

## Electronic Supplementary Information

# Mechanisms for Dehydrogenation and Hydrogenation of N-heterocycles using PNP-Pincer- Supported Iron Catalysts: A Density Functional Study

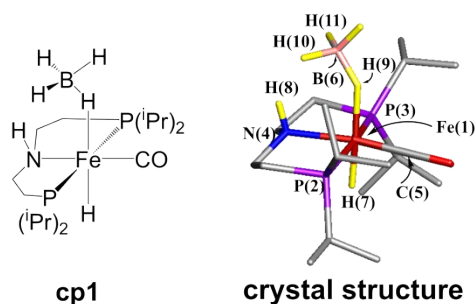
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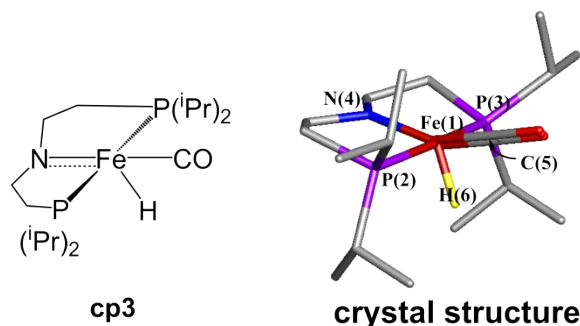
**Table S1** Selected bond distances (Å) and bond angles (°) of X-ray crystal structure and calculated structures in singlet, triplet, and quintet states of **cp1**. The relative free energies in the gas phase are shown in kcal/mol.



|                                                              | Crystal<br>Structure* | B3LYP/BS1 |       |       |
|--------------------------------------------------------------|-----------------------|-----------|-------|-------|
|                                                              |                       | S = 0     | S = 1 | S = 2 |
| <i>Relative Energy (kcal/mol)</i>                            |                       |           |       |       |
| $\Delta G$                                                   |                       | 0.00      | 15.81 | 20.90 |
| <i>Geometry Parameters (<math>\text{\AA}</math>, degree)</i> |                       |           |       |       |
| Fe(1)-H(9)                                                   | 1.70                  | 1.69      | 1.74  | 1.90  |
| Fe(1)-H(7)                                                   | 1.45                  | 1.52      | 1.56  | 1.70  |
| Fe(1)-N(4)                                                   | 2.07                  | 2.12      | 2.13  | 2.30  |
| Fe(1)-P(2)                                                   | 2.22                  | 2.27      | 2.72  | 2.65  |
| Fe(1)-P(3)                                                   | 2.21                  | 2.26      | 2.63  | 2.61  |
| Fe(1)-C(5)                                                   | 1.72                  | 1.75      | 1.79  | 2.12  |
| H(8)-H(10)                                                   | 2.16                  | 2.22      | 2.00  | 2.05  |
| H(8)-H(11)                                                   | 2.43                  | 2.03      | 2.20  | 2.21  |
| H(7)-Fe(1)-C(5)                                              | 87.5                  | 87.6      | 82.0  | 80.7  |
| H(7)-Fe(1)-N(4)                                              | 85.3                  | 88.5      | 89.5  | 99.2  |
| N(4)-Fe(1)-H(9)                                              | 92.2                  | 92.1      | 95.3  | 92.1  |
| N(4)-Fe(1)-B(6)                                              | 77.6                  | 75.0      | 75.7  | 74.1  |
| Fe(1)-H(9)-B(6)                                              | 143.8                 | 140.3     | 132.8 | 129.8 |

\* I. Koehne, T. J. Schmeier, E. A. Bielinski, C. J. Pan, P. O. Lagaditis, W. H. Bernskoetter, M. K. Takase, C. Wurtele, N. Hazari and S. Schneider, *Inorganic chemistry*, 2014, **53**, 2133-2143.

**Table S2** Selected bond distances (Å) and bond angles (°) of X-ray crystal structure and calculated structures in singlet, triplet, and quintet states of **cp3**. The relative free energies in the gas phase are shown in kcal/mol.

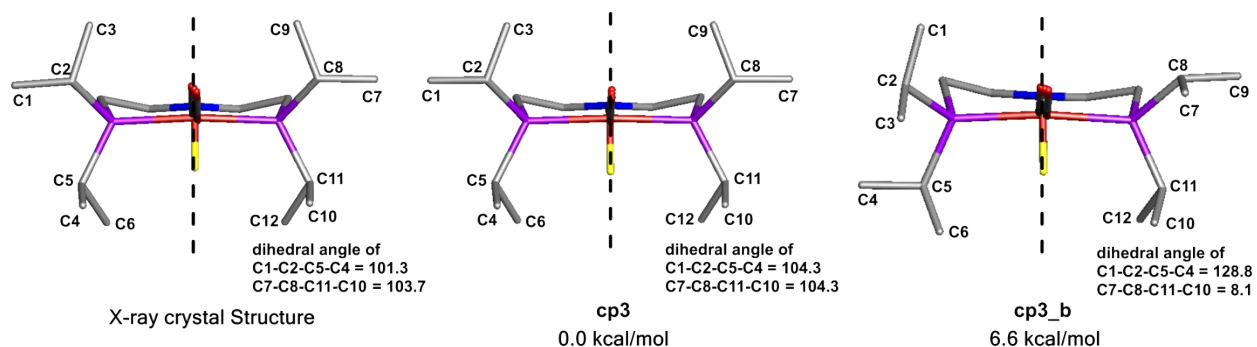


| Crystal<br>Structure*           |       | B3LYP/BS1 |       |       |
|---------------------------------|-------|-----------|-------|-------|
|                                 |       | S = 0     | S = 1 | S = 2 |
| Relative Energy (kcal/mol)      |       |           |       |       |
| ΔG                              |       | 0.00      | 13.21 | 18.84 |
| Geometry Parameters (Å, degree) |       |           |       |       |
| Fe(1)-H(6)                      | 1.41  | 1.50      | 1.58  | 1.66  |
| Fe(1)-N(4)                      | 1.86  | 1.88      | 1.94  | 1.99  |
| Fe(1)-P(2)                      | 2.19  | 2.24      | 2.27  | 2.64  |
| Fe(1)-P(3)                      | 2.17  | 2.24      | 2.27  | 2.64  |
| Fe(1)-C(5)                      | 1.73  | 1.75      | 1.95  | 2.01  |
| H(6)-Fe(1)-C(5)                 | 82.8  | 84.8      | 78.0  | 106.9 |
| H(6)-Fe(1)-N(4)                 | 121.2 | 118.8     | 157.7 | 131.9 |

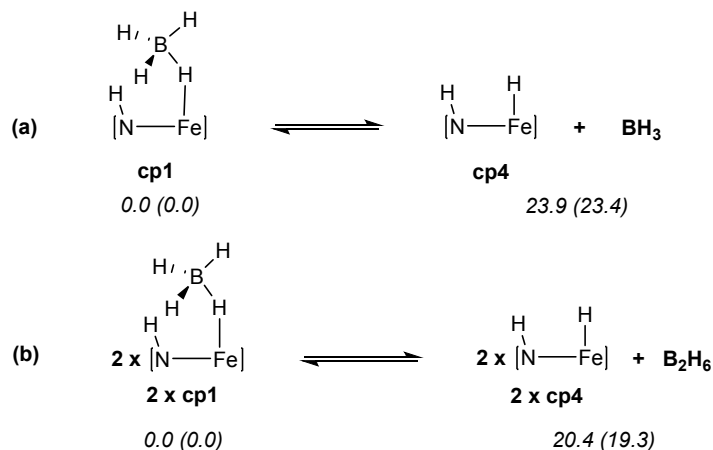
\*S. Chakraborty, W. W. Brennessel and W. D. Jones, *Journal of the American Chemical Society*, 2014, **136**, 8564-8567.

**Table S3** Relative solvent corrected free energies (in kcal/mol) of **cp1** and **cp3** in THF and in *p*-xylene using M06, M06L, and  $\omega$ B97XD functionals on optimized geometry by B3LYP/BS1.

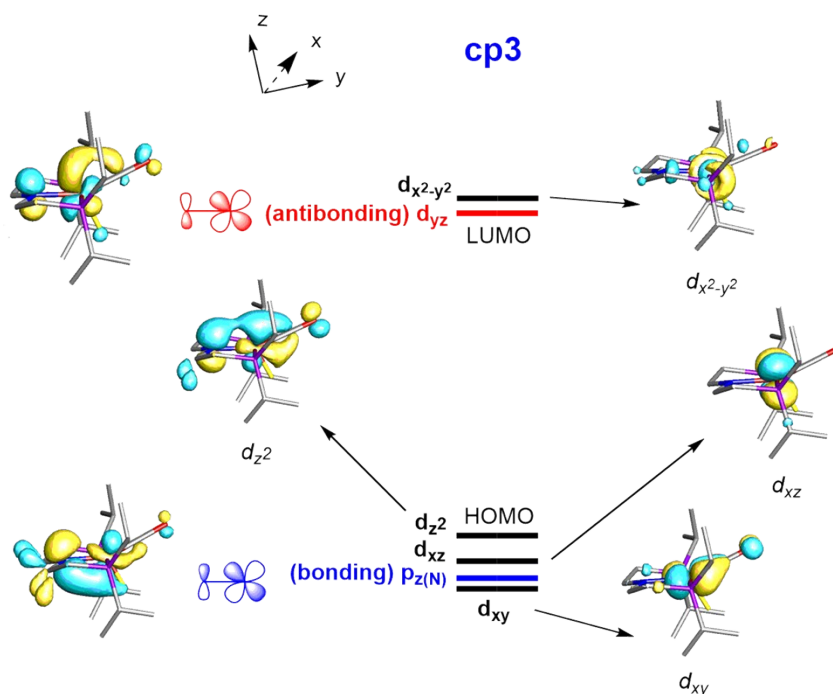
|                        |                    | <b>cp1</b>   |              |              | <b>cp3</b>   |              |              |
|------------------------|--------------------|--------------|--------------|--------------|--------------|--------------|--------------|
|                        |                    | <i>S</i> = 0 | <i>S</i> = 1 | <i>S</i> = 2 | <i>S</i> = 0 | <i>S</i> = 1 | <i>S</i> = 2 |
| <b>THF</b>             | M06/BS2            | 0.00         | 14.28        | 10.38        | 0.00         | 8.68         | 11.40        |
|                        | M06L/BS2           | 0.00         | 27.34        | 34.13        | 0.00         | 18.45        | 31.64        |
|                        | $\omega$ B97XD/BS2 | 0.00         | 20.70        | 18.82        | 0.00         | 12.07        | 18.43        |
| <b><i>p</i>-xylene</b> | M06/BS2            | 0.00         | 14.08        | 11.56        | 0.00         | 8.96         | 12.55        |
|                        | M06L/BS2           | 0.00         | 27.26        | 35.35        | 0.00         | 18.75        | 32.81        |
|                        | $\omega$ B97XD/BS2 | 0.00         | 20.54        | 20.16        | 0.00         | 12.36        | 19.72        |



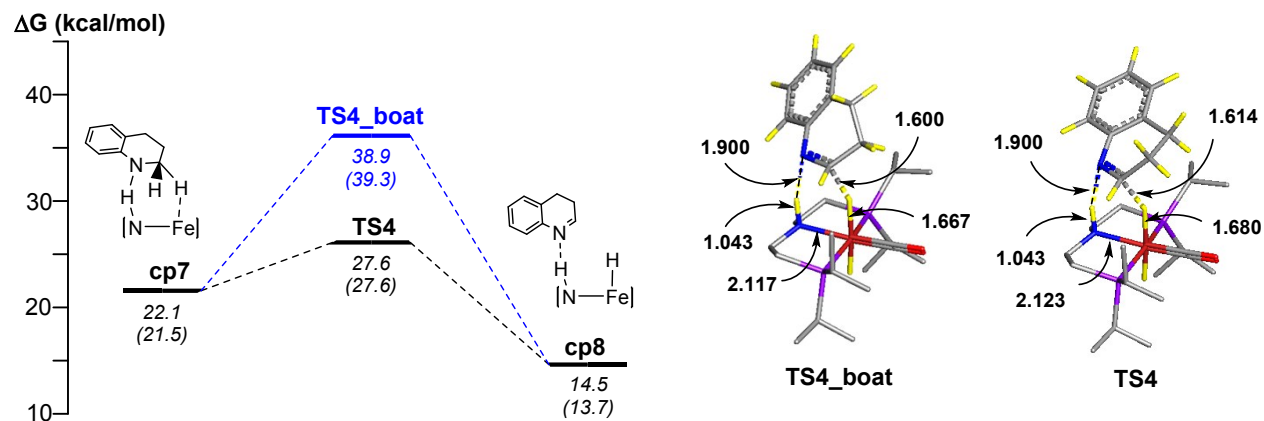
**Fig. S1** Calculated **cp3** complexes with different arrangements of isopropyl groups.



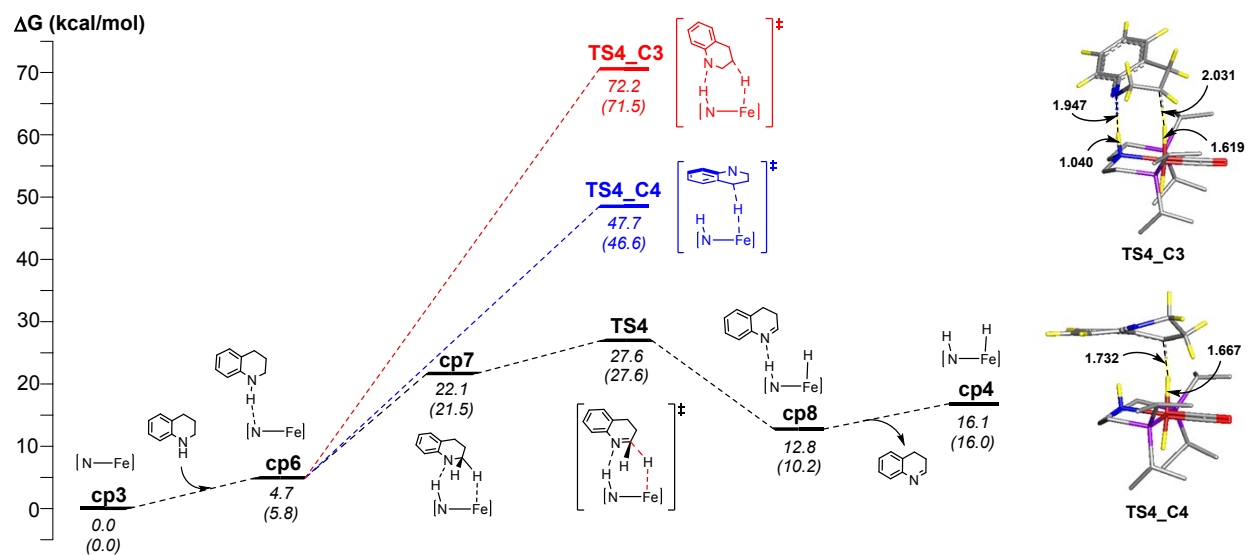
**Fig. S2** (a) Direct dissociation of  $\text{BH}_3$  from **cp1**. (b) Formation of diborane ( $\text{B}_2\text{H}_6$ ) from **cp1**. Solvent corrected free energies in *p*-xylene and in THF (in parenthesis) are shown in kcal/mol.



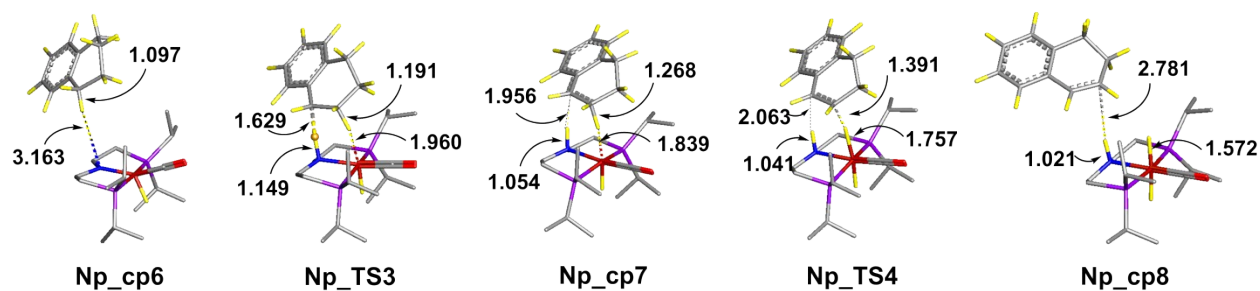
**Fig. S3** Selected molecular orbital (MO) plots of **cp3**.



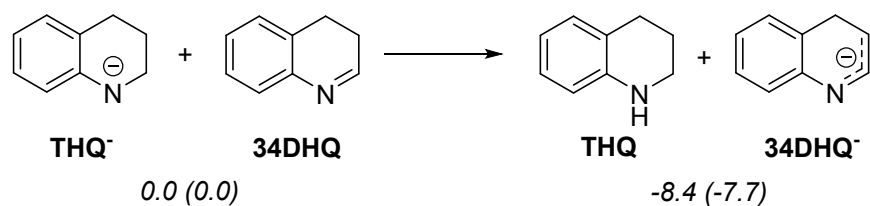
**Fig. S4** The hydride transfer from **cp12** via **TS4** and **TS4\_boat**, the transition state corresponding to **TS4** with the boat conformation on the aliphatic ring of **THQ**. Solvent corrected free energies in *p*-xylene and in THF (in parentheses) are shown in kcal/mol.



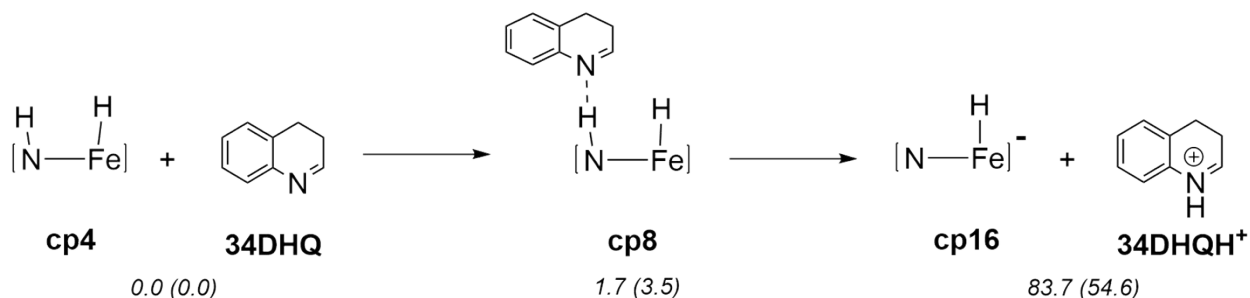
**Fig. S5** Relative free energy profiles for the hydride transfer from C2 (in black), from C3 (in red), and from C4 (in blue) of **THQ** to Fe. Solvent corrected free energies in *p*-xylene and in THF (in parentheses) are shown in kcal/mol.



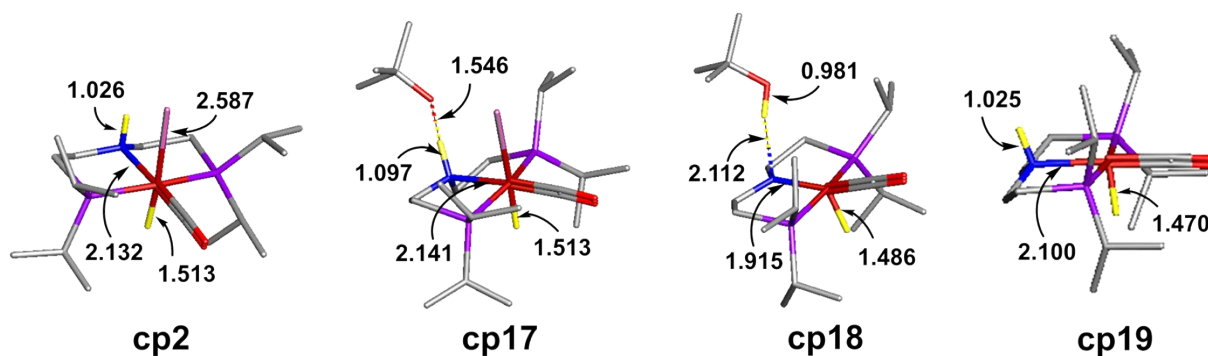
**Fig. S6** Optimized structure of intermediates and transition states in the dehydrogenation of **THN** to **DHN**.



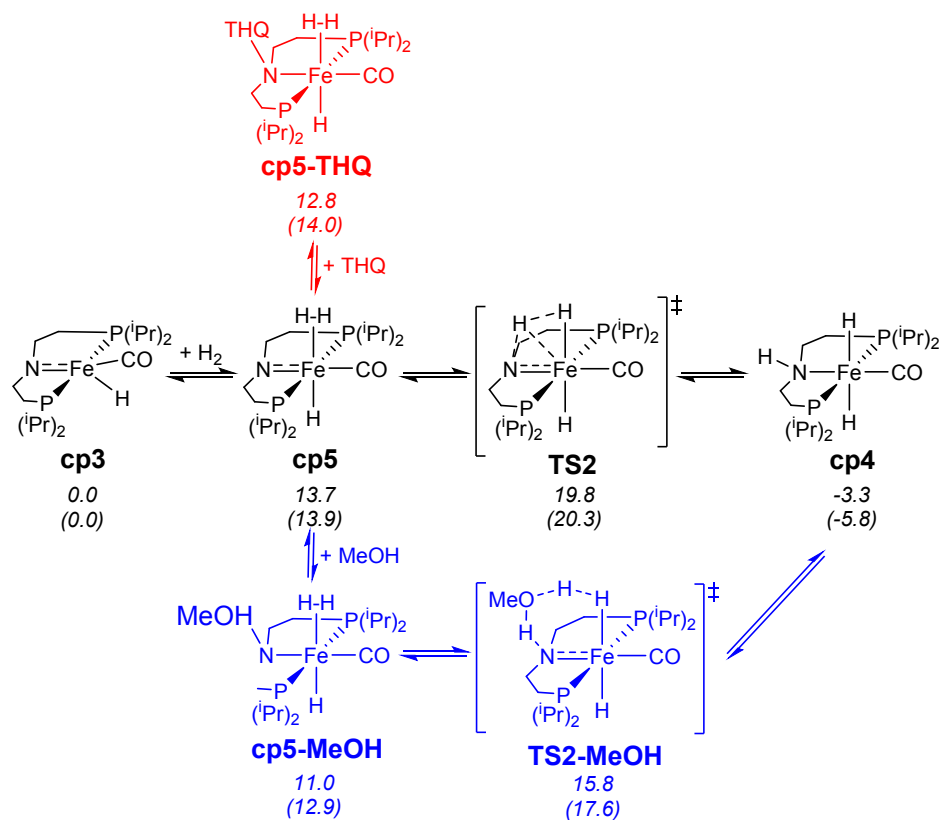
**Fig. S7** The proton-transfer free energy of **34DHQ** relative to **THQ**. Solvent corrected free energies in *p*-xylene and THF (shown in parentheses) are shown in kcal/mol.



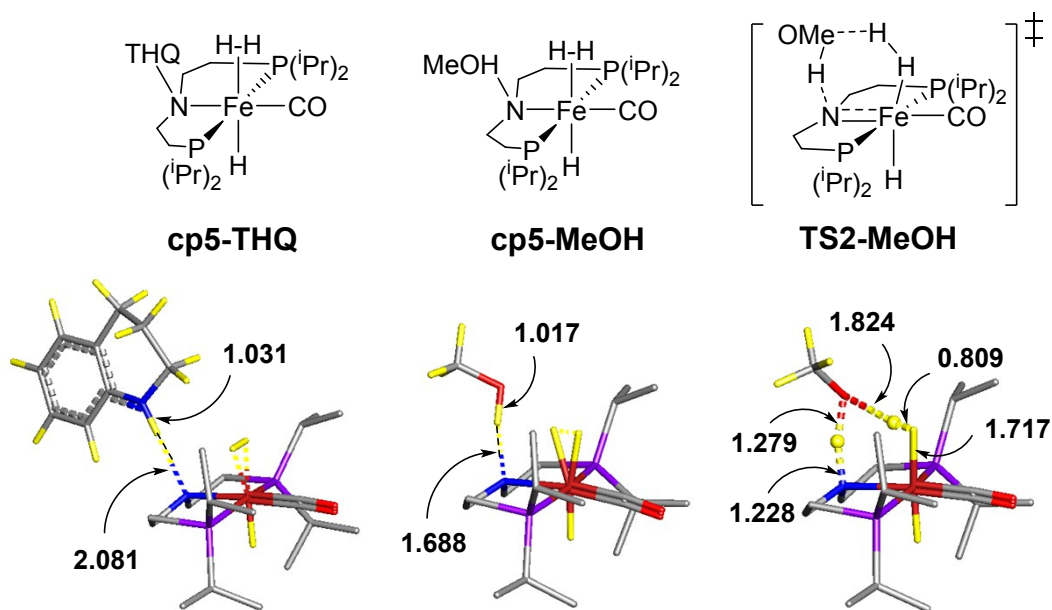
**Fig. S8** Formation of protonated **34DHQ** using **cp4**. Solvent corrected free energies in *p*-xylene and in THF (in parentheses) are shown in kcal/mol.



