -4.253475 |
| C | -0.905325 | -3.773682 | -4.258701 |
| C | -1.329103 | -3.880514 | -2.880041 |
| C | 0.875486 | -3.869351 | -2.871770 |
| C | 2.197462 | -3.812148 | -2.420936 |
| C | -2.653857 | -3.834472 | -2.437470 |
| H | 4.854194 | -3.588360 | 1.370124 |
| H | 4.862623 | -3.590164 | -1.339144 |
| H | -1.605822 | -3.692579 | 5.099846 |
| H | 1.103194 | -3.676563 | 5.106291 |
| H | 2.945745 | -3.718277 | 3.204828 |
| H | -5.325310 | -3.629872 | -1.370883 |
| H | -5.333793 | -3.628783 | 1.338171 |
| H | -3.439559 | -3.753570 | 3.185450 |
| H | 1.135224 | -3.681278 | -5.098505 |
| H | -1.573802 | -3.697040 | -5.108914 |
| H | 2.965932 | -3.721838 | -3.185352 |
| H | -3.419315 | -3.756271 | -3.206226 |
| N | 1.824031 | -3.900117 | 0.006284 |
| N | -0.242152 | -3.956793 | 2.064183 |
| N | -2.290927 | -3.903743 | -0.006741 |
| N | -0.229034 | -3.959108 | -2.064611 |
| Zn | -0.233539 | -3.964617 | -0.000189 |
| C | -3.263819 | 2.989375 | 0.738934 |
| C | -3.269224 | 2.989594 | -0.713151 |
| C | -2.636348 | 4.020804 | -1.414367 |
| C | -1.973022 | 5.090595 | -0.690695 |
| C | -1.967788 | 5.090332 | 0.707461 |
| C | -2.625739 | 4.020381 | 1.435730 |
| C | -3.125885 | 1.615683 | 1.187287 |
| C | -3.046408 | 0.767666 | 0.011731 |
| C | -3.134639 | 1.616039 | -1.162954 |
| C | -2.369881 | 1.323801 | -2.297719 |
| C | -1.842608 | 3.717444 | -2.591581 |
| C | -0.770446 | 5.448407 | -1.420994 |
| C | 0.393015 | 5.793812 | -0.726070 |
| C | 0.398401 | 5.793569 | 0.725475 |
| C | -0.759871 | 5.447945 | 1.428930 |
| C | -0.670547 | 4.598927 | 2.602724 |
| C | -1.823335 | 3.716705 | 2.606969 |
| C | -1.689210 | 2.393408 | 3.038573 |
| C | -2.352823 | 1.323129 | 2.316335 |
| C | -2.193470 | -0.339997 | 0.008414 |
| C | -1.391300 | -0.639641 | 1.178802 |
| C | -1.470092 | 0.170926 | 2.313593 |
| C | -0.261521 | 0.527520 | 3.035658 |
| C | -0.397113 | 1.901410 | 3.483253 |

| | | | |
|---|---|---|---|
| C | 0.713602 | 2.752194 | 3.479768 |
| C | 0.573780 | 4.125724 | 3.031043 |
| C | 1.776200 | 4.483942 | 2.300078 |
| C | 1.690247 | 5.302303 | 1.169321 |
| C | -0.689826 | 4.599706 | -2.595689 |
| C | 3.414610 | 3.039406 | -1.186373 |
| C | 2.642082 | 3.332352 | -2.315007 |
| C | 1.979940 | 2.262265 | -3.038860 |
| C | 2.114854 | 0.938953 | -2.607572 |
| C | 2.917559 | 0.634927 | -1.435394 |
| C | 3.561695 | 1.665587 | 0.713559 |
| C | 3.423368 | 3.039066 | 1.162789 |
| C | 3.333259 | 3.887790 | -0.011363 |
| C | 2.483738 | 4.998852 | -0.008099 |
| C | 1.681579 | 5.302661 | -1.179611 |
| C | 1.759131 | 4.484604 | -2.311188 |
| C | 0.687829 | 2.753168 | -3.483371 |
| C | -0.422868 | 1.902394 | -3.478913 |
| C | -0.283918 | 0.528403 | -3.032623 |
| C | 0.961502 | 0.057411 | -2.602836 |
| C | 1.051734 | -0.784862 | -1.427849 |
| C | 2.258004 | -0.432921 | -0.706734 |
| C | 2.263216 | -0.433214 | 0.690849 |
| C | 2.928125 | 0.634519 | 1.414819 |
| C | 2.659189 | 3.331719 | 2.297167 |
| C | 2.002417 | 2.261425 | 3.025630 |
| C | 2.134086 | 0.938244 | 2.592950 |
| C | 0.980702 | 0.056696 | 2.596554 |
| C | 1.062177 | -0.785295 | 1.420723 |
| C | -0.101854 | -1.119475 | 0.726301 |
| C | -0.107157 | -1.119242 | -0.724965 |
| C | -1.399877 | -0.639277 | -1.167869 |
| C | -1.487083 | 0.171654 | -2.301736 |
| C | 0.551318 | 4.126606 | -3.033328 |
| C | -1.711672 | 2.394274 | -3.024579 |
| C | 3.556303 | 1.665800 | -0.738579 |

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|---|---|---|---|
| C | 3.911882 | 0.685079 | 4.361672 |
| C | 3.912098 | -0.681300 | 4.362121 |
| C | 2.527539 | -1.100368 | 4.345941 |
| C | 2.527192 | 1.103701 | 4.345212 |
| C | -1.004720 | 4.246067 | 3.853386 |
| C | 0.357187 | 4.246062 | 3.966202 |
| C | 0.764419 | 2.868735 | 4.129775 |
| C | -1.433312 | 2.868660 | 3.947439 |
| C | 2.085669 | 2.426345 | 4.248898 |
| C | -4.571332 | -0.682887 | 3.645246 |
| C | -4.571522 | 0.683451 | 3.644665 |
| C | -3.205046 | 1.102818 | 3.865815 |
| C | -3.204735 | -1.101678 | 3.866733 |
| C | -2.755789 | 2.425728 | 3.846051 |
| C | 0.358512 | -4.243685 | 3.969205 |
| C | -1.003408 | -4.244209 | 3.856555 |
| C | -1.432434 | -2.866877 | 3.949662 |
| C | 0.765319 | -2.866109 | 4.131756 |
| C | 2.086434 | -2.423216 | 4.250506 |
| C | -2.755069 | -2.424462 | 3.848032 |
| H | 4.763222 | 1.356457 | 4.354783 |
| H | 4.763648 | -1.352414 | 4.355664 |
| H | -1.666399 | 5.092815 | 3.709880 |
| H | 1.033416 | 5.092931 | 3.934634 |
| H | 2.856002 | 3.194056 | 4.230729 |
| H | -5.408841 | -1.354392 | 3.493018 |
| H | -5.409221 | 1.354591 | 3.491874 |
| H | -3.512533 | 3.192435 | 3.696484 |
| H | 1.035011 | -5.090357 | 3.938162 |
| H | -1.664834 | -5.091278 | 3.713762 |
| H | 2.857012 | -3.190693 | 4.232821 |
| H | -3.511571 | -3.191533 | 3.699112 |
| N | 1.712369 | 0.001542 | 4.360373 |
| N | -0.341273 | 2.057271 | 4.118085 |
| N | -2.403813 | 0.000747 | 4.019072 |
| N | -0.340641 | -2.055010 | 4.119606 |
| Zn | -0.343669 | 0.001138 | 4.171423 |
| C | 0.468507 | 3.216388 | -4.514464 |
| C | 1.667858 | 2.439064 | -4.739672 |
| C | 0.325453 | 3.963286 | -3.339289 |
| C | 2.687308 | 2.438982 | -3.789837 |
| C | 3.369705 | 1.206232 | -3.469327 |
| C | 3.089504 | -0.002268 | -4.164948 |
| C | 3.369107 | -1.210260 | -3.468193 |
| C | -2.016893 | 3.218731 | -3.135615 |
| C | -1.859992 | 2.440118 | -4.345384 |
| C | -0.942610 | 3.964349 | -2.635631 |
| C | -0.641562 | 2.438982 | -5.020952 |
| C | -0.126762 | 1.205786 | -5.570519 |
| C | -0.875985 | -0.001906 | -5.518417 |
| C | -0.127371 | -1.210029 | -5.569406 |
| C | 2.014228 | -0.002469 | -5.166635 |
| C | 1.300048 | 1.205802 | -5.397018 |
| C | 1.299438 | -1.210596 | -5.395890 |
| C | -1.473030 | 3.220405 | -0.346199 |
| C | -2.576929 | 2.443337 | -0.869627 |
| C | -0.665674 | 3.965969 | -1.212425 |
| C | -2.843920 | 2.442997 | -2.236922 |
| C | -3.208026 | 1.208988 | -2.896374 |
| C | -3.391880 | 0.000296 | -2.168210 |
| C | -3.208621 | -1.209171 | -2.895242 |
| C | -2.160246 | -0.001243 | -4.804941 |
| C | -2.599967 | 1.207599 | -4.198462 |
| C | -2.600559 | -1.209294 | -4.197317 |
| C | 1.349171 | 3.219424 | -0.001674 |
| C | 0.509668 | 2.440138 | 0.881498 |
| C | 0.774928 | 3.966407 | -1.036103 |
| C | -0.872326 | 2.440832 | 0.714318 |
| C | -1.611689 | 1.209504 | 0.849509 |
| C | -0.975735 | 0.001291 | 1.235334 |
| C | -1.612281 | -1.206957 | 0.850613 |
| C | -3.111606 | 0.000904 | -0.726082 |
| C | -2.666887 | 1.209969 | -0.122498 |
| C | -2.667515 | -1.207819 | -0.121352 |
| C | 2.549009 | 3.217508 | -2.577736 |

