

Electronic Supplementary Information for:

## Molecular Mechanism of Palladium-Catalysed Cyanoesterification of Methyl Cyanoformate onto Norbornene

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## Corrections of translational entropy proposed by Whitesides (Ref. 25)

Absolute values of experimental entropies in solution are larger than those by using Sacker-Tetrode equation, which is a conventional model for gas phase. Translational entropy in solution is proposed by Whitesides and his co-workers, as follows:

$$S_{trans}^{corrected} = R \ln \left[ \left( \frac{10^{-15/2} V_{free}}{N_A^4 [X]} \right) \left( \frac{2\pi M R T e^{5/3}}{h^2} \right)^{3/2} \right] = R \ln \left[ \left( \frac{10^{-15/2} V_{free}}{N_A^4 [X]} \right) \left( \frac{2\pi M R T e^{3/2}}{h^2} \right)^{3/2} \right] + R \ln V_{free}$$

$$= S_{trans} + R \ln V_{free}$$

$S_{trans}$  refers gas-phase translational entropy and is given by Sacker-Tetrode equation.

$e$ : elementary electric charge,  $1.60217657 \times 10^{-19}$  C

$h$ : Planck's constant,  $6.62606957 \times 10^{-34}$  m<sup>2</sup> kg s<sup>-1</sup>

$R$ : ideal gas constant,  $8.3144621$  J K<sup>-1</sup> mol<sup>-1</sup>

$M$ : molecular weight, g mol<sup>-1</sup>

$N_A$ : Avogadro's number,  $6.0221413 \times 10^{23}$  mol<sup>-1</sup>

$V_{free}$ : "free volume" is defined as " the volume occupied by the center of mass of one molecule of liquid moving randomly in a cage that is defined by its nearest neighbors" by a following equation

$$V_{free} = C_{free} \left\{ \sqrt[3]{\left( \frac{10^{27}}{[X] N_A} \right)} - \sqrt[3]{V_{mole}} \right\}^3$$

Since the density of toluene at 25 °C is 0.8623 g cm<sup>-3</sup> from *CRC Handbook of Chemistry and Physics*, 91st Edition, Haynes, W. M. Ed. 2010, and  $M$  for toluene is 92.14 g mol<sup>-1</sup>, thus  $[X] = 9.3585$  (mol/L).  $V_{mole} = 139.1238$  Å<sup>3</sup> by 1000 times volume calculations by using Gaussian 09 program,  $V_{free}$  is 0.6706 Å<sup>3</sup> when  $C_{free} = 8$ . Then  $R \ln V_{free}$  for toluene in BHandHLYP/def2-TZVP is -46.380 J/mol K.

Thus:

$$H = E_{elec}(a.u.) + ZPE(a.u.) + kT(a.u.)$$

$$S^{corrected} = (S_{trans} + S_{rot} + S_{vib}) \times 4.184 + (-46.380)$$

$$G = H \times 2625.4997 - 383.15 \frac{S^{corrected}}{1000}$$

**Table S1.** Calculated energies and thermal corrections of representative stationary points for the cyanoesterification, calculated at the BHandHLYP/def2-TZVP level at 383.15 K, and 1 atm.

| Species                                 | $E_{\text{elec}}/\text{a.u.}$ | ZPE/a.u. | H/a.u.   | $S^{\text{corrected}}/\text{J}\cdot\text{mol}^{-1}\cdot\text{K}^{-1}$ | G / $\text{kJ}\cdot\text{mol}^{-1}$ | imag.freq./ $\text{cm}^{-1}$ |
|-----------------------------------------|-------------------------------|----------|----------|-----------------------------------------------------------------------|-------------------------------------|------------------------------|
| NBE                                     | -272.648617743                | 0.158027 | 0.167704 | 284.9510353                                                           | -715092.8364                        | —                            |
| toluene                                 | -271.491576638                | 0.131721 | 0.142548 | 328.3432993                                                           | -712206.7646                        | —                            |
| PPh <sub>3</sub>                        | -1036.12674168                | 0.282781 | 0.308693 | 574.3457633                                                           | -2719017.595                        | —                            |
| Pd(PPh <sub>3</sub> ) <sub>2</sub>      | -2200.11818506                | 0.567829 | 0.624092 | 1108.600723                                                           | -5773705.007                        | —                            |
| 2t2P                                    | -2521.39078856                | 0.631925 | 0.69899  | 1245.338027                                                           | -6616893.593                        | —                            |
| <i>endo</i> -3cP-N_CN                   | -1757.87414398                | n.d.     | n.d.     | n.d.                                                                  | n.d.                                | n.d.                         |
| <i>endo</i> -3cP-N_Pd <sub>LP(O)</sub>  | -1757.87515821                | n.d.     | n.d.     | n.d.                                                                  | n.d.                                | n.d.                         |
| <i>endo</i> -3cP-N_Pd <sub>LP(OR)</sub> | -1757.87486739                | n.d.     | n.d.     | n.d.                                                                  | n.d.                                | n.d.                         |
| <i>endo</i> -3cP-N_PPh <sub>3</sub>     | -1757.87505843                | n.d.     | n.d.     | n.d.                                                                  | n.d.                                | n.d.                         |
| <i>endo</i> -3cP-O_COOR                 | -1757.86731005                | n.d.     | n.d.     | n.d.                                                                  | n.d.                                | n.d.                         |
| <i>endo</i> -3cP-O_Pd <sub>LP(O)</sub>  | -1757.87111792                | n.d.     | n.d.     | n.d.                                                                  | n.d.                                | n.d.                         |
| <i>endo</i> -3cP-O_Pd <sub>LP(OR)</sub> | -1757.87036634                | n.d.     | n.d.     | n.d.                                                                  | n.d.                                | n.d.                         |
| <i>endo</i> -3cP-O_PPh <sub>3</sub>     | -1757.86039305                | n.d.     | n.d.     | n.d.                                                                  | n.d.                                | n.d.                         |
| <i>endo</i> -3tP-N_CN                   | -1757.87565242                | n.d.     | n.d.     | n.d.                                                                  | n.d.                                | n.d.                         |
| <i>endo</i> -3tP-N_COOR                 | -1757.87495261                | n.d.     | n.d.     | n.d.                                                                  | n.d.                                | n.d.                         |
| <i>endo</i> -3tP-N_Pd <sub>LP(O)</sub>  | -1757.87892162                | n.d.     | n.d.     | n.d.                                                                  | n.d.                                | n.d.                         |
| <i>endo</i> -3tP-N_Pd <sub>LP(OR)</sub> | -1757.87877589                | n.d.     | n.d.     | n.d.                                                                  | n.d.                                | n.d.                         |
| <i>endo</i> -3tP-O_CN                   | -1757.87564899                | n.d.     | n.d.     | n.d.                                                                  | n.d.                                | n.d.                         |
| <i>endo</i> -3tP-O_COOR                 | -1757.8749883                 | n.d.     | n.d.     | n.d.                                                                  | n.d.                                | n.d.                         |
| <i>endo</i> -3tP-O_Pd <sub>LP(O)</sub>  | -1757.87892285                | n.d.     | n.d.     | n.d.                                                                  | n.d.                                | n.d.                         |
| <i>endo</i> -3tP-O_Pd <sub>LP(OR)</sub> | -1757.87877449                | n.d.     | n.d.     | n.d.                                                                  | n.d.                                | n.d.                         |
| <i>exo</i> -3cP-N_CN                    | -1757.88264699                | n.d.     | n.d.     | n.d.                                                                  | n.d.                                | n.d.                         |
| <i>exo</i> -3cP-N_Pd <sub>LP(O)</sub>   | -1757.88455564                | n.d.     | n.d.     | n.d.                                                                  | n.d.                                | n.d.                         |
| <i>exo</i> -3cP-N_Pd <sub>LP(OR)</sub>  | -1757.88429434                | n.d.     | n.d.     | n.d.                                                                  | n.d.                                | n.d.                         |
| <i>exo</i> -3cP-N_PPh <sub>3</sub>      | -1757.87559684                | n.d.     | n.d.     | n.d.                                                                  | n.d.                                | n.d.                         |
| <i>exo</i> -3cP-O_COOR                  | -1757.87873849                | n.d.     | n.d.     | n.d.                                                                  | n.d.                                | n.d.                         |
| <i>exo</i> -3cP-O_Pd <sub>LP(O)</sub>   | -1757.88414957                | n.d.     | n.d.     | n.d.                                                                  | n.d.                                | n.d.                         |
| <i>exo</i> -3cP-O_Pd <sub>LP(OR)</sub>  | -1757.88329299                | n.d.     | n.d.     | n.d.                                                                  | n.d.                                | n.d.                         |
| <i>exo</i> -3cP-O_PPh <sub>3</sub>      | -1757.86283291                | n.d.     | n.d.     | n.d.                                                                  | n.d.                                | n.d.                         |
| <i>exo</i> -3tP-N_CN                    | -1757.88579332                | n.d.     | n.d.     | n.d.                                                                  | n.d.                                | n.d.                         |
| <i>exo</i> -3tP-N_COOR                  | -1757.88617605                | n.d.     | n.d.     | n.d.                                                                  | n.d.                                | n.d.                         |
| <i>exo</i> -3tP-N_Pd <sub>LP(O)</sub>   | -1757.8908848                 | n.d.     | n.d.     | n.d.                                                                  | n.d.                                | n.d.                         |
| <i>exo</i> -3tP-N_Pd <sub>LP(OR)</sub>  | -1757.8905829                 | n.d.     | n.d.     | n.d.                                                                  | n.d.                                | n.d.                         |

**Table S1.** Continued

| Species                                | $E_{\text{elec}}/\text{a.u.}$ | ZPE/a.u. | H/a.u.   | $S^{\text{corre}}/\text{J}\cdot\text{mol}^{-1}\cdot\text{K}^{-1}$ | G / $\text{kJ}\cdot\text{mol}^{-1}$ | imag. freq/ $\text{cm}^{-1}$ |
|----------------------------------------|-------------------------------|----------|----------|-------------------------------------------------------------------|-------------------------------------|------------------------------|
| <i>exo</i> -3tP-O_CN                   | -1757.89058245                | n.d.     | n.d.     | n.d.                                                              | n.d.                                | n.d.                         |
| <i>exo</i> -3tP-O_COOR                 | -1757.88617687                | n.d.     | n.d.     | n.d.                                                              | n.d.                                | n.d.                         |
| <i>exo</i> -3tP-O_Pd <sub>LP(O)</sub>  | -1757.89058415                | n.d.     | n.d.     | n.d.                                                              | n.d.                                | n.d.                         |
| <i>exo</i> -3tP-O_Pd <sub>LP(OR)</sub> | -1757.89058415                | n.d.     | n.d.     | n.d.                                                              | n.d.                                | n.d.                         |
| <i>exo</i> -3tP-O                      | -1757.89058311                | 0.507282 | 0.557848 | 969.9806193                                                       | -4612916.348                        | —                            |
| <i>exo</i> -3tP-OMe                    | -1757.88984543                | 0.507409 | 0.557909 | 963.1983553                                                       | -4612911.319                        | —                            |
| <i>exo</i> -3cP-O                      | -1757.88380042                | 0.507368 | 0.557874 | 961.7548753                                                       | -4612895.094                        | —                            |
| <i>exo</i> -3cP-OMe                    | -1757.88356014                | 0.50732  | 0.557868 | 965.0142113                                                       | -4612895.854                        | —                            |
| <i>exo</i> -3cP-N                      | -1757.88401412                | 0.50735  | 0.558013 | 969.4115953                                                       | -4612898.272                        | —                            |
| <i>exo</i> -3t-O                       | -721.712167393                | 0.222307 | 0.245972 | 538.5683793                                                       | -1893831.965                        | —                            |
| <i>exo</i> -3t-OMe                     | -721.706507097                | 0.22179  | 0.24568  | 543.9155313                                                       | -1893821.277                        | —                            |
| <i>exo</i> -3c-O                       | -721.724441202                | 0.221713 | 0.245797 | 556.0826033                                                       | -1893872.92                         | —                            |
| <i>exo</i> -3c-OMe                     | -721.723340651                | 0.221839 | 0.245865 | 552.9069473                                                       | -1893868.304                        | —                            |
| <i>exo</i> -3c-N                       | -721.72557262                 | 0.221763 | 0.245732 | 546.6142113                                                       | -1893872.302                        | —                            |
| <i>exo</i> -3c-N'                      | -721.730950855                | 0.221673 | 0.245602 | 547.2710993                                                       | -1893887.251                        | —                            |
| <i>exo</i> -3t2N-O                     | -994.384539728                | 0.382814 | 0.416811 | 688.9831793                                                       | -2608920.879                        | —                            |
| <i>exo</i> -3t2N-OMe                   | -994.383700433                | 0.38279  | 0.416821 | 691.8031953                                                       | -2608919.793                        | —                            |
| <i>exo</i> -3c2N-O                     | -994.384061697                | 0.382299 | 0.416733 | 703.8656673                                                       | -2608926.884                        | —                            |
| <i>exo</i> -3c2N-OMe                   | -994.383721065                | 0.382296 | 0.416764 | 706.8781473                                                       | -2608927.07                         | —                            |
| <i>exo</i> -3c2N-N                     | -994.38406094                 | 0.382296 | 0.416734 | 704.0079233                                                       | -2608926.941                        | —                            |
| <i>exo</i> -3c2N-N'                    | -994.383719255                | 0.382297 | 0.416764 | 706.8446753                                                       | -2608927.05                         | —                            |
| <i>exo</i> -3tT-O                      | -993.212811088                | 0.355791 | 0.391245 | 723.9028433                                                       | -2605995.958                        | —                            |
| <i>exo</i> -3tT-OMe                    | -993.211817099                | 0.355684 | 0.391256 | 731.7603953                                                       | -2605996.611                        | —                            |
| <i>exo</i> -3tTr-O                     | -993.212831848                | 0.355962 | 0.391336 | 721.9447313                                                       | -2605994.575                        | —                            |
| <i>exo</i> -3tTr-OMe                   | -993.212588567                | 0.355953 | 0.39133  | 721.7355313                                                       | -2605993.895                        | —                            |
| <i>exo</i> -3cT-O                      | -993.219313792                | 0.355315 | 0.391171 | 739.1535233                                                       | -2606020.318                        | —                            |
| <i>exo</i> -3cT-OMe                    | -993.219079921                | 0.35535  | 0.391212 | 739.4966113                                                       | -2606019.636                        | —                            |
| <i>exo</i> -3cT-N                      | -993.216530351                | 0.355231 | 0.391157 | 740.1995233                                                       | -2606013.668                        | —                            |
| <i>exo</i> -3cT-N'                     | -993.215455524                | 0.355069 | 0.391134 | 752.3122033                                                       | -2606015.973                        | —                            |
| <i>exo</i> -TS <sub>3_4</sub> tP-O     | -1757.86537581                | 0.50709  | 0.556404 | 941.9143473                                                       | -4612843.708                        | 382.67 i                     |
| <i>exo</i> -TS <sub>3_4</sub> tP-OMe   | -1757.86237713                | 0.507483 | 0.556619 | 934.5630593                                                       | -4612831.422                        | 390.57 i                     |
| <i>exo</i> -TS <sub>3_4</sub> tP-N     | -1757.85326362                | 0.50626  | 0.555881 | 964.6920433                                                       | -4612824.187                        | 480.88 i                     |
| <i>exo</i> -TS <sub>3_4</sub> cP-O     | -1757.86563727                | 0.507118 | 0.556361 | 935.4040433                                                       | -4612841.94                         | 352.19 i                     |
| <i>exo</i> -TS <sub>3_4</sub> cP-OMe   | -1757.86408052                | 0.507095 | 0.556381 | 938.4123393                                                       | -4612839.013                        | 353.84 i                     |
| <i>exo</i> -TS <sub>3_4</sub> cP-N     | -1757.84182893                | 0.506567 | 0.555926 | 946.5251153                                                       | -4612786.281                        | 460.60 i                     |
| <i>exo</i> -TS <sub>3_4</sub> t-O      | -721.704830053                | 0.221569 | 0.244212 | 513.6568433                                                       | -1893809.715                        | 235.38 i                     |