**Fig. S9** Optimized geometries of intermediates in the formation of **cp4** and **cp3** from **cp2**.

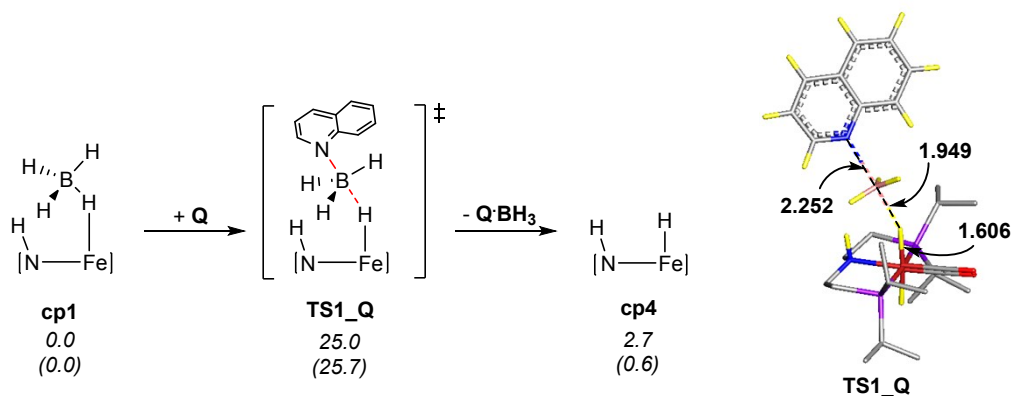


**Fig. S10** Formation of **cp4** from **cp3**. Solvent free energies relative to **cp3** in *p*-xylene and in THF (in parentheses) are given in kcal/mol.

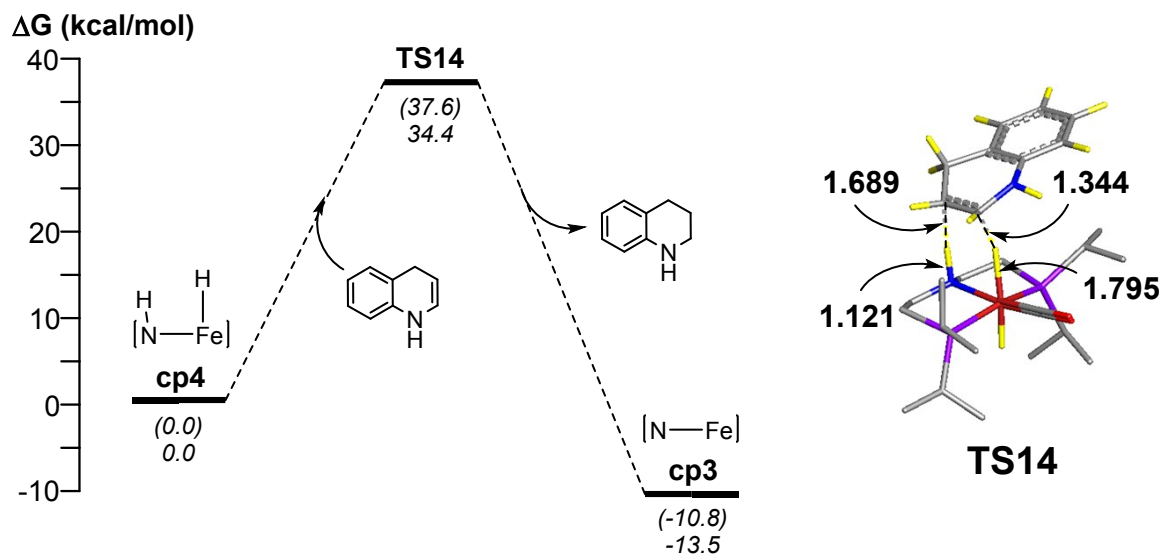


**Fig. S11** The optimized structures of **cp5-THQ**, **cp5-MeOH**, and **TS2-MeOH**.

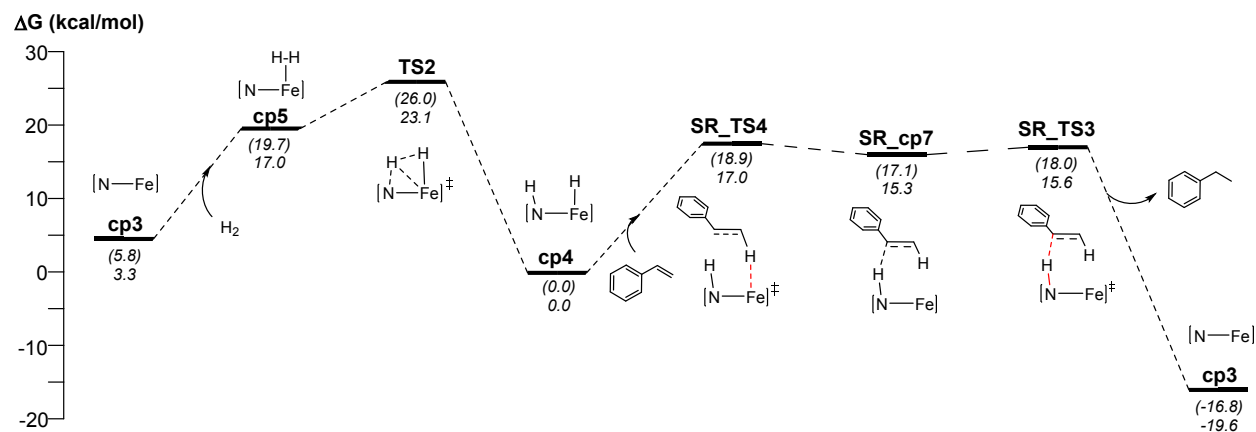




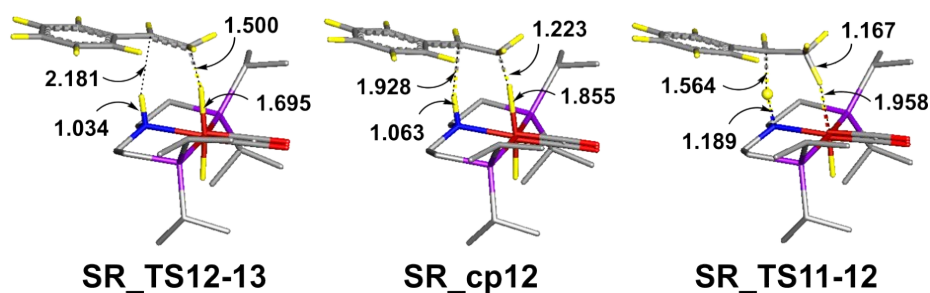
**Fig. S12** Formation of **cp4** from **cp1** with the assistance of quinoline (**Q**). Solvent corrected free energies in *p*-xylene and in THF (in parentheses) are shown in kcal/mol.



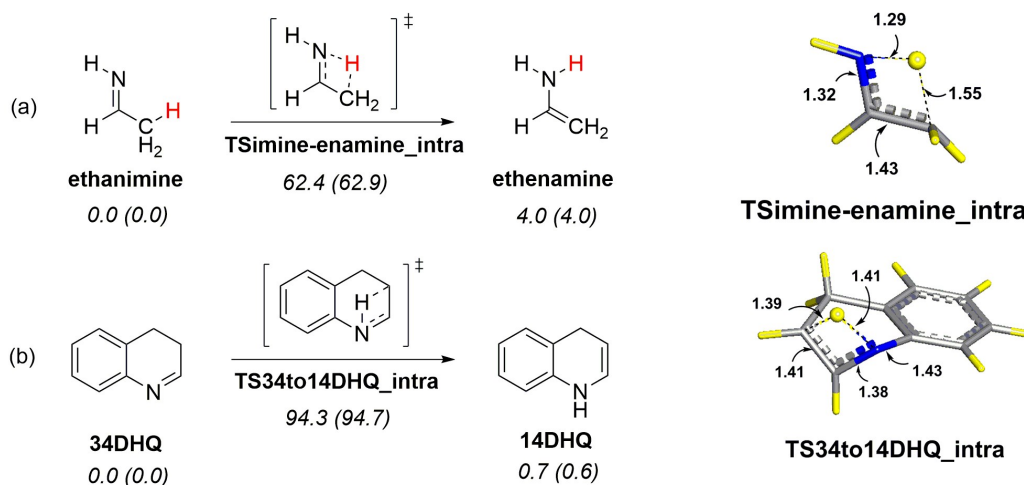
**Fig. S13** Relative free energy profile for the hydrogenation of **14DHQ** to **THQ**. Solvent corrected free energies in THF (in parentheses) and in *p*-xylene are shown in kcal/mol.



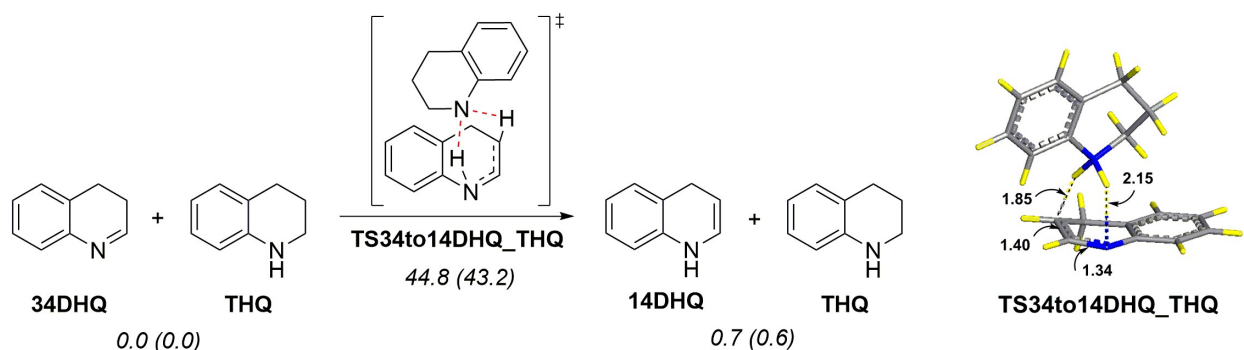
**Fig. S14** Relative free energy profile for hydrogenation of styrene by **cp4**. Solvent corrected free energies in THF (in parenthesis) and in *p*-xylene are shown in kcal/mol.



**Fig. S15** Optimized structure of intermediates and transition states in hydrogenation of styrene.



**Fig. S16** The imine-enamine tautomerization *via* the intramolecular 1,3-H shift: (a) the isomerization of **34DHQ** to **14DHQ** and (b) the isomerization of ethanimine to ethenamine. Solvent corrected free energies in *p*-xylene and in THF (in parentheses) are shown in kcal/mol.



**Fig. S17** The isomerization of **34DHQ** to **14DHQ** using **THQ** as a proton shuttle. Solvent corrected free energies in *p*-xylene and in THF (in parentheses) are shown in kcal/mol.

**Table S4** Relative electronic energies, enthalpies, gas-phase free energies, and free energies with solvent correction in the formation of the active species **cp3** and **cp4** from the starting complexes **cp1** and **cp2** (kcal/mol). The gas phase geometry structures were optimized by B3LYP/BS1. The solvent corrected free energies were calculated in *p*-xylene and THF.

|                                       | B3LYP/BS1                |            |                         | M06/BS2                 |                              |
|---------------------------------------|--------------------------|------------|-------------------------|-------------------------|------------------------------|
|                                       | $\Delta E_{\text{elec}}$ | $\Delta H$ | $\Delta G_{\text{gas}}$ | $\Delta G_{\text{THF}}$ | $\Delta G_{p\text{-xylene}}$ |
| <b>Conversion between cp3 and cp4</b> |                          |            |                         |                         |                              |
| cp3 + H <sub>2</sub> + THQ + MeOH     | 0.00                     | 0.00       | 0.00                    | 0.00                    | 0.00                         |
| cp5 + THQ + MeOH                      | 8.13                     | 10.51      | 19.45                   | 13.88                   | 13.66                        |
| TS2 + THQ + MeOH                      | 13.59                    | 14.62      | 24.64                   | 20.25                   | 19.82                        |
| cp4 + THQ + MeOH                      | -10.36                   | -5.55      | 3.94                    | -5.79                   | -3.31                        |
| cp5-THQ + MeOH                        | 0.62                     | 4.61       | 24.14                   | 14.04                   | 12.77                        |

|                                             |        |        |        |        |        |
|---------------------------------------------|--------|--------|--------|--------|--------|
| cp5-MeOH + THQ                              | -8.16  | -4.02  | 15.93  | 12.92  | 11.02  |
| TS2-MeOH + THQ                              | -3.82  | -2.48  | 18.43  | 17.58  | 15.82  |
| <b>Generation of cp4 from cp1</b>           |        |        |        |        |        |
| cp1 + THQ                                   | 0.00   | 0.00   | 0.00   | 0.00   | 0.00   |
| TS1                                         | 18.07  | 18.05  | 29.97  | 25.32  | 24.74  |
| cp4 + THQ·BH <sub>3</sub>                   | 8.89   | 8.93   | 9.41   | 5.02   | 7.59   |
| cp1 + Q                                     | 0.00   | 0.00   | 0.00   | 0.00   | 0.00   |
| TS1_Q                                       | 17.97  | 17.44  | 27.91  | 25.69  | 25.01  |
| cp4 + Q·BH <sub>3</sub>                     | 2.58   | 2.19   | 2.68   | 0.59   | 2.70   |
| <b>Generation of cp3 from cp2</b>           |        |        |        |        |        |
| cp2 + ·O <sup>t</sup> Bu                    | 0.00   | 0.00   | 0.00   | 0.00   | 0.00   |
| cp17                                        | -37.68 | -36.73 | -25.41 | 6.20   | -2.01  |
| cp18 + Br <sup>-</sup>                      | -36.78 | -34.93 | -33.72 | -9.32  | -11.73 |
| cp19 + Br <sup>-</sup> + ·O <sup>t</sup> Bu | 99.89  | 99.31  | 89.31  | 22.67  | 51.12  |
| cp3 + Br <sup>-</sup> + HO <sup>t</sup> Bu  | -29.09 | -28.72 | -38.07 | -13.84 | -15.04 |

**Table S5.** Relative electronic energies, enthalpies, gas-phase free energies, and free energies with solvent correction in the dehydrogenation of **THQ** to **34DHQ** (kcal/mol). The gas phase geometry structures were optimized by B3LYP/BS1. The solvent corrected free energies were calculated in *p*-xylene and THF.

|             | B3LYP/BS1                |            |                         | M06/BS2                 |                              |
|-------------|--------------------------|------------|-------------------------|-------------------------|------------------------------|
|             | $\Delta E_{\text{elec}}$ | $\Delta H$ | $\Delta G_{\text{gas}}$ | $\Delta G_{\text{THF}}$ | $\Delta G_{p\text{-xylene}}$ |
| cp3 + THQ   | 0.00                     | 0.00       | 0.00                    | 0.00                    | 0.00                         |
| cp6         | -3.93                    | -2.27      | 8.56                    | 5.78                    | 4.66                         |
| TS3         | 17.91                    | 15.96      | 31.25                   | 21.47                   | 21.52                        |
| cp7         | 17.67                    | 17.65      | 32.32                   | 21.47                   | 22.06                        |
| TS4_boat    | 22.36                    | 20.70      | 35.85                   | 39.25                   | 38.85                        |
| TS4         | 21.79                    | 20.57      | 36.40                   | 27.56                   | 27.58                        |
| cp8         | 9.67                     | 8.95       | 19.84                   | 13.68                   | 14.54                        |
| cp4 + 34DHQ | 17.02                    | 14.81      | 15.70                   | 10.18                   | 12.80                        |

**Table S6.** Relative electronic energies, enthalpies, gas-phase free energies, and free energies with solvent correction in the dehydrogenation of **THN** to **DHN** (kcal/mol). The gas phase geometry structures were optimized by B3LYP/BS1. The solvent corrected free energies were calculated in *p*-xylene and THF.

|           | B3LYP/BS1                |            |                         | M06/BS2                 |                              |
|-----------|--------------------------|------------|-------------------------|-------------------------|------------------------------|
|           | $\Delta E_{\text{elec}}$ | $\Delta H$ | $\Delta G_{\text{gas}}$ | $\Delta G_{\text{THF}}$ | $\Delta G_{p\text{-xylene}}$ |
| cp3 + THN | 0.00                     | 0.00       | 0.00                    | 0.00                    | 0.00                         |
| Np_cp6    | -1.05                    | 0.52       | 9.71                    | 6.74                    | 6.62                         |
| Np_TS3    | 39.84                    | 37.76      | 53.09                   | 41.81                   | 42.15                        |
| Np_cp7    | 39.26                    | 38.41      | 52.35                   | 39.31                   | 40.15                        |
| Np_TS4    | 39.40                    | 37.40      | 51.48                   | 38.79                   | 39.55                        |
| Np_cp8    | 17.73                    | 17.41      | 27.89                   | 18.87                   | 21.19                        |
| cp4 + DHN | 20.03                    | 18.09      | 18.94                   | 12.37                   | 15.09                        |

**Table S7.** Relative electronic energies, enthalpies, gas-phase free energies, and free energies with solvent correction in the dehydrogenation of **34DHQ**, **14DHQ** and **12DHQ** to **Q** (kcal/mol). The gas phase geometry structures were optimized by B3LYP/BS1. The solvent corrected free energies were calculated in *p*-xylene and THF.

|                                 | B3LYP/BS1                |            |                         | M06/BS2                 |                              |
|---------------------------------|--------------------------|------------|-------------------------|-------------------------|------------------------------|
|                                 | $\Delta E_{\text{elec}}$ | $\Delta H$ | $\Delta G_{\text{gas}}$ | $\Delta G_{\text{THF}}$ | $\Delta G_{p\text{-xylene}}$ |
| <b>Dehydrogenation of 34DHQ</b> |                          |            |                         |                         |                              |
| cp3                             | 0.00                     | 0.00       | 0.00                    | 0.00                    | 0.00                         |
| TS5                             | 22.03                    | 19.95      | 35.01                   | 22.57                   | 22.80                        |
| cp9                             | 16.37                    | 16.86      | 32.13                   | 16.70                   | 18.38                        |
| TS6                             | 17.02                    | 16.00      | 31.69                   | 18.42                   | 19.45                        |
| cp4                             | -0.63                    | -1.87      | -0.77                   | -5.60                   | -3.36                        |
| <b>Dehydrogenation of 14DHQ</b> |                          |            |                         |                         |                              |
| cp3 + 14DHQ                     | 0.00                     | 0.00       | 0.00                    | 0.00                    | 0.00                         |
| cp10                            | -5.16                    | -3.39      | 7.84                    | 4.80                    | 3.49                         |
| TS7                             | 8.68                     | 6.96       | 20.97                   | 14.72                   | 13.84                        |
| cp11                            | 8.03                     | 9.11       | 23.14                   | 14.63                   | 14.64                        |
| cp12                            | 15.98                    | 16.16      | 31.14                   | 16.91                   | 18.24                        |
| TS8                             | 16.27                    | 14.92      | 29.82                   | 17.52                   | 18.27                        |
| cp13                            | -9.86                    | -9.60      | 2.04                    | -2.47                   | -1.91                        |
| cp4 + Q                         | -2.73                    | -4.16      | -2.48                   | -6.24                   | -4.06                        |
| <b>Dehydrogenation of 12DHQ</b> |                          |            |                         |                         |                              |
| cp3 + 12DHQ                     | 0.00                     | 0.00       | 0.00                    | 0.00                    | 0.00                         |
| cp14                            | -4.35                    | -2.67      | 8.08                    | 5.27                    | 4.02                         |
| TS9                             | 10.84                    | 8.64       | 23.92                   | 16.88                   | 16.03                        |
| cp15                            | 8.89                     | 8.41       | 23.05                   | 14.99                   | 14.84                        |
| TS10                            | 7.53                     | 7.53       | 22.88                   | 15.23                   | 14.95                        |
| cp13                            | -11.79                   | -11.60     | -0.23                   | -4.82                   | -4.31                        |
| cp4 + Q                         | -4.67                    | -6.16      | -4.75                   | -8.59                   | -6.46                        |

**Table S8.** Relative electronic energies, enthalpies, gas-phase free energies, and free energies with solvent correction in the isomerization of **34DHQ** to **14DHQ** and **12DHQ** (kcal/mol). The gas phase geometry structures were optimized by B3LYP/BS1. The solvent corrected free energies were calculated in *p*-xylene and THF.

|                             | B3LYP/BS1                |            |                         | M06/BS2                 |                              |
|-----------------------------|--------------------------|------------|-------------------------|-------------------------|------------------------------|
|                             | $\Delta E_{\text{elec}}$ | $\Delta H$ | $\Delta G_{\text{gas}}$ | $\Delta G_{\text{THF}}$ | $\Delta G_{p\text{-xylene}}$ |
| 34DHQH <sup>+</sup> + 34DHQ | 0.00                     | 0.00       | 0.00                    | 0.00                    | 0.00                         |
| TS11                        | -6.96                    | -8.85      | 1.80                    | 14.57                   | 9.45                         |
| 14DHQ + 34DHQH <sup>+</sup> | 2.10                     | 2.29       | 1.71                    | 0.64                    | 0.70                         |
| 34DHQH <sup>+</sup> + 14DHQ | 0.00                     | 0.00       | 0.00                    | 0.00                    | 0.00                         |
| TS12                        | -7.40                    | -8.37      | 3.35                    | 13.73                   | 9.84                         |

|                            |        |        |        |        |        |
|----------------------------|--------|--------|--------|--------|--------|
| THQ + QH <sup>+</sup>      | -22.51 | -21.62 | -20.78 | -16.93 | -18.20 |
| QH <sup>+</sup> + 14DHQ    | 0.00   | 0.00   | 0.00   | 0.00   | 0.00   |
| TS13                       | 6.24   | 4.29   | 15.83  | 25.86  | 22.25  |
| 12DHQ + QH <sup>+</sup>    | 1.93   | 2.00   | 2.27   | 2.39   | 2.40   |
| 14DHQ + <sup>-</sup> O'Bu  | 0.00   | 0.00   | 0.00   | 0.00   | 0.00   |
| TS15                       | -45.47 | -43.59 | -33.35 | 8.43   | 3.65   |
| 14DHQ <sup>-</sup> + HO'Bu | -24.13 | -23.59 | -23.78 | -13.40 | -14.70 |
| 14DHQ <sup>-</sup> + 14DHQ | 0.00   | 0.00   | 0.00   | 0.00   | 0.00   |
| TS16                       | -7.05  | -9.22  | 1.77   | 16.56  | 11.81  |
| 34DHQ + 14DHQ <sup>-</sup> | -2.10  | -2.29  | -1.71  | -0.64  | -0.70  |
| cp4 + 34DHQ                | 0.00   | 0.00   | 0.00   | 0.00   | 0.00   |
| cp8                        | -7.34  | -5.86  | 4.14   | 3.51   | 1.74   |
| cp16 + 34DHQH <sup>+</sup> | 137.11 | 134.64 | 135.40 | 54.56  | 83.73  |

**Table S9.** Relative electronic energies, enthalpies, gas-phase free energies, and free energies with solvent correction in the hydrogenation of styrene (kcal/mol). The gas phase geometry structures were optimized by B3LYP/BS1. The solvent correction free energies were calculated in *p*-xylene and THF.

|                    | B3LYP/BS1                |            |                         | M06/BS2                 |                              |
|--------------------|--------------------------|------------|-------------------------|-------------------------|------------------------------|
|                    | $\Delta E_{\text{elec}}$ | $\Delta H$ | $\Delta G_{\text{gas}}$ | $\Delta G_{\text{THF}}$ | $\Delta G_{p\text{-xylene}}$ |
| cp4 + styrene      | 0.00                     | 0.00       | 0.00                    | 0.00                    | 0.00                         |
| SR_TS4             | 10.51                    | 10.55      | 23.81                   | 18.87                   | 16.96                        |
| SR_cp7             | 9.02                     | 10.52      | 23.47                   | 17.05                   | 15.33                        |
| SR_TS3             | 10.03                    | 9.40       | 22.99                   | 17.97                   | 15.55                        |
| cp3 + ethylbenzene | -27.74                   | -22.87     | -23.74                  | -16.77                  | -19.55                       |