| | | | |
|---|---|---|---|
| C | 3.135294 | 2.441638 | -1.506387 |
| C | 1.386838 | 3.964321 | -2.351174 |
| C | 2.547659 | 2.442716 | -0.243092 |
| C | 2.452590 | 1.208852 | 0.503181 |
| C | 3.028188 | -0.000282 | 0.024109 |
| C | 2.451994 | -1.208683 | 0.504296 |
| C | 0.482176 | 0.001009 | 1.410995 |
| C | 1.193168 | 1.208884 | 1.188938 |
| C | 1.192553 | -1.207421 | 1.189983 |
| C | 3.647491 | -0.001069 | -1.307659 |
| C | 3.645784 | 1.207111 | -2.058825 |
| C | 3.645176 | -1.209955 | -2.057690 |
| C | 1.347550 | -3.219170 | 0.001328 |
| C | 2.546446 | -2.443310 | -0.240807 |
| C | 3.134070 | -2.443713 | -1.504101 |
| C | 0.772941 | -3.966847 | -1.032384 |
| C | -1.474649 | -3.219058 | -0.343200 |
| C | -0.873550 | -2.438777 | 0.716571 |
| C | 0.508442 | -2.438614 | 0.883731 |
| C | -0.667667 | -3.965859 | -1.208708 |
| C | -2.018506 | -3.219737 | -3.132599 |
| C | -2.845144 | -2.442742 | -2.234631 |
| C | -2.578173 | -2.441931 | -0.867335 |
| C | -0.944608 | -3.965435 | -2.631915 |
| C | 0.466892 | -3.219936 | -4.511443 |
| C | -0.642788 | -2.442454 | -5.018675 |
| C | -1.861201 | -2.442319 | -4.343091 |
| C | 0.323452 | -3.965669 | -3.335576 |
| C | 2.547395 | -3.220294 | -2.574723 |
| C | 2.686081 | -2.442967 | -3.787548 |
| C | 1.666625 | -2.443421 | -4.737377 |
| C | 1.384840 | -3.966306 | -2.347459 |

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| | | | |
|---|---|---|---|
| C | 3.646198 | 2.279470 | 4.059767 |
| C | 4.181025 | 1.021937 | 4.094185 |
| C | 3.075680 | 0.099439 | 4.223043 |
| C | 2.212789 | 2.129301 | 4.173650 |
| C | -2.289230 | 3.653992 | 4.160214 |
| C | -1.029582 | 4.183609 | 4.126171 |
| C | -0.105661 | 3.075253 | 4.224027 |
| C | -2.138370 | 2.220254 | 4.273869 |
| C | 1.286867 | 3.177231 | 4.158304 |
| C | -3.646092 | -2.279292 | 4.060062 |
| C | -4.180918 | -1.021757 | 4.094418 |
| C | -3.075567 | -0.099250 | 4.223152 |
| C | -2.212677 | -2.129114 | 4.173862 |
| C | -3.185137 | 1.294145 | 4.244850 |
| C | 2.289340 | -3.653808 | 4.160376 |
| C | 1.029691 | -4.183425 | 4.126400 |
| C | 0.105774 | -3.075062 | 4.224213 |
| C | 2.138484 | -2.220062 | 4.273942 |
| C | 3.185249 | -1.293955 | 4.244831 |
| C | -1.286757 | -3.177045 | 4.158546 |
| H | 4.164783 | 3.226386 | 3.960321 |
| H | 5.224173 | 0.734166 | 4.026232 |
| H | -3.237752 | 4.175404 | 4.096725 |
| H | -0.742033 | 5.224678 | 4.030521 |
| H | 1.693944 | 4.180659 | 4.057196 |
| H | -4.164684 | -3.226214 | 3.960713 |
| H | -5.224070 | -0.733994 | 4.026500 |
| H | -4.191555 | 1.701297 | 4.180987 |
| H | 3.237860 | -4.175224 | 4.096895 |
| H | 0.742138 | -5.224500 | 4.030827 |
| H | 4.191665 | -1.701110 | 4.180943 |
| H | -1.693835 | -4.180479 | 4.057507 |
| N | 1.896051 | 0.798831 | 4.272946 |
| N | -0.805925 | 1.900967 | 4.331530 |
| N | -1.895936 | -0.798638 | 4.273052 |
| N | 0.806040 | -1.900769 | 4.331620 |
| Zn | 0.000058 | 0.000099 | 4.327282 |
| C | 1.258589 | 3.243446 | -2.133837 |
| C | 2.114706 | 2.679944 | -3.132539 |
| C | 1.617773 | 2.373315 | -4.445442 |
| C | 0.228926 | 2.579353 | -4.785081 |
| C | -0.612142 | 3.164609 | -3.788793 |
| C | -0.092427 | 3.538655 | -2.502393 |
| C | -1.157012 | 3.450924 | -1.540521 |
| C | -0.905422 | 3.018703 | -0.186065 |
| C | 0.451055 | 2.752733 | 0.176766 |
| C | 1.522253 | 2.915716 | -0.766990 |
| C | 2.577180 | 2.003028 | -0.415737 |
| C | 3.377313 | 1.358181 | -1.430923 |
| C | 3.121815 | 1.713705 | -2.791895 |
| C | 3.194544 | 0.738858 | -3.859599 |
| C | 2.328929 | 1.197551 | -4.907377 |
| C | -1.989552 | 2.750917 | -3.618055 |
| C | -2.340190 | 3.009531 | -2.252165 |
| C | 0.796110 | 1.667847 | 1.066367 |
| C | 2.137752 | 1.271265 | 0.755706 |
| C | 2.567869 | -0.059901 | 0.971650 |
| C | 3.564382 | -0.624648 | 0.089810 |
| C | 3.869121 | 0.023499 | -1.175832 |
| C | 3.754912 | -0.991373 | -2.228203 |
| C | 3.354672 | -0.663223 | -3.587622 |
| C | 2.528142 | -1.619411 | -4.321766 |
| C | 1.717292 | -1.131250 | -5.426379 |
| C | 1.696812 | 0.276027 | -5.777683 |
| C | 0.395746 | 0.601925 | -6.314909 |
| C | -0.389512 | 1.673823 | -5.725095 |
| C | -1.717550 | 1.131261 | -5.426220 |
| C | -2.528337 | 1.619393 | -4.321548 |
| C | -3.354826 | 0.663184 | -3.587388 |
| C | -3.754983 | 0.991283 | -2.227931 |
| C | -3.315877 | 2.220290 | -1.595064 |
| C | -3.191100 | 1.991818 | -0.174667 |
| C | -1.933337 | 2.269190 | 0.497716 |
| C | -1.564939 | 1.068265 | 1.243432 |
| C | -0.180913 | 0.707282 | 1.486081 |
| C | 0.181083 | -0.707512 | 1.486038 |
| C | 1.565096 | -1.068483 | 1.243296 |
| C | 1.933443 | -2.269377 | 0.497504 |
| C | 3.191160 | -1.991970 | -0.174945 |

| | | | |
|---|---|---|---|
| C | 3.315841 | -2.220399 | -1.595355 |
| C | 2.340131 | -3.009636 | -2.252424 |
| C | 1.989407 | -2.750963 | -3.618281 |
| C | 0.611984 | -3.164638 | -3.788942 |
| C | -0.229143 | -2.579354 | -4.785167 |
| C | 0.389230 | -1.673795 | -5.725199 |
| C | -0.396062 | -0.601865 | -6.314923 |
| C | -1.697103 | -0.275998 | -5.777603 |
| C | -2.329164 | -1.197549 | -4.907281 |
| C | -3.194704 | -0.738887 | -3.859423 |
| C | -3.121906 | -1.713773 | -2.791764 |
| C | -3.377322 | -1.358300 | -1.430764 |
| C | -3.869105 | -0.023627 | -1.175587 |
| C | -3.564290 | 0.624481 | 0.090054 |
| C | -2.567723 | 0.059695 | 0.971808 |
| C | -2.137628 | -1.271467 | 0.755791 |
| C | -0.795964 | -1.668059 | 1.066353 |
| C | -0.450966 | -2.752910 | 0.176688 |
| C | 0.905487 | -3.018881 | -0.186228 |
| C | 1.156997 | -3.451050 | -1.540718 |
| C | 0.092350 | -3.538736 | -2.502522 |
| C | -1.617971 | -2.373324 | -4.445430 |
| C | -2.114823 | -2.680004 | -3.132509 |
| C | -2.577126 | -2.003183 | -0.415651 |
| C | -1.522218 | -2.915848 | -0.767007 |
| C | -1.258645 | -3.243538 | -2.133879 |
| N | -0.000036 | -0.000064 | -2.134994 |
| Sc | -1.592211 | 0.594064 | -1.146199 |
| Sc | -0.000130 | -0.000061 | -4.097926 |
| Sc | 1.592226 | -0.594120 | -1.146303 |