**Table S1.** Continued

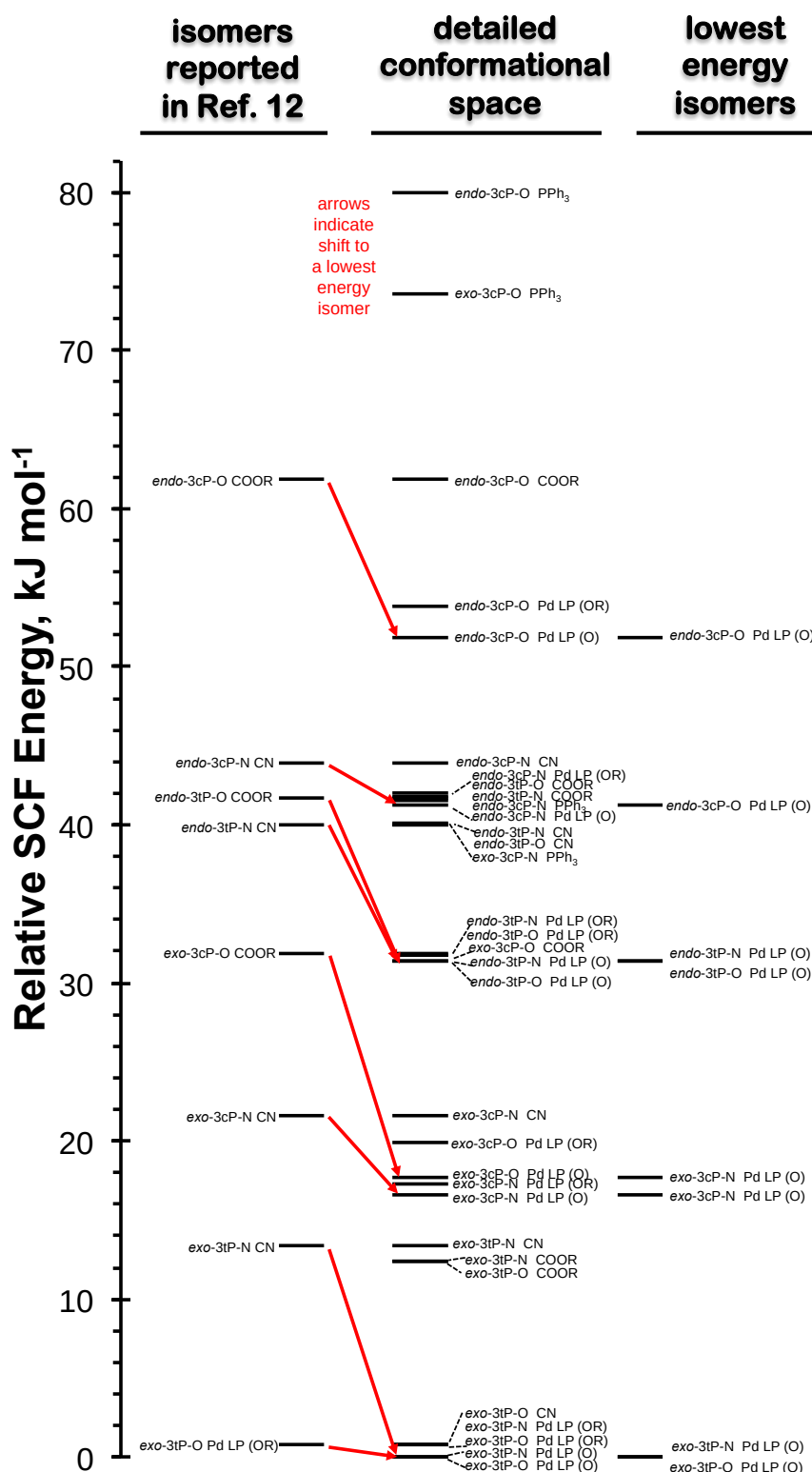
| Species                               | $E_{\text{elec}}/\text{a.u.}$ | ZPE/a.u. | H/a.u.   | $S^{\text{corre}}/\text{J}\cdot\text{mol}^{-1}\cdot\text{K}^{-1}$ | G / $\text{kJ}\cdot\text{mol}^{-1}$ | imag. freq / $\text{cm}^{-1}$ |
|---------------------------------------|-------------------------------|----------|----------|-------------------------------------------------------------------|-------------------------------------|-------------------------------|
| <i>exo</i> -TS <sub>3_4</sub> t-OMe   | -721.703365326                | 0.221607 | 0.244232 | 513.0627153                                                       | -1893805.489                        | 248.36 i                      |
| <i>exo</i> -TS <sub>3_4</sub> t-N     | -721.685178786                | 0.221135 | 0.243811 | 521.2466193                                                       | -1893763.22                         | 398.78 i                      |
| <i>exo</i> -TS <sub>3_4</sub> t-N'    | -721.686747992                | 0.221392 | 0.243967 | 516.9956753                                                       | -1893764.627                        | 423.31 i                      |
| <i>exo</i> -TS <sub>3_4</sub> c-O     | -721.686442478                | 0.220909 | 0.243725 | 516.2216353                                                       | -1893765.432                        | 395.66 i                      |
| <i>exo</i> -TS <sub>3_4</sub> c-OMe   | -721.684403586                | 0.220986 | 0.243802 | 516.1379553                                                       | -1893759.643                        | 405.09 i                      |
| <i>exo</i> -TS <sub>3_4</sub> c-N     | -721.662114746                | 0.221307 | 0.243925 | 516.2676593                                                       | -1893700.007                        | 396.80 i                      |
| <i>exo</i> -TS <sub>3_4</sub> c-N'    | -721.662114746                | 0.221307 | 0.243925 | 516.2676593                                                       | -1893700.007                        | 396.80 i                      |
| <i>exo</i> -TS <sub>3_4</sub> t2N-O   | -994.36903939                 | 0.382187 | 0.415157 | 670.1719153                                                       | -2608878.965                        | 359.76 i                      |
| <i>exo</i> -TS <sub>3_4</sub> t2N-OMe | -994.367524793                | 0.382225 | 0.415198 | 669.6196273                                                       | -2608874.569                        | 359.42 i                      |
| <i>exo</i> -TS <sub>3_4</sub> t2N-N   | -994.355988133                | 0.381614 | 0.414756 | 679.0168913                                                       | -2608850.645                        | 459.38 i                      |
| <i>exo</i> -TS <sub>3_4</sub> t2N-N'  | -994.355611463                | 0.381653 | 0.414786 | 678.2093793                                                       | -2608849.165                        | 457.90 i                      |
| <i>exo</i> -TS <sub>3_4</sub> c2N-O   | -994.362587773                | 0.382566 | 0.415225 | 660.4566673                                                       | -2608857.13                         | 361.15 i                      |
| <i>exo</i> -TS <sub>3_4</sub> c2N-OMe | -994.360288385                | 0.382603 | 0.415283 | 662.3436513                                                       | -2608851.566                        | 362.45 i                      |
| <i>exo</i> -TS <sub>3_4</sub> c2N-N   | -994.34155629                 | 0.381836 | 0.414768 | 670.7953313                                                       | -2608808.989                        | 445.22 i                      |
| <i>exo</i> -TS <sub>3_4</sub> c2N-N'  | -994.341448015                | 0.381862 | 0.41479  | 670.1593633                                                       | -2608808.335                        | 442.42 i                      |
| <i>exo</i> -TS <sub>3_4</sub> tT-O    | -993.201689296                | 0.355149 | 0.389748 | 714.6896753                                                       | -2605968.844                        | 329.51 i                      |
| <i>exo</i> -TS <sub>3_4</sub> tT-OMe  | -993.200946998                | 0.35498  | 0.389765 | 728.8650673                                                       | -2605972.725                        | 329.04 i                      |
| <i>exo</i> -TS <sub>3_4</sub> tT-N    | -993.187002359                | 0.35463  | 0.389234 | 713.6018353                                                       | -2605932.579                        | 442.15 i                      |
| <i>exo</i> -TS <sub>3_4</sub> tT-N'   | -993.185382149                | 0.354467 | 0.389184 | 719.1581873                                                       | -2605931.013                        | 439.73 i                      |
| <i>exo</i> -TS <sub>3_4</sub> tTr-O   | -993.202936509                | 0.355272 | 0.389696 | 706.4471953                                                       | -2605968.774                        | 326.50 i                      |
| <i>exo</i> -TS <sub>3_4</sub> tTr-OMe | -993.201397577                | 0.355327 | 0.389716 | 704.8028833                                                       | -2605963.906                        | 333.07 i                      |
| <i>exo</i> -TS <sub>3_4</sub> tTr-N   | -993.186423401                | 0.354797 | 0.389328 | 712.6060433                                                       | -2605929.992                        | 441.51 i                      |
| <i>exo</i> -TS <sub>3_4</sub> tTr-N'  | -993.186041012                | 0.354981 | 0.389395 | 711.0035713                                                       | -2605927.715                        | 435.63 i                      |
| <i>exo</i> -TS <sub>3_4</sub> cT-O    | -993.165591611                | 0.354536 | 0.389029 | 708.6688993                                                       | -2605875.26                         | 384.46 i                      |
| <i>exo</i> -TS <sub>3_4</sub> cT-OMe  | -993.165004535                | 0.354438 | 0.389029 | 715.8193553                                                       | -2605876.715                        | 386.05 i                      |
| <i>exo</i> -TS <sub>3_4</sub> cT-N    | -993.190496521                | 0.355354 | 0.389522 | 695.4139873                                                       | -2605932.127                        | 447.09 i                      |
| <i>exo</i> -TS <sub>3_4</sub> cT-N'   | -993.188483401                | 0.355409 | 0.38959  | 697.8825473                                                       | -2605927.464                        | 448.10 i                      |
| <i>exo</i> -4tP-O                     | -1757.92370378                | 0.509967 | 0.559143 | 952.4496593                                                       | -4612986.14                         | —                             |
| <i>exo</i> -4tP-OMe                   | -1757.90689855                | 0.510136 | 0.559336 | 951.0522033                                                       | -4612940.532                        | —                             |
| <i>exo</i> -4tP-N                     | -1757.88646181                | 0.508604 | 0.5583   | 956.7759153                                                       | -4612895.811                        | —                             |
| <i>exo</i> -4cP-O                     | -1757.91788393                | 0.510267 | 0.55928  | 933.3078593                                                       | -4612962.378                        | —                             |
| <i>exo</i> -4cP-OMe                   | -1757.91062831                | 0.510249 | 0.559377 | 936.4667793                                                       | -4612944.332                        | —                             |
| <i>exo</i> -4cP-N                     | -1757.86800124                | 0.508578 | 0.558017 | 948.1234033                                                       | -4612844.839                        | —                             |
| <i>exo</i> -4t-O                      | -721.766582563                | 0.225556 | 0.247596 | 502.0838993                                                       | -1893948.059                        | —                             |
| <i>exo</i> -4t-N                      | -721.727775017                | 0.223731 | 0.246435 | 517.9119713                                                       | -1893860.074                        | —                             |
| <i>exo</i> -4t-N'                     | -721.728870975                | 0.223899 | 0.246547 | 515.7111873                                                       | -1893861.373                        | —                             |