### xyz coordinates

|            |              |              |              |   |              |              |              |
|------------|--------------|--------------|--------------|---|--------------|--------------|--------------|
| <b>cp1</b> |              |              |              | C | -2.777535000 | 1.977242000  | 2.049600000  |
| FE         | -0.026204000 | -0.090042000 | -0.041966000 | C | -3.119939000 | -0.473250000 | 2.528914000  |
| P          | -2.271823000 | 0.181582000  | -0.102006000 | C | -3.331821000 | -1.074721000 | -1.021125000 |
| P          | 2.243933000  | 0.115209000  | -0.030227000 | C | -4.823954001 | -0.718612000 | -1.105633000 |
| O          | -0.088216000 | -2.334636000 | 1.806645000  | C | -3.120393000 | -2.520549000 | -0.544905000 |
| N          | 0.016402000  | 1.660138000  | -1.238082000 | C | 2.983043000  | 0.770592000  | 1.576568000  |
| C          | -2.458834000 | 1.694841000  | -1.185476000 | C | 4.416239001  | 1.315627000  | 1.472130000  |
| C          | -1.178122000 | 2.525660000  | -1.099051000 | C | 2.876565000  | -0.278463000 | 2.696555000  |
| C          | 1.267283000  | 2.443910000  | -1.121212000 | C | 3.448701000  | -1.257437000 | -0.542395000 |
| C          | 2.480190000  | 1.521218000  | -1.233613000 | C | 4.018821000  | -1.101011000 | -1.961089000 |
| C          | -0.064401000 | -1.461581000 | 1.037986000  | C | 2.796544000  | -2.640104000 | -0.369289000 |
| C          | -3.225540000 | 0.629218000  | 1.462778000  | B | -0.032116000 | -1.020996000 | -2.691941000 |

|   |              |              |              |
|---|--------------|--------------|--------------|
| H | -0.017859000 | 0.800146000  | 1.191574000  |
| H | -0.007854000 | 1.219191000  | -2.163541000 |
| H | -2.598504000 | 1.335568000  | -2.209992000 |
| H | -3.332043000 | 2.300418000  | -0.922774000 |
| H | -1.175485000 | 3.310876000  | -1.870151000 |
| H | -1.106040000 | 3.017824000  | -0.125002000 |
| H | 1.247277000  | 2.945247000  | -0.147404000 |
| H | 1.307682000  | 3.226208000  | -1.894159000 |
| H | 3.408521000  | 2.079944000  | -1.084446000 |
| H | 2.510176000  | 1.085551000  | -2.235451000 |
| H | -4.275653001 | 0.723667000  | 1.157961000  |
| H | -3.340187000 | 2.183214000  | 2.967644000  |
| H | -2.957135000 | 2.812909000  | 1.366332000  |
| H | -1.712798000 | 1.959505000  | 2.300875000  |
| H | -3.715862000 | -0.197957000 | 3.406974000  |
| H | -2.084706000 | -0.606319000 | 2.855087000  |
| H | -3.484961000 | -1.439169000 | 2.172162000  |
| H | -2.896162000 | -1.009050000 | -2.025249000 |
| H | -5.328064001 | -1.401058000 | -1.799530000 |
| H | -4.994724001 | 0.300235000  | -1.468914000 |
| H | -5.322988001 | -0.819560000 | -0.135660000 |
| H | -3.627392000 | -3.207278000 | -1.232292000 |
| H | -3.534791000 | -2.696436000 | 0.453027000  |
| H | -2.061304000 | -2.786115000 | -0.533033000 |
| H | 2.310298000  | 1.598263000  | 1.833622000  |
| H | 4.732457001  | 1.711595000  | 2.444196000  |
| H | 4.508640001  | 2.128297000  | 0.746123000  |
| H | 5.133461001  | 0.535614000  | 1.195037000  |
| H | 3.207166000  | 0.155374000  | 3.647115000  |
| H | 3.515604000  | -1.146532000 | 2.498175000  |
| H | 1.852424000  | -0.633648000 | 2.827154000  |
| H | 4.284450001  | -1.184090000 | 0.164325000  |
| H | 4.711997001  | -1.925526000 | -2.164258000 |
| H | 4.575155001  | -0.167128000 | -2.086613000 |
| H | 3.226430000  | -1.140099000 | -2.714099000 |
| H | 3.527425000  | -3.423622000 | -0.601709000 |
| H | 1.945045000  | -2.755272000 | -1.045614000 |

|   |              |              |              |
|---|--------------|--------------|--------------|
| H | 2.441675000  | -2.807802000 | 0.651153000  |
| H | -0.046497000 | -1.094493000 | -1.404726000 |
| H | -0.970095000 | -0.330730000 | -3.057292000 |
| H | 1.030001000  | -0.540860000 | -3.040303000 |
| H | -0.154699000 | -2.182061000 | -3.013048000 |

# TS1

|    |              |              |              |
|----|--------------|--------------|--------------|
| FE | 1.590506658  | 0.032440546  | 0.063018862  |
| C  | 2.630134629  | -0.050361175 | 1.450046280  |
| O  | 3.304335041  | -0.111266611 | 2.402414075  |
| N  | 0.212663308  | 0.117579323  | -1.569103824 |
| C  | 0.246764705  | 1.396333317  | -2.312177655 |
| C  | 0.222473812  | 2.575191160  | -1.340542726 |
| P  | 1.476555651  | 2.261958249  | 0.016125959  |
| C  | 0.700984029  | 3.224016482  | 1.443578938  |
| C  | 0.375899776  | 4.695894144  | 1.141743807  |
| C  | 1.476338789  | 3.094295561  | 2.764478450  |
| C  | 2.987737634  | 3.282507680  | -0.486872118 |
| C  | 3.339023943  | 3.120564807  | -1.974008336 |
| C  | 4.207884051  | 2.914221253  | 0.374377063  |
| C  | 0.291702762  | -1.042988684 | -2.483669966 |
| C  | 0.337984369  | -2.345648936 | -1.685380130 |
| P  | 1.658565059  | -2.163623780 | -0.370920982 |
| C  | 1.237997500  | -3.532068855 | 0.860288060  |
| C  | -0.137048146 | -3.322328662 | 1.511330211  |
| C  | 2.318447460  | -3.654212803 | 1.950046101  |
| C  | 3.173319886  | -2.818439015 | -1.302202175 |
| C  | 3.167299047  | -4.327668790 | -1.591864393 |
| C  | 4.506663413  | -2.370050039 | -0.683876811 |
| B  | -1.733654259 | 0.032968554  | 1.213745810  |
| C  | -6.002032534 | -0.247376886 | -1.530692146 |
| C  | -5.379089497 | -0.569456286 | -0.318772944 |
| C  | -4.634784689 | 0.429675631  | 0.336919613  |
| C  | -4.541888852 | 1.713728401  | -0.222293473 |
| C  | -5.178034527 | 2.011617745  | -1.423235623 |
| C  | -5.911770072 | 1.026070250  | -2.088444805 |
| C  | -5.539697838 | -1.950695126 | 0.289576144  |

|   |              |              |              |            |              |              |              |
|---|--------------|--------------|--------------|------------|--------------|--------------|--------------|
| C | -4.505294416 | -2.229533198 | 1.386886444  | H          | 3.329368928  | -4.915013307 | -0.682282511 |
| C | -4.376435763 | -1.021053721 | 2.311857026  | H          | 4.703730870  | -2.860264906 | 0.274608497  |
| N | -3.922915320 | 0.144941046  | 1.534539194  | H          | 4.512201880  | -1.289993961 | -0.524071608 |
| H | 2.737451904  | 0.165591092  | -0.984706214 | H          | 5.333933447  | -2.626331312 | -1.356911467 |
| H | -0.669861764 | 0.063168766  | -1.057704435 | H          | 0.304365409  | -0.067114207 | 1.011055467  |
| H | -0.596609861 | 1.458626224  | -3.017881265 | H          | -1.818182802 | -0.846441027 | 0.404819248  |
| H | 1.171273186  | 1.401302813  | -2.896247576 | H          | -1.711744611 | 1.168626808  | 0.832375863  |
| H | -0.758943013 | 2.630840265  | -0.856944307 | H          | -1.563571506 | -0.218529285 | 2.371104847  |
| H | 0.381284476  | 3.519295946  | -1.871266108 | H          | -6.576356269 | -1.018678050 | -2.039529556 |
| H | -0.240821191 | 2.676024858  | 1.567298214  | H          | -3.962076567 | 2.474099556  | 0.294151531  |
| H | -0.201595768 | 5.127581289  | 1.968266559  | H          | -5.100130862 | 3.012413072  | -1.838399618 |
| H | -0.216153048 | 4.819102050  | 0.229590483  | H          | -6.408255787 | 1.248331866  | -3.028111426 |
| H | 1.283335660  | 5.300732671  | 1.037135743  | H          | -5.476087958 | -2.712258486 | -0.496434193 |
| H | 2.404934551  | 3.674820421  | 2.750099817  | H          | -3.525471468 | -2.432442018 | 0.943797800  |
| H | 1.725075548  | 2.056349024  | 2.995051447  | H          | -3.633410003 | -1.201892298 | 3.092314947  |
| H | 0.867674038  | 3.485160315  | 3.588796545  | H          | -6.550944555 | -2.038193363 | 0.712547737  |
| H | 2.729150763  | 4.334300161  | -0.308511047 | H          | -4.791931510 | -3.110394242 | 1.970630420  |
| H | 4.241488548  | 3.698780640  | -2.205460550 | H          | -5.343788046 | -0.816630582 | 2.797478473  |
| H | 2.545340132  | 3.478873845  | -2.636765137 | H          | -3.842832054 | 0.970296407  | 2.118423031  |
| H | 3.541002718  | 2.070639253  | -2.207830406 |            |              |              |              |
| H | 4.496764956  | 1.874503285  | 0.196250004  | <b>cp4</b> |              |              |              |
| H | 4.022783847  | 3.029174532  | 1.444806973  | FE         | -0.001174732 | -0.041994048 | -0.089389567 |
| H | 5.057858737  | 3.555460177  | 0.111489368  | C          | 0.034465241  | -1.684167552 | 0.468617217  |
| H | 1.207191212  | -0.924353482 | -3.073343068 | O          | 0.062396899  | -2.796157319 | 0.825706936  |
| H | -0.556677673 | -1.045589192 | -3.185672533 | N          | -0.032298874 | 1.968386513  | -0.837398652 |
| H | 0.511175823  | -3.199473956 | -2.349365838 | C          | -1.265772312 | 2.704629272  | -0.487988674 |
| H | -0.621643045 | -2.504667498 | -1.184698433 | C          | -2.491418461 | 1.852256261  | -0.809208499 |
| H | 1.211919223  | -4.469860454 | 0.290009424  | P          | -2.218205551 | 0.130529810  | -0.113247720 |
| H | -0.319356430 | -4.118961683 | 2.242964854  | C          | -3.228397120 | -0.893713224 | -1.338803988 |
| H | -0.953776612 | -3.353462558 | 0.784816339  | C          | -4.705073947 | -0.490054222 | -1.474239623 |
| H | -0.189215708 | -2.359176346 | 2.024036576  | C          | -3.088893707 | -2.410029472 | -1.131850621 |
| H | 2.419834159  | -2.722378043 | 2.513721578  | C          | -3.223449008 | 0.116487421  | 1.488891492  |
| H | 3.300395710  | -3.908787199 | 1.543499288  | C          | -2.948226358 | 1.356395588  | 2.354153382  |
| H | 2.041560342  | -4.444589358 | 2.657674492  | C          | -2.934791157 | -1.156204791 | 2.303279422  |
| H | 3.076792238  | -2.286278034 | -2.258551836 | C          | 1.186462317  | 2.733977302  | -0.498549365 |
| H | 3.978003546  | -4.578096751 | -2.286324908 | C          | 2.427916957  | 1.921462806  | -0.860947489 |
| H | 2.231440336  | -4.668473034 | -2.047024898 | P          | 2.214962839  | 0.199950439  | -0.146490523 |



|   |              |              |              |
|---|--------------|--------------|--------------|
| C | 3.345221807  | -0.852722581 | -1.233982475 |
| C | 2.889416669  | -0.853538593 | -2.701783284 |
| C | 3.424722681  | -2.296884677 | -0.708589064 |
| C | 3.146430344  | 0.387336293  | 1.491297342  |
| C | 4.673210173  | 0.515140628  | 1.372405076  |
| C | 2.749029688  | -0.669307054 | 2.533768867  |
| H | 0.018543141  | 0.583332344  | 1.351405793  |
| H | -0.033909199 | 1.791885240  | -1.841289914 |
| H | -1.309091128 | 3.670574781  | -1.015822208 |
| H | -1.216052635 | 2.909794037  | 0.584858808  |
| H | -2.598851330 | 1.749431634  | -1.896146656 |
| H | -3.404176839 | 2.329620794  | -0.439400219 |
| H | -2.710465957 | -0.649436389 | -2.275974359 |
| H | -5.162499822 | -1.022707298 | -2.316535903 |
| H | -4.836096611 | 0.581581266  | -1.654619700 |
| H | -5.280351868 | -0.752979590 | -0.580111149 |
| H | -3.633687201 | -2.749458401 | -0.244822578 |
| H | -2.044939586 | -2.713700853 | -1.030412047 |
| H | -3.513508268 | -2.941138307 | -1.992099009 |
| H | -4.283005489 | 0.124787040  | 1.202122511  |
| H | -3.504317348 | 1.280283277  | 3.296061740  |
| H | -3.260471327 | 2.286759537  | 1.869428546  |
| H | -1.882748836 | 1.428779768  | 2.594005323  |
| H | -1.885995036 | -1.181615421 | 2.612939392  |
| H | -3.139830221 | -2.073421200 | 1.746159130  |
| H | -3.556529284 | -1.169923768 | 3.206510328  |
| H | 1.151671062  | 2.918522986  | 0.580059448  |
| H | 1.192649984  | 3.710787925  | -1.007664516 |
| H | 3.334577358  | 2.417724706  | -0.499746896 |
| H | 2.514342240  | 1.841108337  | -1.949511876 |
| H | 4.346141983  | -0.404889595 | -1.180574540 |
| H | 3.535281441  | -1.518483636 | -3.287356884 |
| H | 2.946434803  | 0.138239586  | -3.161215454 |
| H | 1.857045402  | -1.203996787 | -2.786569526 |
| H | 2.438895940  | -2.770909840 | -0.708031597 |
| H | 3.823777401  | -2.352889961 | 0.307522585  |
| H | 4.082158565  | -2.891871976 | -1.353399071 |

|   |              |              |              |
|---|--------------|--------------|--------------|
| H | 2.748044604  | 1.347035331  | 1.849144483  |
| H | 5.101315091  | 0.794852350  | 2.342261177  |
| H | 4.981496427  | 1.277153412  | 0.648607740  |
| H | 5.135929114  | -0.432278500 | 1.077306612  |
| H | 3.109020922  | -1.668017493 | 2.267307419  |
| H | 1.663655794  | -0.714295418 | 2.642853520  |
| H | 3.185371945  | -0.413993616 | 3.507054918  |
| H | -0.048847470 | -0.517432251 | -1.586786178 |

## TS2

|    |              |              |              |
|----|--------------|--------------|--------------|
| FE | -0.009964902 | -0.091708038 | -0.186491499 |
| C  | 0.026581279  | -1.749736049 | 0.367146359  |
| O  | 0.058560603  | -2.843196021 | 0.768946141  |
| N  | -0.039763169 | 1.835518815  | -1.026897793 |
| C  | -1.220997234 | 2.627525151  | -0.746286941 |
| C  | -2.494663523 | 1.800513519  | -0.932990752 |
| P  | -2.245880815 | 0.147090677  | -0.103998664 |
| C  | -3.341491807 | -0.955398905 | -1.179825967 |
| C  | -4.802664706 | -0.490449446 | -1.294076493 |
| C  | -3.271823734 | -2.449749588 | -0.827331663 |
| C  | -3.123163008 | 0.262937269  | 1.559191418  |
| C  | -2.793402720 | 1.569744255  | 2.299073994  |
| C  | -2.786720913 | -0.942234558 | 2.453301143  |
| C  | 1.169160849  | 2.617147519  | -0.867939579 |
| C  | 2.409668510  | 1.770471823  | -1.160207893 |
| P  | 2.230411934  | 0.189780943  | -0.188261739 |
| C  | 3.408791194  | -1.001503494 | -1.053151523 |
| C  | 2.926945277  | -1.327835472 | -2.476780769 |
| C  | 3.612789245  | -2.302543596 | -0.257114194 |
| C  | 3.056393645  | 0.648426529  | 1.444332751  |
| C  | 4.574832327  | 0.871518149  | 1.353322340  |
| C  | 2.692296966  | -0.289054077 | 2.606446867  |
| H  | 0.008971624  | 0.381902297  | 1.258795336  |
| H  | -0.061736326 | 0.571084892  | -1.750516796 |
| H  | -1.268230588 | 3.511309840  | -1.408883110 |
| H  | -1.191070390 | 3.021578021  | 0.288345421  |
| H  | -2.643603797 | 1.591350478  | -1.998908469 |

|            |              |              |              |   |              |              |              |
|------------|--------------|--------------|--------------|---|--------------|--------------|--------------|
| H          | -3.381647065 | 2.330674989  | -0.572563524 | C | 0.008227329  | -1.644461793 | 0.600264648  |
| H          | -2.862684181 | -0.828649504 | -2.160986843 | O | 0.038313891  | -2.629512777 | 1.222091794  |
| H          | -5.326151212 | -1.088182554 | -2.049549560 | N | -0.021922316 | 1.819054431  | -0.995000549 |
| H          | -4.889139377 | 0.559563968  | -1.587704020 | C | -1.141831349 | 2.656850944  | -0.611143348 |
| H          | -5.342974966 | -0.623062308 | -0.350518656 | C | -2.468186014 | 1.921931107  | -0.815398579 |
| H          | -3.791367908 | -2.667993782 | 0.111295867  | P | -2.252747860 | 0.206298973  | -0.130138912 |
| H          | -2.244263872 | -2.807903651 | -0.736818980 | C | -3.324141559 | -0.816537431 | -1.307531395 |
| H          | -3.764934120 | -3.037200792 | -1.610721648 | C | -4.825449253 | -0.494106636 | -1.246468020 |
| H          | -4.198669212 | 0.255723310  | 1.339545995  | C | -3.073221188 | -2.331513279 | -1.235390509 |
| H          | -3.312339690 | 1.583945746  | 3.264684311  | C | -3.180893107 | 0.238734640  | 1.508082112  |
| H          | -3.106557137 | 2.458762610  | 1.744288563  | C | -2.642275452 | 1.333101677  | 2.443919952  |
| H          | -1.719051879 | 1.647401064  | 2.491396548  | C | -3.177150291 | -1.122880430 | 2.220984757  |
| H          | -1.719161424 | -0.953036543 | 2.690593334  | C | 1.193041643  | 2.592214382  | -0.834108182 |
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| H          | 2.438258620  | 1.513084485  | -2.223658418 | C | 3.048677366  | 0.636333374  | 1.419499099  |
| H          | 4.373794857  | -0.482150249 | -1.126402781 | C | 4.570271118  | 0.842775392  | 1.340599083  |
| H          | 3.653722938  | -1.984757366 | -2.968738560 | C | 2.667047212  | -0.284019586 | 2.589808489  |
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| H          | -3.728300334 | -1.046591755 | 3.165729911  | C | -2.772642789 | 2.720777129  | 0.436919720  |
| H          | 1.314185631  | 2.983570232  | 0.203431102  | C | -4.808315803 | 1.263480182  | 0.047227020  |
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| H | 5.369148007 | 2.175069751  | -0.190027699 |
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## cp2

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| N  | -0.018924402 | 0.301148560  | 2.050535781  |
| C  | 1.172811836  | 0.937521957  | 2.652818806  |
| C  | 2.451032398  | 0.362180443  | 2.041602184  |
| P  | 2.272207249  | 0.305075112  | 0.178117328  |
| C  | 3.363094379  | -1.170455829 | -0.252658267 |
| C  | 4.850383565  | -0.991460783 | 0.086754008  |
| C  | 3.160855180  | -1.678163007 | -1.688553265 |
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| C  | 3.160108252  | 1.995362972  | -1.927761293 |
| C  | -1.277090430 | 0.836265150  | 2.615414353  |
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| N  | -0.313396874 | -0.776470366 | -1.327973460 |
| C  | -1.031062945 | -0.111345532 | -2.439935614 |
| C  | -2.138189570 | 0.763664605  | -1.858244464 |
| P  | -1.481924617 | 1.660828814  | -0.355102928 |
| C  | -2.895080164 | 1.362416289  | 0.855139650  |
| C  | -4.252835092 | 1.900912239  | 0.377003090  |
| C  | -2.604296863 | 1.796588724  | 2.298812041  |
| C  | -1.616221030 | 3.474045084  | -0.879723583 |
| C  | -0.751661908 | 3.771800917  | -2.115427651 |
| C  | -1.284120361 | 4.464299211  | 0.248263513  |
| C  | 0.591246959  | -1.808832594 | -1.873148676 |
| C  | 1.681699603  | -2.172828920 | -0.865959234 |
| P  | 2.445021561  | -0.573721135 | -0.305951932 |
| C  | 3.732856633  | -1.028654803 | 1.011248992  |
| C  | 3.468457509  | -2.376450096 | 1.703290623  |
| C  | 3.871086402  | 0.093250580  | 2.054704109  |
| C  | 3.529133299  | -0.060388876 | -1.770534504 |
| C  | 4.481942422  | -1.133352282 | -2.318749371 |
| C  | 4.279536099  | 1.244071764  | -1.457748843 |
| BR | 0.116163650  | -0.676952286 | 2.176212424  |
| C  | -3.112715964 | -2.995804889 | -0.328607227 |
| C  | -2.117317585 | -3.940347443 | 0.397092318  |
| C  | -3.489409659 | -3.632370604 | -1.698395767 |

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| C | -4.403032622 | -2.894724520 | 0.529822607  |
| O | -2.579068561 | -1.743609936 | -0.510546039 |
| H | 0.971641919  | 1.428597927  | -1.301206751 |
| H | -1.128768144 | -1.303007968 | -0.816055594 |
| H | -1.484744242 | -0.869319037 | -3.096781370 |
| H | -0.310912405 | 0.474863163  | -3.022965772 |
| H | -2.908711267 | 0.071717362  | -1.498392865 |
| H | -2.553720512 | 1.448796867  | -2.604845651 |
| H | -2.926155301 | 0.262551581  | 0.820369434  |
| H | -5.048284666 | 1.535037647  | 1.038273474  |
| H | -4.497768254 | 1.573328995  | -0.637793754 |
| H | -4.291343186 | 2.997467876  | 0.401330569  |
| H | -2.632583580 | 2.886159923  | 2.420161571  |
| H | -1.635623696 | 1.423513758  | 2.637133450  |
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| H | -2.668716940 | 3.614444124  | -1.161995242 |
| H | -0.908684916 | 4.809143383  | -2.439977049 |
| H | -0.993975914 | 3.118350741  | -2.958861657 |
| H | 0.309955473  | 3.637051090  | -1.891037457 |
| H | -0.259573080 | 4.331381681  | 0.606749088  |
| H | -1.954290466 | 4.357038378  | 1.104241933  |
| H | -1.378196495 | 5.495196222  | -0.118749638 |
| H | 1.050964726  | -1.432988313 | -2.798317853 |
| H | 0.009465078  | -2.702676366 | -2.145592783 |
| H | 2.393319116  | -2.893624912 | -1.283580082 |
| H | 1.221535412  | -2.609947145 | 0.024245657  |
| H | 4.684682424  | -1.112246021 | 0.469562947  |
| H | 4.258090084  | -2.567075564 | 2.441947767  |
| H | 3.468009392  | -3.213057702 | 0.997558728  |
| H | 2.507385753  | -2.360702376 | 2.224644397  |
| H | 2.938910980  | 0.204812210  | 2.615027779  |
| H | 4.108121381  | 1.058731499  | 1.598908464  |
| H | 4.675967693  | -0.152747294 | 2.759861344  |
| H | 2.786069665  | 0.171810634  | -2.542565752 |
| H | 5.018758558  | -0.749343970 | -3.195997994 |
| H | 3.952252660  | -2.038800197 | -2.629533806 |
| H | 5.239074925  | -1.425810392 | -1.582095357 |

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| H | 5.043634264  | 1.095742572  | -0.685705974 |
| H | 3.592232322  | 2.021350654  | -1.113639788 |
| H | 4.792125733  | 1.614172252  | -2.354896383 |
| H | -1.806504739 | -3.481135061 | 1.340514632  |
| H | -1.217710309 | -4.075685201 | -0.217407709 |
| H | -2.536510628 | -4.936564871 | 0.603446796  |
| H | -2.591651697 | -3.718233345 | -2.323786168 |
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| H | -3.940914683 | -4.632127480 | -1.611217164 |
| H | -4.903355066 | -3.862621755 | 0.682890165  |
| H | -5.110228221 | -2.213119308 | 0.042052841  |
| H | -4.153638567 | -2.473378627 | 1.509772731  |