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| | | | |
|---|---|---|---|
| C | -4.267024 | 4.543300 | -0.694545 |
| C | -4.234949 | 4.154763 | -2.004958 |
| C | -4.440434 | 2.724025 | -2.023752 |
| C | -4.489899 | 3.350764 | 0.091443 |
| C | -4.686194 | 0.838677 | 4.117981 |
| C | -4.626121 | 2.148683 | 3.733693 |
| C | -4.680653 | 2.164697 | 2.288148 |
| C | -4.778151 | 0.050774 | 2.908385 |
| C | -4.551170 | 3.303476 | 1.487482 |
| C | -4.662723 | -3.976595 | 0.383863 |
| C | -4.674516 | -3.588896 | 1.694906 |
| C | -4.759169 | -2.145823 | 1.705213 |
| C | -4.738645 | -2.771416 | -0.410762 |
| C | -4.769564 | -1.345604 | 2.852336 |
| C | -4.474354 | -0.262615 | -4.434549 |
| C | -4.555185 | -1.571363 | -4.050798 |
| C | -4.703547 | -1.577576 | -2.611817 |
| C | -4.576395 | 0.534157 | -3.231312 |
| C | -4.449228 | 1.924947 | -3.171240 |
| C | -4.716493 | -2.721432 | -1.808231 |
| H | -4.145290 | 5.541016 | -0.287961 |
| H | -4.082672 | 4.771716 | -2.883514 |
| H | -4.651868 | 0.432462 | 5.122553 |
| H | -4.535246 | 3.028189 | 4.361311 |
| H | -4.447477 | 4.252624 | 2.008646 |
| H | -4.600534 | -4.981895 | -0.017408 |
| H | -4.624373 | -4.213587 | 2.579689 |
| H | -4.728450 | -1.867782 | 3.805548 |
| H | -4.338800 | 0.136023 | -5.433594 |
| H | -4.497947 | -2.457575 | -4.672831 |
| H | -4.303874 | 2.438351 | -4.118965 |
| H | -4.660022 | -3.676724 | -2.325347 |
| N | -4.593286 | 2.265013 | -0.740449 |
| N | -4.795641 | 0.882217 | 1.818234 |
| N | -4.797129 | -1.678774 | 0.416388 |
| N | -4.739096 | -0.288681 | -2.146871 |
| Zn | -4.747978 | 0.297013 | -0.163609 |
| C | -0.156967 | -1.255110 | 3.385648 |
| C | -1.096434 | -0.380356 | 2.740596 |
| C | -0.683079 | 0.979559 | 2.976851 |
| C | 0.847562 | -0.441874 | 4.016353 |
| C | 0.525935 | 0.932741 | 3.765441 |
| C | 2.206520 | -0.875627 | 4.086784 |
| C | 2.513161 | -2.186209 | 3.607044 |
| C | 0.178012 | -2.521826 | 2.824197 |
| C | 1.508656 | -2.995815 | 2.984389 |
| C | -0.520699 | -2.936252 | 1.632086 |
| C | -1.717223 | -0.744574 | 1.522031 |
| C | -1.437722 | -2.043682 | 0.990829 |
| C | -1.995619 | 0.282459 | 0.580948 |
| C | -0.935607 | 2.024179 | 2.027004 |
| C | -1.618856 | 1.650323 | 0.820698 |
| C | 0.036047 | 3.092953 | 1.912888 |
| C | 1.547697 | 1.904868 | 3.580588 |
| C | 1.280664 | 2.966635 | 2.643910 |
| C | 3.227945 | 0.119524 | 4.003569 |
| C | 2.902295 | 1.496088 | 3.746374 |
| C | 4.481050 | -0.163911 | 3.369032 |
| C | 3.768264 | -2.465980 | 2.965165 |
| C | 4.744181 | -1.440764 | 2.801337 |
| C | 2.138466 | -3.786066 | 1.950603 |
| C | 3.538576 | -3.447905 | 1.940656 |
| C | 0.048638 | -3.813992 | 0.627354 |
| C | 1.447848 | -4.173483 | 0.754308 |
| C | -1.411510 | -2.308909 | -0.420416 |
| C | -0.524969 | -3.426357 | -0.672779 |
| C | -1.938844 | 0.041236 | -0.830928 |
| C | -1.621527 | -1.240795 | -1.361000 |
| C | -1.319280 | 2.254295 | -0.465409 |
| C | -1.510157 | 1.242869 | -1.475753 |
| C | 0.345422 | 3.713058 | 0.614989 |
| C | -0.308249 | 3.267860 | -0.605936 |
| C | 2.336974 | 3.511693 | 1.844552 |
| C | 1.778917 | 3.928582 | 0.587295 |
| C | 3.955609 | 2.064731 | 2.950665 |
| C | 4.941668 | 1.040662 | 2.717680 |
| C | 3.689275 | 3.054695 | 1.968218 |
| C | 5.718576 | 1.007219 | 1.513206 |
| C | 5.550733 | -1.472134 | 1.608289 |
| C | 6.105273 | -0.286541 | 0.988070 |
| C | 4.275960 | -3.439504 | 0.727583 |

| | | | |
|---|---|---|---|
| C | 5.301603 | -2.447704 | 0.589189 |
| C | 2.223611 | -4.207611 | -0.456521 |
| C | 3.622593 | -3.859883 | -0.465939 |
| C | 0.299746 | -3.382494 | -1.871892 |
| C | 1.664239 | -3.817905 | -1.740325 |
| C | -0.910219 | -1.286877 | -2.584423 |
| C | 0.067542 | -2.326733 | -2.817407 |
| C | -0.720887 | 1.192504 | -2.662734 |
| C | -0.462722 | -0.090456 | -3.235020 |
| C | 0.480375 | 3.204993 | -1.803980 |
| C | 0.259086 | 2.211745 | -2.828679 |
| C | 2.568681 | 3.854456 | -0.615272 |
| C | 1.890419 | 3.529656 | -1.819883 |
| C | 4.482065 | 3.065650 | 0.784464 |
| C | 5.478800 | 2.050509 | 0.552933 |
| C | 3.932824 | 3.453426 | -0.484113 |
| C | 5.536644 | 1.805970 | -0.879622 |
| C | 4.564079 | 2.670109 | -1.506677 |
| C | 6.176680 | -0.537452 | -0.458417 |
| C | 5.640184 | -1.865997 | -0.680458 |
| C | 5.846929 | 0.506581 | -1.414866 |
| C | 3.929880 | -3.269434 | -1.738233 |
| C | 2.727022 | -3.229215 | -2.519513 |
| C | 4.912087 | -2.241600 | -1.866125 |
| C | 1.126191 | -1.748709 | -3.607220 |
| C | 0.798266 | -0.373708 | -3.860576 |
| C | 2.477411 | -2.166249 | -3.441453 |
| C | 1.512951 | 1.933825 | -3.465148 |
| C | 2.519304 | 2.753214 | -2.848135 |
| C | 3.851921 | 2.269840 | -2.679145 |
| C | 1.818616 | 0.622832 | -3.946364 |
| C | 5.129910 | 0.127607 | -2.598580 |
| C | 4.699984 | -1.232511 | -2.842091 |
| C | 3.504286 | -1.191280 | -3.630212 |
| C | 4.176285 | 1.000301 | -3.238022 |
| C | 3.177313 | 0.187488 | -3.868841 |
| N | 2.007904 | -0.136128 | 0.113843 |
| Sc | 1.119178 | -1.920110 | -0.148060 |
| Sc | 0.845879 | 1.469545 | 0.457123 |
| Sc | 4.004260 | 0.036695 | 0.038083 |

----------sbpc-c60----------

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| | | | |
|---|---|---|---|
| C | -3.534515 | 3.109031 | -0.715814 |
| C | -3.534519 | 3.109039 | 0.715794 |
| C | -4.490932 | 2.378764 | 1.426130 |
| C | -5.456732 | 1.677570 | 0.704519 |
| C | -5.456723 | 1.677556 | -0.704534 |
| C | -4.490918 | 2.378741 | -1.426147 |
| C | -2.328337 | 3.795502 | -1.145930 |
| C | -2.328340 | 3.795511 | 1.145908 |
| H | -4.464288 | 2.350029 | 2.512156 |
| H | -6.213324 | 1.105446 | 1.236245 |
| H | -6.213307 | 1.105418 | -1.236258 |
| H | -4.464263 | 2.349984 | -2.512173 |
| C | 1.940641 | 3.617030 | -2.457133 |
| C | 0.703625 | 3.489794 | -3.169939 |
| C | 0.664189 | 2.851373 | -4.411839 |
| C | 1.860708 | 2.374043 | -4.946097 |
| C | 3.078502 | 2.507942 | -4.247866 |
| C | 3.128966 | 3.118290 | -2.995625 |
| C | 1.625455 | 4.158655 | -1.146513 |
| C | -0.350227 | 3.970012 | -2.291448 |
| H | -0.279663 | 2.723828 | -4.935050 |
| H | 1.855327 | 1.877786 | -5.913763 |
| H | 3.990187 | 2.113037 | -4.689883 |
| H | 4.058712 | 3.191881 | -2.437894 |
| C | 0.703607 | 3.489810 | 3.169934 |
| C | 1.940627 | 3.617038 | 2.457133 |
| C | 3.128952 | 3.118316 | 2.995643 |
| C | 3.078479 | 2.507974 | 4.247888 |
| C | 1.860678 | 2.374064 | 4.946104 |
| C | 0.664162 | 2.851387 | 4.411832 |
| C | -0.350241 | 3.970033 | 2.291439 |
| C | 1.625447 | 4.158639 | 1.146502 |
| H | 4.058704 | 3.191914 | 2.437925 |
| H | 3.990163 | 2.113083 | 4.689919 |
| H | 1.855287 | 1.877802 | 5.913768 |
| H | -0.279696 | 2.723831 | 4.935030 |
| N | 0.291338 | 4.474084 | 1.188711 |
| N | -1.757600 | 4.288352 | -0.000013 |
| N | 0.291344 | 4.474092 | -1.188729 |
| N | -1.666795 | 3.713933 | 2.309236 |
| N | -1.666782 | 3.713913 | -2.309255 |
| N | 2.316644 | 4.081990 | -0.000003 |
| B | -0.446660 | 5.014113 | -0.000007 |
| Cl | -0.614562 | 6.882822 | -0.000004 |
| C | -0.080316 | 1.164629 | 0.724361 |
| C | -0.080321 | 1.164627 | -0.724330 |
| C | -1.174241 | 0.650103 | -1.422542 |
| C | -2.309523 | 0.116433 | -0.698063 |
| C | -2.309516 | 0.116429 | 0.698106 |
| C | -1.174229 | 0.650095 | 1.422579 |
| C | 1.266841 | 0.874777 | 1.172494 |
| C | 2.100949 | 0.698409 | 0.000005 |
| C | 1.266831 | 0.874776 | -1.172475 |
| C | 1.471929 | 0.083468 | -2.304429 |
| C | -0.964579 | -0.169001 | -2.600006 |
| C | -2.803395 | -1.037120 | -1.424419 |
| C | -3.279268 | -2.150971 | -0.726196 |
| C | -3.279260 | -2.150976 | 0.726228 |
| C | -2.803381 | -1.037131 | 1.424455 |
| C | -1.971402 | -1.215340 | 2.600604 |
| C | -0.964557 | -0.169019 | 2.600033 |
| C | 0.335745 | -0.449730 | 3.029950 |
| C | 1.471949 | 0.083451 | 2.304436 |
| C | 3.112592 | -0.264988 | -0.000001 |
| C | 3.325269 | -1.091144 | 1.174979 |
| C | 2.519534 | -0.918764 | 2.305643 |
| C | 2.029260 | -2.076398 | 3.031820 |
| C | 0.678985 | -1.785962 | 3.480273 |
| C | -0.290300 | -2.794000 | 3.480506 |
| C | -1.640767 | -2.503821 | 3.032911 |
| C | -2.131619 | -3.661148 | 2.306844 |