**Table S1.** Continued

| Species                                            | $E_{\text{elec}}/\text{a.u.}$ | ZPE/a.u. | H/a.u.   | $S^{\text{corre}}/\text{J}\cdot\text{mol}^{-1}\cdot\text{K}^{-1}$ | $G/\text{kJ}\cdot\text{mol}^{-1}$ | imag. freq/ $\text{cm}^{-1}$ |
|----------------------------------------------------|-------------------------------|----------|----------|-------------------------------------------------------------------|-----------------------------------|------------------------------|
| <i>exo</i> -4c-O                                   | -721.723779114                | 0.22359  | 0.246359 | 520.5060513                                                       | -1893851.146                      | —                            |
| <i>exo</i> -4c-OMe                                 | -721.729839183                | 0.224085 | 0.246646 | 514.9831713                                                       | -1893862.888                      | —                            |
| <i>exo</i> -4c-N                                   | -721.681091148                | 0.223036 | 0.245638 | 515.7111873                                                       | -1893740.58                       | —                            |
| <i>exo</i> -4c-N'                                  | -721.681096043                | 0.223035 | 0.245636 | 515.6567953                                                       | -1893740.579                      | —                            |
| <i>exo</i> -4t2N-O                                 | -994.428410204                | 0.385308 | 0.418148 | 678.5148113                                                       | -2609021.992                      | —                            |
| <i>exo</i> -4t2N-OMe                               | -994.428410668                | 0.385307 | 0.418147 | 678.5064433                                                       | -2609021.995                      | —                            |
| <i>exo</i> -4t2N-N                                 | -994.390654668                | 0.383625 | 0.417047 | 692.2215953                                                       | -2608935.426                      | —                            |
| <i>exo</i> -4t2N-N'                                | -994.390089167                | 0.383605 | 0.417049 | 693.7320193                                                       | -2608934.567                      | —                            |
| <i>exo</i> -4c2N-O                                 | -994.40804888                 | 0.385657 | 0.418161 | 659.9169313                                                       | -2608960.457                      | —                            |
| <i>exo</i> -4c2N-OMe                               | -994.399162958                | 0.385495 | 0.418199 | 669.5401313                                                       | -2608941.14                       | —                            |
| <i>exo</i> -4c2N-N                                 | -994.363242683                | 0.383605 | 0.416609 | 671.8287793                                                       | -2608856.845                      | —                            |
| <i>exo</i> -4c2N-N'                                | -994.362825313                | 0.383635 | 0.416631 | 670.9082993                                                       | -2608855.26                       | —                            |
| <i>exo</i> -4tT-O                                  | -993.264437408                | 0.358588 | 0.392869 | 718.8109153                                                       | -2606117.945                      | —                            |
| <i>exo</i> -4tT-N                                  | -993.224309658                | 0.356944 | 0.391726 | 726.4299793                                                       | -2606022.826                      | —                            |
| <i>exo</i> -4tT-N'                                 | -993.223666158                | 0.356827 | 0.391727 | 733.1662193                                                       | -2606024.022                      | —                            |
| <i>exo</i> -4tTr-O                                 | -993.263631847                | 0.358653 | 0.392789 | 709.0663793                                                       | -2606112.135                      | —                            |
| <i>exo</i> -4tTr-OMe                               | -993.263631499                | 0.358653 | 0.392789 | 709.1291393                                                       | -2606112.159                      | —                            |
| <i>exo</i> -4tTr-N                                 | -993.223509312                | 0.357082 | 0.391898 | 727.4425073                                                       | -2606020.299                      | —                            |
| <i>exo</i> -4tTr-N'                                | -993.225026377                | 0.357227 | 0.391997 | 724.4718673                                                       | -2606022.503                      | —                            |
| <i>exo</i> -4cT-O                                  | -993.186572421                | 0.356292 | 0.390867 | 710.9826513                                                       | -2605921.795                      | —                            |
| <i>exo</i> -4cT-N                                  | -993.235246094                | 0.358547 | 0.392472 | 691.2509073                                                       | -2606031.893                      | —                            |
| <i>exo</i> -4cT-N'                                 | -993.235246442                | 0.358546 | 0.392473 | 691.3178513                                                       | -2606031.92                       | —                            |
| <i>exo</i> -TS <sub>LFR</sub> -O                   | -1757.89720092                | 0.509007 | 0.557847 | 952.9098993                                                       | -4612922.656                      | 21.15 i                      |
| <i>exo</i> -TS <sub>LFR</sub> -OMe                 | -1757.89193006                | 0.508699 | 0.557667 | 958.8637313                                                       | -4612912.38                       | 13.21 i                      |
| <i>exo</i> -TS <sub>rot</sub> -O                   | -1757.89257329                | 0.508738 | 0.557675 | 951.1191473                                                       | -4612910.978                      | 92.23 i                      |
| <i>exo</i> -4tP- $\pi$ O1                          | -1757.89726386                | 0.508807 | 0.558798 | 975.9511873                                                       | -4612929.678                      | —                            |
| <i>exo</i> -4tP- $\pi$ O2                          | -1757.8920923                 | 0.508661 | 0.558631 | 979.0724513                                                       | -4612918.118                      | —                            |
| <i>exo</i> -4t2P-O <sup>a</sup>                    | -2794.03002282                | 0.797188 | 0.873107 | 1339.080547                                                       | -7331852.696                      | —                            |
| <i>exo</i> -4t2P-OMe <sup>a</sup>                  | -2794.022927                  | 0.797126 | 0.873155 | 1341.657891                                                       | -7331835.091                      | —                            |
| <i>exo</i> -TS <sub>4_5t</sub> P-O                 | -1757.86428141                | 0.509071 | 0.557989 | 958.7131073                                                       | -4612837.909                      | 351.60 i                     |
| <i>exo</i> -TS <sub>4_5t</sub> P-OMe               | -1757.8614901                 | 0.509008 | 0.557975 | 959.2779473                                                       | -4612830.999                      | 349.78 i                     |
| <i>exo</i> -TS <sub>4_5t</sub> P-N                 | -1757.85564473                | 0.507943 | 0.557044 | 956.7382593                                                       | -4612819.919                      | 275.33 i                     |
| <i>exo</i> -TS <sub>4_5t</sub> P-O <sup>a</sup>    | -2793.98433128                | 0.795664 | 0.871452 | 1372.008627                                                       | -7331753.696                      | 337.54 i                     |
| <i>exo</i> -TS <sub>4_5t</sub> 2P-OMe <sup>a</sup> | -2793.97908788                | 0.795676 | 0.871465 | 1369.586091                                                       | -7331738.936                      | 335.20 i                     |
| <i>exo</i> -5tP-O                                  | -1757.93652771                | 0.511315 | 0.560803 | 997.6996193                                                       | -4613029.249                      | —                            |
| <i>exo</i> -5tP-OMe                                | -1757.9346617                 | 0.511474 | 0.560965 | 1004.594851                                                       | -4613026.149                      | —                            |

**Table S1.** Continued

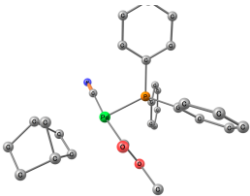
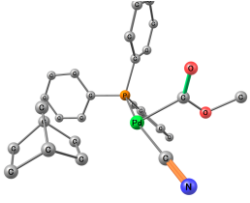
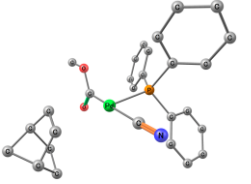
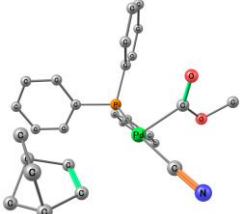
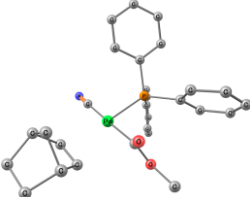
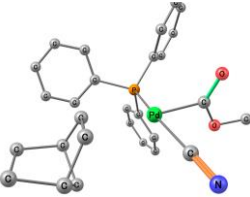
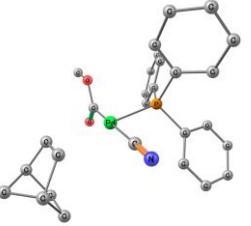
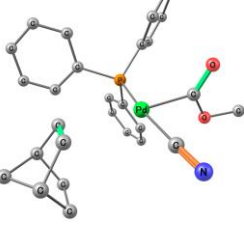
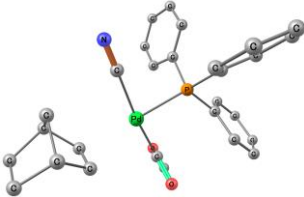
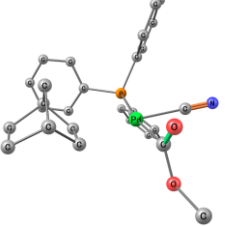
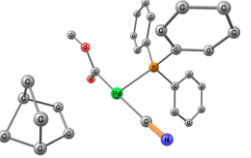
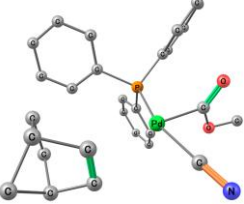
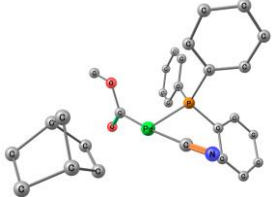
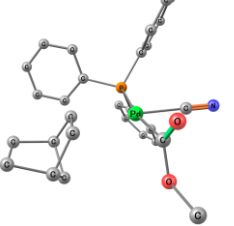
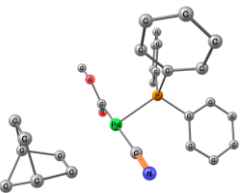
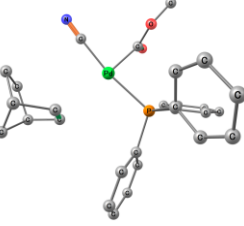
| Species                             | $E_{elec}/a.u.$ | ZPE/a.u. | H/a.u.   | $S^{corre}/J\cdot mol^{-1}\cdot K^{-1}$ | G / $kJ\cdot mol^{-1}$ | imag. freq/ $cm^{-1}$ |
|-------------------------------------|-----------------|----------|----------|-----------------------------------------|------------------------|-----------------------|
| <i>exo</i> -5-O                     | -593.961459544  | 0.22627  | 0.245575 | 451.3110593                             | -1558379.725           | —                     |
| <i>exo</i> -5-OMe                   | -593.959589256  | 0.226409 | 0.245714 | 452.3528753                             | -1558374.484           | —                     |
| <i>endo</i> -3tP-O                  | -1757.87843506  | 0.507277 | 0.557935 | 968.3404913                             | -4612883.61            | —                     |
| <i>endo</i> -TS <sub>3_4</sub> tP-O | -1757.84994636  | 0.507178 | 0.556428 | 938.9311553                             | -4612801.761           | 390.05 i              |
| <i>endo</i> -4tP-O                  | -1757.92243819  | 0.509888 | 0.559057 | 953.0061313                             | -4612983.464           | —                     |
| <i>endo</i> -TS <sub>4_5</sub> tP-O | -1757.85838097  | 0.509216 | 0.558012 | 960.6754033                             | -4612822.728           | 339.78 i              |
| <i>endo</i> -5tP-O                  | -1757.93275834  | 0.511629 | 0.561084 | 1003.440067                             | -4613019.99            | —                     |
| <i>endo</i> -5-O                    | -593.959153816  | 0.226438 | 0.245685 | 450.1186193                             | -1558372.484           | —                     |