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|    |              |              |              |
|----|--------------|--------------|--------------|
| FE | 0.370702555  | 0.700249118  | 0.191837513  |
| P  | -1.684023595 | 1.603839336  | 0.005833586  |
| P  | 2.397697537  | -0.220511636 | -0.045538016 |
| O  | 0.817119028  | 1.567569734  | 2.943186095  |
| N  | -0.118863917 | -0.353601667 | -1.330328504 |
| C  | 0.631363735  | 1.217203204  | 1.845012759  |
| C  | -2.433470812 | 0.537455487  | -1.317882488 |
| C  | -1.286302703 | -0.023401746 | -2.163157665 |
| C  | 0.872028291  | -1.033978271 | -2.174677409 |
| C  | 2.090189750  | -1.494837404 | -1.365138878 |
| C  | -1.822493182 | 3.376196722  | -0.607801431 |
| C  | -1.203100213 | 3.547295606  | -2.003852697 |
| C  | -1.183081014 | 4.354059847  | 0.391507178  |
| C  | -2.924317860 | 1.554382464  | 1.425178745  |
| C  | -2.771011294 | 0.264714284  | 2.250153131  |
| C  | -4.383076754 | 1.757869610  | 0.981603671  |
| C  | 3.810286214  | 0.837245884  | -0.693685344 |
| C  | 3.445236000  | 1.511810878  | -2.025308808 |
| C  | 4.236740719  | 1.883839073  | 0.347969129  |
| C  | 3.182591157  | -1.169234409 | 1.381092411  |
| C  | 2.149280416  | -2.083108182 | 2.061111574  |
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| C  | -1.974066255 | -3.727347154 | -0.215225702 |

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| C | -0.647081493 | -4.479101842 | -0.022459373 |
| C | -2.420968799 | -3.793269871 | -1.685126918 |
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| O | -1.835428363 | -2.364327296 | 0.199084937  |
| H | 0.950927725  | 2.015868872  | -0.184733387 |
| H | -2.929131979 | -0.290208635 | -0.801414902 |
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| H | -1.003202771 | 0.702965797  | -2.944312914 |
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| H | 2.961978382  | -1.668254237 | -2.004859906 |
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| H | -1.713541363 | 2.944333187  | -2.760289141 |
| H | -0.145996585 | 3.264952392  | -1.997282308 |
| H | -1.300301699 | 5.383887968  | 0.034496142  |
| H | -0.113535676 | 4.149628114  | 0.498718667  |
| H | -1.638347926 | 4.298037444  | 1.384997235  |
| H | -2.638867430 | 2.398825059  | 2.066091437  |
| H | -3.521163904 | 0.247884072  | 3.049978316  |
| H | -1.784721057 | 0.204646351  | 2.715985040  |
| H | -2.901000962 | -0.634928510 | 1.641138900  |
| H | -5.037193095 | 1.798871281  | 1.860211241  |
| H | -4.728394899 | 0.927190363  | 0.357424067  |
| H | -4.532201892 | 2.685787481  | 0.421141516  |
| H | 4.650822980  | 0.155166652  | -0.877389696 |
| H | 4.289713998  | 2.114882710  | -2.378994712 |
| H | 2.581221333  | 2.171084159  | -1.902419779 |
| H | 3.210203496  | 0.783659256  | -2.807243688 |
| H | 5.051242654  | 2.499133550  | -0.051406837 |
| H | 4.594721387  | 1.430450195  | 1.277353976  |
| H | 3.401433464  | 2.546967478  | 0.593990768  |
| H | 3.448955718  | -0.385873695 | 2.102324144  |
| H | 2.585788707  | -2.534306871 | 2.959551132  |
| H | 1.836249360  | -2.901754298 | 1.404404320  |

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| H | 1.252986724  | -1.533239435 | 2.358607343  |
| H | 4.846910132  | -2.463506782 | 1.900341156  |
| H | 5.251298204  | -1.302756779 | 0.635664865  |
| H | 4.251985271  | -2.714835239 | 0.257970460  |
| H | -1.138229056 | -1.892985215 | -0.305731268 |
| H | -0.315067155 | -4.398704822 | 1.016972983  |
| H | 0.133235892  | -4.058650200 | -0.667330853 |
| H | -0.748089688 | -5.540805829 | -0.273385569 |
| H | -1.658648875 | -3.361770351 | -2.343810834 |
| H | -3.349815264 | -3.231494758 | -1.824239820 |
| H | -2.591820229 | -4.827032190 | -2.005404873 |
| H | -3.243760658 | -5.366223458 | 0.462272527  |
| H | -3.992070356 | -3.759226237 | 0.579687188  |
| H | -2.747659173 | -4.240233001 | 1.745202309  |

**cp19**

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| P  | -2.277694100 | -0.056945530 | 0.071840317  |
| O  | 0.000103943  | 1.109808414  | -2.823218097 |
| N  | 0.000004742  | -0.670396445 | 1.864882784  |
| C  | 0.000039600  | 0.641081044  | -1.765691285 |
| C  | 2.486130343  | -0.653963996 | 1.831276668  |
| C  | 1.231434599  | -0.289850300 | 2.623540073  |
| C  | -1.231335098 | -0.289601965 | 2.623579629  |
| C  | -2.486094062 | -0.653653639 | 1.831404829  |
| C  | 3.329958130  | 1.488956475  | -0.052127555 |
| C  | 2.873296831  | 2.573283376  | 0.937344312  |
| C  | 3.371276609  | 2.033287691  | -1.489915592 |
| C  | 3.146331981  | -1.340445738 | -0.986809979 |
| C  | 2.313072101  | -2.633219059 | -1.036117861 |
| C  | 4.604542515  | -1.620586364 | -0.590968231 |
| C  | -3.330019753 | 1.488937694  | -0.052379572 |
| C  | -2.873341044 | 2.573523130  | 0.936811806  |
| C  | -3.371540483 | 2.032898788  | -1.490306395 |
| C  | -3.146260547 | -1.340640692 | -0.986535791 |
| C  | -2.312982554 | -2.633409949 | -1.035499062 |

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| C | -4.604490423 | -1.620734174 | -0.590730636 |
| H | -0.000234775 | 1.427063869  | 0.293105194  |
| H | 2.620739070  | -1.741747810 | 1.813264187  |
| H | 3.376334017  | -0.232477290 | 2.307788343  |
| H | 1.232712942  | -0.776284434 | 3.607683280  |
| H | 1.177735003  | 0.789460645  | 2.784547191  |
| H | -1.177481966 | 0.789721402  | 2.784481515  |
| H | -1.232628020 | -0.775939998 | 3.607772959  |
| H | -3.376243162 | -0.232076305 | 2.307941079  |
| H | -2.620795496 | -1.741430404 | 1.813467285  |
| H | 4.341486210  | 1.170739225  | 0.231622370  |
| H | 3.533800624  | 3.442116671  | 0.852727364  |
| H | 2.915956086  | 2.237247636  | 1.977930739  |
| H | 1.853001199  | 2.904032659  | 0.722312000  |
| H | 4.031411110  | 2.905786119  | -1.527558074 |
| H | 2.382046227  | 2.354665874  | -1.828529869 |
| H | 3.757913529  | 1.304361249  | -2.207673891 |
| H | 3.133583916  | -0.902241784 | -1.992758559 |
| H | 2.769619108  | -3.349551565 | -1.726317744 |
| H | 1.291794004  | -2.447602457 | -1.389397093 |
| H | 2.257056329  | -3.123985339 | -0.057490098 |
| H | 5.042261748  | -2.346161439 | -1.284501532 |
| H | 4.677318418  | -2.048478918 | 0.414590056  |
| H | 5.227441852  | -0.722992992 | -0.624777556 |
| H | -4.341493877 | 1.170737272  | 0.231566403  |
| H | -3.533996642 | 3.442242869  | 0.852173777  |
| H | -1.853134678 | 2.904393785  | 0.721524034  |
| H | -2.915737356 | 2.237648726  | 1.977463677  |
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| H | -3.758451739 | 1.303831130  | -2.207776996 |
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| H | -3.133458819 | -0.902673180 | -1.992584153 |
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| H | -1.291667017 | -2.447880895 | -1.388714576 |
| H | -5.042092157 | -2.346585563 | -1.284052462 |
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**cp5-THQ**

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H 0.415558892 3.661704806 3.446517810  
H 1.465449221 4.470564667 -1.045820014  
H 3.006379227 3.802753210 -2.885600588  
H 1.437878829 3.006788646 -3.054185458  
H 2.822445398 2.097499917 -2.434093738  
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| H | 0.378024122  | -0.470156706 | 1.376984849  |
| H | -7.395117657 | -0.276918892 | 0.299966485  |
| H | -3.151296629 | -0.728664225 | -2.197851398 |
| H | -5.272548974 | -0.472834581 | -3.430501771 |
| H | -7.429153263 | -0.248610085 | -2.183988860 |
| H | -6.171178934 | -0.996744441 | 2.354099051  |
| H | -4.037234666 | -2.221514193 | 2.370301149  |
| H | -1.866799547 | -1.036673825 | 2.242408122  |
| H | -5.341174917 | 0.548363810  | 2.352848415  |
| H | -3.942312954 | -0.983013673 | 3.629708240  |
| H | -2.701627812 | 0.516782247  | 2.104418309  |
| H | -1.984614504 | -0.567612941 | -0.106065343 |

**cp5-MeOH**

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| FE | -0.076651000 | -0.178690000 | 0.152871000  |
| C  | -0.223697000 | -1.647683000 | 1.108206000  |
| N  | 0.080977000  | 1.452781000  | -1.128715000 |
| P  | 2.156064000  | -0.323219000 | -0.183348000 |
| P  | -2.300017000 | 0.155907000  | -0.059002000 |
| C  | 2.477397000  | 1.015971000  | -1.433976000 |
| C  | 3.288625000  | 0.201002000  | 1.233272000  |
| C  | 2.931945000  | -1.860807000 | -0.946484000 |
| C  | -2.342113000 | 1.810549000  | -0.898638000 |
| C  | -3.462645000 | 0.358464000  | 1.411963000  |
| C  | -3.212924000 | -0.943933000 | -1.289100000 |
| O  | -0.346390000 | -2.664274000 | 1.661327000  |
| C  | -1.136794000 | 1.829975000  | -1.837271000 |
| C  | 1.147324000  | 1.329663000  | -2.119369000 |
| C  | 2.861914000  | -3.092588000 | -0.030040000 |
| C  | 2.320524000  | -2.179366000 | -2.320043000 |
| C  | 3.014782000  | -0.519938000 | 2.563032000  |
| C  | 4.785568001  | 0.184451000  | 0.886297000  |
| C  | -4.713660001 | -0.638598000 | -1.426353000 |
| C  | -2.961829000 | -2.447139000 | -1.088103000 |
| C  | -3.769328000 | -0.972973000 | 2.119384000  |
| C  | -2.921192000 | 1.378696000  | 2.427661000  |
| O  | 1.093594000  | 3.156775000  | 0.719603000  |

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| C | 1.389730000  | 4.432424001  | 0.204318000  |
| H | -0.196755000 | -1.047087000 | -1.061859000 |
| H | 2.813609000  | 1.893077000  | -0.873413000 |
| H | 3.259830000  | 0.740244000  | -2.148409000 |
| H | 1.255625000  | 2.268726000  | -2.692774000 |
| H | 0.918721000  | 0.544458000  | -2.866043000 |
| H | -1.337971000 | 1.149005000  | -2.690930000 |
| H | -1.039513000 | 2.836468000  | -2.283376000 |
| H | -3.283589000 | 1.997768000  | -1.426280000 |
| H | -2.222578000 | 2.581090000  | -0.130845000 |
| H | 3.987722000  | -1.599168000 | -1.097132000 |
| H | 2.829634000  | -3.047439000 | -2.755241000 |
| H | 2.419226000  | -1.349734000 | -3.025561000 |
| H | 1.256736000  | -2.416590000 | -2.230273000 |
| H | 3.338464000  | -3.947119000 | -0.524672000 |
| H | 1.827411000  | -3.371258000 | 0.188494000  |
| H | 3.376411000  | -2.936500000 | 0.921242000  |
| H | 2.972737000  | 1.246237000  | 1.357253000  |
| H | 5.360190001  | 0.661952000  | 1.688479000  |
| H | 5.004316001  | 0.725134000  | -0.039935000 |
| H | 5.166161001  | -0.837395000 | 0.780389000  |
| H | 3.564951000  | -0.023866000 | 3.371027000  |
| H | 3.339294000  | -1.564603000 | 2.543109000  |
| H | 1.953627000  | -0.504326000 | 2.825552000  |
| H | -2.719364000 | -0.659797000 | -2.227940000 |
| H | -5.125528001 | -1.184392000 | -2.282969000 |
| H | -4.915677001 | 0.424470000  | -1.589736000 |
| H | -5.275180001 | -0.955812000 | -0.541805000 |
| H | -3.386779000 | -3.006154000 | -1.930101000 |
| H | -3.430864000 | -2.827089000 | -0.175667000 |
| H | -1.893684000 | -2.666802000 | -1.038344000 |
| H | -4.398151001 | 0.755892000  | 0.996507000  |
| H | -3.669551000 | 1.550557000  | 3.209692000  |
| H | -2.686707000 | 2.347438000  | 1.978615000  |
| H | -2.015144000 | 1.008149000  | 2.918361000  |
| H | -4.422608001 | -0.791735000 | 2.980862000  |
| H | -2.857445000 | -1.450159000 | 2.492061000  |

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| H | -4.278358001 | -1.687053000 | 1.467992000  |
| H | -0.309701000 | 0.902910000  | 1.440769000  |
| H | 0.656726000  | 2.597982000  | -0.005963000 |
| H | 0.484466000  | 0.847439000  | 1.386879000  |
| H | 0.495657000  | 4.970826001  | -0.152109000 |
| H | 2.111618000  | 4.403860001  | -0.631137000 |
| H | 1.838013000  | 5.037502001  | 1.000885000  |

**TS2-MeOH**

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| FE | -0.030903000 | -0.165375000 | 0.115426000  |
| C  | -0.077329000 | -1.459200000 | 1.298551000  |
| N  | 0.035747000  | 1.233066000  | -1.445400000 |
| P  | 2.223426000  | -0.207761000 | -0.194267000 |
| P  | -2.278589000 | 0.044958000  | -0.087995000 |
| C  | 2.454225000  | 0.875483000  | -1.694082000 |
| C  | 3.276779000  | 0.683019000  | 1.085373000  |
| C  | 3.128376000  | -1.794328000 | -0.651774000 |
| C  | -2.396458000 | 1.547834000  | -1.178677000 |
| C  | -3.440637000 | 0.419596000  | 1.347804000  |
| C  | -3.160718000 | -1.259334000 | -1.130956000 |
| O  | -0.124926000 | -2.368116000 | 2.023303000  |
| C  | -1.225276000 | 1.471786000  | -2.158537000 |
| C  | 1.111181000  | 0.982313000  | -2.418881000 |
| C  | 3.184209000  | -2.811498000 | 0.498747000  |
| C  | 2.527237000  | -2.439344000 | -1.911123000 |
| C  | 3.056041000  | 0.198129000  | 2.527018000  |
| C  | 4.771068001  | 0.752266000  | 0.736012000  |
| C  | -4.674714001 | -1.039207000 | -1.283072000 |
| C  | -2.842137000 | -2.705244000 | -0.717156000 |
| C  | -3.638590000 | -0.800715000 | 2.263856000  |
| C  | -2.963850000 | 1.625571000  | 2.174593000  |
| O  | 0.969551000  | 2.944217000  | 0.091631000  |
| C  | 0.261423000  | 4.079804000  | 0.470235000  |
| H  | -0.131484000 | -1.246802000 | -0.923867000 |
| H  | 2.735737000  | 1.865678000  | -1.325241000 |
| H  | 3.243867000  | 0.505240000  | -2.355566000 |
| H  | 1.159382000  | 1.803402000  | -3.153232000 |

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|---|--------------|--------------|--------------|
| H | 0.897606000  | 0.060021000  | -2.978466000 |
| H | -1.402447000 | 0.658793000  | -2.881142000 |
| H | -1.168734000 | 2.402009000  | -2.746858000 |
| H | -3.356029000 | 1.623586000  | -1.701116000 |
| H | -2.289842000 | 2.433634000  | -0.545143000 |
| H | 4.153997000  | -1.480168000 | -0.887488000 |
| H | 3.110345000  | -3.326675000 | -2.184173000 |
| H | 2.534300000  | -1.763090000 | -2.770798000 |
| H | 1.492764000  | -2.749247000 | -1.737823000 |
| H | 3.709153000  | -3.715204000 | 0.167279000  |
| H | 2.182307000  | -3.109437000 | 0.819746000  |
| H | 3.717001000  | -2.425415000 | 1.371067000  |
| H | 2.845288000  | 1.690628000  | 1.008922000  |
| H | 5.286256001  | 1.421553000  | 1.434852000  |
| H | 4.944318001  | 1.139391000  | -0.273045000 |
| H | 5.254998001  | -0.228077000 | 0.810952000  |
| H | 3.538009000  | 0.893026000  | 3.224577000  |
| H | 3.486580000  | -0.791820000 | 2.706924000  |
| H | 1.994034000  | 0.154782000  | 2.782360000  |
| H | -2.693007000 | -1.099162000 | -2.111575000 |
| H | -5.073745001 | -1.722361000 | -2.041592000 |
| H | -4.925024001 | -0.021209000 | -1.597570000 |
| H | -5.210169001 | -1.244756000 | -0.350786000 |
| H | -3.270545000 | -3.400027000 | -1.449037000 |
| H | -3.265136000 | -2.959271000 | 0.259118000  |
| H | -1.764598000 | -2.875039000 | -0.676125000 |
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| H | -3.702248000 | 1.848082000  | 2.953329000  |
| H | -2.835532000 | 2.530963000  | 1.575652000  |
| H | -2.011536000 | 1.416621000  | 2.671333000  |
| H | -4.290716001 | -0.531783000 | 3.102764000  |
| H | -2.687666000 | -1.145497000 | 2.682033000  |
| H | -4.102685000 | -1.643696000 | 1.746677000  |
| H | -0.053020000 | 0.942994000  | 1.426070000  |
| H | 0.397440000  | 2.191785000  | -0.769381000 |
| H | 0.332075000  | 1.460304000  | 0.938268000  |
| H | -0.415844000 | 3.907925000  | 1.334691000  |

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| H | -0.374767000 | 4.490985001 | -0.340516000 |
| H | 0.934961000  | 4.900276001 | 0.772770000  |

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| FE | -1.463214966 | 0.101590647  | 0.176298407  |
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| O  | -2.118744437 | 0.165414804  | 3.017443757  |
| N  | -0.354744313 | -0.055501426 | -1.352198162 |
| C  | -1.858991922 | 0.143841238  | 1.878401769  |
| C  | -0.523073559 | -2.538812908 | -1.340015602 |
| C  | -0.223173600 | -1.277127620 | -2.158574637 |
| C  | 0.057799465  | 1.087575731  | -2.178130797 |
| C  | 0.163179765  | 2.372895048  | -1.351932890 |
| C  | -3.450146768 | -2.647181748 | -0.821278079 |
| C  | -3.733310291 | -1.941008499 | -2.156487034 |
| C  | -4.606839673 | -2.425750241 | 0.166670706  |
| C  | -1.558333617 | -3.316099556 | 1.334869763  |
| C  | -0.242256584 | -3.036886646 | 2.079785564  |
| C  | -1.653874518 | -4.796542748 | 0.930686032  |
| C  | -2.585462782 | 3.336971032  | -0.722430546 |
| C  | -3.088084706 | 2.786562964  | -2.066444117 |
| C  | -3.734943045 | 3.418212555  | 0.295023743  |
| C  | -0.493357181 | 3.398701122  | 1.347212129  |
| C  | 0.621178755  | 2.680312668  | 2.125753535  |
| C  | -0.032080238 | 4.794205897  | 0.894435894  |
| C  | 6.337492070  | -0.552122919 | -0.551085393 |
| C  | 5.187595703  | -0.434130194 | 0.234048283  |
| C  | 3.938470478  | -0.252258156 | -0.406868744 |
| C  | 3.895573708  | -0.210396780 | -1.813644374 |
| C  | 5.055290891  | -0.337682026 | -2.571101823 |
| C  | 6.291701696  | -0.508837707 | -1.944491272 |
| C  | 5.270459048  | -0.514777685 | 1.748624772  |
| C  | 4.021708136  | 0.062862844  | 2.428731074  |
| C  | 2.763706582  | -0.468678946 | 1.739611559  |
| N  | 2.775587230  | -0.068210727 | 0.339863925  |
| H  | -2.925106059 | 0.323482692  | -0.026103468 |

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| H | 0.371601959  | -2.839116993 | -0.784266609 |
| H | -0.813801972 | -3.379923430 | -1.978405802 |
| H | 0.794088219  | -1.351733676 | -2.579204936 |
| H | -0.898948060 | -1.232530265 | -3.031044294 |
| H | -0.652492561 | 1.231309470  | -3.010972822 |
| H | 1.030950945  | 0.888917076  | -2.657439527 |
| H | 0.112949963  | 3.269307895  | -1.978846670 |
| H | 1.122530650  | 2.384267861  | -0.823806704 |
| H | -3.353935754 | -3.722262298 | -1.019319338 |
| H | -4.700894736 | -2.271422268 | -2.552141173 |
| H | -2.975209273 | -2.165440619 | -2.912186922 |
| H | -3.770979401 | -0.856168724 | -2.022598818 |
| H | -5.551651630 | -2.748345161 | -0.285758850 |
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| H | -4.479602101 | -2.989491945 | 1.095915211  |
| H | -2.378586516 | -3.089690695 | 2.028215746  |
| H | -0.167880783 | -3.687997097 | 2.958214722  |
| H | -0.179698138 | -2.001501325 | 2.421717680  |
| H | 0.631313723  | -3.240576393 | 1.450648807  |
| H | -1.507126577 | -5.433890539 | 1.810448690  |
| H | -0.879640576 | -5.064459518 | 0.203087457  |
| H | -2.625247250 | -5.055135975 | 0.500530903  |
| H | -2.192716164 | 4.347274698  | -0.894814282 |
| H | -3.935806744 | 3.385583719  | -2.419183605 |
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| H | -4.553108808 | 4.023129485  | -0.112557187 |
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| H | -4.126613873 | 2.420024520  | 0.514200184  |
| H | -1.346391307 | 3.518141091  | 2.027291602  |
| H | 0.980488499  | 3.323880596  | 2.937243141  |
| H | 1.479172511  | 2.443473469  | 1.487311173  |
| H | 0.263747934  | 1.749140185  | 2.571001597  |
| H | 0.293889024  | 5.378516082  | 1.762644972  |
| H | -0.824176662 | 5.362299770  | 0.398939593  |
| H | 0.818928803  | 4.730629229  | 0.207773716  |
| H | 7.294145712  | -0.684367749 | -0.048927366 |

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| H | 2.936916311 | -0.073411512 | -2.306680929 |
| H | 4.990478557 | -0.302424798 | -3.655483822 |
| H | 7.201761462 | -0.604549437 | -2.528656610 |
| H | 6.170368871 | 0.003710612  | 2.100745212  |
| H | 4.025265751 | 1.156928446  | 2.356449984  |
| H | 1.861394481 | -0.061431300 | 2.203850963  |
| H | 5.389540955 | -1.564981202 | 2.053059056  |
| H | 4.007538401 | -0.197751164 | 3.492527961  |
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### TS3

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| FE | 0.825989183  | 0.356281054  | 0.166717910  |
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| O  | 1.676624086  | 1.308442770  | 2.790448155  |
| N  | 0.149721784  | -0.418630360 | -1.617026305 |
| C  | -0.602443672 | 0.510183018  | -2.491210087 |
| C  | -1.641651429 | 1.297158282  | -1.694247379 |
| P  | -0.868932526 | 1.854462272  | -0.093990207 |
| C  | -2.372754350 | 1.933808067  | 1.043020255  |
| C  | -3.455325188 | 2.932905525  | 0.602649967  |
| C  | -2.019291171 | 2.116068781  | 2.527402360  |
| C  | -0.379182688 | 3.652895083  | -0.392036577 |
| C  | 0.369635850  | 3.853910597  | -1.719334602 |
| C  | 0.445482555  | 4.227996254  | 0.771258152  |
| C  | 1.113377311  | -1.175074804 | -2.448895449 |
| C  | 2.061187850  | -2.006571090 | -1.582514222 |
| P  | 2.692848982  | -0.893658592 | -0.233338058 |
| C  | 3.598365256  | -2.052579410 | 0.949858448  |
| C  | 2.666040087  | -3.091586260 | 1.592072931  |
| C  | 4.351613096  | -1.281381150 | 2.048412697  |
| C  | 4.067444238  | 0.053158128  | -1.126029685 |
| C  | 5.269194410  | -0.807940998 | -1.548121252 |
| C  | 4.530299442  | 1.327417914  | -0.400064422 |
| C  | -4.971271960 | -1.548804001 | 0.554266647  |
| C  | -2.799500860 | -1.934333502 | -0.500199452 |
| C  | -3.476468746 | -1.915182052 | -1.748590444 |