| | | | |
|---|---|---|---|
| C | -2.935162 | -3.487722 | 1.174820 |
| C | -1.971424 | -1.215322 | -2.600575 |
| C | -0.879697 | -5.462597 | -1.174513 |
| C | -1.084556 | -4.666790 | -2.306209 |
| C | 0.053250 | -4.130696 | -3.031331 |
| C | 1.353526 | -4.410856 | -2.599630 |
| C | 1.565463 | -5.236645 | -1.424846 |
| C | 0.469868 | -5.752858 | 0.725786 |
| C | -0.879687 | -5.462605 | 1.174504 |
| C | -1.713698 | -5.282378 | -0.000001 |
| C | -2.721566 | -4.313613 | 0.000007 |
| C | -2.935175 | -3.487715 | -1.174800 |
| C | -2.131638 | -3.661130 | -2.306830 |
| C | -0.290329 | -2.793975 | -3.480501 |
| C | 0.678955 | -1.785937 | -3.480270 |
| C | 2.029232 | -2.076376 | -3.031826 |
| C | 2.360424 | -3.364592 | -2.599710 |
| C | 3.193962 | -3.543986 | -1.425056 |
| C | 2.702917 | -4.701236 | -0.699113 |
| C | 2.702923 | -4.701243 | 0.699079 |
| C | 1.565474 | -5.236655 | 1.424818 |
| C | -1.084538 | -4.666807 | 2.306207 |
| C | 0.053275 | -4.130717 | 3.031323 |
| C | 1.353549 | -4.410875 | 2.599611 |
| C | 2.360447 | -3.364610 | 2.599689 |
| C | 3.193972 | -3.543997 | 1.425025 |
| C | 3.667070 | -2.428487 | 0.725971 |
| C | 3.667066 | -2.428480 | -0.725999 |
| C | 3.325263 | -1.091131 | -1.174993 |
| C | 2.519513 | -0.918748 | -2.305648 |
| C | -1.640793 | -2.503800 | -3.032894 |
| C | 0.335720 | -0.449703 | -3.029947 |
| C | 0.469863 | -5.752852 | -0.725808 |

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| | | | |
|---|---|---|---|
| C | -2.974563 | -0.714544 | 3.850344 |
| C | -2.973232 | 0.719793 | 3.850375 |
| C | -4.046282 | 1.430870 | 3.308615 |
| C | -5.122881 | 0.709235 | 2.792634 |
| C | -5.124222 | -0.699913 | 2.792647 |
| C | -4.048978 | -1.423581 | 3.308603 |
| C | -1.676725 | -1.146010 | 4.342793 |
| C | -1.674617 | 1.148835 | 4.342861 |
| H | -4.027819 | 2.517038 | 3.281627 |
| H | -5.971591 | 1.241294 | 2.369471 |
| H | -5.973958 | -1.230359 | 2.369514 |
| H | -4.032565 | -2.509781 | 3.281603 |
| C | 2.527990 | -2.480809 | 3.590506 |
| C | 1.287897 | -3.197710 | 3.665698 |
| C | 1.175034 | -4.480113 | 3.124638 |
| C | 2.305824 | -5.052097 | 2.540838 |
| C | 3.523594 | -4.347612 | 2.466495 |
| C | 3.643252 | -3.054466 | 2.976240 |
| C | 2.287688 | -1.149678 | 4.126083 |
| C | 0.305078 | -2.297673 | 4.246328 |
| H | 0.226200 | -5.008694 | 3.157004 |
| H | 2.244023 | -6.052972 | 2.120279 |
| H | 4.381018 | -4.817713 | 1.990742 |
| H | 4.573326 | -2.498195 | 2.894655 |
| C | 1.293732 | 3.194826 | 3.665140 |
| C | 2.532427 | 2.475517 | 3.589751 |
| C | 3.648530 | 3.046769 | 2.974770 |
| C | 3.531106 | 4.339921 | 2.464540 |
| C | 2.314752 | 5.046826 | 2.539237 |
| C | 1.183109 | 4.477288 | 3.123775 |
| C | 0.309323 | 2.296740 | 4.246095 |
| C | 2.289787 | 1.145017 | 4.125840 |
| H | 4.577480 | 2.488653 | 2.892968 |
| H | 4.389182 | 4.808155 | 1.988122 |
| H | 2.254759 | 6.047706 | 2.118425 |
| H | 0.235372 | 5.007800 | 3.156558 |
| N | 1.013477 | 1.183180 | 4.624376 |
| N | -1.038998 | 0.000820 | 4.741063 |
| N | 1.011291 | -1.185385 | 4.624549 |
| N | -1.031507 | 2.315642 | 4.182898 |
| N | -1.035779 | -2.314018 | 4.182938 |
| N | 2.962319 | -0.002963 | 3.948416 |
| B | 0.362643 | -0.000467 | 5.266191 |
| Cl | 0.470543 | -0.000432 | 7.140904 |
| C | 0.810307 | 3.217694 | -4.386261 |
| C | 2.023644 | 2.441709 | -4.247985 |
| C | 0.326332 | 3.964787 | -3.305658 |
| C | 2.718637 | 2.443269 | -3.040530 |
| C | 3.279201 | 1.211573 | -2.532697 |
| C | 3.216853 | 0.002306 | -3.278986 |
| C | 3.281444 | -1.205147 | -2.529973 |
| C | -1.970490 | 3.215300 | -3.798278 |
| C | -1.463509 | 2.436745 | -4.907312 |
| C | -1.092332 | 3.963707 | -3.006099 |
| C | -0.100732 | 2.438379 | -5.196241 |
| C | 0.554741 | 1.205636 | -5.569653 |
| C | -0.174509 | -0.003683 | -5.740116 |
| C | 0.557032 | -1.211233 | -5.566964 |
| C | 2.481948 | 0.000172 | -4.551400 |
| C | 1.866533 | 1.207317 | -4.982991 |
| C | 1.868838 | -1.209105 | -4.980289 |
| C | -2.271759 | 3.218419 | -0.972640 |
| C | -3.171228 | 2.439412 | -1.796671 |
| C | -1.246596 | 3.966043 | -1.563753 |
| C | -3.024219 | 2.438334 | -3.182092 |
| C | -3.176043 | 1.203866 | -3.918494 |
| C | -3.564455 | -0.004132 | -3.275503 |
| C | -3.173742 | -1.212843 | -3.915771 |
| C | -1.612374 | -0.004710 | -5.435533 |
| C | -2.211956 | 1.203374 | -4.984404 |
| C | -2.209641 | -1.212911 | -4.981661 |
| C | 0.323032 | 3.218150 | 0.182959 |
| C | -0.737273 | 2.441167 | 0.784300 |
| C | 0.077842 | 3.967180 | -0.972618 |
| C | -2.009421 | 2.441566 | 0.219879 |
| C | -2.756158 | 1.207260 | 0.136034 |
| C | -2.262123 | 0.001583 | 0.698355 |
| C | -2.753836 | -1.206285 | 0.138705 |

| | | | |
|---|---|---|---|
| C | -3.720904 | -0.002627 | -1.814142 |
| C | -3.476881 | 1.206940 | -1.106611 |
| C | -3.474578 | -1.210146 | -1.103921 |
| C | 2.228197 | 3.221740 | -1.923837 |
| C | 2.472376 | 2.444787 | -0.727993 |
| C | 1.049962 | 3.967153 | -2.049047 |
| C | 1.535883 | 2.441372 | 0.300254 |
| C | 1.228249 | 1.210314 | 0.986107 |
| C | 1.922674 | 0.005571 | 0.700620 |
| C | 1.230535 | -1.199823 | 0.988810 |
| C | -0.922928 | 0.003550 | 1.296179 |
| C | -0.175256 | 1.209674 | 1.282909 |
| C | -0.172960 | -1.201195 | 1.285635 |
| C | 2.911556 | 0.005283 | -0.384186 |
| C | 3.128688 | 1.213217 | -1.103249 |
| C | 3.130959 | -1.203849 | -1.100542 |
| C | 0.329164 | -3.211150 | 0.190180 |
| C | 1.540524 | -2.431833 | 0.305753 |
| C | 2.477032 | -2.435833 | -0.722481 |
| C | 0.085389 | -3.963273 | -0.963669 |
| C | -2.265648 | -3.219033 | -0.965378 |
| C | -2.004750 | -2.438949 | 0.225347 |
| C | -0.732615 | -2.434836 | 0.789724 |
| C | -1.239049 | -3.966010 | -1.554823 |
| C | -1.964379 | -3.221719 | -3.791049 |
| C | -3.019593 | -2.445381 | -3.176600 |
| C | -3.166612 | -2.443610 | -1.791175 |
| C | -1.084787 | -3.966641 | -2.997158 |
| C | 0.816435 | -3.220128 | -4.379010 |
| C | -0.096088 | -2.444386 | -5.190757 |
| C | -1.458858 | -2.444698 | -4.901807 |
| C | 0.333880 | -3.965702 | -3.296708 |
| C | 2.234322 | -3.215944 | -1.916565 |
| C | 2.723251 | -2.439055 | -3.035023 |
| C | 2.028284 | -2.441549 | -4.242514 |
| C | 1.057499 | -3.963874 | -2.040080 |