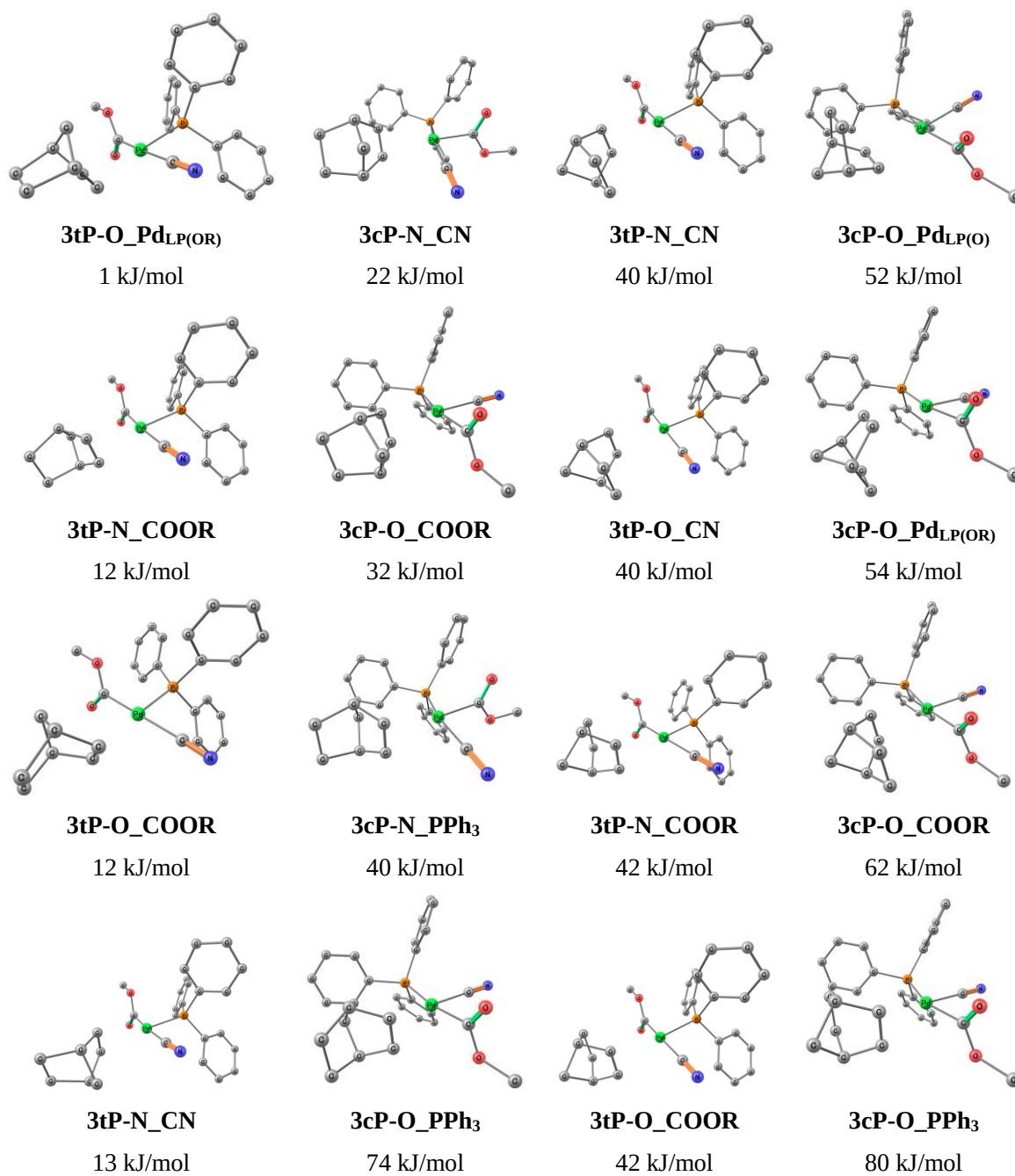
**Figure S1.** Results of conformational analysis of the Pd<sup>II</sup> coordinated NBE  $\pi$ -complex along an axis formed by the centroid of the olefin bond and the Pd centre. The orientation of the NBE (indicated with underlined superscripts) is defined as the methylene (for *exo*) or ethylene (for *endo*) bridge position being eclipsed with cyanide (CN), ester (COOR), phosphane (PPh<sub>3</sub>), Pd 4d<sub>z<sup>2</sup></sub> lone pair (Pd LP) with the ester pointing its carbonyl (O) and carboxylate (OR) group pointing toward the olefin.



**Table S2.** Optimized structures with relative energies from conformational analysis shown in Figure S1.

| <i>Exo-isomers</i>                                                                                                                       |                                                                                                                                           | <i>Endo-isomers</i>                                                                                                                        |                                                                                                                                           |
|------------------------------------------------------------------------------------------------------------------------------------------|-------------------------------------------------------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------------------------------------------------------|-------------------------------------------------------------------------------------------------------------------------------------------|
| <i>trans</i>                                                                                                                             | <i>cis</i>                                                                                                                                | <i>trans</i>                                                                                                                               | <i>cis</i>                                                                                                                                |
|  <p><b>3tP-O_Pd<sub>LP</sub>(O)</b><br/>0 kJ/mol</p>    |  <p><b>3cP-N_Pd<sub>LP</sub>(O)</b><br/>17 kJ/mol</p>    |  <p><b>3tP-N_Pd<sub>LP</sub>(O)</b><br/>31 kJ/mol</p>    |  <p><b>3cP-N_Pd<sub>LP</sub>(O)</b><br/>41 kJ/mol</p>  |
|  <p><b>3tP-N_Pd<sub>LP</sub>(O)</b><br/>0 kJ/mol</p>    |  <p><b>3cP-N_Pd<sub>LP</sub>(OR)</b><br/>17 kJ/mol</p>   |  <p><b>3tP-O_Pd<sub>LP</sub>(O)</b><br/>31 kJ/mol</p>    |  <p><b>3cP-N_Pd<sub>LP</sub>(OR)</b><br/>42 kJ/mol</p> |
|  <p><b>3tP-O_CN</b><br/>1 kJ/mol</p>                  |  <p><b>3cP-O_Pd<sub>LP</sub>(O)</b><br/>18 kJ/mol</p>  |  <p><b>3tP-N_Pd<sub>LP</sub>(OR)</b><br/>32 kJ/mol</p> |  <p><b>3cP-N_PPh<sub>3</sub></b><br/>42 kJ/mol</p>   |
|  <p><b>3tP-N_Pd<sub>LP</sub>(OR)</b><br/>1 kJ/mol</p> |  <p><b>3cP-O_Pd<sub>LP</sub>(OR)</b><br/>20 kJ/mol</p> |  <p><b>3tP-O_Pd<sub>LP</sub>(OR)</b><br/>32 kJ/mol</p> |  <p><b>3cP-N_CN</b><br/>44 kJ/mol</p>                |

**Table S2.** Continued

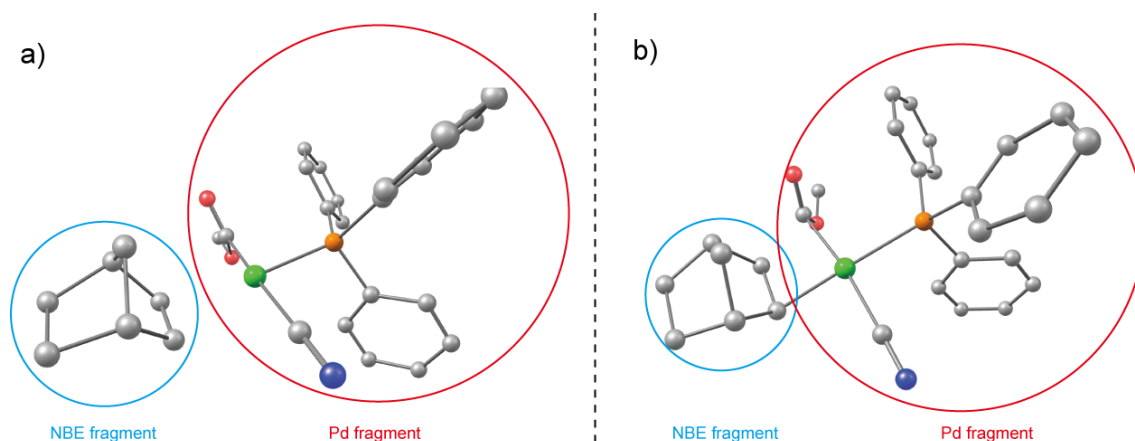


## Discussion of the importance of the conformational analysis results in Figure S1 and Table S2

Compelling evidence was provided<sup>12</sup> for the NBE substrate coordination being the source of exclusive *exo* selectivity in cyanoesterification reaction catalysed by  $4d^8$   $Pd^{II}$  complexes. The electron-configuration is of note here, since the main reason for the selectivity is the formation of a  $C-H\cdots Pd\ 4d_{z^2}$  agostic interaction. In order to further substantiate, the unexpectedly early origin of regioselectivity, we carried out a conformational analysis, where the methylene bridgehead groups of NBE was rotated around the olefin centroid and Pd axis in four steps. The initial structures were constructed with the methylene bridge eclipsing the cyanide (CN), ester (COOR), phosphane ( $PPh_3$ ) ligands, or the Pd  $4d_{z^2}$  double occupied orbital (Pd LP). The left-hand side of Fig. S1 shows the eight energy levels reported in the previous study,<sup>12</sup> where the  $\pi$ -complexes were constructed in a somewhat arbitrary manner. Each of these complexes underwent a 4-fold rotation around the  $Pd\cdots$ olefin centroid axis that resulted 32 individual structures as summarized in the middle of Fig. S1. The red arrows indicate the drop in energy for each arrangement of the olefin (*exo/endo*) and the CN (**N**)/COOR (**O**) vs.  $PPh_3$  (**P**) ligands being *cis* (**c**) or *trans* (**t**) in comparison to the published structures.<sup>12</sup> For the sake of clarity, the right hand side of Fig. S1 summarizes the lowest energy structures of *exo*- and *endo*-isomers for each ligand arrangement. As can be seen from the distribution of the lowest energy structures, the most stable  $\pi$ -complexes are obtained when the bridgehead group is eclipsed with the double occupied Pd  $4d$  orbital (Pd LP), which is approximately perpendicular to the olefin double bond and the plane formed by the  $[Pd(PPh_3)(CN)(COOR)]$  coordination environment. The energy levels as shown on the right-hand side of Fig. S1 unambiguously support the clear separation of the *exo* and *endo* isomers. It also shows that the scrambling of the CN/COOR and  $PPh_3$  ligands to form *cis* (**3c**) or *trans* (**3t**) isomers would not be feasible due to considerable 20 and 10  $\text{kJ mol}^{-1}$  energetic differences for the group of *exo-3* and *endo-3* complexes, respectively. The lowest energy isomers for the *exo-3tP-O* and *exo-3tP-N* complexes are mirror images of each other due to the methylene bridgehead group of the olefin located *trans* to the  $PPh_3$  ligand pointing to the opposite sides of the  $[Pd(PPh_3)(CN)(COOR)]$  coordination plane.

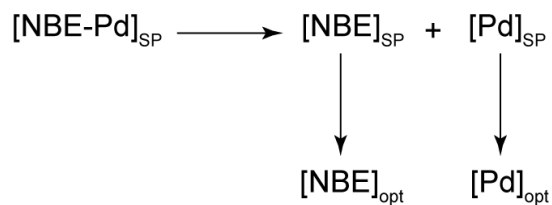
In addition to using the interatomic distances as a criterion for olefin/ $Pd^{II}$  interaction (Table S2) for describing the origin of regioselectivity in cyanoesterification reaction, we examined the binding energy between NBE and the  $[Pd^{II}(PPh_3)(CN)(COOR)]$  fragment using energy decomposition analysis (EDA, page S13-S15).<sup>27</sup> These were calculated to be -84 and -58  $\text{kJ mol}^{-1}$  for *exo*- and *endo*- $\pi$ -complexes, respectively, which clearly shows the approx. 30  $\text{kJ mol}^{-1}$  energetic preference for the *exo*-isomer over the *endo*- $\pi$ -complex as can also be seen from the potential energy diagram in Fig. S1. The energies of the optimized structures of the unsaturated  $[Pd^{II}(PPh_3)(CN)(COOR)]$  fragments from the *exo*- and *endo*-complexes show negligible differences in their deformation energies (19-20  $\text{kJ mol}^{-1}$ ). However, the deformation destabilization energies of NBE in *exo*- and *endo*- $\pi$ -complexes are 11 and 19  $\text{kJ mol}^{-1}$ . These results indicate that about 8  $\text{kJ mol}^{-1}$  more structural distortion is needed for the NBE substrate to coordinate to the Pd fragment in the *endo*- than in the *exo*-isomer. This is due to the less favorable interaction of the ethylene bridgehead Pd lone pair or neighboring ligand than the methylene bridgehead in *exo*-isomer.

**Table S3:** Energy decomposition analyses at the BHandHLYP/def2-TZVP level.



**Figure S3.** a) Fragments in *exo*-3tP-O. b) Fragments in *exo*-TS<sub>3\_4</sub>tP-O.

Both interaction and deformation energies are calculated as follows,



$$\text{Interaction energy: INT} = \{E [\text{NBE}]_{\text{SP}} + E [\text{Pd}]_{\text{SP}}\} - E [\text{NBE-Pd}]_{\text{SP}}$$

$$\text{Deformation energy of NBE: DEF}_{\text{NBE}} = E [\text{NBE}]_{\text{SP}} - E [\text{NBE}]_{\text{opt}}$$

$$\text{Deformation energy of Pd: DEF}_{\text{PD}} = E [\text{Pd}]_{\text{SP}} - E [\text{Pd}]_{\text{opt}}$$

| <i>exo</i> -3tP-O                             |                |
|-----------------------------------------------|----------------|
| $E [\text{NBE-Pd}]_{\text{SP}} / \text{a.u.}$ | -1757.89058311 |
| $E [\text{NBE}]_{\text{SP}} / \text{a.u.}$    | -272.644478175 |
| $E [\text{Pd}]_{\text{SP}} / \text{a.u.}$     | -1485.21413706 |
| $E [\text{NBE}]_{\text{opt}} / \text{a.u.}$   | -272.648618708 |
| $E [\text{Pd}]_{\text{opt}} / \text{a.u.}$    | -1485.22174656 |
| INT / kJ·mol <sup>-1</sup>                    | 83.9           |
| DEF <sub>NBE</sub> / kJ·mol <sup>-1</sup>     | 10.9           |
| DEF <sub>PD</sub> / kJ·mol <sup>-1</sup>      | 20.0           |