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| C | -4.847067779 | -1.705949949 | -1.838763009 |
| C | -5.615174777 | -1.518105618 | -0.683922156 |
| C | -2.925133005 | -1.763000219 | 2.034480371  |
| C | -1.593231549 | -2.514144433 | 1.977664806  |
| C | -0.769867539 | -2.089478076 | 0.756283406  |
| N | -1.435504862 | -2.149659497 | -0.498152732 |
| C | -3.592586093 | -1.742660814 | 0.671687038  |
| H | 1.608018003  | 1.445340066  | -0.465181178 |
| H | -0.631686274 | -1.232515263 | -1.226693845 |
| H | -1.106132322 | -0.052297155 | -3.292747636 |
| H | 0.106107198  | 1.194203912  | -2.974840056 |
| H | -2.479047679 | 0.640930869  | -1.436351571 |
| H | -2.040947787 | 2.129663967  | -2.282442326 |
| H | -2.787619836 | 0.925904124  | 0.920007013  |
| H | -4.361467960 | 2.777910867  | 1.199084702  |
| H | -3.733959094 | 2.811339629  | -0.448232103 |
| H | -3.140645413 | 3.970629581  | 0.756535104  |
| H | -1.667784031 | 3.130032424  | 2.743154109  |
| H | -1.248285743 | 1.415479460  | 2.857576491  |
| H | -2.911192625 | 1.947979723  | 3.141928656  |
| H | -1.325950538 | 4.203074832  | -0.456333508 |
| H | 0.616240814  | 4.915061784  | -1.841733343 |
| H | -0.225831350 | 3.555476153  | -2.586544943 |
| H | 1.305687731  | 3.287490363  | -1.733323772 |
| H | 1.406793178  | 3.713720666  | 0.858310912  |
| H | -0.064518388 | 4.147507718  | 1.734074119  |
| H | 0.647810652  | 5.290406284  | 0.591794387  |
| H | 1.689456211  | -0.470954755 | -3.065641442 |
| H | 0.571497655  | -1.834700279 | -3.143462799 |
| H | 2.859111490  | -2.453828987 | -2.184433940 |
| H | 1.502322221  | -2.819986011 | -1.111741456 |
| H | 4.330697381  | -2.589243085 | 0.333478917  |
| H | 3.252967486  | -3.758242550 | 2.234426810  |
| H | 2.154081814  | -3.717175007 | 0.856197924  |
| H | 1.908777947  | -2.612089127 | 2.219888074  |
| H | 3.673640409  | -0.650962546 | 2.631797456  |
| H | 5.144057416  | -0.645134503 | 1.648864117  |

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| H | 4.821152796  | -1.991089821 | 2.739124532  |
| H | 3.544442485  | 0.378707404  | -2.034768106 |
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**cp7**

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| FE | 0.815852189  | 0.349727578  | 0.161194934  |
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| C  | 1.212040146  | -1.056339587 | -2.525563194 |
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| C | 4.298873258  | -1.315967164 | 2.072784171  |
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| C | 4.523453199  | 1.393228948  | -0.271542664 |
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| H | 2.958868848  | -2.326636479 | -2.254873130 |

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| O               | 1.717556589  | 1.004688827  | 2.864370240  | H | -4.255104960 | 2.644797181  | 1.227533728  |
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| C               | -1.428233155 | 1.590161571  | -1.689097344 | H | -1.651382598 | 3.047192538  | 2.843086868  |
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| H          | 1.465342237  | 3.542701641  | -1.476714827 | N | 0.290906526  | -0.221090563 | -1.835949423 |
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| H          | 0.901076648  | 5.211900098  | 1.122682095  | P | -0.819192439 | 1.853296935  | -0.053694256 |
| H          | 1.891762626  | -0.181826052 | -3.071180052 | C | -2.395829050 | 1.801643756  | 0.982116015  |
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| H          | 3.482615296  | -1.093575413 | 2.644678767  | P | 2.728519111  | -0.844774930 | -0.264016088 |
| H          | 5.007033710  | -1.136066093 | 1.750143123  | C | 3.492463148  | -2.203453842 | 0.807056151  |
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| H          | 3.823399289  | 0.307540876  | -1.921072226 | C | 4.101127449  | -1.631523098 | 2.100507437  |
| H          | 6.139847211  | -0.520247552 | -1.948892373 | C | 4.220882956  | 0.173866492  | -0.838053514 |
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| H          | 3.914840264  | 1.726932536  | 0.107047451  | C | -2.988669705 | -1.897241624 | -0.606932908 |
| H          | 5.486118720  | 1.619234767  | -0.711851737 | C | -3.818629398 | -1.762920229 | -1.738769416 |
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| H          | -3.083664046 | -3.708686860 | 1.605796788  | N | -1.632268285 | -2.164047301 | -0.822050990 |
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| H          | -1.870021166 | -0.961692714 | 2.185545688  | H | 1.663062619  | 1.499294577  | -0.453435499 |
| H          | -1.178308620 | -2.509690975 | 2.645003582  | H | -0.416361843 | -0.966453889 | -1.657440573 |
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|            |              |              |              | H | -1.923668649 | 2.357328867  | -2.249487103 |
| <b>TS4</b> |              |              |              |   |              |              |              |
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| H | 1.483370080  | 3.539319136  | 1.057989810  |
| H | 0.063468774  | 3.812625430  | 2.070615979  |
| H | 0.721356343  | 5.140604616  | 1.107409502  |
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| H | 4.299914758  | -2.641960528 | 0.207015347  |
| H | 3.007294984  | -4.088824105 | 1.751501388  |
| H | 2.091887561  | -3.819757588 | 0.270652850  |
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| H | 3.349977684  | -1.106686990 | 2.698399134  |
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| H | 4.501937121  | -2.448606497 | 2.711733267  |
| H | 3.818442731  | 0.635711919  | -1.749296652 |
| H | 6.198954112  | 0.010305426  | -1.712409030 |
| H | 5.244857231  | -1.458811076 | -1.916384321 |
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| H | 5.042448373  | 0.968199744  | 1.039700860  |
| H | 3.698776248  | 1.910961649  | 0.370831138  |
| H | 5.308457861  | 1.990517246  | -0.372069979 |
| H | -0.131130634 | -0.932533633 | 0.621805984  |
| H | -5.388802117 | -1.437082698 | 1.776682641  |
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| H | -6.820043654 | -1.192078594 | -0.236575979 |

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| H | -1.670763007 | -3.766915491 | 1.550411736 |
| H | 0.111756936  | -2.769682578 | 0.032422706 |
| H | -0.682375493 | -2.567539927 | 2.389577099 |
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| C  | -0.233672326 | 1.166540348  | -2.236391316 |
| C  | -0.230615803 | 2.417920528  | -1.359148393 |
| P  | 1.170774436  | 2.266446337  | -0.119662926 |
| C  | 0.427731132  | 3.181339748  | 1.359670342  |
| C  | 0.174129989  | 4.681558671  | 1.145690034  |
| C  | 1.176562876  | 2.918229039  | 2.675270786  |
| C  | 2.477035716  | 3.444314539  | -0.811882705 |
| C  | 2.859649790  | 3.079113854  | -2.254287511 |
| C  | 3.730922793  | 3.481060108  | 0.076851273  |
| C  | -0.120791653 | -1.271323400 | -2.209094070 |
| C  | 0.077559559  | -2.493211847 | -1.313333439 |
| P  | 1.552568000  | -2.149186947 | -0.213391656 |
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| C  | 2.943065903  | -2.918390168 | -1.244077638 |
| C  | 2.924391257  | -4.451838008 | -1.341589708 |
| C  | 4.336674430  | -2.393044695 | -0.864966715 |
| C  | -6.591089774 | -0.547277669 | 0.065834672  |
| C  | -5.295585472 | -0.511135788 | 0.581536836  |
| C  | -4.235415495 | -0.113800137 | -0.259899478 |
| C  | -4.492229470 | 0.234405431  | -1.590894253 |
| C  | -5.793567858 | 0.203904250  | -2.089975063 |
| C  | -6.845721015 | -0.189173364 | -1.260874308 |
| C  | -4.958615480 | -0.920641110 | 1.997846538  |
| C  | -3.754490045 | -0.118897517 | 2.508735953  |

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| C | -2.669144266 | -0.071140570 | 1.459197174  |
| N | -2.890548594 | -0.067425418 | 0.193371979  |
| H | 2.436573843  | 0.149781012  | -1.249470205 |
| H | -1.142161656 | 1.134200035  | -2.860029115 |
| H | 0.632428233  | 1.164020079  | -2.904610304 |
| H | -1.168805575 | 2.471141764  | -0.795353195 |
| H | -0.162465549 | 3.323434335  | -1.970739282 |
| H | -0.544266260 | 2.676461292  | 1.442930035  |
| H | -0.415822863 | 5.086467358  | 1.976830961  |
| H | -0.376248831 | 4.887111698  | 0.221496110  |
| H | 1.111138988  | 5.247411833  | 1.111933288  |
| H | 2.157663003  | 3.402459475  | 2.695286568  |
| H | 1.320951080  | 1.847954417  | 2.837244135  |
| H | 0.600562554  | 3.320236323  | 3.517978126  |
| H | 2.021558938  | 4.442998604  | -0.819852206 |
| H | 3.643583891  | 3.757108492  | -2.612524168 |
| H | 2.014105602  | 3.166481030  | -2.944169539 |
| H | 3.235785362  | 2.053297434  | -2.305205896 |
| H | 4.189195779  | 2.490742475  | 0.151258141  |
| H | 3.515296410  | 3.826666099  | 1.091299502  |
| H | 4.473804463  | 4.163903119  | -0.352661617 |
| H | 0.708026745  | -1.180717127 | -2.919601750 |
| H | -1.051437858 | -1.363353520 | -2.790993038 |
| H | 0.199812943  | -3.401169823 | -1.913583393 |
| H | -0.805302617 | -2.631533074 | -0.681769411 |
| H | 1.176645983  | -4.348677297 | 0.786340072  |
| H | -0.067132531 | -3.735139243 | 2.858246402  |
| H | -0.870925978 | -3.060931899 | 1.437425081  |
| H | 0.115428821  | -2.010134298 | 2.460705922  |
| H | 2.732956609  | -2.381135842 | 2.566709966  |
| H | 3.435088555  | -3.713538524 | 1.642363067  |
| H | 2.350415953  | -4.055877540 | 2.991614686  |
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| H | 1.944123795  | -4.846991826 | -1.628475515 |
| H | 3.209025855  | -4.921015042 | -0.394265059 |
| H | 4.664083992  | -2.756989172 | 0.114033589  |

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| H | 4.344446770  | -1.301260409 | -0.844251521 |
| H | 5.075078781  | -2.731315610 | -1.602146514 |
| H | 0.457742119  | -0.013828467 | 1.175891710  |
| H | -7.411304599 | -0.854267132 | 0.710799548  |
| H | -3.658009669 | 0.533521077  | -2.218401383 |
| H | -5.985345836 | 0.482330497  | -3.122037433 |
| H | -7.861715878 | -0.217948168 | -1.643637515 |
| H | -4.708927806 | -1.992133934 | 2.013859571  |
| H | -5.822864632 | -0.792086580 | 2.656980392  |
| H | -4.053343523 | 0.917275422  | 2.733207079  |
| H | -3.357696017 | -0.535674870 | 3.439379757  |
| H | -1.622044453 | -0.018265309 | 1.766537387  |
| H | -0.979805305 | -0.072058716 | -0.805837149 |

# TS5

|    |              |              |              |
|----|--------------|--------------|--------------|
| FE | -0.768742000 | 0.350966000  | -0.116945000 |
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| O  | -0.904869000 | 0.671561000  | -3.014532000 |
| N  | -0.547597000 | -0.086209000 | 1.832223000  |
| C  | 0.215786000  | 0.859379000  | 2.679833000  |
| C  | 1.445453000  | 1.395370000  | 1.946900000  |
| P  | 0.970406000  | 1.779567000  | 0.188719000  |
| C  | 2.614742000  | 1.617517000  | -0.716959000 |
| C  | 3.774548000  | 2.387799000  | -0.063968000 |
| C  | 2.531274000  | 1.931817000  | -2.220022000 |
| C  | 0.580584000  | 3.625852000  | 0.145690000  |
| C  | -0.244295000 | 4.092675000  | 1.355449000  |
| C  | -0.133069000 | 4.028582000  | -1.156719000 |
| C  | -1.731189000 | -0.547983000 | 2.591371000  |
| C  | -2.580766000 | -1.500690000 | 1.750246000  |
| P  | -2.751867000 | -0.743674000 | 0.058514000  |
| C  | -3.338783000 | -2.176580000 | -1.018528000 |
| C  | -2.249560000 | -3.251680000 | -1.158695000 |
| C  | -3.795562000 | -1.712096000 | -2.412548000 |
| C  | -4.264190001 | 0.366722000  | 0.286953000  |
| C  | -5.580463001 | -0.388664000 | 0.534205000  |
| C  | -4.432772001 | 1.431644000  | -0.809598000 |

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| C | 2.162926000  | -2.174191000 | 2.397656000  | H          | -1.377484000 | -2.857201000 | -1.688563000 |
| C | 1.078245000  | -2.209510000 | 0.125063000  | H          | -2.995706000 | -1.183566000 | -2.940260000 |
| C | 0.959397000  | -2.313879000 | 1.625318000  | H          | -4.665712001 | -1.053400000 | -2.370280000 |
| N | 3.351732000  | -1.831550000 | 1.976045000  | H          | -4.072837000 | -2.582824000 | -3.017750000 |
| C | 4.840603001  | -1.576309000 | 0.110150000  | H          | -3.998362000 | 0.899521000  | 1.209990000  |
| C | 5.127663001  | -1.609808000 | -1.249794000 | H          | -6.363025001 | 0.319897000  | 0.828823000  |
| C | 4.110479000  | -1.883571000 | -2.172925000 | H          | -5.500336001 | -1.134617000 | 1.330879000  |
| C | 3.533832000  | -1.803257000 | 0.587128000  | H          | -5.930855001 | -0.898516000 | -0.368789000 |
| C | 2.500420000  | -2.046186000 | -0.350892000 | H          | -4.724781001 | 0.994598000  | -1.768674000 |
| C | 2.811806000  | -2.102329000 | -1.714608000 | H          | -3.509845000 | 1.995267000  | -0.959336000 |
| H | -1.592734000 | 1.570358000  | 0.055181000  | H          | -5.221598001 | 2.135180000  | -0.518824000 |
| H | 0.203168000  | -1.133027000 | 1.834421000  | H          | 0.477831000  | -1.293329000 | -0.256185000 |
| H | 0.534096000  | 0.353491000  | 3.605706000  | H          | 0.589657000  | -3.033422000 | -0.405779000 |
| H | -0.443742000 | 1.684131000  | 2.977884000  | H          | 0.261612000  | -3.061045000 | 2.011577000  |
| H | 2.218086000  | 0.620220000  | 1.904995000  | H          | 2.071845000  | -2.318856000 | 3.479359000  |
| H | 1.874893000  | 2.253977000  | 2.472479000  | H          | 5.615977001  | -1.391948000 | 0.847784000  |
| H | 2.826496000  | 0.547473000  | -0.617455000 | H          | 6.143890001  | -1.436174000 | -1.593982000 |
| H | 4.707554001  | 2.145451000  | -0.584633000 | H          | 4.327911001  | -1.924100000 | -3.236472000 |
| H | 3.913937000  | 2.124221000  | 0.987616000  | H          | 2.015432000  | -2.305985000 | -2.428845000 |
| H | 3.637337000  | 3.472989000  | -0.130971000 |            |              |              |              |
| H | 2.438912000  | 3.007375000  | -2.403958000 | <b>cp9</b> |              |              |              |
| H | 1.695517000  | 1.427589000  | -2.710618000 | FE         | -0.703841000 | 0.335934000  | -0.106336000 |
| H | 3.452233000  | 1.595600000  | -2.708308000 | C          | -0.755149000 | 0.523104000  | -1.844918000 |
| H | 1.554177000  | 4.131409000  | 0.183668000  | O          | -0.800897000 | 0.642722000  | -3.002881000 |
| H | -0.441913000 | 5.167699001  | 1.271052000  | N          | -0.557687000 | -0.035910000 | 1.941407000  |
| H | 0.270873000  | 3.929893000  | 2.306092000  | C          | 0.239429000  | 0.947042000  | 2.726380000  |
| H | -1.210369000 | 3.579293000  | 1.391493000  | C          | 1.510110000  | 1.346085000  | 1.978488000  |
| H | -1.124889000 | 3.570623000  | -1.206273000 | P          | 1.071667000  | 1.716448000  | 0.204135000  |
| H | 0.415285000  | 3.733521000  | -2.053619000 | C          | 2.719891000  | 1.508482000  | -0.679722000 |
| H | -0.259842000 | 5.117206001  | -1.186795000 | C          | 3.903506000  | 2.203924000  | 0.012846000  |
| H | -2.329254000 | 0.320173000  | 2.902876000  | C          | 2.662959000  | 1.884480000  | -2.169842000 |
| H | -1.409584000 | -1.055068000 | 3.515591000  | C          | 0.747232000  | 3.578209000  | 0.123125000  |
| H | -3.542813000 | -1.704989000 | 2.231164000  | C          | -0.016607000 | 4.123541000  | 1.339371000  |
| H | -2.060473000 | -2.455711000 | 1.634949000  | C          | 0.006908000  | 3.968441000  | -1.168144000 |
| H | -4.197693001 | -2.619516000 | -0.497354000 | C          | -1.840452000 | -0.318421000 | 2.636385000  |
| H | -2.638590000 | -4.096812000 | -1.737744000 | C          | -2.710751000 | -1.268709000 | 1.815311000  |
| H | -1.911213000 | -3.643768000 | -0.195675000 | P          | -2.750973000 | -0.643321000 | 0.056592000  |

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|---|--------------|--------------|--------------|------------|--------------|--------------|--------------|
| C | -3.417705000 | -2.120531000 | -0.912410000 | H          | -1.647073000 | -0.740084000 | 3.633726000  |
| C | -2.444761000 | -3.309106000 | -0.908146000 | H          | -3.708031000 | -1.356380000 | 2.258737000  |
| C | -3.768933000 | -1.748065000 | -2.363914000 | H          | -2.266348000 | -2.268389000 | 1.811539000  |
| C | -4.203588001 | 0.568642000  | 0.132956000  | H          | -4.337463001 | -2.426946000 | -0.397274000 |
| C | -5.575461001 | -0.079205000 | 0.381183000  | H          | -2.925425000 | -4.177044000 | -1.373668000 |
| C | -4.256220001 | 1.547496000  | -1.051424000 | H          | -2.131111000 | -3.609060000 | 0.095363000  |
| N | 3.147508000  | -1.969701000 | 1.947639000  | H          | -1.547410000 | -3.079195000 | -1.488510000 |
| C | 1.946013000  | -2.430451000 | 2.302840000  | H          | -2.901823000 | -1.339235000 | -2.892194000 |
| C | 0.940020000  | -2.267717000 | 0.049139000  | H          | -4.577683001 | -1.017312000 | -2.427657000 |
| C | 0.856527000  | -2.655634000 | 1.461621000  | H          | -4.094000000 | -2.644052000 | -2.904987000 |
| C | 4.997062001  | -1.619162000 | -1.213720000 | H          | -3.938112000 | 1.158845000  | 1.020125000  |
| C | 3.999305000  | -1.859215000 | -2.175718000 | H          | -6.318052001 | 0.698226000  | 0.594224000  |
| C | 2.693899000  | -2.091830000 | -1.756670000 | H          | -5.574581001 | -0.767828000 | 1.231948000  |
| C | 4.685663001  | -1.633050000 | 0.136450000  | H          | -5.928773001 | -0.630162000 | -0.495983000 |
| C | 3.365272000  | -1.886884000 | 0.587339000  | H          | -4.552094001 | 1.054979000  | -1.982191000 |
| C | 2.353309000  | -2.094602000 | -0.395325000 | H          | -3.288117000 | 2.025973000  | -1.210497000 |
| H | -1.493991000 | 1.594296000  | 0.136051000  | H          | -4.996201001 | 2.330708000  | -0.849119000 |
| H | -0.013126000 | -0.927923000 | 1.949373000  | H          | -0.014463000 | -3.187391000 | 1.837267000  |
| H | 0.493321000  | 0.521732000  | 3.707885000  | H          | 0.337019000  | -1.191092000 | -0.176361000 |
| H | -0.397742000 | 1.818761000  | 2.897524000  | H          | 0.367631000  | -2.900515000 | -0.631825000 |
| H | 2.212718000  | 0.504354000  | 1.968026000  | H          | 1.832301000  | -2.659794000 | 3.366373000  |
| H | 2.006183000  | 2.181864000  | 2.481875000  | H          | 6.020601001  | -1.434274000 | -1.530530000 |
| H | 2.885175000  | 0.429073000  | -0.619813000 | H          | 4.244531001  | -1.862202000 | -3.233862000 |
| H | 4.828329001  | 1.949837000  | -0.516465000 | H          | 1.911864000  | -2.265941000 | -2.494287000 |
| H | 4.028822000  | 1.883013000  | 1.050015000  | H          | 5.447128001  | -1.474085000 | 0.894439000  |
| H | 3.809424000  | 3.295883000  | -0.001618000 |            |              |              |              |
| H | 2.611020000  | 2.969115000  | -2.312629000 | <b>TS6</b> |              |              |              |
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| H | 3.575715000  | 1.532828000  | -2.661977000 | C          | -0.741748000 | 0.486510000  | -1.841215000 |
| H | 1.740946000  | 4.043963000  | 0.111964000  | O          | -0.758785000 | 0.559818000  | -3.005659000 |
| H | -0.163995000 | 5.203778001  | 1.224821000  | N          | -0.567306000 | -0.023173000 | 1.961280000  |
| H | 0.518393000  | 3.967413000  | 2.280471000  | C          | 0.205365000  | 0.985734000  | 2.734028000  |
| H | -1.006421000 | 3.662241000  | 1.418090000  | C          | 1.472547000  | 1.393112000  | 1.985055000  |
| H | -1.003057000 | 3.549577000  | -1.167836000 | P          | 1.034714000  | 1.737843000  | 0.203309000  |
| H | 0.511401000  | 3.621728000  | -2.072119000 | C          | 2.698750000  | 1.542477000  | -0.657402000 |
| H | -0.076302000 | 5.059947001  | -1.230321000 | C          | 3.866804000  | 2.265019000  | 0.034177000  |
| H | -2.353663000 | 0.637994000  | 2.781598000  | C          | 2.650213000  | 1.896794000  | -2.153109000 |