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| | | | |
|---|---|---|---|
| C | -3.253869 | -0.738311 | -3.724819 |
| C | -3.259603 | 0.695338 | -3.718959 |
| C | -4.300088 | 1.398679 | -3.105762 |
| C | -5.339016 | 0.669143 | -2.526070 |
| C | -5.332649 | -0.740978 | -2.531090 |
| C | -4.287414 | -1.456267 | -3.116597 |
| C | -1.982208 | -1.161583 | -4.288130 |
| C | -1.993187 | 1.134300 | -4.283456 |
| H | -4.283698 | 2.485076 | -3.073830 |
| H | -6.161572 | 1.195036 | -2.046297 |
| H | -6.150288 | -1.277813 | -2.054992 |
| H | -4.259476 | -2.542648 | -3.091699 |
| C | 2.263163 | -2.452043 | -3.715538 |
| C | 1.023646 | -3.172928 | -3.710027 |
| C | 0.932296 | -4.424048 | -3.093898 |
| C | 2.082136 | -4.959045 | -2.511497 |
| C | 3.301126 | -4.250245 | -2.517315 |
| C | 3.400291 | -2.988717 | -3.105172 |
| C | 1.994763 | -1.139184 | -4.279842 |
| C | 0.011713 | -2.295878 | -4.277244 |
| H | -0.017377 | -4.951990 | -3.062259 |
| H | 2.035951 | -5.933378 | -2.029974 |
| H | 4.173936 | -4.689855 | -2.039507 |
| H | 4.328390 | -2.423457 | -3.080430 |
| C | 0.987059 | 3.182694 | -3.715403 |
| C | 2.231411 | 2.470180 | -3.705999 |
| C | 3.358234 | 3.017257 | -3.086363 |
| C | 3.244581 | 4.281289 | -2.505998 |
| C | 2.021168 | 4.982298 | -2.515909 |
| C | 0.880928 | 4.436430 | -3.106588 |
| C | -0.013584 | 2.294143 | -4.283968 |
| C | 1.979621 | 1.154797 | -4.272746 |
| H | 4.289467 | 2.457907 | -3.048746 |
| H | 4.109342 | 4.728304 | -2.020547 |
| H | 1.963951 | 5.958780 | -2.039915 |
| H | -0.072841 | 4.957491 | -3.085838 |
| N | 0.679899 | 1.190225 | -4.717485 |
| N | -1.372083 | -0.010028 | -4.723510 |
| N | 0.693232 | -1.186911 | -4.717377 |
| N | -1.348546 | 2.303064 | -4.144219 |
| N | -1.323380 | -2.321656 | -4.142533 |
| N | 2.669411 | 0.011870 | -4.134416 |
| B | 0.002229 | -0.002211 | -5.325815 |
| Cl | 0.007983 | -0.002267 | -7.211648 |
| C | 0.003521 | -0.001417 | 5.578305 |
| C | -0.989156 | 1.007722 | 5.367914 |
| C | -2.305991 | 0.666077 | 4.904685 |
| C | -2.653747 | -0.700839 | 4.592462 |
| C | -1.664364 | -1.704564 | 4.830918 |
| C | -0.373847 | -1.364836 | 5.365023 |
| C | 0.580914 | -2.333049 | 4.899481 |
| C | 1.939251 | -1.951419 | 4.587337 |
| C | 2.313067 | -0.593310 | 4.829864 |
| C | 1.373477 | 0.353454 | 5.366136 |
| C | 1.734501 | 1.664833 | 4.901894 |
| C | 0.723873 | 2.650135 | 4.591771 |
| C | -0.639019 | 2.295322 | 4.833809 |
| C | -1.705760 | 2.724819 | 3.952214 |
| C | -2.761245 | 1.760054 | 4.068319 |
| C | -1.503839 | -2.841198 | 3.947386 |
| C | -0.139475 | -3.271998 | 4.061371 |
| C | 3.215737 | 0.116494 | 3.946434 |
| C | 2.907035 | 1.513368 | 4.062719 |
| C | 3.124282 | 2.395103 | 2.975263 |
| C | 2.247998 | 3.532491 | 2.808647 |
| C | 0.983766 | 3.587736 | 3.523319 |
| C | -0.066807 | 3.862479 | 2.539185 |
| C | -1.430624 | 3.379719 | 2.702902 |
| C | -2.171180 | 2.962240 | 1.512615 |
| C | -3.281406 | 2.035691 | 1.673662 |
| C | -3.631272 | 1.508093 | 2.978995 |
| C | -4.179144 | 0.181495 | 2.810486 |
| C | -3.596030 | -0.942458 | 3.523745 |
| C | -3.310178 | -1.988680 | 2.537519 |
| C | -2.209858 | -2.928874 | 2.698302 |

| | | | |
|---|---|---|---|
| C | -1.477593 | -3.358403 | 1.507142 |
| C | -0.120266 | -3.858422 | 1.667409 |
| C | 0.513583 | -3.899516 | 2.972267 |
| C | 1.936666 | -3.710294 | 2.803223 |
| C | 2.620215 | -2.645286 | 3.518063 |
| C | 3.381760 | -1.871782 | 2.532504 |
| C | 3.643587 | -0.448568 | 2.696148 |
| C | 3.649599 | 0.403064 | 1.507137 |
| C | 3.405919 | 1.828893 | 1.669436 |
| C | 2.659322 | 2.617669 | 0.682676 |
| C | 1.990033 | 3.693908 | 1.397874 |
| C | 0.567282 | 3.905142 | 1.232851 |
| C | -0.096142 | 3.276575 | 0.150106 |
| C | -1.468118 | 2.866924 | 0.262463 |
| C | -1.643269 | 1.729982 | -0.615132 |
| C | -2.648120 | 0.741755 | -0.376923 |
| C | -3.591837 | 0.997002 | 0.685245 |
| C | -4.191169 | -0.120849 | 1.399091 |
| C | -3.663644 | -1.458503 | 1.231986 |
| C | -2.788139 | -1.716817 | 0.148007 |
| C | -1.746836 | -2.699455 | 0.258644 |
| C | -0.674651 | -2.280671 | -0.618097 |
| C | 0.683046 | -2.657069 | -0.379707 |
| C | 0.934223 | -3.604685 | 0.679878 |
| C | 2.202775 | -3.566433 | 1.392243 |
| C | 3.097797 | -2.440595 | 1.226403 |
| C | 2.881563 | -1.550351 | 0.145323 |
| C | 3.211701 | -0.157122 | 0.258125 |
| C | 2.314448 | 0.563785 | -0.618460 |
| C | 1.962799 | 1.927768 | -0.377375 |
| C | 0.608417 | 2.320889 | -0.678300 |
| C | -0.360157 | 1.370213 | -1.145591 |
| C | -2.312738 | -0.627409 | -0.679161 |
| C | -1.004830 | -0.988864 | -1.146083 |
| C | 1.700740 | -1.681114 | -0.681782 |
| C | 1.360210 | -0.367068 | -1.147570 |
| C | -0.001767 | 0.004729 | -1.360733 |
| N | 0.001923 | 0.001602 | 2.098200 |
| Sc | 0.984054 | -1.697015 | 2.070996 |
| Sc | -1.959899 | 0.000759 | 2.072532 |
| Sc | 0.987987 | 1.698084 | 2.071904 |

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| | | | |
|---|---|---|---|
| C | -3.098597 | -4.474145 | 0.246971 |
| C | -2.668488 | -4.434018 | 1.614671 |
| C | -3.496041 | -3.898168 | 2.604798 |
| C | -4.756335 | -3.433614 | 2.230489 |
| C | -5.180819 | -3.477098 | 0.886840 |
| C | -4.354693 | -3.983240 | -0.116478 |
| C | -1.973540 | -4.946645 | -0.543435 |
| C | -1.285538 | -4.880659 | 1.643533 |
| H | -3.153124 | -3.837662 | 3.634083 |
| H | -5.420756 | -3.017988 | 2.984375 |
| H | -6.165921 | -3.095582 | 0.628710 |
| H | -4.667710 | -3.989202 | -1.157110 |
| C | 1.630851 | -4.164777 | -3.075868 |
| C | 0.233045 | -4.252750 | -3.384006 |
| C | -0.276261 | -3.673772 | -4.548161 |
| C | 0.614267 | -3.033333 | -5.409489 |
| C | 1.988167 | -2.949026 | -5.108093 |
| C | 2.507065 | -3.500930 | -3.937077 |
| C | 1.810501 | -4.706160 | -1.738429 |
| C | -0.424356 | -4.850261 | -2.233224 |
| H | -1.341276 | -3.711870 | -4.760837 |
| H | 0.241747 | -2.573779 | -6.321820 |
| H | 2.650452 | -2.425245 | -5.793075 |
| H | 3.559714 | -3.404969 | -3.685161 |
| C | 2.145334 | -4.103670 | 2.682080 |
| C | 3.110465 | -4.048049 | 1.623110 |
| C | 4.324655 | -3.380591 | 1.802088 |
| C | 4.578521 | -2.793812 | 3.041475 |
| C | 3.628877 | -2.846888 | 4.082115 |
| C | 2.403694 | -3.490422 | 3.910851 |
| C | 0.950319 | -4.730355 | 2.140719 |
| C | 2.496745 | -4.646283 | 0.449127 |
| H | 5.041694 | -3.317058 | 0.988031 |
| H | 5.518069 | -2.271459 | 3.205639 |
| H | 3.853231 | -2.365036 | 5.030765 |
| H | 1.656731 | -3.504723 | 4.699788 |
| N | 1.297796 | -5.149488 | 0.881482 |
| N | -1.013030 | -5.302347 | 0.367171 |
| N | 0.587531 | -5.214586 | -1.382147 |
| N | -0.324275 | -4.667698 | 2.555429 |
| N | -1.709178 | -4.797457 | -1.850938 |
| N | 2.795676 | -4.503028 | -0.851430 |
| B | 0.329330 | -5.824689 | -0.039195 |
| Cl | 0.448384 | -7.698117 | -0.021624 |
| C | -3.260327 | 2.081573 | 2.671518 |
| C | -3.763643 | 2.980058 | 1.669284 |
| C | -3.103559 | 4.249530 | 1.835456 |
| C | -2.283366 | 2.786784 | 3.456396 |
| C | -2.184573 | 4.120595 | 2.943170 |
| C | -1.136764 | 2.116883 | 3.983344 |
| C | -1.047573 | 0.704144 | 3.795217 |
| C | -3.111956 | 0.689690 | 2.407451 |
| C | -2.025416 | 0.003013 | 3.015701 |
| C | -3.561519 | 0.200896 | 1.130246 |
| C | -4.136686 | 2.517712 | 0.379589 |
| C | -4.050552 | 1.108662 | 0.135549 |
| C | -3.922959 | 3.378278 | -0.735604 |
| C | -2.844276 | 5.115335 | 0.722192 |
| C | -3.277621 | 4.657429 | -0.571394 |
| C | -1.645036 | 5.928813 | 0.759168 |
| C | -0.945159 | 4.817035 | 2.940329 |
| C | -0.697234 | 5.704855 | 1.832863 |
| C | 0.083409 | 2.855977 | 4.073953 |
| C | 0.180417 | 4.191547 | 3.549896 |
| C | 1.348883 | 2.213114 | 3.878834 |
| C | 0.223739 | 0.063188 | 3.593557 |
| C | 1.429068 | 0.823272 | 3.589642 |
| C | -1.362673 | -1.077216 | 2.325219 |
| C | 0.030157 | -1.030368 | 2.683199 |
| C | -2.974788 | -0.941614 | 0.463682 |