**Table S3.** Continued

| <i>endo</i> -3tP-O                        |                |
|-------------------------------------------|----------------|
| $E$ [NBE-Pd] <sub>SP</sub> / a.u.         | -1757.87843506 |
| $E$ [NBE] <sub>SP</sub> / a.u.            | -272.641598036 |
| $E$ [Pd] <sub>SP</sub> / a.u.             | -1485.21462768 |
| $E$ [NBE] <sub>opt</sub> / a.u.           | -272.64861831  |
| $E$ [Pd] <sub>opt</sub> / a.u.            | -1485.22174213 |
| INT / kJ·mol <sup>-1</sup>                | 58.3           |
| DEF <sub>NBE</sub> / kJ·mol <sup>-1</sup> | 18.7           |
| DEF <sub>Pd</sub> / kJ·mol <sup>-1</sup>  | 18.7           |
| <i>exo</i> -TS <sub>3_4</sub> tP-O        |                |
| $E$ [NBE-Pd] <sub>SP</sub> / a.u.         | -1757.86537536 |
| $E$ [NBE] <sub>SP</sub> / a.u.            | -272.612517183 |
| $E$ [Pd] <sub>SP</sub> / a.u.             | -1485.18009955 |
| $E$ [NBE] <sub>opt</sub> / a.u.           | -272.648618708 |
| $E$ [Pd] <sub>opt</sub> / a.u.            | -1485.22174656 |
| INT / kJ·mol <sup>-1</sup>                | 191.0          |
| DEF <sub>NBE</sub> / kJ·mol <sup>-1</sup> | 94.8           |
| DEF <sub>Pd</sub> / kJ·mol <sup>-1</sup>  | 109.3          |
| <i>exo</i> -TS <sub>3_4</sub> tP-OMe      |                |
| $E$ [NBE-Pd] <sub>SP</sub> / a.u.         | -1757.86237656 |
| $E$ [NBE] <sub>SP</sub> / a.u.            | -272.611346593 |
| $E$ [Pd] <sub>SP</sub> / a.u.             | -1485.17817528 |
| $E$ [NBE] <sub>opt</sub> / a.u.           | -1485.22174656 |
| $E$ [Pd] <sub>opt</sub> / a.u.            | -272.648618708 |
| INT / kJ·mol <sup>-1</sup>                | 191.3          |
| DEF <sub>NBE</sub> / kJ·mol <sup>-1</sup> | 97.9           |
| DEF <sub>Pd</sub> / kJ·mol <sup>-1</sup>  | 114.4          |
| <i>exo</i> -TS <sub>3_4</sub> tP-N        |                |
| $E$ [NBE-Pd] <sub>SP</sub> / a.u.         | -1757.85326362 |
| $E$ [NBE] <sub>SP</sub> / a.u.            | -272.612202295 |
| $E$ [Pd] <sub>SP</sub> / a.u.             | -1485.20073027 |
| $E$ [NBE] <sub>opt</sub> / a.u.           | -272.648618634 |
| $E$ [Pd] <sub>opt</sub> / a.u.            | -1485.22174656 |
| INT / kJ·mol <sup>-1</sup>                | 105.9          |
| DEF <sub>NBE</sub> / kJ·mol <sup>-1</sup> | 95.6           |
| DEF <sub>Pd</sub> / kJ·mol <sup>-1</sup>  | 55.2           |

### Energy Decomposition Analyses (EDA) for $\pi$ -complexes.

In our previous theoretical investigations<sup>12</sup>, we explained the *exo*-selectivity by the Gibbs energy preference of *exo*- $\pi$ -complex over *endo*- $\pi$ -complex. We examined the interaction energy between NBE and the Pd<sup>II</sup> complex using energy decomposition analysis (EDA, Table S2).

**Table S4.** Energy decomposition analyses for both *exo*- and *endo*- $\pi$ -complexes. Energies are in kJ mol<sup>-1</sup>.

|                                      | <i>exo</i> -3tP-O | <i>exo</i> -3tP-O | $\Delta E$ |
|--------------------------------------|-------------------|-------------------|------------|
| Interaction/ kJ mol <sup>-1</sup>    | -84               | -58               | -26        |
| Pd deformation kJ mol <sup>-1</sup>  | 20                | 19                | 1          |
| NBE deformation kJ mol <sup>-1</sup> | 11                | 19                | -8         |

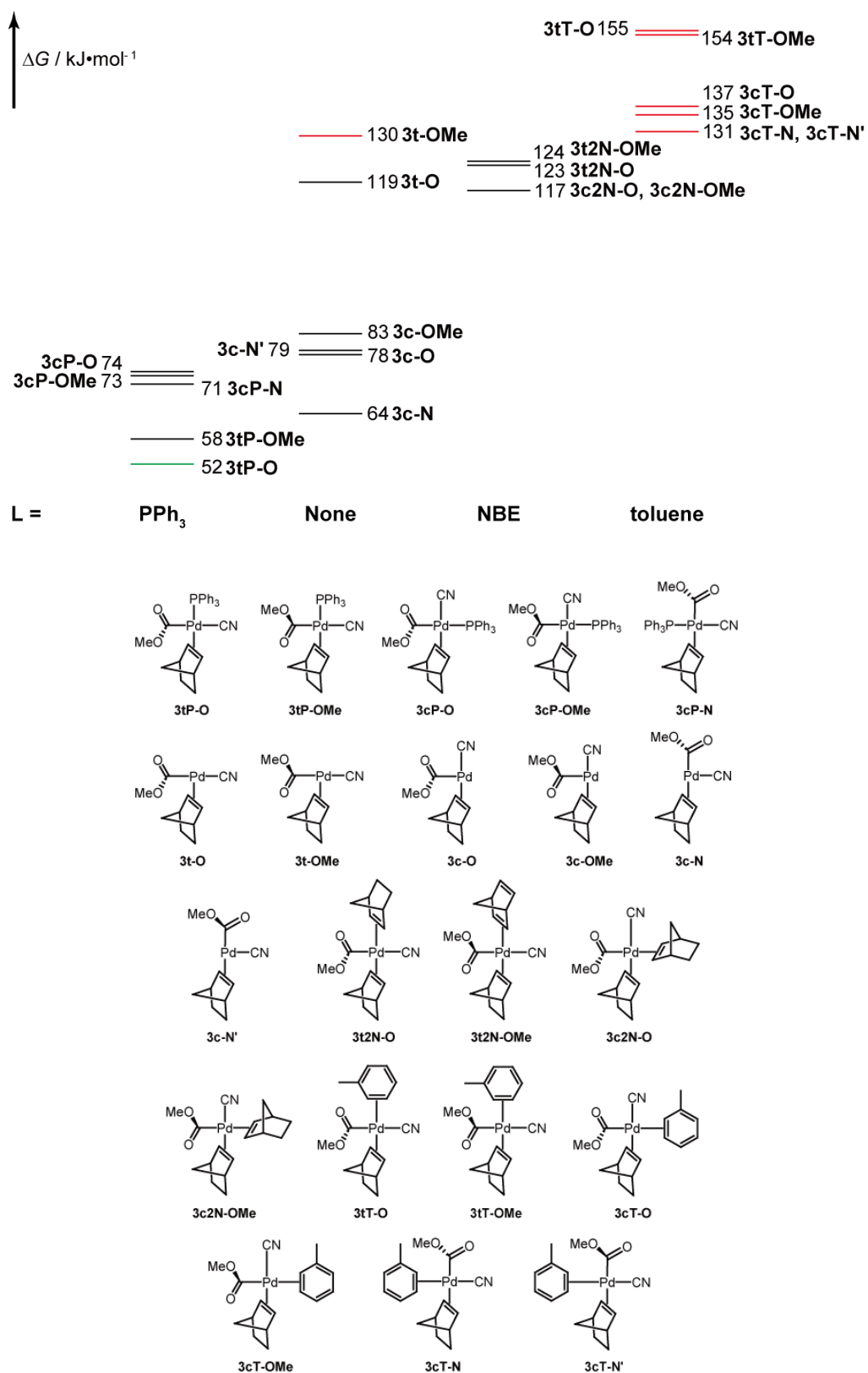
The EDA shows that the binding energies between a NBE and a Pd<sup>II</sup> complex are -84 and -58 kJ mol<sup>-1</sup> for *exo*- and *endo*- $\pi$ -complexes, respectively. The deformation destabilization energies of NBE for *exo*- and *endo*- $\pi$ -complexes are 11 and 19 kJ mol<sup>-1</sup>, respectively. These results indicate that the binding energy is attributed more to the stability of the *exo*- $\pi$ -complex than the deformation destabilization.

### Energy Decomposition Analyses (EDA) for several transition states for migratory insertion.

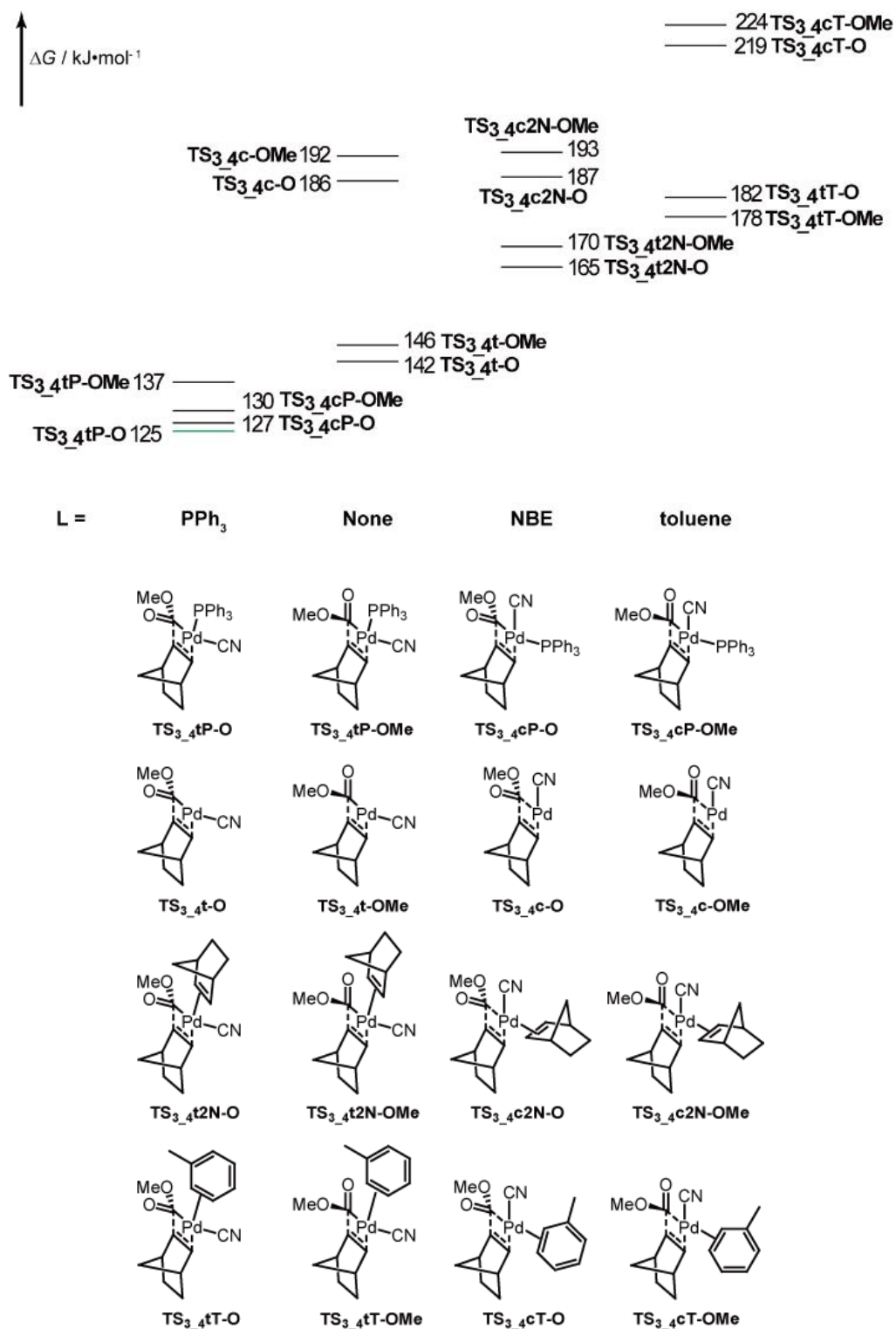
**Table S5.** Energy decomposition analyses for each transition state of migratory insertion. Energies are in kJ mol<sup>-1</sup>.

|                                      | <i>exo</i> -TS <sub>3_4</sub> tP-O | <i>exo</i> -TS <sub>3_4</sub> tP-OMe | <i>exo</i> -TS <sub>3_4</sub> tP-N |
|--------------------------------------|------------------------------------|--------------------------------------|------------------------------------|
| Interaction/ kJ mol <sup>-1</sup>    | -191                               | -191                                 | -106                               |
| Pd deformation kJ mol <sup>-1</sup>  | 109                                | 114                                  | 55                                 |
| NBE deformation kJ mol <sup>-1</sup> | 95                                 | 98                                   | 96                                 |
| Total                                | 13                                 | 21                                   | 45                                 |

This results shows that the deformation destabilizations of NBE fragment are similar in energy. In addition, deformation destabilization of Pd fragment for *exo*-TS<sub>3\_4</sub>tP-N is lowest (55 kJ mol<sup>-1</sup>) in energy than others (109 and 114 kJ mol<sup>-1</sup>). However, Interaction energy between both fragments in *exo*-TS<sub>3\_4</sub>tP-N is very small. Comprehensively, *exo*-TS<sub>3\_4</sub>tP-N has a large destabilization.