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| C | 0.703012000  | 3.598642000  | 0.101413000  | H           | 0.471205000  | 4.014663000  | 2.253755000  |
| C | -0.065569000 | 4.152727000  | 1.310574000  | H           | -1.050015000 | 3.681210000  | 1.394787000  |
| C | -0.042546000 | 3.965158000  | -1.193762000 | H           | -1.045628000 | 3.530295000  | -1.187811000 |
| C | -1.851985000 | -0.319398000 | 2.644694000  | H           | 0.466918000  | 3.615254000  | -2.093927000 |
| C | -2.705908000 | -1.279369000 | 1.817688000  | H           | -0.141254000 | 5.054732001  | -1.268170000 |
| P | -2.739575000 | -0.653828000 | 0.056842000  | H           | -2.375559000 | 0.633058000  | 2.777588000  |
| C | -3.387461000 | -2.142704000 | -0.908717000 | H           | -1.666299000 | -0.732742000 | 3.647374000  |
| C | -2.389208000 | -3.309649000 | -0.914245000 | H           | -3.705037000 | -1.375775000 | 2.255315000  |
| C | -3.754358000 | -1.776669000 | -2.358134000 | H           | -2.254201000 | -2.276117000 | 1.817694000  |
| C | -4.214167001 | 0.533633000  | 0.125711000  | H           | -4.297589001 | -2.469219000 | -0.388779000 |
| C | -5.578935001 | -0.130326000 | 0.369883000  | H           | -2.853195000 | -4.189276001 | -1.374971000 |
| C | -4.272807001 | 1.509980000  | -1.060287000 | H           | -2.058121000 | -3.601122000 | 0.086357000  |
| N | 3.190715000  | -2.016080000 | 1.942851000  | H           | -1.504294000 | -3.056225000 | -1.504138000 |
| C | 1.989818000  | -2.458240000 | 2.304159000  | H           | -2.899661000 | -1.345460000 | -2.888836000 |
| C | 1.001490000  | -2.325419000 | 0.063983000  | H           | -4.580807001 | -1.065670000 | -2.416759000 |
| C | 0.905101000  | -2.693175000 | 1.448757000  | H           | -4.060071000 | -2.679198000 | -2.899934000 |
| C | 5.014050001  | -1.573774000 | -1.214829000 | H           | -3.959388000 | 1.129486000  | 1.012204000  |
| C | 4.005933000  | -1.794635000 | -2.175339000 | H           | -6.332531001 | 0.638098000  | 0.577631000  |
| C | 2.708099000  | -2.047994000 | -1.758585000 | H           | -5.573368001 | -0.816687000 | 1.222639000  |
| C | 4.716594001  | -1.624154000 | 0.135013000  | H           | -5.922288001 | -0.688444000 | -0.506759000 |
| C | 3.400417000  | -1.901784000 | 0.586402000  | H           | -4.563131001 | 1.013518000  | -1.990811000 |
| C | 2.379270000  | -2.098047000 | -0.390533000 | H           | -3.306664000 | 1.993511000  | -1.216508000 |
| H | -1.522318000 | 1.597155000  | 0.166809000  | H           | -5.018704001 | 2.288580000  | -0.861234000 |
| H | -0.009814000 | -0.894964000 | 1.969108000  | H           | 0.010632000  | -3.175515000 | 1.834463000  |
| H | 0.458178000  | 0.587124000  | 3.727539000  | H           | 0.279954000  | -1.088513000 | -0.195683000 |
| H | -0.448295000 | 1.849553000  | 2.880234000  | H           | 0.373740000  | -2.867294000 | -0.637878000 |
| H | 2.184993000  | 0.560239000  | 1.981256000  | H           | 1.869326000  | -2.671139000 | 3.369342000  |
| H | 1.958860000  | 2.237937000  | 2.482717000  | H           | 6.032225001  | -1.372579000 | -1.537917000 |
| H | 2.877789000  | 0.466243000  | -0.581401000 | H           | 4.244316001  | -1.764076000 | -3.234563000 |
| H | 4.800912001  | 2.019227000  | -0.483068000 | H           | 1.920734000  | -2.204004000 | -2.493390000 |
| H | 3.987706000  | 1.963264000  | 1.077801000  | H           | 5.481499001  | -1.475752000 | 0.891331000  |
| H | 3.755993000  | 3.354943000  | 0.003153000  |             |              |              |              |
| H | 2.575514000  | 2.978107000  | -2.309808000 | <b>cp10</b> |              |              |              |
| H | 1.817260000  | 1.415497000  | -2.671105000 | FE          | 1.397686545  | 0.108571787  | 0.177894552  |
| H | 3.575475000  | 1.560466000  | -2.633008000 | P           | 1.106471408  | 2.330253044  | -0.014297074 |
| H | 1.692481000  | 4.073111000  | 0.083316000  | P           | 1.717263584  | -2.097793912 | -0.105948031 |
| H | -0.224456000 | 5.229838001  | 1.182072000  | O           | 2.220799100  | 0.155355658  | 2.976870561  |

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|---|--------------|--------------|--------------|---|--------------|--------------|--------------|
| N | 0.235020526  | -0.023951896 | -1.322370735 | H | 2.143377304  | 4.360608926  | -0.861796987 |
| C | 1.891543319  | 0.138545322  | 1.856564751  | H | 3.821340467  | 3.396474208  | -2.460862284 |
| C | -0.251835704 | 2.411537722  | -1.280462303 | H | 2.177834601  | 2.874168751  | -2.841168480 |
| C | -0.180423405 | 1.135933597  | -2.125318181 | H | 3.287972391  | 1.763191268  | -2.019106689 |
| C | 0.122381576  | -1.227867898 | -2.159370472 | H | 4.521008274  | 3.990790748  | -0.166377853 |
| C | 0.407689188  | -2.503057318 | -1.359073859 | H | 4.098049317  | 2.378068134  | 0.437548261  |
| C | 2.525519712  | 3.341159638  | -0.722489205 | H | 3.443693058  | 3.824684379  | 1.221882367  |
| C | 2.972715526  | 2.808211463  | -2.092747024 | H | 1.377181343  | 3.524520865  | 2.053068486  |
| C | 3.710668913  | 3.385357977  | 0.255809253  | H | -0.891826750 | 3.316920759  | 3.072615704  |
| C | 0.496572348  | 3.407923000  | 1.408417482  | H | -0.218814148 | 1.741224416  | 2.635121281  |
| C | -0.583957615 | 2.687187693  | 2.229968632  | H | -1.480141227 | 2.475884730  | 1.637589657  |
| C | 0.018406592  | 4.805339733  | 0.979309218  | H | -0.271766988 | 5.386750551  | 1.861923869  |
| C | 3.343030596  | -2.659749236 | -0.866532635 | H | -0.859730768 | 4.744459496  | 0.327385202  |
| C | 3.610704695  | -1.974828217 | -2.215983907 | H | 0.790104415  | 5.374667006  | 0.453868283  |
| C | 4.513933294  | -2.425533686 | 0.101802303  | H | 3.244339583  | -3.737675080 | -1.047071211 |
| C | 1.455592532  | -3.345087343 | 1.284332725  | H | 4.572453523  | -2.314000093 | -2.618320154 |
| C | 0.200678727  | -3.008167808 | 2.106038569  | H | 3.654589862  | -0.887961647 | -2.099984557 |
| C | 1.428948009  | -4.812873033 | 0.825649107  | H | 2.843160688  | -2.209281145 | -2.958964264 |
| C | -6.267781360 | -0.242658025 | -0.324780243 | H | 5.450257347  | -2.764641929 | -0.356134523 |
| C | -5.056965090 | -0.389841460 | 0.356062147  | H | 4.395455083  | -2.968253326 | 1.044528674  |
| C | -3.862257698 | -0.422716445 | -0.397504304 | H | 4.615355215  | -1.360891460 | 0.334124770  |
| C | -3.922042887 | -0.328789623 | -1.797986169 | H | 2.325007487  | -3.200861458 | 1.938433994  |
| C | -5.143808761 | -0.193911736 | -2.450899347 | H | 0.106199071  | -3.708911781 | 2.943434718  |
| C | -6.329308452 | -0.145065771 | -1.715630496 | H | -0.714578903 | -3.087877068 | 1.509977581  |
| C | -5.037177019 | -0.536409347 | 1.871960970  | H | 0.247185283  | -1.998491266 | 2.518925854  |
| C | -3.642127024 | -0.401331791 | 2.428788564  | H | 1.316093801  | -5.471406647 | 1.694594361  |
| C | -2.562269885 | -0.423928358 | 1.635252462  | H | 2.343882744  | -5.112709711 | 0.307327418  |
| N | -2.632103014 | -0.545416299 | 0.250630895  | H | 0.582145104  | -5.008843189 | 0.158794292  |
| H | 2.843985596  | 0.315852286  | -0.109081455 | H | -7.187243596 | -0.208548206 | 0.256298335  |
| H | -1.196105764 | 2.429182785  | -0.725641449 | H | -2.999469863 | -0.365749543 | -2.370534865 |
| H | -0.212108599 | 3.314416022  | -1.898685520 | H | -5.166261424 | -0.123606256 | -3.534973836 |
| H | -1.165797294 | 0.955999913  | -2.586982139 | H | -7.286649125 | -0.035565290 | -2.215983198 |
| H | 0.516388051  | 1.283347604  | -2.968462319 | H | -5.470870538 | -1.511242282 | 2.156128321  |
| H | 0.814116621  | -1.161113426 | -3.017039720 | H | -5.707369105 | 0.211323869  | 2.322049298  |
| H | -0.885768943 | -1.298980297 | -2.602832588 | H | -3.510189789 | -0.316619417 | 3.502263575  |
| H | 0.673955811  | -3.342376914 | -2.010191131 | H | -1.552922237 | -0.354298240 | 2.024970034  |
| H | -0.487120519 | -2.788569900 | -0.795485690 | H | -1.773667761 | -0.367356784 | -0.268609109 |

**TS7**

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| FE | 0.970719098  | 0.387078286  | 0.080967505  |
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| O  | 2.261444842  | 1.337749555  | 2.518665600  |
| N  | 0.048520028  | -0.308307901 | -1.610665634 |
| C  | -0.592974293 | 0.695435084  | -2.483188970 |
| C  | -1.396344155 | 1.695369367  | -1.650288360 |
| P  | -0.367489929 | 2.202406114  | -0.184039931 |
| C  | -1.684191910 | 2.639524483  | 1.090853310  |
| C  | -2.750122746 | 3.624738586  | 0.584315063  |
| C  | -1.108571643 | 3.097737265  | 2.440423727  |
| C  | 0.441230732  | 3.837906676  | -0.658711486 |
| C  | 0.992293644  | 3.830919762  | -2.093780380 |
| C  | 1.556850365  | 4.233599455  | 0.324543895  |
| C  | 0.787158095  | -1.279090877 | -2.439241905 |
| C  | 1.453981743  | -2.329810615 | -1.551765742 |
| P  | 2.344988105  | -1.418228825 | -0.198003322 |
| C  | 2.696947506  | -2.739292382 | 1.100465959  |
| C  | 1.406864961  | -3.349688299 | 1.674583569  |
| C  | 3.582968724  | -2.204528347 | 2.238829690  |
| C  | 4.007803492  | -1.040169457 | -1.009846413 |
| C  | 4.886635587  | -2.276927449 | -1.258106517 |
| C  | 4.802170741  | 0.078256963  | -0.315751171 |
| C  | -5.356622758 | -1.743125379 | 0.558682915  |
| C  | -3.092785015 | -1.647128459 | -0.314279073 |
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| C  | -3.445698009 | -1.514829526 | 2.214243365  |
| C  | -2.029825450 | -0.987344945 | 2.209007449  |
| C  | -1.304857738 | -1.059671291 | 1.069165885  |
| N  | -1.723515445 | -1.472225120 | -0.160758202 |
| C  | -3.985442832 | -1.621373356 | 0.792205618  |
| H  | 1.992849540  | 1.155898435  | -0.664262415 |
| H  | -0.854371687 | -0.920331674 | -1.053167499 |
| H  | -1.262965701 | 0.197037917  | -3.201941482 |

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| H | 0.175415083  | 1.213860271  | -3.072030741 |
| H | -2.286692496 | 1.199771473  | -1.248992274 |
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| H | -2.334750514 | 4.622799471  | 0.405451323  |
| H | -0.687581182 | 4.106682607  | 2.381897296  |
| H | -0.332574076 | 2.424428897  | 2.812312489  |
| H | -1.909780018 | 3.125529583  | 3.187414002  |
| H | -0.357184166 | 4.589058886  | -0.604062277 |
| H | 1.454022596  | 4.800599429  | -2.313074551 |
| H | 0.214804059  | 3.662546615  | -2.843791536 |
| H | 1.761153778  | 3.060979255  | -2.213789257 |
| H | 2.398520661  | 3.538813380  | 0.253103741  |
| H | 1.224870280  | 4.248909604  | 1.364677859  |
| H | 1.926131121  | 5.235833541  | 0.077709356  |
| H | 1.538767657  | -0.753479816 | -3.047218811 |
| H | 0.102637800  | -1.773834896 | -3.146774595 |
| H | 2.112556696  | -2.987996581 | -2.127833169 |
| H | 0.679150128  | -2.944561654 | -1.085198821 |
| H | 3.244261550  | -3.533368371 | 0.575755604  |
| H | 1.669900919  | -4.145439636 | 2.380954837  |
| H | 0.765504146  | -3.791029235 | 0.907950720  |
| H | 0.809976642  | -2.610237939 | 2.215560571  |
| H | 3.108800832  | -1.363247922 | 2.753338999  |
| H | 4.564485419  | -1.875058196 | 1.889523551  |
| H | 3.747167436  | -2.995150922 | 2.979808625  |
| H | 3.685656182  | -0.647792596 | -1.983757798 |
| H | 5.738493286  | -2.004942780 | -1.891735177 |
| H | 4.349592355  | -3.085495305 | -1.763477690 |
| H | 5.293584918  | -2.675849193 | -0.323721014 |
| H | 5.183652196  | -0.231967470 | 0.661324350  |
| H | 4.189177570  | 0.970215348  | -0.173412652 |
| H | 5.667423545  | 0.351963933  | -0.930837239 |
| H | -6.034126007 | -1.713872803 | 1.410766398  |
| H | -2.940960530 | -1.869976954 | -2.449573504 |

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| H | -5.379528132 | -2.108729164 | -2.818571643 |
| H | -6.948358704 | -2.016298151 | -0.875887674 |
| H | -3.494875930 | -2.503665009 | 2.708664755  |
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| H | -1.578519782 | -0.633520168 | 3.130703807  |
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**cp11**

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| FE | 0.913099000  | 0.392604000  | 0.087791000  |
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| O  | 1.903129000  | 1.342907000  | 2.661215000  |
| N  | 0.215964000  | -0.271243000 | -1.753315000 |
| C  | -0.453970000 | 0.747115000  | -2.592480000 |
| C  | -1.462751000 | 1.537300000  | -1.760532000 |
| P  | -0.658563000 | 2.031608000  | -0.155098000 |
| C  | -2.138961000 | 2.175496000  | 0.997894000  |
| C  | -3.272420000 | 3.066059000  | 0.463951000  |
| C  | -1.761313000 | 2.567831000  | 2.435071000  |
| C  | -0.045681000 | 3.797017000  | -0.413865000 |
| C  | 0.636916000  | 3.997897000  | -1.776538000 |
| C  | 0.901983000  | 4.245330001  | 0.712322000  |
| C  | 1.144821000  | -1.078793000 | -2.570498000 |
| C  | 1.878810000  | -2.088965000 | -1.690004000 |
| P  | 2.562644000  | -1.163476000 | -0.226868000 |
| C  | 3.044622000  | -2.519451000 | 0.991020000  |
| C  | 1.843765000  | -3.381187000 | 1.418891000  |
| C  | 3.754307000  | -1.949437000 | 2.231724000  |
| C  | 4.188083001  | -0.479722000 | -0.905273000 |
| C  | 5.253244001  | -1.547848000 | -1.200109000 |
| C  | 4.769876001  | 0.674930000  | -0.073327000 |
| C  | -5.148349001 | -1.893420000 | 0.649693000  |
| C  | -2.951514000 | -1.816128000 | -0.396778000 |
| C  | -3.598495000 | -1.925695000 | -1.649154000 |
| C  | -4.983053001 | -2.014891000 | -1.747875000 |
| C  | -5.774584001 | -1.988763000 | -0.595693000 |
| C  | -3.102601000 | -1.819488000 | 2.153809000  |
| C  | -1.697161000 | -1.276117000 | 2.055872000  |

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| N | -1.574180000 | -1.666326000 | -0.357789000 |
| C | -3.759752000 | -1.824396000 | 0.777724000  |
| H | 1.846502000  | 1.355208000  | -0.556131000 |
| H | -0.569823000 | -0.929258000 | -1.368797000 |
| H | -0.967939000 | 0.260665000  | -3.435619000 |
| H | 0.309470000  | 1.409883000  | -3.014224000 |
| H | -2.303510000 | 0.886082000  | -1.498978000 |
| H | -1.856953000 | 2.390438000  | -2.321004000 |
| H | -2.488561000 | 1.136248000  | 1.028652000  |
| H | -4.135118000 | 2.998587000  | 1.136317000  |
| H | -3.613638000 | 2.764400000  | -0.530065000 |
| H | -2.980677000 | 4.121493000  | 0.420045000  |
| H | -1.463827000 | 3.619143000  | 2.506343000  |
| H | -0.951786000 | 1.951328000  | 2.833061000  |
| H | -2.630516000 | 2.432808000  | 3.088320000  |
| H | -0.944045000 | 4.426983001  | -0.388736000 |
| H | 0.970345000  | 5.038020001  | -1.868542000 |
| H | -0.031519000 | 3.794633000  | -2.617741000 |
| H | 1.518744000  | 3.356050000  | -1.870898000 |
| H | 1.831701000  | 3.669978000  | 0.686502000  |
| H | 0.467279000  | 4.131598000  | 1.707474000  |
| H | 1.157521000  | 5.303085001  | 0.579389000  |
| H | 1.857049000  | -0.405149000 | -3.064119000 |
| H | 0.594316000  | -1.603006000 | -3.365886000 |
| H | 2.645196000  | -2.629774000 | -2.254655000 |
| H | 1.157376000  | -2.817920000 | -1.309319000 |
| H | 3.751049000  | -3.164199000 | 0.452126000  |
| H | 2.194122000  | -4.173068000 | 2.090787000  |
| H | 1.344571000  | -3.866566000 | 0.576649000  |
| H | 1.091116000  | -2.798456000 | 1.957016000  |
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| H | 3.859690000  | -0.050040000 | -1.861268000 |
| H | 6.086999001  | -1.097620000 | -1.750749000 |
| H | 4.869420001  | -2.373125000 | -1.807921000 |



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| H | 4.023571000  | 1.451714000  | 0.104111000  |
| H | 5.612491001  | 1.126107000  | -0.610101000 |
| H | -5.755066001 | -1.888211000 | 1.554363000  |
| H | -2.979224000 | -1.942911000 | -2.543461000 |
| H | -5.447474001 | -2.100209000 | -2.727663000 |
| H | -6.856804001 | -2.051213000 | -0.664130000 |
| H | -3.103323000 | -2.843896000 | 2.575253000  |
| H | 0.029953000  | -1.094989000 | 0.862706000  |
| H | -1.169354000 | -0.954907000 | 2.948521000  |
| H | -3.708382000 | -1.228060000 | 2.856681000  |

# cp12

|    |              |              |              |
|----|--------------|--------------|--------------|
| FE | 0.156697548  | -0.755268937 | 0.142714815  |
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| O  | 0.242126120  | -2.464500185 | 2.498622688  |
| N  | 0.079136987  | 0.565964761  | -1.496007769 |
| C  | 1.316008392  | 0.596788702  | -2.324483523 |
| C  | 2.564564148  | 0.672479735  | -1.447055684 |
| P  | 2.395726728  | -0.541255910 | -0.038945295 |
| C  | 3.440209332  | 0.287492802  | 1.298186124  |
| C  | 4.873231840  | 0.648631141  | 0.874388992  |
| C  | 3.436048884  | -0.470511488 | 2.635978505  |
| C  | 3.397073188  | -2.056218089 | -0.562683255 |
| C  | 3.158835020  | -2.447190663 | -2.029943906 |
| C  | 3.113132183  | -3.261535576 | 0.349727474  |
| C  | -1.117341387 | 0.431287900  | -2.374825422 |
| C  | -2.387370208 | 0.195439841  | -1.560034561 |
| P  | -2.045206334 | -1.115275750 | -0.278235594 |
| C  | -3.383886606 | -0.799713381 | 1.004815036  |
| C  | -3.415312242 | -1.850246658 | 2.127358539  |
| C  | -4.787100208 | -0.581994273 | 0.415679641  |
| C  | -2.538526105 | -2.766103235 | -1.057942194 |
| C  | -1.943128832 | -3.955949877 | -0.284656836 |
| C  | -2.165780705 | -2.880249259 | -2.544361535 |
| C  | 1.200507442  | 3.481402497  | 0.337519692  |

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| C | -0.060460749 | 2.965703185  | 0.687955167  |
| C | -1.230686867 | 3.451328394  | 0.013394944  |
| C | -1.035975136 | 4.310845724  | -1.105872856 |
| C | 0.223325875  | 4.760863988  | -1.460462383 |
| C | 1.356732462  | 4.375008874  | -0.716455275 |
| C | -0.246427011 | 1.909173994  | 1.721300950  |
| C | -1.560058601 | 2.031316639  | 2.356461371  |
| C | -2.594907146 | 2.590440850  | 1.638044495  |
| N | -2.504383806 | 3.184226615  | 0.425947048  |
| H | 0.364181279  | -1.927908711 | -0.786475944 |
| H | 1.284304832  | 1.449248514  | -3.016969943 |
| H | 1.323195261  | -0.319541092 | -2.920702931 |
| H | 2.633561029  | 1.670037468  | -1.003740780 |
| H | 3.466496454  | 0.515091115  | -2.046540188 |
| H | 2.887063943  | 1.222095181  | 1.453405861  |
| H | 5.351741576  | 1.247322890  | 1.658066161  |
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# TS9

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| N | -1.293483253 | -0.138196519 | 1.136647108  |
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| C | 4.464690612  | -0.842242579 | 0.523544094  |
| C | 3.159526559  | -0.895715471 | 0.010048879  |
| C | 2.538696320  | 0.265368825  | -0.502724499 |

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|---|--------------|--------------|--------------|
| C | 3.268134429  | 1.465149341  | -0.501368270 |
| C | 4.561222228  | 1.519769546  | 0.001054546  |
| C | 1.131461888  | 0.203412290  | -0.982589109 |
| C | 0.606582186  | -1.152725108 | -1.180474939 |
| C | 1.269396916  | -2.228868039 | -0.679549704 |
| N | 2.468706777  | -2.105584768 | -0.036805995 |
| H | -5.220226074 | -2.382177405 | 0.463106455  |
| H | -2.938230733 | -2.199496292 | 1.418788139  |
| H | -4.787406559 | 1.512488399  | -1.309095827 |
| H | -6.145545230 | -0.516572867 | -0.899585866 |
| H | -1.676015607 | 1.890995044  | -1.410576196 |
| H | -0.447951537 | 2.993547092  | 0.405535068  |
| H | 0.315707382  | 0.983102893  | 1.761513327  |
| H | -1.714298854 | 2.626724199  | 1.570484330  |
| H | -2.825057585 | 2.923991268  | -0.583871147 |
| H | 6.166193029  | 0.397488399  | 0.914338903  |
| H | 4.929853425  | -1.744720747 | 0.910646581  |
| H | 2.806030714  | 2.361462528  | -0.906748361 |
| H | 5.110708443  | 2.454826041  | -0.009168825 |
| H | 0.431390031  | 0.710438199  | -0.118656499 |
| H | -0.926607274 | -0.963378990 | 1.593974640  |
| H | 0.898833964  | -3.241898748 | -0.790015445 |
| H | 2.956612776  | -2.941363541 | 0.252490074  |
| H | -0.317320705 | -1.306708154 | -1.724065577 |
| H | 0.919752574  | 0.898722128  | -1.802250838 |

#### TS13

|   |             |              |              |
|---|-------------|--------------|--------------|
| C | 2.485423828 | 2.863062506  | -0.019823521 |
| C | 3.315729359 | 1.850877072  | -0.475332588 |
| C | 3.027812763 | 0.516676772  | -0.144036358 |
| C | 1.889241055 | 0.194612206  | 0.639312942  |
| C | 1.070366445 | 1.249549190  | 1.089923647  |
| C | 1.361734227 | 2.566507667  | 0.771049593  |
| C | 1.589067243 | -1.208048061 | 0.924076077  |
| C | 2.622787974 | -2.166862978 | 0.623890528  |
| C | 3.701445390 | -1.798490279 | -0.125630734 |
| N | 3.871890465 | -0.510240654 | -0.540747079 |

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|---|--------------|--------------|--------------|
| C | -4.546675459 | 1.077527046  | 0.430595410  |
| C | -4.193328233 | -0.247899734 | 0.632068271  |
| C | -2.987680334 | -0.757952759 | 0.115777020  |
| C | -2.138746783 | 0.113348838  | -0.616629511 |
| C | -2.501856615 | 1.452367611  | -0.825238958 |
| C | -3.698571774 | 1.923773601  | -0.303057474 |
| C | -2.588243369 | -2.135659448 | 0.257381119  |
| C | -0.451854415 | -1.656154779 | -0.834036124 |
| C | -1.399435988 | -2.580259040 | -0.219796245 |
| N | -0.967309589 | -0.400418010 | -1.148482299 |
| H | 2.714906360  | 3.893881516  | -0.269201801 |
| H | 4.194108574  | 2.082842111  | -1.070973967 |
| H | 0.203710171  | 1.014956099  | 1.701064740  |
| H | 0.727780600  | 3.367931496  | 1.134604463  |
| H | 0.970062273  | -1.399620268 | 1.802767199  |
| H | 2.538506657  | -3.191866624 | 0.963196926  |
| H | 4.484305753  | -2.492916747 | -0.406623311 |
| H | 4.709156574  | -0.268249554 | -1.053075391 |
| H | -5.478508837 | 1.460308959  | 0.832084688  |
| H | -4.846616438 | -0.912383504 | 1.189661208  |
| H | -1.848535606 | 2.109173906  | -1.392681440 |
| H | -3.979264024 | 2.959317267  | -0.465772003 |
| H | 0.519114342  | -1.500804510 | 0.053621535  |
| H | -3.275193496 | -2.825810514 | 0.738525507  |
| H | -1.101988512 | -3.618210563 | -0.120508572 |
| H | 0.200942647  | -2.061915182 | -1.613383096 |
| H | -0.407845144 | 0.216124216  | -1.721659536 |