| | | | |
|---|---|---|---|
| C | -1.796443 | -1.546187 | 1.043092 |
| C | -3.723826 | 0.573298 | -1.157568 |
| C | -3.088455 | -0.717779 | -0.982667 |
| C | -3.571535 | 2.859468 | -2.027476 |
| C | -3.428714 | 1.456968 | -2.255090 |
| C | -2.510998 | 4.922080 | -1.778970 |
| C | -2.691871 | 3.796021 | -2.664996 |
| C | -0.870680 | 6.206766 | -0.459705 |
| C | -1.278426 | 5.664344 | -1.745883 |
| C | 0.628319 | 5.864093 | 1.314247 |
| C | 0.529646 | 6.127046 | -0.094843 |
| C | 1.507599 | 4.374193 | 3.028738 |
| C | 2.240436 | 3.150526 | 3.233020 |
| C | 1.751659 | 5.184197 | 1.888603 |
| C | 3.273746 | 2.729584 | 2.330912 |
| C | 2.481498 | 0.403001 | 2.699160 |
| C | 3.458174 | 1.306075 | 2.122366 |
| C | 1.027878 | -1.396031 | 1.747856 |
| C | 2.261830 | -0.674602 | 1.784765 |
| C | -0.774568 | -1.978053 | 0.129755 |
| C | 0.619994 | -1.907765 | 0.485366 |
| C | -2.011000 | -1.086793 | -1.884934 |
| C | -0.875206 | -1.745810 | -1.300258 |
| C | -2.450628 | 1.028939 | -3.190633 |
| C | -1.727905 | -0.207657 | -2.983731 |
| C | -1.651083 | 3.356055 | -3.540646 |
| C | -1.572884 | 1.960681 | -3.835593 |
| C | -0.250096 | 5.215905 | -2.640154 |
| C | -0.439954 | 4.105430 | -3.540723 |
| C | 1.558664 | 5.665181 | -0.991417 |
| C | 1.152025 | 5.248626 | -2.286036 |
| C | 2.800100 | 4.807621 | 1.000695 |
| C | 3.544024 | 3.589851 | 1.209592 |
| C | 2.703709 | 5.038447 | -0.413251 |
| C | 3.900687 | 3.062408 | -0.098096 |
| C | 3.364349 | 3.960970 | -1.092004 |
| C | 3.826479 | 0.768796 | 0.802141 |
| C | 3.049935 | -0.439159 | 0.609704 |
| C | 4.011467 | 1.648632 | -0.341086 |
| C | 1.375152 | -1.645499 | -0.703167 |
| C | 0.460565 | -1.525700 | -1.798244 |
| C | 2.582662 | -0.888999 | -0.675480 |
| C | -0.394244 | -0.014643 | -3.499593 |
| C | -0.301185 | 1.318042 | -4.020287 |
| C | 0.725574 | -0.645322 | -2.889584 |
| C | 0.829031 | 3.468467 | -3.741043 |
| C | 1.813315 | 4.177718 | -2.971902 |
| C | 2.900724 | 3.485949 | -2.357498 |
| C | 0.919748 | 2.055912 | -3.933837 |
| C | 3.556777 | 1.192135 | -1.623939 |
| C | 2.883823 | -0.076938 | -1.798984 |
| C | 1.973994 | 0.045292 | -2.899750 |
| C | 3.039258 | 2.093749 | -2.623177 |
| C | 2.065831 | 1.386558 | -3.405333 |
| N | -0.121197 | 2.087960 | 0.086241 |
| Sc | -1.248966 | 0.454088 | -0.230710 |
| Sc | -0.895523 | 3.925528 | -0.140894 |
| Sc | 1.803800 | 1.841796 | 0.597732 |

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| | | | |
|---|---|---|---|
| C | 0.129579 | -1.176253 | -4.637121 |
| C | 1.149824 | -0.194226 | -4.645240 |
| C | 0.531298 | 1.079267 | -4.626816 |
| C | -0.871342 | 0.884719 | -4.608268 |
| C | -1.119395 | -0.509568 | -4.613767 |
| C | 0.321187 | -2.442378 | -4.107242 |
| C | 2.414787 | -0.414133 | -4.123643 |
| C | 1.133757 | 2.203729 | -4.086140 |
| C | -1.751651 | 1.793658 | -4.043994 |
| C | -2.254509 | -1.077436 | -4.058185 |
| C | -3.277818 | -0.117057 | -3.660015 |
| C | -3.028616 | 1.261139 | -3.653231 |
| C | -1.148181 | 3.067538 | -3.669254 |
| C | 0.239405 | 3.257076 | -3.689525 |
| C | 3.147508 | 0.766287 | -3.753682 |
| C | 2.538703 | 2.027588 | -3.735858 |
| C | 2.687712 | -1.801420 | -3.765543 |
| C | 1.676583 | -2.770687 | -3.758355 |
| C | -0.907192 | -3.126634 | -3.719134 |
| C | -2.141021 | -2.464053 | -3.695742 |
| H | -3.784631 | 1.923600 | -3.239375 |
| H | 0.642722 | 4.185262 | -3.292433 |
| H | 4.162297 | 0.674255 | -3.374823 |
| H | 1.909706 | -3.760460 | -3.373884 |
| H | -3.003392 | -2.988296 | -3.291666 |
| C | -1.985599 | 4.087262 | -3.123997 |
| N | -2.700990 | 4.886300 | -2.674671 |
| C | -4.505876 | -0.608659 | -3.122538 |
| N | -5.486406 | -1.051082 | -2.680991 |
| C | -0.817939 | -4.457405 | -3.209444 |
| N | -0.700077 | -5.536378 | -2.792218 |
| C | 3.982093 | -2.137281 | -3.265171 |
| N | 5.045100 | -2.366437 | -2.853300 |
| C | 3.259156 | 3.145459 | -3.216538 |
| N | 3.804884 | 4.078494 | -2.787866 |
| C | -0.767612 | 0.875832 | -1.217939 |
| C | -1.053624 | -0.542886 | -1.213117 |
| C | -2.149368 | -1.033347 | -0.498963 |
| C | -2.999038 | -0.119168 | 0.239091 |
| C | -2.723141 | 1.251971 | 0.233173 |
| C | -1.585662 | 1.758428 | -0.509405 |
| C | 0.670542 | 1.042988 | -1.198889 |
| C | 1.273946 | -0.273712 | -1.181058 |
| C | 0.207385 | -1.254162 | -1.189994 |
| C | 0.331493 | -2.432063 | -0.449589 |
| C | -2.023063 | -2.256855 | 0.269469 |
| C | -3.396099 | -0.776387 | 1.470428 |
| C | -3.497800 | -0.035879 | 2.652064 |
| C | -3.210285 | 1.387678 | 2.646299 |
| C | -2.831972 | 2.021369 | 1.459136 |
| C | -1.763492 | 3.004517 | 1.469081 |
| C | -0.993320 | 2.842471 | 0.249646 |
| C | 0.395884 | 3.003839 | 0.269420 |

| | | | |
|---|---|---|---|
| C | 1.243535 | 2.086189 | -0.467986 |
| C | 2.429535 | -0.504016 | -0.430761 |
| C | 3.026692 | 0.577951 | 0.329503 |
| C | 2.443497 | 1.849460 | 0.311672 |
| C | 2.335740 | 2.618565 | 1.537675 |
| C | 1.071393 | 3.331833 | 1.511553 |
| C | 0.330473 | 3.483095 | 2.687497 |
| C | -1.111931 | 3.316724 | 2.665827 |
| C | -1.506440 | 2.661144 | 3.899300 |
| C | -2.535919 | 1.714603 | 3.889552 |
| C | -2.792297 | -2.096496 | 1.490106 |
| C | -0.648366 | -1.056187 | 5.438438 |
| C | -1.220401 | -2.097739 | 4.702015 |
| C | -0.372218 | -3.012489 | 3.959773 |
| C | 1.016672 | -2.852249 | 3.980829 |
| C | 1.610402 | -1.770406 | 4.745421 |
| C | 1.080436 | 0.533463 | 5.454313 |
| C | -0.184012 | 1.245963 | 5.428673 |
| C | -1.252588 | 0.263660 | 5.418747 |
| C | -2.406497 | 0.493363 | 4.663614 |
| C | -3.000975 | -0.588022 | 3.899232 |
| C | -2.418834 | -1.859425 | 3.917961 |
| C | -1.046197 | -3.339969 | 2.716716 |
| C | -0.306420 | -3.496315 | 1.540693 |
| C | 1.135693 | -3.330042 | 1.562536 |
| C | 1.784881 | -3.012959 | 2.759415 |
| C | 2.853171 | -2.029438 | 2.769395 |
| C | 2.744742 | -1.262012 | 3.996637 |
| C | 3.021813 | 0.108491 | 3.991268 |
| C | 2.174258 | 1.023337 | 4.734140 |
| C | -0.308234 | 2.421973 | 4.683062 |
| C | 0.826797 | 2.929919 | 3.934235 |
| C | 2.045276 | 2.244392 | 3.959949 |
| C | 2.812947 | 2.084496 | 2.738311 |
| C | 3.416946 | 0.764283 | 2.757907 |
| C | 3.523724 | 0.024562 | 1.576155 |
| C | 3.235880 | -1.398579 | 1.581985 |
| C | 2.560298 | -1.726070 | 0.339863 |
| C | 1.531198 | -2.673653 | 0.329697 |
| C | -2.310939 | -2.626929 | 2.690609 |
| C | -0.803685 | -2.941783 | 0.295346 |
| C | 0.793518 | -0.889115 | 5.459945 |