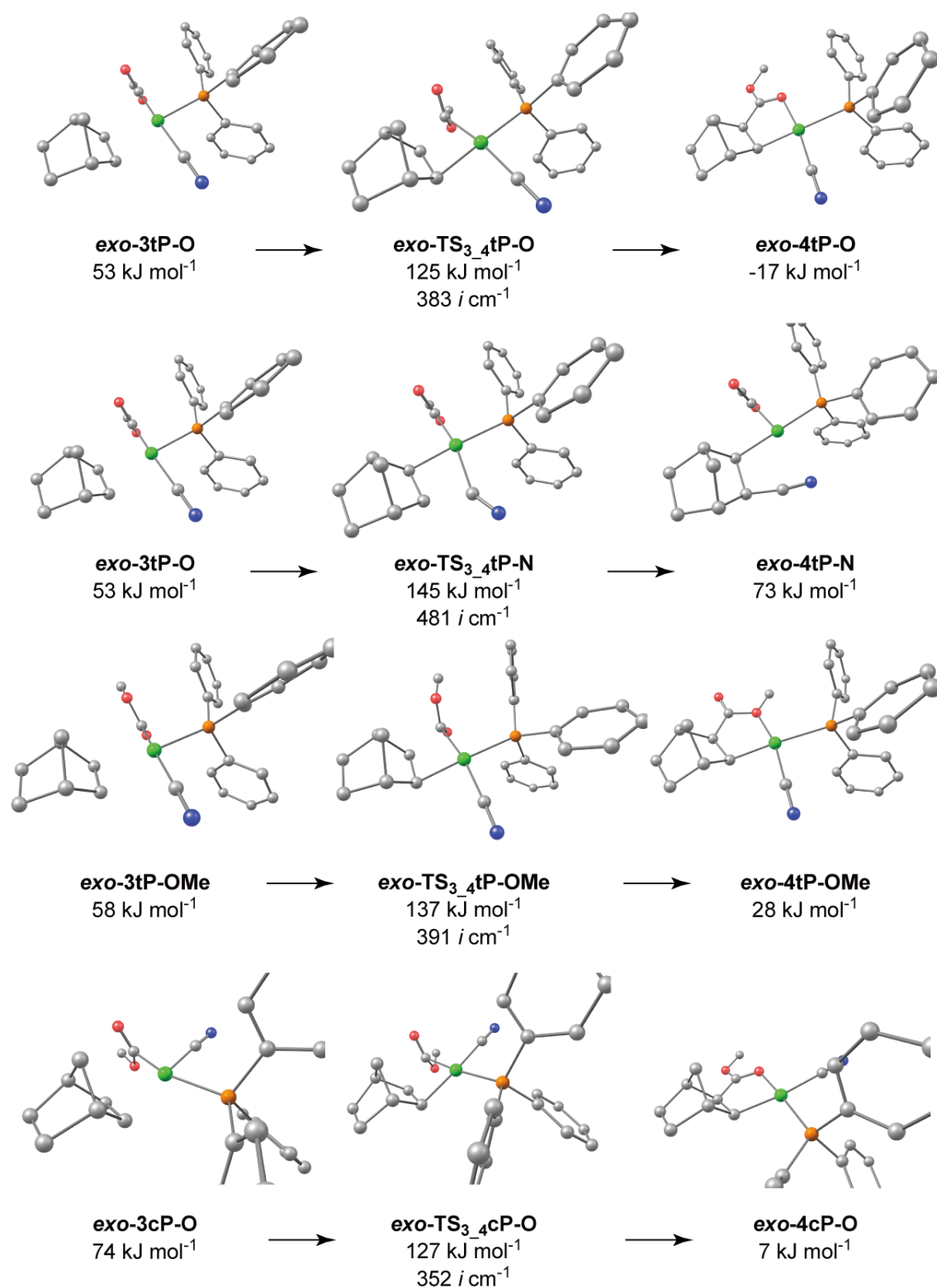


**Figure S4.** Relative Gibbs free energy levels of *exo*- $\pi$ -complexes **3** calculated at BHandHLYP/def2-TZVP level of theory.



**Figure S5.** Potential energy map for all transition states of the migratory insertion of NBE into the Pd–COOMe bond for unsaturated (L = none) Pd(COOMe)(CN)(NBE) complex, and alternative coordination environments (L = second NBE, or solvent toluene) calculated at BHandHLYP/def2-TZVP level of theory.





**Figure S6.** Possible structures for migratory insertion and these relative Gibbs free energies at the BHandHLYP/def2-TZVP level.