#### TS15

|   |             |              |              |
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| C | 3.572188000 | -0.618310000 | 0.245586000  |
| C | 2.548846000 | 0.319834000  | 0.102399000  |
| C | 1.223484000 | -0.126539000 | -0.205207000 |
| C | 1.022972000 | -1.528446000 | -0.337999000 |
| C | 2.060609000 | -2.436762000 | -0.180243000 |
| C | 3.357567000 | -1.993925000 | 0.112617000  |
| C | 2.841733000 | 1.805522000  | 0.293970000  |
| C | 1.632746000 | 2.634027000  | -0.062554000 |

|   |              |              |              |
|---|--------------|--------------|--------------|
| C | 0.439754000  | 2.051594000  | -0.344319000 |
| N | 0.154802000  | 0.712175000  | -0.393951000 |
| C | -3.127578000 | -0.196996000 | 0.083004000  |
| C | -3.433765000 | 1.306992000  | 0.254332000  |
| C | -2.518183000 | -0.750747000 | 1.387962000  |
| C | -4.429528001 | -0.968725000 | -0.277030000 |
| O | -2.234046000 | -0.385610000 | -0.994608000 |
| H | 4.576217001  | -0.255632000 | 0.474387000  |
| H | 0.017700000  | -1.862499000 | -0.581197000 |
| H | 1.860631000  | -3.502146000 | -0.292168000 |
| H | 4.177328000  | -2.698582000 | 0.234036000  |
| H | 3.723312000  | 2.092851000  | -0.312586000 |
| H | 3.168749000  | 1.993338000  | 1.339108000  |
| H | 1.720841000  | 3.718853000  | -0.067401000 |
| H | -0.413383000 | 2.696546000  | -0.574221000 |
| H | -1.343084000 | 0.065939000  | -0.781054000 |
| H | -3.827134000 | 1.711388000  | -0.685127000 |
| H | -2.517525000 | 1.851359000  | 0.502909000  |
| H | -4.172054000 | 1.489863000  | 1.047045000  |
| H | -1.574999000 | -0.240013000 | 1.602557000  |
| H | -2.304370000 | -1.818866000 | 1.272642000  |
| H | -3.197609000 | -0.623842000 | 2.241983000  |
| H | -4.289202001 | -1.433773000 | -1.255828000 |
| H | -5.304980001 | -0.311039000 | -0.333217000 |
| H | -4.656745001 | -1.759207000 | 0.447538000  |

#### TS16

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| C | 3.337757000 | 0.958519000  | -1.319924000 |
| C | 2.736814000 | -0.171815000 | -0.762797000 |
| C | 3.237991000 | -0.691233000 | 0.459548000  |
| C | 4.335186001 | -0.048677000 | 1.063585000  |
| C | 4.926162001 | 1.074832000  | 0.489935000  |
| C | 4.426076001 | 1.589507000  | -0.708818000 |
| C | 1.604943000 | -0.905371000 | -1.463406000 |
| C | 0.788143000 | -1.713550000 | -0.453594000 |
| C | 1.561889000 | -2.252574000 | 0.633303000  |
| N | 2.696308000 | -1.807060000 | 1.113209000  |

|   |              |              |              |
|---|--------------|--------------|--------------|
| C | -4.756286001 | 0.624857000  | -0.076707000 |
| C | -3.408885000 | 0.917766000  | 0.136103000  |
| C | -2.458478000 | -0.148053000 | 0.153714000  |
| C | -2.944256000 | -1.468155000 | -0.027160000 |
| C | -4.293766001 | -1.727336000 | -0.232896000 |
| C | -5.221148001 | -0.680401000 | -0.264658000 |
| C | -2.967309000 | 2.359076000  | 0.373287000  |
| C | -1.463661000 | 2.463081000  | 0.440743000  |
| C | -0.680189000 | 1.362573000  | 0.428336000  |
| N | -1.114147000 | 0.061321000  | 0.336438000  |
| H | 2.941133000  | 1.354763000  | -2.254054000 |
| H | 4.698631001  | -0.461402000 | 2.000902000  |
| H | 5.771471001  | 1.553449000  | 0.980654000  |
| H | 4.872470001  | 2.471659000  | -1.161788000 |
| H | 2.039547000  | -1.552529000 | -2.249204000 |
| H | 0.965203000  | -0.185244000 | -1.992544000 |
| H | -0.174639000 | -0.862683000 | 0.050248000  |
| H | 0.136295000  | -2.460684000 | -0.919674000 |
| H | 1.127531000  | -3.093803000 | 1.187085000  |
| H | -5.467775001 | 1.451576000  | -0.091096000 |
| H | -2.227929000 | -2.284252000 | -0.000811000 |
| H | -4.625504001 | -2.755427000 | -0.369529000 |
| H | -6.278725001 | -0.874453000 | -0.425624000 |
| H | -3.437391000 | 2.744632000  | 1.300359000  |
| H | -3.376356000 | 3.007606000  | -0.423972000 |
| H | -1.009312000 | 3.447532000  | 0.520827000  |
| H | 0.404309000  | 1.461160000  | 0.489124000  |

# **Np\_cp6**

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| FE | -1.566877761 | -0.332069347 | 0.200450987  |
| P  | -0.500172213 | -2.299767745 | 0.209093836  |
| P  | -2.596735030 | 1.600671312  | -0.246515863 |
| O  | -2.289320251 | -0.379529450 | 3.025928592  |
| N  | -0.490413333 | 0.069997370  | -1.294033449 |
| C  | -2.002924499 | -0.363042655 | 1.892737968  |
| C  | 0.873201387  | -1.992920694 | -1.003505704 |
| C  | 0.412772274  | -0.881190806 | -1.953612532 |

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| C | -1.486347500 | 2.338119335  | -1.542939916 |
| C | -1.411080776 | -3.804353356 | -0.454629138 |
| C | -1.984493904 | -3.532388970 | -1.853946007 |
| C | -2.519704798 | -4.252741465 | 0.511047779  |
| C | 0.350115484  | -2.955764987 | 1.757360468  |
| C | 1.194539897  | -1.859893925 | 2.429945546  |
| C | 1.180984769  | -4.231109820 | 1.542378962  |
| C | -4.304660756 | 1.551293128  | -1.029600850 |
| C | -4.309375210 | 0.692626138  | -2.303753167 |
| C | -5.354180659 | 1.046500329  | -0.026751994 |
| C | -2.762680788 | 2.940424400  | 1.070560547  |
| C | -1.425813297 | 3.163388895  | 1.798974614  |
| C | -3.339880188 | 4.272456303  | 0.564526913  |
| C | 6.289923343  | 0.057649746  | -0.465736580 |
| C | 5.271499039  | 0.800910437  | 0.149811991  |
| C | 4.166148099  | 1.212433530  | -0.618013801 |
| C | 4.120510711  | 0.871289841  | -1.978694511 |
| C | 5.136316583  | 0.132096470  | -2.579362710 |
| C | 6.230889680  | -0.279923111 | -1.815186893 |
| C | 5.372178233  | 1.127743641  | 1.630609072  |
| C | 4.453383592  | 2.278635532  | 2.058441548  |
| C | 3.038297104  | 2.053488801  | 1.515659794  |
| C | 3.042694443  | 2.044008007  | -0.018677943 |
| H | -2.857203056 | -1.058222907 | -0.007551424 |
| H | 1.737855030  | -1.647217662 | -0.428280805 |
| H | 1.176393910  | -2.895076746 | -1.545682000 |
| H | 1.300179290  | -0.356230877 | -2.344340006 |
| H | -0.080524946 | -1.326055077 | -2.836651245 |
| H | -1.284464834 | 0.842276971  | -3.102546119 |
| H | 0.234182696  | 1.570887198  | -2.602351423 |
| H | -2.027619295 | 2.951095264  | -2.271726433 |
| H | -0.780204821 | 2.992435604  | -1.021828320 |
| H | -0.668067748 | -4.607718360 | -0.539422063 |
| H | -2.532836341 | -4.412808220 | -2.209363670 |
| H | -1.201402751 | -3.314098193 | -2.585720755 |
| H | -2.673922565 | -2.683741804 | -1.830402949 |

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| H | -3.043416177 | -5.124221502 | 0.101420248  |
| H | -3.252967755 | -3.452824758 | 0.655066272  |
| H | -2.130562880 | -4.536286514 | 1.494009046  |
| H | -0.481384521 | -3.188920923 | 2.435055337  |
| H | 1.588377096  | -2.228135372 | 3.384226417  |
| H | 0.608733909  | -0.959894354 | 2.630248148  |
| H | 2.053134654  | -1.574898084 | 1.811691552  |
| H | 1.628278560  | -4.550680721 | 2.490961051  |
| H | 2.002426665  | -4.059756148 | 0.837558204  |
| H | 0.582909955  | -5.066110766 | 1.167169561  |
| H | -4.548505962 | 2.583657658  | -1.311247582 |
| H | -5.316000856 | 0.677025535  | -2.737929396 |
| H | -4.017135693 | -0.337259553 | -2.079531077 |
| H | -3.627572101 | 1.081284896  | -3.065852192 |
| H | -6.341903817 | 1.013006166  | -0.501019617 |
| H | -5.436024179 | 1.690106564  | 0.854805866  |
| H | -5.105793278 | 0.036225785  | 0.313401337  |
| H | -3.463043388 | 2.509583472  | 1.797679405  |
| H | -1.571140108 | 3.851362753  | 2.639705636  |
| H | -0.675636096 | 3.611489936  | 1.137814705  |
| H | -1.013994579 | 2.230561940  | 2.191035704  |
| H | -3.400363124 | 4.991887119  | 1.389538796  |
| H | -4.346549539 | 4.165435801  | 0.151224769  |
| H | -2.702971990 | 4.716965142  | -0.208425362 |
| H | 7.144360044  | -0.256574578 | 0.130323179  |
| H | 3.270828352  | 1.200007640  | -2.573538180 |
| H | 5.076269144  | -0.119796085 | -3.634550204 |
| H | 7.033347494  | -0.854710106 | -2.269166407 |
| H | 6.415038196  | 1.352732747  | 1.885119380  |
| H | 4.845354076  | 3.229025782  | 1.670799202  |
| H | 2.351148186  | 2.825652131  | 1.879762817  |
| H | 5.109756861  | 0.230628863  | 2.211324948  |
| H | 4.444489587  | 2.362475733  | 3.151131118  |
| H | 2.656801800  | 1.093847923  | 1.889678705  |
| H | 2.077730584  | 1.681850508  | -0.393859280 |
| H | 3.143890898  | 3.078102539  | -0.381247895 |

# Np\_TS3

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| O  | 1.823280000  | 1.328759000  | 2.751750000  |
| N  | 0.124965000  | -0.476716000 | -1.528561000 |
| C  | -0.603390000 | 0.437552000  | -2.444386000 |
| C  | -1.575308000 | 1.316032000  | -1.660769000 |
| P  | -0.722112000 | 1.924059000  | -0.117491000 |
| C  | -2.200955000 | 2.154145000  | 1.038389000  |
| C  | -3.266023000 | 3.141488000  | 0.532215000  |
| C  | -1.805447000 | 2.467400000  | 2.490289000  |
| C  | -0.159771000 | 3.681935000  | -0.520523000 |
| C  | 0.514081000  | 3.791204000  | -1.897377000 |
| C  | 0.770628000  | 4.243275001  | 0.567607000  |
| C  | 0.994008000  | -1.371761000 | -2.335256000 |
| C  | 1.935515000  | -2.180847000 | -1.442661000 |
| P  | 2.687117000  | -0.998639000 | -0.215840000 |
| C  | 3.524799000  | -2.122451000 | 1.045623000  |
| C  | 2.506089000  | -2.979816000 | 1.813045000  |
| C  | 4.394888001  | -1.330784000 | 2.038185000  |
| C  | 4.105042000  | -0.256148000 | -1.224592000 |
| C  | 5.228610001  | -1.245041000 | -1.576394000 |
| C  | 4.674219001  | 1.047114000  | -0.639256000 |
| C  | -5.213378001 | -1.482403000 | 0.523993000  |
| C  | -3.861482000 | -1.797644000 | 0.677827000  |
| C  | -3.031245000 | -1.979085000 | -0.463333000 |
| C  | -3.651954000 | -1.904027000 | -1.732074000 |
| C  | -5.007852001 | -1.619562000 | -1.870822000 |
| C  | -5.797931001 | -1.383338000 | -0.741335000 |
| C  | -3.257771000 | -2.079017000 | 2.035642000  |
| C  | -1.837113000 | -1.518540000 | 2.150861000  |
| C  | -0.936521000 | -1.990703000 | 0.984464000  |
| C  | -1.603504000 | -2.256635000 | -0.307222000 |
| H  | 1.722434000  | 1.389237000  | -0.572249000 |
| H  | -0.683523000 | -1.176185000 | -1.107930000 |
| H  | -1.155756000 | -0.147216000 | -3.195559000 |
| H  | 0.130590000  | 1.050290000  | -2.978600000 |

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|---|--------------|--------------|--------------|
| H | -2.428693000 | 0.710835000  | -1.337539000 |
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| H | -2.649736000 | 1.153304000  | 1.021375000  |
| H | -4.160287000 | 3.070313000  | 1.161839000  |
| H | -3.575473000 | 2.934757000  | -0.496344000 |
| H | -2.918531000 | 4.178690000  | 0.583469000  |
| H | -1.417904000 | 3.485984000  | 2.592821000  |
| H | -1.047109000 | 1.779176000  | 2.871536000  |
| H | -2.685727000 | 2.390631000  | 3.138936000  |
| H | -1.074544000 | 4.286192001  | -0.546778000 |
| H | 0.814905000  | 4.830311001  | -2.075384000 |
| H | -0.151837000 | 3.500782000  | -2.715026000 |
| H | 1.412443000  | 3.168372000  | -1.945064000 |
| H | 1.698691000  | 3.666801000  | 0.614523000  |
| H | 0.317818000  | 4.229384001  | 1.561970000  |
| H | 1.028201000  | 5.283328001  | 0.335261000  |
| H | 1.572037000  | -0.761703000 | -3.040329000 |
| H | 0.368341000  | -2.049260000 | -2.935847000 |
| H | 2.677198000  | -2.719932000 | -2.041718000 |
| H | 1.361573000  | -2.922503000 | -0.879210000 |
| H | 4.174094000  | -2.796018000 | 0.471002000  |
| H | 3.035148000  | -3.641301000 | 2.508734000  |
| H | 1.904954000  | -3.611874000 | 1.154358000  |
| H | 1.825176000  | -2.354660000 | 2.398246000  |
| H | 3.806699000  | -0.581187000 | 2.576026000  |
| H | 5.229203001  | -0.821024000 | 1.551345000  |
| H | 4.819487001  | -2.015179000 | 2.781722000  |
| H | 3.586099000  | 0.015388000  | -2.153677000 |
| H | 5.905460001  | -0.791529000 | -2.309662000 |
| H | 4.854252001  | -2.176619000 | -2.011936000 |
| H | 5.830463001  | -1.502425000 | -0.699121000 |
| H | 5.245462001  | 0.873398000  | 0.277300000  |
| H | 3.877633000  | 1.759434000  | -0.414379000 |
| H | 5.355155001  | 1.509065000  | -1.363826000 |
| H | -0.131057000 | -1.118931000 | 0.889694000  |
| H | -5.826758001 | -1.344909000 | 1.413232000  |
| H | -3.043355000 | -2.070680000 | -2.619637000 |

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| H | -5.448560001 | -1.568794000 | -2.863849000 |
| H | -6.851830001 | -1.140760000 | -0.843366000 |
| H | -3.222236000 | -3.169936000 | 2.183674000  |
| H | -3.894398000 | -1.679303000 | 2.834199000  |
| H | -1.891402000 | -0.427128000 | 2.155106000  |
| H | -1.382998000 | -1.803359000 | 3.108232000  |
| H | -0.296355000 | -2.819110000 | 1.301698000  |
| H | -1.235884000 | -3.117425000 | -0.869429000 |

# **Np\_cp7**

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| FE | 0.886022313  | 0.347441025  | 0.149716979  |
| C  | 1.353107563  | 0.875718152  | 1.747848199  |
| O  | 1.668638932  | 1.223853615  | 2.816503217  |
| N  | 0.178513864  | -0.450442679 | -1.639602805 |
| C  | -0.576722426 | 0.493618814  | -2.505034895 |
| C  | -1.610942971 | 1.257964856  | -1.684884529 |
| P  | -0.820232838 | 1.837014524  | -0.095235664 |
| C  | -2.335340960 | 1.951043430  | 1.029193701  |
| C  | -3.480536266 | 2.824108908  | 0.489441086  |
| C  | -1.990369346 | 2.334179241  | 2.477469752  |
| C  | -0.341191909 | 3.639206142  | -0.408448520 |
| C  | 0.323960156  | 3.854500365  | -1.777185910 |
| C  | 0.570799417  | 4.182030707  | 0.704829542  |
| C  | 1.158689314  | -1.211032762 | -2.459555719 |
| C  | 2.107896758  | -2.022093999 | -1.577736399 |
| P  | 2.736135555  | -0.890459849 | -0.234713981 |
| C  | 3.604480060  | -2.060087225 | 0.965395381  |
| C  | 2.633009811  | -3.052907924 | 1.622028895  |
| C  | 4.377489989  | -1.294134787 | 2.054136286  |
| C  | 4.150776682  | 0.000670145  | -1.126326611 |
| C  | 5.347912981  | -0.889490799 | -1.498580945 |
| C  | 4.612005165  | 1.287312039  | -0.422301469 |
| C  | -5.078829874 | -1.375839927 | 0.524540030  |
| C  | -3.755691954 | -1.787356131 | 0.677456026  |
| C  | -2.956792474 | -2.083602671 | -0.467712964 |
| C  | -3.590834215 | -2.027616639 | -1.733780367 |
| C  | -4.920939978 | -1.638277529 | -1.865893824 |

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| C | -5.671945415 | -1.283905229 | -0.739987279 |
| C | -3.152448468 | -2.096812744 | 2.028799466  |
| C | -1.686261479 | -1.658675937 | 2.137934126  |
| C | -0.846259536 | -2.095823294 | 0.908767209  |
| C | -1.577491576 | -2.459182417 | -0.280841288 |
| H | 1.644663283  | 1.441911263  | -0.562203011 |
| H | -0.523465986 | -1.150269939 | -1.280957740 |
| H | -1.070956562 | -0.055007833 | -3.320502361 |
| H | 0.147480361  | 1.178883804  | -2.954406092 |
| H | -2.427409550 | 0.581794937  | -1.409882302 |
| H | -2.043214618 | 2.075265228  | -2.270414371 |
| H | -2.689954659 | 0.913298684  | 1.028667297  |
| H | -4.359848355 | 2.711109182  | 1.133860499  |
| H | -3.783486664 | 2.540865019  | -0.522249211 |
| H | -3.219567685 | 3.887902361  | 0.485015936  |
| H | -1.738842416 | 3.396160988  | 2.562592530  |
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| H | -2.857146402 | 2.156276501  | 3.124301146  |
| H | -1.282353423 | 4.202630017  | -0.399712910 |
| H | 0.584318032  | 4.912886587  | -1.895192523 |
| H | -0.331138858 | 3.586575092  | -2.611388983 |
| H | 1.245769750  | 3.270243950  | -1.856774845 |
| H | 1.527958952  | 3.653388414  | 0.705465735  |
| H | 0.133924561  | 4.082150130  | 1.701077059  |
| H | 0.770030340  | 5.246716627  | 0.534602456  |
| H | 1.723981935  | -0.486478558 | -3.055659878 |
| H | 0.630028267  | -1.868659012 | -3.164953343 |
| H | 2.905648353  | -2.471247107 | -2.178850663 |
| H | 1.558156311  | -2.835693471 | -1.095361142 |
| H | 4.321950270  | -2.631642640 | 0.362768178  |
| H | 3.191633194  | -3.729928162 | 2.278713173  |
| H | 2.101326497  | -3.672748867 | 0.894896130  |
| H | 1.891222040  | -2.532387689 | 2.234758541  |
| H | 3.717512828  | -0.631590890 | 2.622032998  |
| H | 5.192113186  | -0.691625094 | 1.646753347  |
| H | 4.820474788  | -2.006142858 | 2.759984949  |
| H | 3.653773072  | 0.311411526  | -2.055089392 |

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| H | 6.025165559  | -0.341206495 | -2.163554145 |
| H | 5.052352735  | -1.805991739 | -2.019252583 |
| H | 5.927367670  | -1.178055928 | -0.615749902 |
| H | 5.161406791  | 1.078452973  | 0.499981081  |
| H | 3.761299955  | 1.926016597  | -0.176206861 |
| H | 5.285520483  | 1.847223210  | -1.081895534 |
| H | -0.094686481 | -1.085650336 | 0.755833436  |
| H | -5.668980595 | -1.157450585 | 1.413330594  |
| H | -3.014574866 | -2.289365564 | -2.620114514 |
| H | -5.373360256 | -1.600514262 | -2.854295869 |
| H | -6.704806842 | -0.963967318 | -0.841572197 |
| H | -3.202183295 | -3.186951507 | 2.176810246  |
| H | -3.744871390 | -1.646187371 | 2.834148439  |
| H | -1.640751908 | -0.571986440 | 2.243414522  |
| H | -1.239278796 | -2.070107890 | 3.051194973  |
| H | -0.071106172 | -2.816229283 | 1.171920745  |
| H | -1.120412603 | -3.131019937 | -1.005640848 |

#### Np\_TS4

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| FE | 0.892743570  | 0.345564184  | 0.142112954  |
| C  | 1.313582184  | 0.795704526  | 1.772772632  |
| O  | 1.589968786  | 1.081404236  | 2.871236227  |
| N  | 0.237089052  | -0.372098337 | -1.714501867 |
| C  | -0.489736388 | 0.622790766  | -2.544815738 |
| C  | -1.555033246 | 1.329926472  | -1.711589885 |
| P  | -0.816104601 | 1.820474303  | -0.067537504 |
| C  | -2.360269461 | 1.830631273  | 1.020811834  |
| C  | -3.535713842 | 2.661676224  | 0.480004168  |
| C  | -2.063511455 | 2.189890226  | 2.485743011  |
| C  | -0.370583907 | 3.650573054  | -0.242383513 |
| C  | 0.281900598  | 3.983803363  | -1.593140255 |
| C  | 0.542608507  | 4.115476793  | 0.904791555  |
| C  | 1.247564147  | -1.089716384 | -2.534862872 |
| C  | 2.168179406  | -1.940353335 | -1.658691045 |
| P  | 2.753616457  | -0.863169440 | -0.250653337 |
| C  | 3.599620247  | -2.077813670 | 0.921295416  |
| C  | 2.621286170  | -3.104080621 | 1.511607002  |