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| | | | |
|---|---|---|---|
| C | -0.013033 | -1.553437 | 4.783669 |
| C | 1.143141 | -0.742159 | 4.870867 |
| C | 0.723270 | 0.603028 | 4.997713 |
| C | -0.692043 | 0.622113 | 4.995667 |
| C | -1.147238 | -0.711826 | 4.867879 |
| C | -0.020701 | -2.767549 | 4.117084 |
| C | 2.360356 | -1.093725 | 4.311151 |
| C | 1.484812 | 1.677043 | 4.566703 |
| C | -1.435005 | 1.706998 | 4.559976 |
| C | -2.367395 | -1.044212 | 4.303585 |
| C | -3.247833 | 0.093845 | 4.061745 |
| C | -2.790272 | 1.413321 | 4.177037 |
| C | -0.648783 | 2.906474 | 4.296805 |
| C | 0.753273 | 2.885339 | 4.302001 |
| C | 3.263198 | -0.003168 | 4.060691 |
| C | 2.849017 | 1.330215 | 4.181607 |
| C | 2.418396 | -2.462939 | 3.810495 |
| C | 1.268608 | -3.257926 | 3.710995 |
| C | -1.344678 | -3.217332 | 3.700952 |
| C | -2.468477 | -2.385077 | 3.794643 |
| H | -3.452785 | 2.219998 | 3.873684 |
| H | 1.285517 | 3.780449 | 3.989950 |
| H | 4.255565 | -0.203674 | 3.665288 |
| H | 1.349080 | -4.227990 | 3.227095 |
| H | -3.407545 | -2.731485 | 3.371319 |
| C | -1.327389 | 4.087678 | 3.869215 |
| N | -1.917562 | 5.022183 | 3.507787 |
| C | -4.563833 | -0.150618 | 3.565309 |
| N | -5.627518 | -0.392924 | 3.162727 |
| C | -1.466151 | -4.487415 | 3.059988 |
| N | -1.520164 | -5.524888 | 2.537669 |
| C | 3.654463 | -2.950532 | 3.288365 |
| N | 4.679557 | -3.308721 | 2.872479 |
| C | 3.737220 | 2.376611 | 3.788365 |
| N | 4.426891 | 3.257188 | 3.470414 |
| C | 3.139870 | -2.199028 | -1.015712 |
| C | 2.367456 | -2.047766 | 0.196352 |
| C | 3.921912 | -1.137389 | -1.485182 |
| C | 2.408596 | -0.848942 | 0.902231 |
| C | 1.195040 | -0.308170 | 1.464998 |
| C | -0.035284 | -1.012725 | 1.396079 |
| C | -1.213427 | -0.224713 | 1.468696 |
| C | 3.154316 | -1.574652 | -3.786519 |
| C | 2.339602 | -2.664599 | -3.293688 |
| C | 3.929910 | -0.819823 | -2.900090 |
| C | 2.333581 | -2.972304 | -1.935581 |
| C | 1.089327 | -3.313600 | -1.283955 |
| C | -0.126045 | -3.433482 | -2.013415 |
| C | -1.327076 | -3.229100 | -1.279169 |
| C | -0.080685 | -2.277195 | 0.652514 |
| C | 1.111285 | -2.742554 | 0.034487 |
| C | -1.303853 | -2.657721 | 0.038248 |
| C | 3.251257 | 1.251953 | -4.050732 |
| C | 2.444551 | 0.466874 | -4.959263 |
| C | 3.979854 | 0.623655 | -3.035342 |
| C | 2.396960 | -0.919038 | -4.830201 |
| C | 1.139026 | -1.612092 | -4.990542 |
| C | -0.046521 | -0.923863 | -5.368823 |
| C | -1.275415 | -1.528694 | -4.985864 |
| C | -0.118058 | -3.109513 | -3.447011 |
| C | 1.103797 | -2.690638 | -4.041694 |
| C | -1.310633 | -2.606837 | -4.036297 |
| C | 3.296950 | 2.378390 | -1.442823 |
| C | 2.539366 | 3.020402 | -2.495334 |
| C | 4.002655 | 1.198003 | -1.703635 |
| C | 2.516533 | 2.467745 | -3.773641 |
| C | 1.280516 | 2.438445 | -4.522022 |
| C | 0.093572 | 3.041356 | -4.022318 |
| C | -1.134117 | 2.521360 | -4.516593 |

| | | | |
|---|---|---|---|
| C | 0.004035 | 0.538581 | -5.505228 |
| C | 1.236204 | 1.202434 | -5.254004 |
| C | -1.178500 | 1.285395 | -5.248753 |
| C | 3.226480 | 0.246039 | 0.433369 |
| C | 2.490979 | 1.464039 | 0.691868 |
| C | 3.967261 | 0.109611 | -0.746699 |
| C | 2.525674 | 2.510362 | -0.226344 |
| C | 1.317544 | 3.245277 | -0.523593 |
| C | 0.100285 | 2.989679 | 0.165726 |
| C | -1.098808 | 3.329734 | -0.518636 |
| C | 0.116744 | 3.623395 | -2.672904 |
| C | 1.325168 | 3.558975 | -1.925946 |
| C | -1.090275 | 3.643256 | -1.920838 |
| C | 0.063946 | 1.882489 | 1.128995 |
| C | 1.244928 | 1.120018 | 1.334069 |
| C | -1.165388 | 1.203469 | 1.338818 |
| C | -3.137231 | 2.602055 | -1.429448 |
| C | -2.353795 | 2.680894 | -0.215741 |
| C | -2.388166 | 1.633993 | 0.702785 |
| C | -3.923069 | 1.472812 | -1.687320 |
| C | -3.180468 | 1.474995 | -4.037635 |
| C | -2.361918 | 2.636700 | -3.763375 |
| C | -2.341169 | 3.189726 | -2.485231 |
| C | -3.945997 | 0.898026 | -3.019003 |
| C | -3.278143 | -1.352577 | -3.773120 |
| C | -2.482126 | -0.750395 | -4.820660 |
| C | -2.433907 | 0.635657 | -4.949694 |
| C | -3.995307 | -0.545429 | -2.883530 |
| C | -3.295927 | -1.977303 | -1.002060 |
| C | -2.548046 | -2.803687 | -1.925260 |
| C | -2.538797 | -2.495970 | -3.283448 |
| C | -4.003574 | -0.862993 | -1.468623 |
| C | -3.204627 | 0.468842 | 0.444347 |
| C | -2.463731 | -0.680048 | 0.911142 |
| C | -2.509984 | -1.880916 | 0.207622 |
| C | -3.959076 | 0.384231 | -0.730731 |

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| | | | |
|---|---|---|---|
| C | -0.424786 | -1.120887 | -4.880295 |
| C | 0.688412 | -0.247744 | -4.937788 |
| C | 0.204057 | 1.082677 | -4.905035 |
| C | -1.207910 | 1.030825 | -4.825905 |
| C | -1.597061 | -0.330533 | -4.811900 |
| C | -0.341797 | -2.395990 | -4.345345 |
| C | 1.945745 | -0.593084 | -4.471412 |
| C | 0.939245 | 2.143593 | -4.400725 |
| C | -1.970383 | 2.030240 | -4.242052 |
| C | -2.762614 | -0.777214 | -4.210069 |
| C | -3.667452 | 0.284461 | -3.788991 |
| C | -3.279339 | 1.631805 | -3.804319 |
| C | -1.224368 | 3.236138 | -3.900780 |
| C | 0.173603 | 3.285171 | -3.982087 |
| C | 2.808976 | 0.507922 | -4.141942 |
| C | 2.332536 | 1.825204 | -4.107649 |
| C | 2.091708 | -2.000455 | -4.116362 |
| C | 0.987081 | -2.859495 | -4.051939 |
| C | -1.615913 | -2.951072 | -3.904171 |
| C | -2.774618 | -2.166360 | -3.837583 |
| H | -3.949550 | 2.368706 | -3.368706 |
| H | 0.684023 | 4.169275 | -3.608739 |
| H | 3.823683 | 0.314993 | -3.804194 |
| H | 1.134692 | -3.867380 | -3.672605 |
| H | -3.668696 | -2.597908 | -3.395002 |
| C | -1.930160 | 4.336150 | -3.325740 |
| N | -2.542727 | 5.201873 | -2.848652 |
| C | -4.912097 | -0.075444 | -3.189678 |
| N | -5.906315 | -0.412027 | -2.689047 |
| C | -1.642059 | -4.282625 | -3.389544 |
| N | -1.619162 | -5.368588 | -2.974115 |
| C | 3.370486 | -2.472604 | -3.691476 |
| N | 4.426403 | -2.818173 | -3.348144 |
| C | 3.190418 | 2.864180 | -3.635287 |
| N | 3.856383 | 3.733105 | -3.243124 |
| C | -0.326837 | 0.083071 | 5.317800 |
| C | -1.211545 | 1.138848 | 4.930507 |
| C | -2.458641 | 0.851973 | 4.276016 |
| C | -2.841070 | -0.503405 | 3.952318 |
| C | -1.960725 | -1.549367 | 4.367114 |
| C | -0.749985 | -1.263230 | 5.086208 |
| C | 0.204191 | -2.298678 | 4.795911 |
| C | 1.613224 | -2.004647 | 4.684343 |
| C | 2.027248 | -0.662048 | 4.943636 |
| C | 1.077482 | 0.352145 | 5.305071 |
| C | 1.582481 | 1.623946 | 4.864411 |
| C | 0.695479 | 2.656410 | 4.382333 |
| C | -0.707779 | 2.384075 | 4.421338 |
| C | -1.598230 | 2.838683 | 3.374492 |
| C | -2.714934 | 1.936946 | 3.349898 |
| C | -1.735030 | -2.722111 | 3.548756 |
| C | -0.434487 | -3.223978 | 3.882438 |
| C | 3.093852 | -0.037850 | 4.190964 |
| C | 2.857008 | 1.377614 | 4.219603 |
| C | 3.299312 | 2.210840 | 3.162721 |
| C | 2.526321 | 3.388584 | 2.835268 |
| C | 1.173404 | 3.542302 | 3.346564 |
| C | 0.301664 | 3.831694 | 2.203807 |
| C | -1.096926 | 3.432668 | 2.167253 |
| C | -1.672671 | 3.015446 | 0.890855 |
| C | -2.850950 | 2.162946 | 0.904607 |
| C | -3.432801 | 1.702319 | 2.151636 |
| C | -4.024002 | 0.400054 | 1.937885 |
| C | -3.626776 | -0.730446 | 2.761634 |
| C | -3.249946 | -1.821746 | 1.858644 |
| C | -2.246623 | -2.814607 | 2.209966 |
| C | -1.372316 | -3.328619 | 1.157499 |
| C | -0.088479 | -3.895640 | 1.536995 |
| C | 0.336531 | -3.923123 | 2.922509 |
| C | 1.775869 | -3.819343 | 2.968723 |
| C | 2.404664 | -2.770457 | 3.750065 |
| C | 3.354114 | -2.078800 | 2.874867 |
| C | 3.674411 | -0.669221 | 3.039067 |
| C | 3.912979 | 0.137977 | 1.843769 |
| C | 3.734513 | 1.579551 | 1.930013 |