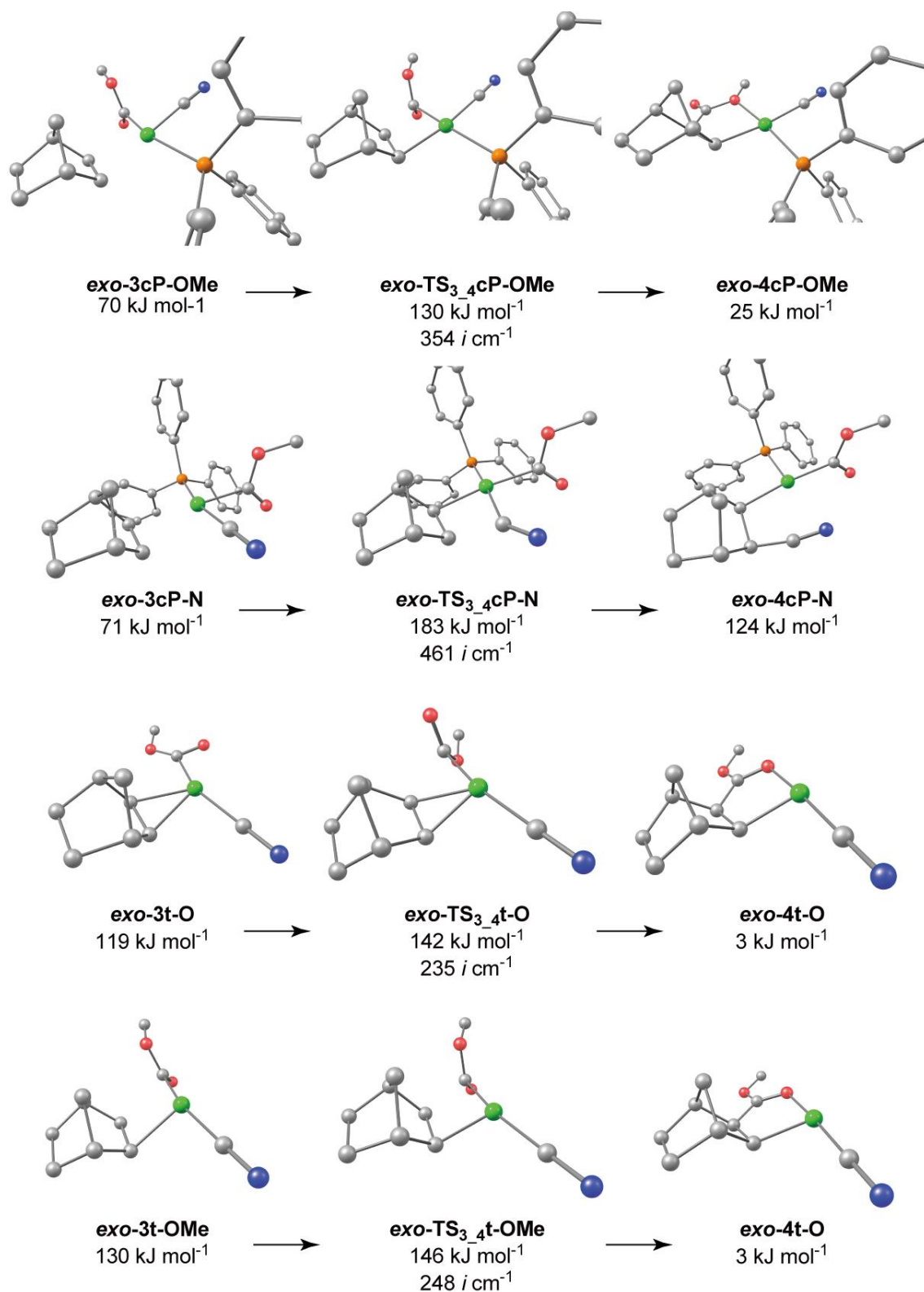


Figure S6. Continued

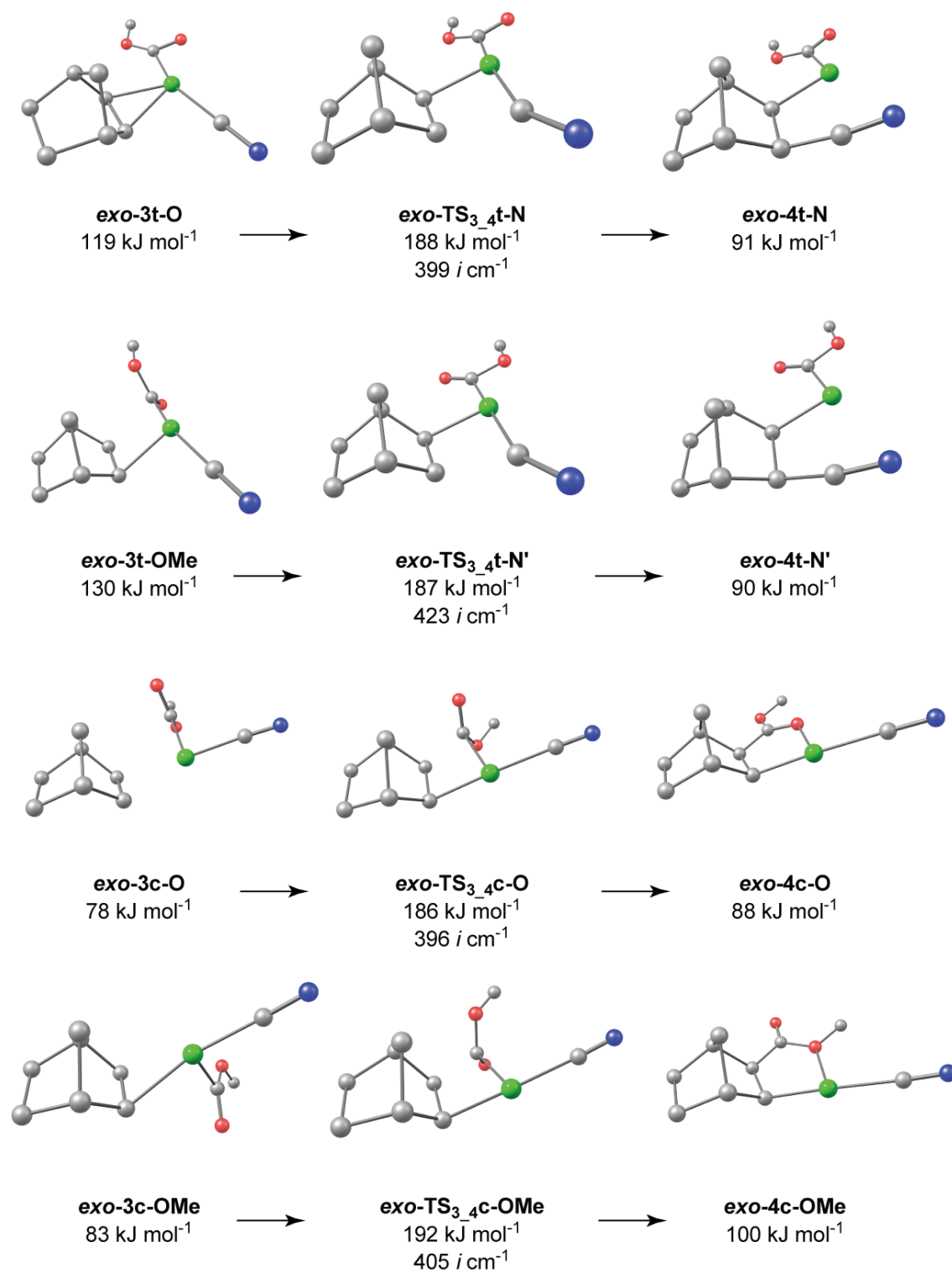


Figure S6. Continued

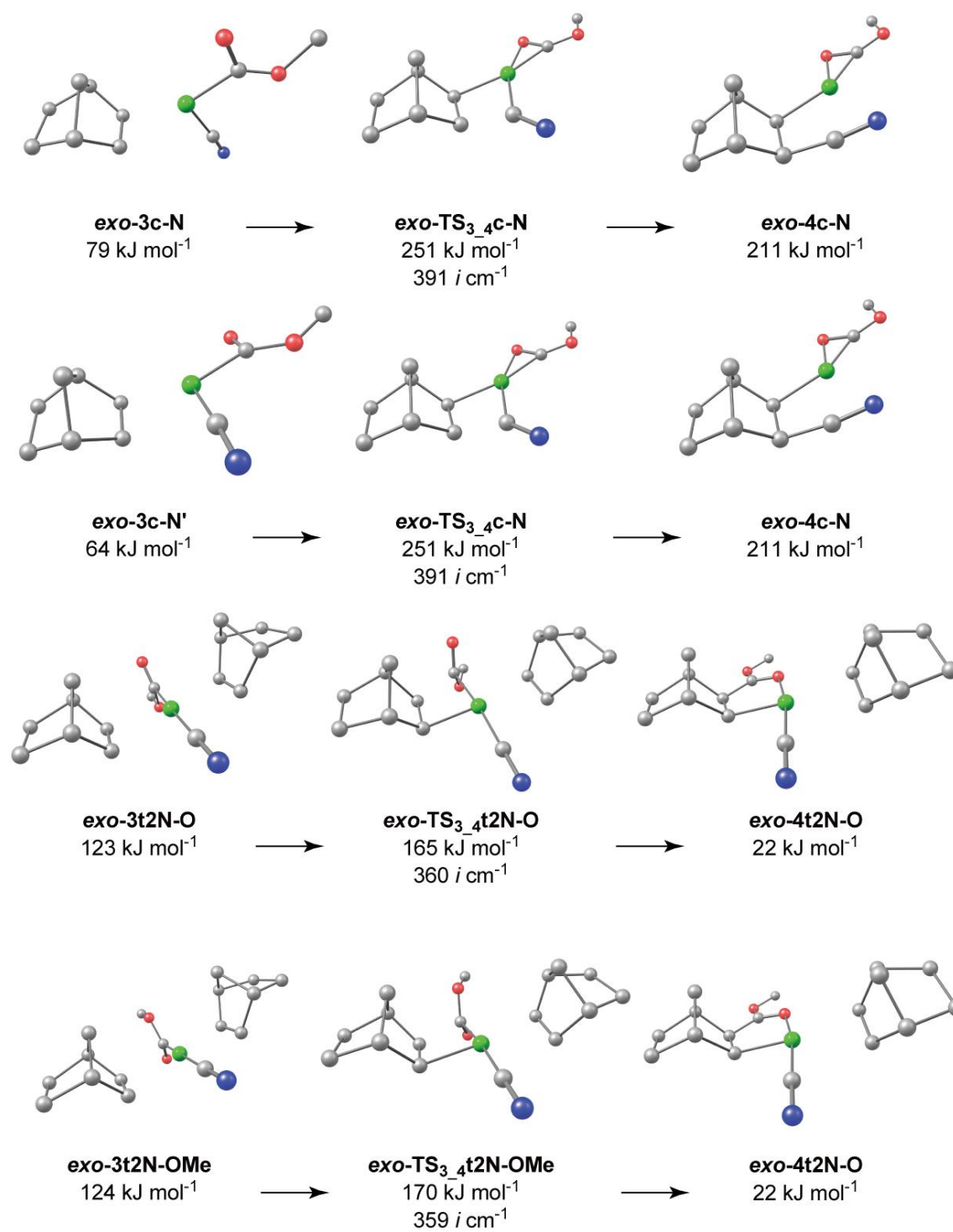


Figure S6. Continued

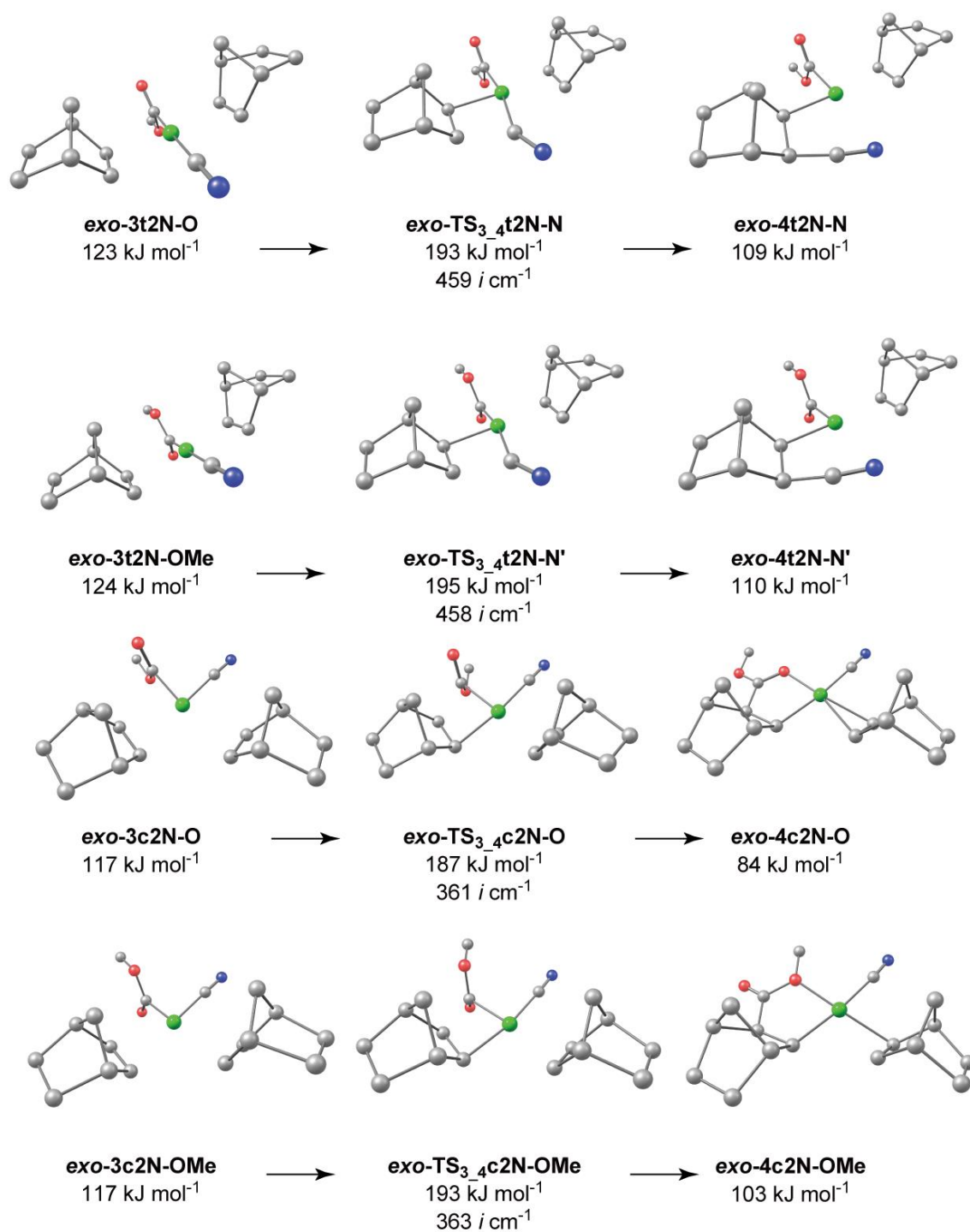


Figure S6. Continued

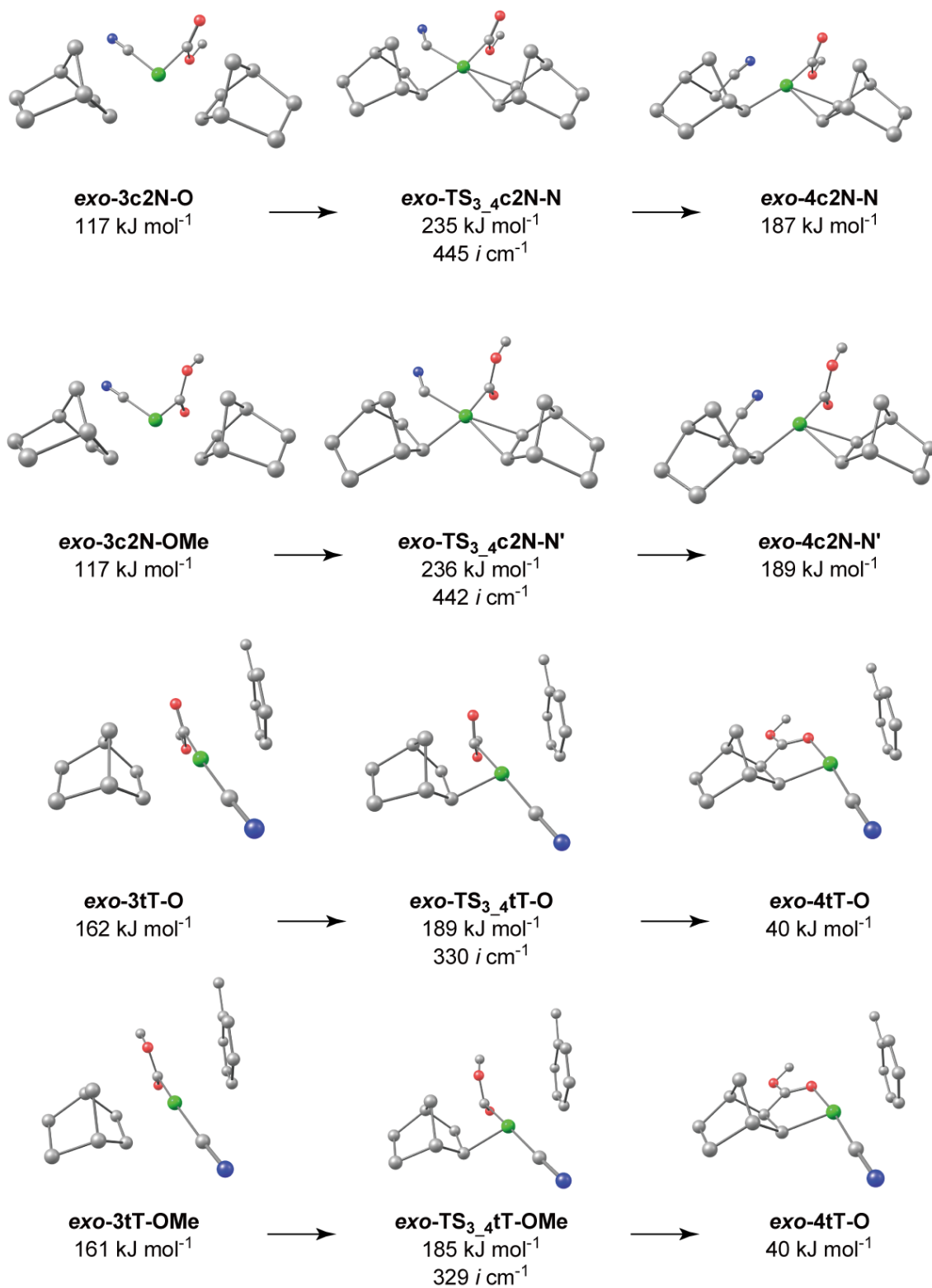


Figure S6. Continued

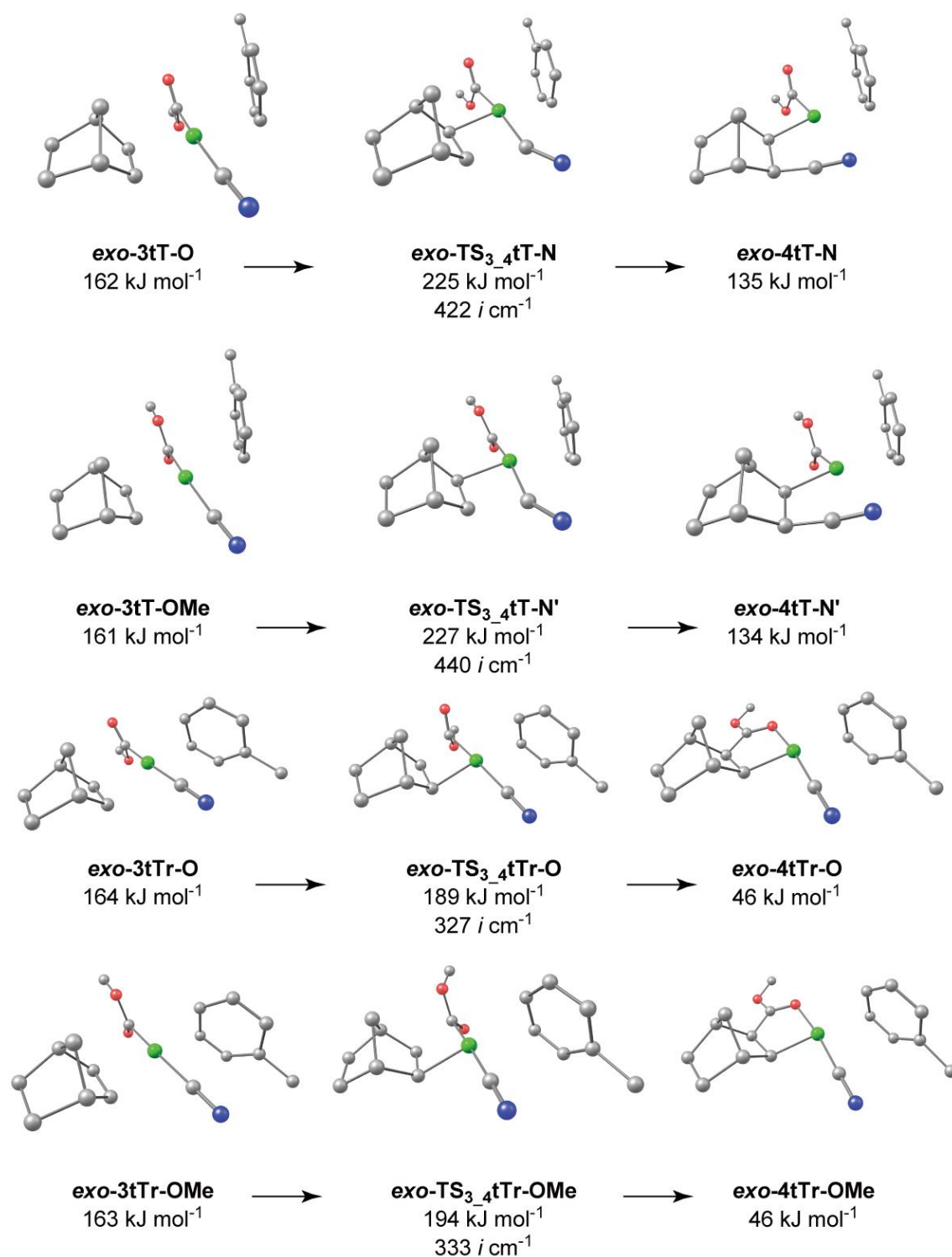
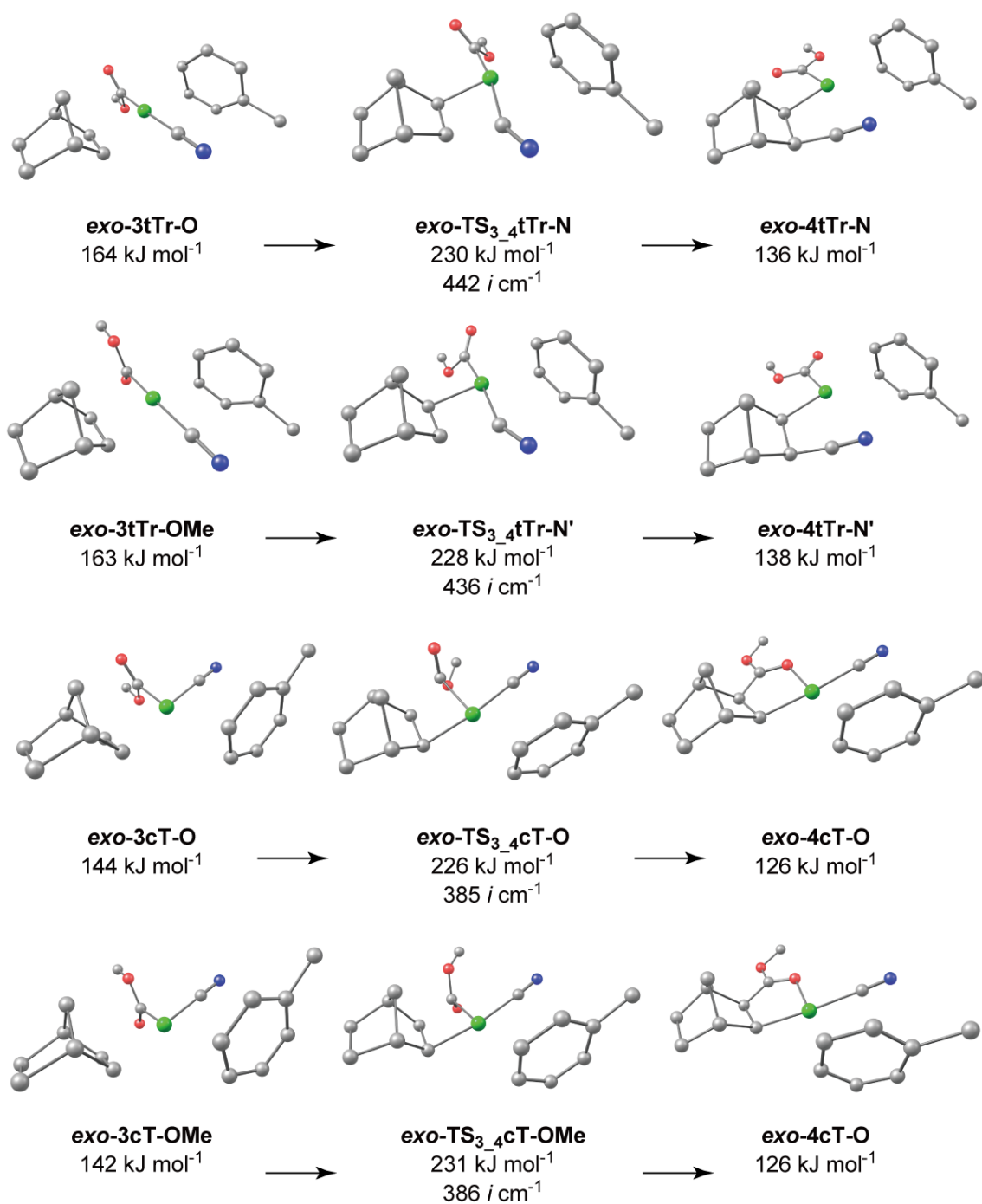