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|---|--------------|--------------|--------------|---------------|--------------|--------------|--------------|
| C | 4.335325044  | -1.350097869 | 2.060696816  | H             | 1.604219417  | -2.774437969 | -1.229371883 |
| C | 4.192985337  | 0.058739979  | -1.072038067 | H             | 4.338289758  | -2.618132619 | 0.315730044  |
| C | 5.404379977  | -0.814357846 | -1.438281242 | H             | 3.166627961  | -3.798116042 | 2.161638525  |
| C | 4.628410133  | 1.324740448  | -0.316220586 | H             | 2.121685333  | -3.703547821 | 0.745523873  |
| C | -5.081410273 | -1.390677341 | 0.551458035  | H             | 1.854409434  | -2.613011154 | 2.117727936  |
| C | -3.760226609 | -1.824256982 | 0.648327250  | H             | 3.648753955  | -0.733447249 | 2.648395580  |
| C | -2.992660049 | -2.047521774 | -0.531295602 | H             | 5.140349166  | -0.707282092 | 1.698543545  |
| C | -3.642547863 | -1.889585015 | -1.776985336 | H             | 4.784348049  | -2.085775435 | 2.737963433  |
| C | -4.970567118 | -1.475465811 | -1.856116342 | H             | 3.721775323  | 0.397504764  | -2.004354229 |
| C | -5.695036318 | -1.201102390 | -0.692445282 | H             | 6.097720171  | -0.242582141 | -2.065973790 |
| C | -3.123665922 | -2.215656410 | 1.963144227  | H             | 5.128455209  | -1.715300210 | -1.995642600 |
| C | -1.646555508 | -1.805411719 | 2.053684972  | H             | 5.960185428  | -1.128532253 | -0.549042807 |
| C | -0.860301464 | -2.165933420 | 0.771822980  | H             | 5.159851767  | 1.089955657  | 0.610473997  |
| C | -1.613523857 | -2.460040281 | -0.393865926 | H             | 3.766367301  | 1.947523864  | -0.068621867 |
| H | 1.658812867  | 1.478796705  | -0.529908640 | H             | 5.311573708  | 1.911283224  | -0.942012997 |
| H | -0.463681727 | -1.076040995 | -1.403977851 | H             | -0.068705925 | -1.026764837 | 0.670122929  |
| H | -0.950513189 | 0.129767273  | -3.414302752 | H             | -5.652015392 | -1.226812714 | 1.464062544  |
| H | 0.249430324  | 1.337354022  | -2.917263534 | H             | -3.084697254 | -2.091349288 | -2.690124568 |
| H | -2.372323785 | 0.633102145  | -1.497265527 | H             | -5.440231824 | -1.357870717 | -2.829801313 |
| H | -1.979816784 | 2.175235336  | -2.261271854 | H             | -6.726242956 | -0.865137560 | -0.749903818 |
| H | -2.662021565 | 0.777201456  | 0.986724945  | H             | -3.188561644 | -3.311039740 | 2.053361126  |
| H | -4.417914916 | 2.498324285  | 1.109590902  | H             | -3.685371930 | -1.799678006 | 2.807811574  |
| H | -3.812598521 | 2.382536822  | -0.540098218 | H             | -1.577332738 | -0.731466921 | 2.242801835  |
| H | -3.322986493 | 3.736157697  | 0.496466878  | H             | -1.177701564 | -2.294825713 | 2.915806059  |
| H | -1.866564921 | 3.260399216  | 2.605433281  | H             | -0.019758288 | -2.833388784 | 0.945506645  |
| H | -1.205295404 | 1.642415699  | 2.883812129  | H             | -1.162942855 | -3.034757100 | -1.201804407 |
| H | -2.933149724 | 1.952222865  | 3.109272599  |               |              |              |              |
| H | -1.319882301 | 4.197513156  | -0.181730892 | <b>Np_cp8</b> |              |              |              |
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| H | -0.374289226 | 3.771874144  | -2.442470520 | C             | 2.961051910  | 0.305364134  | 1.072258332  |
| H | 1.212045236  | 3.422188955  | -1.722999878 | O             | 3.856464670  | 0.451627977  | 1.808309852  |
| H | 1.505924196  | 3.600652930  | 0.855332857  | N             | -0.056749133 | -0.207074495 | -1.319235694 |
| H | 0.115764868  | 3.927692111  | 1.892579177  | C             | -0.263568607 | 0.929624805  | -2.243623616 |
| H | 0.725570291  | 5.193309639  | 0.819980024  | C             | -0.262525032 | 2.243775172  | -1.465066028 |
| H | 1.831896054  | -0.333357507 | -3.069836778 | P             | 1.213225719  | 2.247928767  | -0.305389965 |
| H | 0.749950549  | -1.710942898 | -3.294033542 | C             | 0.521223674  | 3.277565284  | 1.121856050  |
| H | 2.984051149  | -2.363455758 | -2.254740804 | C             | 0.136839305  | 4.721679246  | 0.763953139  |

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| C | 1.388441219  | 3.226608708  | 2.389211813  | H | 1.809515862  | 2.965421885  | -3.247727935 |
| C | 2.441168141  | 3.386699668  | -1.180189770 | H | 3.104707648  | 1.915124002  | -2.642513412 |
| C | 2.709153984  | 2.934990482  | -2.624749649 | H | 4.233481491  | 2.496310496  | -0.312001653 |
| C | 3.767675389  | 3.481301598  | -0.407944930 | H | 3.642778134  | 3.892476472  | 0.596949402  |
| C | -0.006236134 | -1.495584517 | -2.043974992 | H | 4.466049665  | 4.133496905  | -0.945796682 |
| C | 0.271982481  | -2.635753478 | -1.066492155 | H | 0.805118691  | -1.415527509 | -2.774736424 |
| P | 1.749659709  | -2.145916401 | -0.022512078 | H | -0.941868373 | -1.671754309 | -2.597569023 |
| C | 1.555751027  | -3.221534525 | 1.516487178  | H | 0.427049305  | -3.576810718 | -1.604381652 |
| C | 0.282662844  | -2.874669723 | 2.304243249  | H | -0.589559763 | -2.777460808 | -0.405991603 |
| C | 2.785588797  | -3.103782488 | 2.434634271  | H | 1.476131045  | -4.260034439 | 1.168875389  |
| C | 3.151352870  | -2.952630576 | -1.007938820 | H | 0.218143427  | -3.508323043 | 3.196724638  |
| C | 3.187903766  | -4.488266818 | -0.970362073 | H | -0.631102205 | -3.039210141 | 1.724669924  |
| C | 4.529652057  | -2.346536413 | -0.700754101 | H | 0.295266398  | -1.827629749 | 2.619070956  |
| C | -6.866061997 | 0.338862494  | -0.032306024 | H | 2.938105604  | -2.070392296 | 2.760201779  |
| C | -5.585927747 | 0.199581980  | 0.502574374  | H | 3.705211733  | -3.441704247 | 1.950039878  |
| C | -4.772695370 | -0.876379565 | 0.078277628  | H | 2.641118269  | -3.719008436 | 3.330471712  |
| C | -5.275969426 | -1.790975696 | -0.857455180 | H | 2.891955729  | -2.640581710 | -2.029258839 |
| C | -6.559228979 | -1.642107807 | -1.383594662 | H | 3.908818336  | -4.863081299 | -1.706559005 |
| C | -7.355378422 | -0.572094239 | -0.973736809 | H | 2.219039555  | -4.942680903 | -1.203625580 |
| C | -5.057636001 | 1.115425358  | 1.588346102  | H | 3.504653502  | -4.861728199 | 0.008618957  |
| C | -3.537675994 | 1.323861262  | 1.495957254  | H | 4.880371216  | -2.604926272 | 0.303309429  |
| C | -2.815019431 | 0.015303468  | 1.274374481  | H | 4.499750747  | -1.258178014 | -0.783368378 |
| C | -3.412028535 | -0.994711433 | 0.617152380  | H | 5.270635909  | -2.728174124 | -1.413576375 |
| H | 2.508467756  | 0.075060121  | -1.297957704 | H | 0.608446101  | 0.069800702  | 1.198246538  |
| H | -1.201836311 | 0.809682641  | -2.807698108 | H | -7.492027216 | 1.166301753  | 0.294100684  |
| H | 0.565282847  | 0.909640737  | -2.956282448 | H | -4.650457356 | -2.621185965 | -1.177693140 |
| H | -1.167797345 | 2.310860655  | -0.849709066 | H | -6.934801560 | -2.357031491 | -2.110064850 |
| H | -0.271948182 | 3.099234058  | -2.148208658 | H | -8.354762630 | -0.446680643 | -1.380476343 |
| H | -0.397727062 | 2.719199028  | 1.345443159  | H | -5.284583491 | 0.657726148  | 2.563361329  |
| H | -0.418154429 | 5.178762918  | 1.591940685  | H | -5.581560131 | 2.076969845  | 1.567993425  |
| H | -0.496008923 | 4.781539452  | -0.127818795 | H | -3.303113817 | 2.011572516  | 0.666906480  |
| H | 1.021567774  | 5.343300357  | 0.590195670  | H | -3.172091317 | 1.813616751  | 2.405007551  |
| H | 2.321891434  | 3.785714335  | 2.271213857  | H | -1.787179893 | -0.078647725 | 1.619523184  |
| H | 1.637633367  | 2.198591298  | 2.659930654  | H | -0.848005322 | -0.237098052 | -0.674785772 |
| H | 0.845430045  | 3.678954934  | 3.227947129  | H | -2.881192120 | -1.928441884 | 0.440040740  |
| H | 1.978363204  | 4.381490620  | -1.212459037 |   |              |              |              |
| H | 3.447189891  | 3.600407583  | -3.088119627 |   |              |              |              |

SR\_TS4



|    |              |              |              |   |              |              |              |
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| FE | 0.816009000  | 0.431042000  | -0.115690000 | H | 3.947641000  | -4.131906000 | -1.766004000 |
| C  | 1.641437000  | 1.323161000  | -1.374112000 | H | 3.618744000  | -3.936835000 | -0.042081000 |
| O  | 2.209630000  | 1.940706000  | -2.184308000 | H | 4.895318001  | -2.986457000 | -0.820136000 |
| N  | -0.228955000 | -0.686237000 | 1.221720000  | H | 4.256433001  | -1.088123000 | -2.518956000 |
| C  | 0.550127000  | -1.601262000 | 2.091965000  | H | 2.551937000  | -0.814105000 | -2.899266000 |
| C  | 1.619566000  | -2.344141000 | 1.291575000  | H | 3.355523000  | -2.298192000 | -3.430076000 |
| P  | 2.420433000  | -1.143720000 | 0.109613000  | H | 4.648457001  | -1.608498000 | 0.948064000  |
| C  | 2.874930000  | -2.300130000 | -1.317286000 | H | 4.830428001  | 0.032048000  | 2.819750000  |
| C  | 3.889300000  | -3.397070000 | -0.954828000 | H | 3.410614000  | -0.996797000 | 3.014006000  |
| C  | 3.280398000  | -1.574552000 | -2.610037000 | H | 3.222421000  | 0.666892000  | 2.428670000  |
| C  | 4.053142000  | -0.687016000 | 0.931220000  | H | 4.243279001  | 1.311519000  | 0.075320000  |
| C  | 3.857601000  | -0.222760000 | 2.383537000  | H | 5.040336001  | 0.063677000  | -0.890338000 |
| C  | 4.816430001  | 0.381324000  | 0.130971000  | H | 5.770123001  | 0.602337000  | 0.624144000  |
| C  | -1.231794000 | 0.014999000  | 2.064500000  | H | -0.708529000 | 0.509960000  | 2.890741000  |
| C  | -2.022608000 | 1.032676000  | 1.245812000  | H | -1.922319000 | -0.718959000 | 2.505241000  |
| P  | -0.840956000 | 1.948852000  | 0.138491000  | H | -2.607951000 | 1.692844000  | 1.893383000  |
| C  | -1.962568000 | 2.430799000  | -1.302049000 | H | -2.727288000 | 0.504609000  | 0.595024000  |
| C  | -1.253106000 | 3.232760000  | -2.405683000 | H | -2.213490000 | 1.446845000  | -1.718488000 |
| C  | -3.274046000 | 3.118035000  | -0.886344000 | H | -1.895337000 | 3.284130000  | -3.292346000 |
| C  | -0.444108000 | 3.569847000  | 1.019377000  | H | -0.303687000 | 2.784162000  | -2.705974000 |
| C  | 0.758404000  | 4.282827001  | 0.376973000  | H | -1.058410000 | 4.263428001  | -2.091560000 |
| C  | -0.188581000 | 3.370833000  | 2.522090000  | H | -3.092876000 | 4.107816000  | -0.453476000 |
| C  | -3.599870000 | -3.194596000 | 0.504506000  | H | -3.846760000 | 2.529649000  | -0.164830000 |
| C  | -2.987670000 | -2.248568000 | -0.360201000 | H | -3.909100000 | 3.264505000  | -1.767745000 |
| C  | -3.856206000 | -1.285916000 | -0.934570000 | H | -1.334003000 | 4.202226001  | 0.905515000  |
| C  | -4.960487001 | -3.171027000 | 0.782628000  | H | 0.909428000  | 5.257362001  | 0.855990000  |
| C  | -5.793454001 | -2.199893000 | 0.212094000  | H | 0.631370000  | 4.455312001  | -0.693839000 |
| C  | -5.222967001 | -1.264121000 | -0.651393000 | H | 1.669153000  | 3.692954000  | 0.513379000  |
| C  | -1.545343000 | -2.286160000 | -0.576261000 | H | 0.654576000  | 2.692564000  | 2.687646000  |
| C  | -0.891896000 | -1.561883000 | -1.694329000 | H | -1.060640000 | 2.975072000  | 3.049879000  |
| H  | 1.555583000  | 1.209432000  | 0.918291000  | H | 0.062503000  | 4.333815001  | 2.981647000  |
| H  | -0.867272000 | -1.414314000 | 0.531457000  | H | -0.251781000 | -0.647595000 | -1.352180000 |
| H  | -0.126892000 | -2.327420000 | 2.568128000  | H | -2.975417000 | -3.962544000 | 0.957722000  |
| H  | 1.012053000  | -1.014889000 | 2.894358000  | H | -3.459683000 | -0.554448000 | -1.633822000 |
| H  | 1.148174000  | -3.123255000 | 0.683498000  | H | -5.380833001 | -3.921094000 | 1.449140000  |
| H  | 2.339141000  | -2.835564000 | 1.954482000  | H | -6.857152001 | -2.181576000 | 0.429634000  |
| H  | 1.909283000  | -2.785688000 | -1.510587000 | H | -5.849356001 | -0.509027000 | -1.121996000 |

|   |              |              |              |
|---|--------------|--------------|--------------|
| H | -1.109617000 | -3.264351000 | -0.361535000 |
| H | -1.576308000 | -1.110473000 | -2.420032000 |
| H | -0.170335000 | -2.166110000 | -2.251960000 |

# **SR\_cp7**

|    |              |              |              |
|----|--------------|--------------|--------------|
| FE | -0.801683000 | 0.446585000  | 0.109779000  |
| C  | -1.611777000 | 1.351447000  | 1.364835000  |
| O  | -2.164638000 | 1.971927000  | 2.183772000  |
| N  | 0.230871000  | -0.695703000 | -1.283732000 |
| C  | -0.612426000 | -1.553624000 | -2.156711000 |
| C  | -1.666378000 | -2.293703000 | -1.335208000 |
| P  | -2.432397000 | -1.096732000 | -0.121341000 |
| C  | -2.881530000 | -2.274182000 | 1.289797000  |
| C  | -3.908894000 | -3.357877000 | 0.924532000  |
| C  | -3.266496000 | -1.562184000 | 2.596372000  |
| C  | -4.074158000 | -0.612259000 | -0.911023000 |
| C  | -3.902394000 | -0.146927000 | -2.365847000 |
| C  | -4.798989001 | 0.468470000  | -0.091725000 |
| C  | 1.219704000  | 0.037628000  | -2.121102000 |
| C  | 2.039955000  | 1.006714000  | -1.274593000 |
| P  | 0.887178000  | 1.925775000  | -0.133202000 |
| C  | 2.040507000  | 2.346600000  | 1.301959000  |
| C  | 1.355984000  | 3.109111000  | 2.448153000  |
| C  | 3.350053000  | 3.039328000  | 0.889591000  |
| C  | 0.533488000  | 3.577851000  | -0.975429000 |
| C  | -0.642294000 | 4.307739001  | -0.303665000 |
| C  | 0.259754000  | 3.426945000  | -2.480327000 |
| C  | 3.495106000  | -3.278969000 | -0.458418000 |
| C  | 2.917840000  | -2.331538000 | 0.436461000  |
| C  | 3.810379000  | -1.345058000 | 0.944831000  |
| C  | 4.833807001  | -3.233988000 | -0.820952000 |
| C  | 5.685756001  | -2.241619000 | -0.316595000 |
| C  | 5.153382001  | -1.306252000 | 0.573870000  |
| C  | 1.522047000  | -2.409352000 | 0.773659000  |
| C  | 0.834838000  | -1.556171000 | 1.724189000  |
| H  | -1.508292000 | 1.231535000  | -0.966492000 |
| H  | 0.784759000  | -1.359023000 | -0.665256000 |

|   |              |              |              |
|---|--------------|--------------|--------------|
| H | 0.018348000  | -2.271767000 | -2.701187000 |
| H | -1.089959000 | -0.904599000 | -2.896065000 |
| H | -1.184471000 | -3.082168000 | -0.746962000 |
| H | -2.402912000 | -2.773860000 | -1.987345000 |
| H | -1.917786000 | -2.769880000 | 1.465110000  |
| H | -3.961004000 | -4.105197000 | 1.724676000  |
| H | -3.655616000 | -3.885245000 | -0.000373000 |
| H | -4.913826001 | -2.938447000 | 0.810867000  |
| H | -4.241703001 | -1.071029000 | 2.522893000  |
| H | -2.531096000 | -0.807436000 | 2.883429000  |
| H | -3.333889000 | -2.294316000 | 3.409479000  |
| H | -4.686818001 | -1.522399000 | -0.916587000 |
| H | -4.878209001 | 0.136949000  | -2.776618000 |
| H | -3.494550000 | -0.930720000 | -3.011109000 |
| H | -3.243494000 | 0.724763000  | -2.422219000 |
| H | -4.208793001 | 1.388705000  | -0.051908000 |
| H | -5.000858001 | 0.154844000  | 0.935405000  |
| H | -5.761534001 | 0.704921000  | -0.559871000 |
| H | 0.659399000  | 0.579070000  | -2.889008000 |
| H | 1.883453000  | -0.676639000 | -2.627750000 |
| H | 2.637075000  | 1.668264000  | -1.909942000 |
| H | 2.735912000  | 0.442448000  | -0.644498000 |
| H | 2.290713000  | 1.345879000  | 1.674969000  |
| H | 2.014347000  | 3.123174000  | 3.324317000  |
| H | 0.409959000  | 2.652690000  | 2.747340000  |
| H | 1.160041000  | 4.152151000  | 2.178544000  |
| H | 3.170842000  | 4.049839000  | 0.506656000  |
| H | 3.900861000  | 2.478988000  | 0.129522000  |
| H | 4.005485000  | 3.138543000  | 1.762581000  |
| H | 1.442579000  | 4.180465000  | -0.853576000 |
| H | -0.774984000 | 5.295353001  | -0.760811000 |
| H | -0.496844000 | 4.454952001  | 0.768713000  |
| H | -1.568467000 | 3.742477000  | -0.439892000 |
| H | -0.608512000 | 2.783718000  | -2.655648000 |
| H | 1.113781000  | 3.015794000  | -3.026130000 |
| H | 0.039510000  | 4.409800001  | -2.912825000 |
| H | 0.193058000  | -0.632482000 | 1.244920000  |

|   |             |              |              |
|---|-------------|--------------|--------------|
| H | 2.857726000 | -4.063310000 | -0.863148000 |
| H | 3.449449000 | -0.618536000 | 1.667946000  |
| H | 5.223608001 | -3.984069000 | -1.505999000 |
| H | 6.732583001 | -2.207234000 | -0.602365000 |
| H | 5.795866001 | -0.536611000 | 0.997272000  |
| H | 1.009042000 | -3.318333000 | 0.461915000  |
| H | 1.479790000 | -1.005564000 | 2.414735000  |
| H | 0.054881000 | -2.057570000 | 2.302195000  |

### SR\_TS3

|    |              |              |              |
|----|--------------|--------------|--------------|
| FE | 0.798943000  | 0.470265000  | -0.095493000 |
| C  | 1.630528000  | 1.362158000  | -1.336321000 |
| O  | 2.186484000  | 1.960672000  | -2.171438000 |
| N  | -0.272527000 | -0.674704000 | 1.309905000  |
| C  | 0.569451000  | -1.538797000 | 2.174532000  |
| C  | 1.602907000  | -2.291743000 | 1.339638000  |
| C  | -3.374952000 | -3.329538000 | 0.404030000  |
| C  | -2.893719000 | -2.374766000 | -0.528016000 |
| C  | -3.819743000 | -1.386160000 | -0.949137000 |
| C  | -4.677963001 | -3.292833000 | 0.888279000  |
| C  | -5.568043001 | -2.298941000 | 0.467566000  |
| C  | -5.123252001 | -1.351650000 | -0.459078000 |
| C  | -1.529421000 | -2.460785000 | -1.012545000 |
| C  | -0.880091000 | -1.554937000 | -1.856791000 |
| H  | 1.492693000  | 1.224790000  | 1.049058000  |
| H  | -0.816972000 | -1.299021000 | 0.690289000  |
| H  | -0.058792000 | -2.244354000 | 2.738932000  |
| H  | 1.066400000  | -0.884619000 | 2.895767000  |
| H  | 1.102041000  | -3.063087000 | 0.743678000  |
| H  | 2.329559000  | -2.796489000 | 1.984243000  |
| H  | 1.836265000  | -2.732456000 | -1.471162000 |
| H  | 3.833245000  | -4.139107000 | -1.731154000 |
| H  | 3.513034000  | -3.934015000 | -0.006622000 |
| H  | 4.816011001  | -3.022977000 | -0.786526000 |
| H  | 4.239627001  | -1.120873000 | -2.485504000 |
| H  | 2.546471000  | -0.770299000 | -2.853345000 |
| H  | 3.283205000  | -2.286006000 | -3.398309000 |

|   |              |              |              |
|---|--------------|--------------|--------------|
| P | 2.390187000  | -1.094315000 | 0.135628000  |
| C | 2.816145000  | -2.275674000 | -1.280427000 |
| C | 3.797671000  | -3.402490000 | -0.920031000 |
| C | 3.242728000  | -1.563941000 | -2.574177000 |
| C | 4.047733000  | -0.662458000 | 0.927574000  |
| C | 3.895468000  | -0.228332000 | 2.393891000  |
| C | 4.779910001  | 0.429593000  | 0.129759000  |
| C | -1.234670000 | 0.094086000  | 2.141582000  |
| C | -2.039052000 | 1.065775000  | 1.282584000  |
| P | -0.869028000 | 1.955261000  | 0.128809000  |
| C | -2.029604000 | 2.356445000  | -1.308891000 |
| C | -1.337713000 | 3.058579000  | -2.488333000 |
| C | -3.320160000 | 3.093419000  | -0.914174000 |
| C | -0.531506000 | 3.622790000  | 0.950303000  |
| C | 0.634829000  | 4.352310001  | 0.262086000  |
| C | -0.244599000 | 3.491161000  | 2.454433000  |
| H | 4.647298001  | -1.581004000 | 0.905102000  |
| H | 4.878388001  | 0.033299000  | 2.802844000  |
| H | 3.482364000  | -1.020861000 | 3.025510000  |
| H | 3.248536000  | 0.650603000  | 2.473357000  |
| H | 4.199058001  | 1.356558000  | 0.120489000  |
| H | 4.967270001  | 0.141374000  | -0.907605000 |
| H | 5.749913001  | 0.642261000  | 0.594255000  |
| H | -0.646732000 | 0.640062000  | 2.884658000  |
| H | -1.907014000 | -0.590928000 | 2.677806000  |
| H | -2.624616000 | 1.743132000  | 1.912201000  |
| H | -2.745879000 | 0.506111000  | 0.660757000  |
| H | -2.304096000 | 1.348101000  | -1.642944000 |
| H | -2.003099000 | 3.059427000  | -3.359644000 |
| H | -0.406626000 | 2.566182000  | -2.776560000 |
| H | -1.111235000 | 4.104843000  | -2.258065000 |
| H | -3.116909000 | 4.118728000  | -0.586938000 |
| H | -3.867568000 | 2.585040000  | -0.115490000 |
| H | -3.989170000 | 3.160286000  | -1.780195000 |
| H | -1.445737000 | 4.217626001  | 0.828433000  |
| H | 0.774829000  | 5.340467001  | 0.716175000  |
| H | 0.473717000  | 4.499040001  | -0.808387000 |

|   |              |              |              |
|---|--------------|--------------|--------------|
| H | 1.561993000  | 3.785717000  | 0.385594000  |
| H | 0.626557000  | 2.851573000  | 2.627703000  |
| H | -1.093029000 | 3.084043000  | 3.012555000  |
| H | -0.024188000 | 4.479701001  | 2.874016000  |
| H | -0.073528000 | -0.475196000 | -1.199154000 |
| H | -2.699826000 | -4.113361000 | 0.741966000  |
| H | -3.519136000 | -0.652759000 | -1.691824000 |

|   |              |              |              |
|---|--------------|--------------|--------------|
| H | -5.004024001 | -4.046815000 | 1.600826000  |
| H | -6.585481001 | -2.269304000 | 0.845512000  |
| H | -5.803503001 | -0.580475000 | -0.813256000 |
| H | -0.972982000 | -3.338874000 | -0.686077000 |
| H | -1.476904000 | -0.845047000 | -2.425510000 |
| H | -0.022781000 | -1.914175000 | -2.419062000 |