| | | | |
|---|---|---|---|
| C | 3.187536 | 2.367310 | 0.823138 |
| C | 2.486120 | 3.500359 | 1.399466 |
| C | 1.124811 | 3.783745 | 1.012159 |
| C | 0.597976 | 3.167671 | -0.149888 |
| C | -0.794178 | 2.834359 | -0.230617 |
| C | -0.902907 | 1.677908 | -1.091623 |
| C | -1.987533 | 0.758254 | -0.982290 |
| C | -3.062645 | 1.104103 | -0.085670 |
| C | -3.824841 | 0.048887 | 0.556193 |
| C | -3.361503 | -1.317117 | 0.504869 |
| C | -2.357629 | -1.668035 | -0.430392 |
| C | -1.408363 | -2.700615 | -0.134170 |
| C | -0.192394 | -2.378096 | -0.848093 |
| C | 1.088997 | -2.822736 | -0.397183 |
| C | 1.117541 | -3.740526 | 0.717313 |
| C | 2.261554 | -3.742843 | 1.614792 |
| C | 3.237756 | -2.677230 | 1.557362 |
| C | 3.243643 | -1.817229 | 0.432237 |
| C | 3.634698 | -0.441516 | 0.559437 |
| C | 2.931260 | 0.296742 | -0.466623 |
| C | 2.626226 | 1.685205 | -0.317679 |
| C | 1.362660 | 2.147384 | -0.837123 |
| C | 0.420286 | 1.229190 | -1.411043 |
| C | -1.697391 | -0.636931 | -1.203812 |
| C | -0.358731 | -1.086287 | -1.452947 |
| C | 2.200569 | -1.916095 | -0.566818 |
| C | 2.014521 | -0.600275 | -1.112512 |
| C | 0.722959 | -0.158865 | -1.531289 |
| N | 0.199055 | -0.036523 | 1.891408 |
| Sc | 1.074487 | -1.789878 | 2.045158 |
| Sc | -1.741638 | 0.097769 | 1.608665 |
| Sc | 1.292659 | 1.592401 | 2.030481 |

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| | | | |
|---|---|---|---|
| C | -0.526807 | -1.035329 | -5.498858 |
| C | 0.609775 | -0.194597 | -5.579826 |
| C | 0.166564 | 1.148908 | -5.513297 |
| C | -1.243259 | 1.137931 | -5.389947 |
| C | -1.672759 | -0.211467 | -5.383415 |
| C | -0.465018 | -2.318813 | -4.980556 |
| C | 1.869770 | -0.583044 | -5.154826 |
| C | 0.948721 | 2.179497 | -5.015694 |
| C | -1.956257 | 2.150258 | -4.766782 |
| C | -2.830249 | -0.631513 | -4.747935 |
| C | -3.687474 | 0.449250 | -4.279332 |
| C | -3.260978 | 1.784275 | -4.289458 |
| C | -1.163868 | 3.326940 | -4.430019 |
| C | 0.231758 | 3.335445 | -4.554342 |
| C | 2.775386 | 0.486897 | -4.836936 |
| C | 2.340345 | 1.816773 | -4.770634 |
| C | 1.984658 | -1.997996 | -4.819951 |
| C | 0.857244 | -2.824352 | -4.730974 |
| C | -1.740687 | -2.841486 | -4.504514 |
| C | -2.872067 | -2.023789 | -4.391000 |
| H | -3.893788 | 2.533395 | -3.820255 |
| H | 0.780595 | 4.195284 | -4.178650 |
| H | 3.794249 | 0.259372 | -4.534850 |
| H | 0.985603 | -3.839476 | -4.364192 |
| H | -3.763194 | -2.432187 | -3.921475 |
| C | -1.814917 | 4.431950 | -3.802359 |
| N | -2.380917 | 5.299388 | -3.273532 |
| C | -4.915256 | 0.115045 | -3.631966 |
| N | -5.895069 | -0.202359 | -3.091983 |
| C | -1.791081 | -4.176356 | -4.000036 |
| N | -1.790793 | -5.264851 | -3.590612 |
| C | 3.261518 | -2.510122 | -4.437556 |
| N | 4.318835 | -2.885934 | -4.132652 |
| C | 3.243562 | 2.825644 | -4.317605 |
| N | 3.947343 | 3.673691 | -3.946504 |
| C | -2.628076 | -0.168918 | 4.866440 |
| C | -3.311808 | 0.644177 | 3.898042 |
| C | -2.737205 | 1.964159 | 3.936082 |
| C | -1.624960 | 0.641418 | 5.502422 |
| C | -1.689406 | 1.953714 | 4.930514 |
| C | -0.376789 | 0.081159 | 5.913404 |
| C | -0.200968 | -1.329468 | 5.769626 |
| C | -2.404431 | -1.557151 | 4.641346 |
| C | -1.205924 | -2.135221 | 5.142257 |
| C | -2.960669 | -2.139215 | 3.445622 |
| C | -3.793614 | 0.096436 | 2.680735 |
| C | -3.624056 | -1.313327 | 2.481807 |
| C | -3.781556 | 0.916177 | 1.516272 |
| C | -2.672268 | 2.789710 | 2.765360 |
| C | -3.216761 | 2.241943 | 1.553171 |
| C | -1.546319 | 3.692039 | 2.628054 |
| C | -0.515110 | 2.734289 | 4.750648 |
| C | -0.467257 | 3.583848 | 3.587735 |
| C | 0.785024 | 0.908343 | 5.825830 |
| C | 0.718301 | 2.220729 | 5.244152 |
| C | 2.064586 | 0.348523 | 5.506864 |
| C | 1.083046 | -1.886716 | 5.440455 |
| C | 2.217062 | -1.043675 | 5.263687 |
| C | -0.547979 | -3.200499 | 4.420848 |
| C | 0.870941 | -3.037853 | 4.606737 |
| C | -2.378272 | -3.275593 | 2.760035 |
| C | -1.089964 | -3.759632 | 3.216814 |
| C | -3.417291 | -1.887482 | 1.181136 |
| C | -2.673883 | -3.124744 | 1.327074 |
| C | -3.544578 | 0.363080 | 0.213302 |
| C | -3.324542 | -1.034257 | 0.023606 |
| C | -2.619840 | 2.507106 | 0.255060 |
| C | -2.818773 | 1.330522 | -0.558348 |
| C | -0.945059 | 3.974227 | 1.316117 |
| C | -1.456026 | 3.340755 | 0.111708 |
| C | 0.773066 | 3.812904 | 2.909292 |
| C | 0.491959 | 4.007794 | 1.513712 |
| C | 1.957982 | 2.471623 | 4.561471 |
| C | 2.800968 | 1.315399 | 4.724227 |
| C | 2.004981 | 3.243718 | 3.371589 |
| C | 3.750150 | 0.927789 | 3.721361 |
| C | 3.190601 | -1.430992 | 4.273162 |
| C | 4.017814 | -0.486872 | 3.547930 |
| C | 1.782139 | -3.382245 | 3.574789 |

| | | | |
|---|---|---|---|
| C | 2.956146 | -2.570599 | 3.437671 |
| C | -0.148734 | -4.155338 | 2.203837 |
| C | 1.270164 | -3.978346 | 2.387821 |
| C | -1.676278 | -3.449167 | 0.320339 |
| C | -0.431909 | -3.997653 | 0.787124 |
| C | -2.427596 | -1.435127 | -1.001408 |
| C | -1.593753 | -2.604239 | -0.837125 |
| C | -1.850114 | 0.923445 | -1.522619 |
| C | -1.698231 | -0.471887 | -1.770991 |
| C | -0.504369 | 2.921573 | -0.877429 |
| C | -0.710294 | 1.754817 | -1.695857 |
| C | 1.444991 | 3.581002 | 0.519833 |
| C | 0.923112 | 3.074332 | -0.700447 |
| C | 2.968733 | 2.903908 | 2.380477 |
| C | 3.820769 | 1.752381 | 2.545066 |
| C | 2.692346 | 3.061620 | 0.980423 |
| C | 4.064758 | 1.191482 | 1.226644 |
| C | 3.352694 | 2.003956 | 0.269860 |
| C | 4.274142 | -1.057639 | 2.216794 |
| C | 3.578789 | -2.328850 | 2.165366 |
| C | 4.256559 | -0.220467 | 1.027695 |
| C | 1.863259 | -3.724917 | 1.104550 |
| C | 0.819373 | -3.720763 | 0.121683 |
| C | 2.999315 | -2.871356 | 0.962413 |
| C | -0.346090 | -2.340306 | -1.507354 |
| C | -0.413758 | -1.027816 | -2.076478 |
| C | 0.883947 | -2.866639 | -1.020542 |
| C | 0.570044 | 1.202512 | -2.020834 |
| C | 1.580560 | 2.019566 | -1.412648 |
| C | 2.783631 | 1.437583 | -0.909886 |
| C | 0.745815 | -0.203967 | -2.167226 |
| C | 3.693303 | -0.768086 | -0.173028 |
| C | 3.102761 | -2.087825 | -0.216636 |
| C | 2.063453 | -2.083266 | -1.202233 |
| C | 2.995997 | 0.047496 | -1.135689 |
| C | 1.992725 | -0.763933 | -1.761013 |
| N | 0.177266 | -0.060917 | 1.920330 |
| Sc | -0.908868 | -1.747519 | 1.830253 |
| Sc | -0.713133 | 1.726121 | 1.709905 |
| Sc | 2.161748 | -0.159172 | 2.211733 |