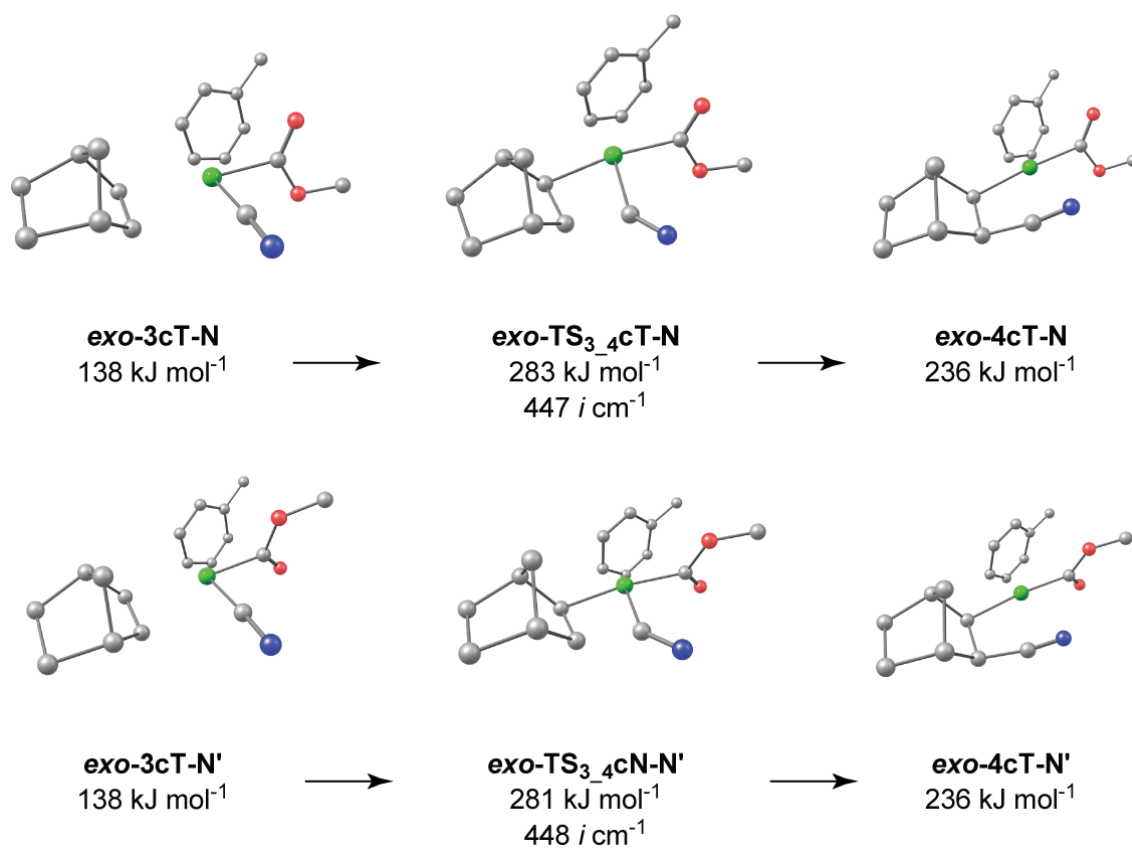
Figure S6. Continued



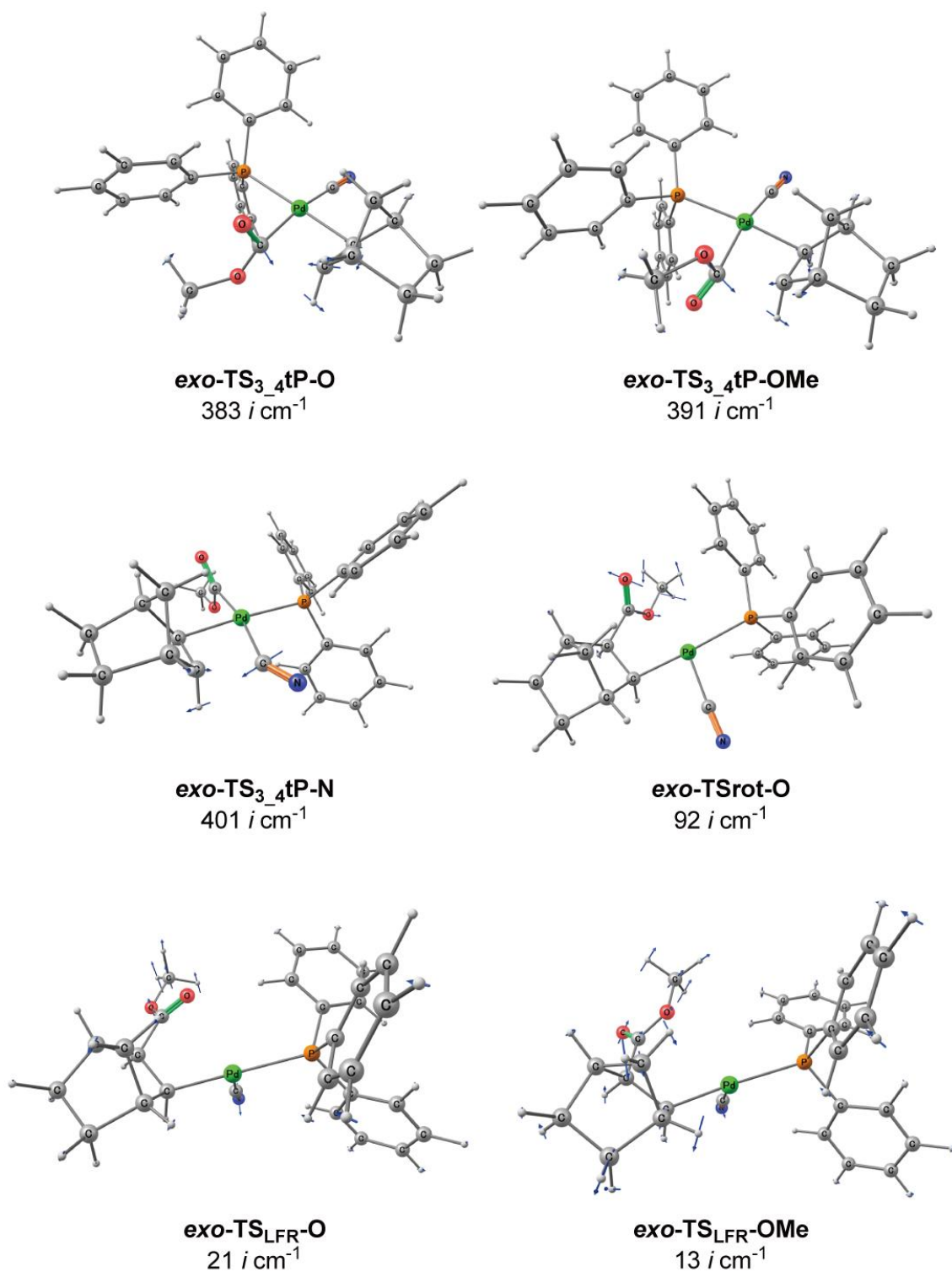


**Figure S6.** Continued

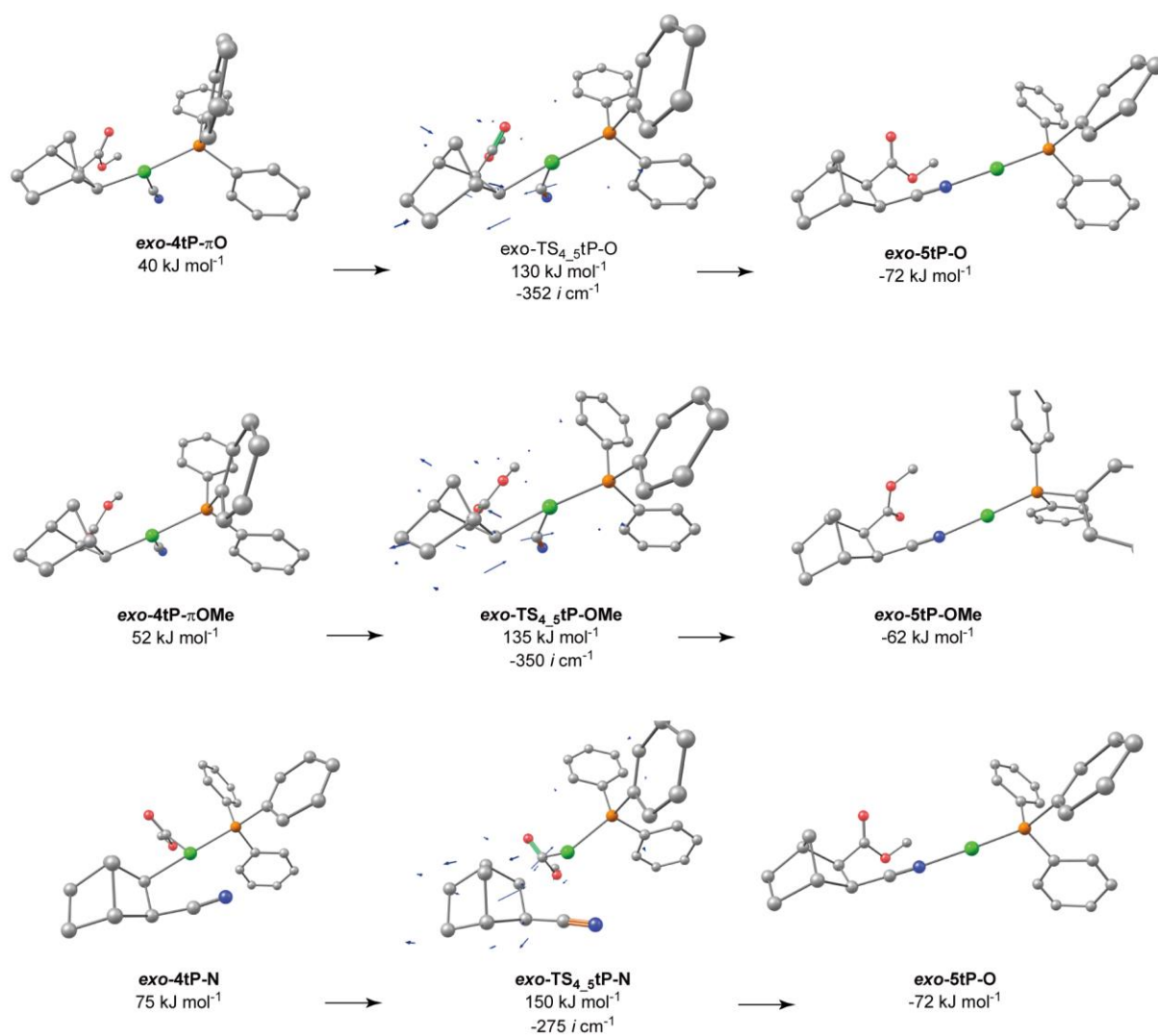




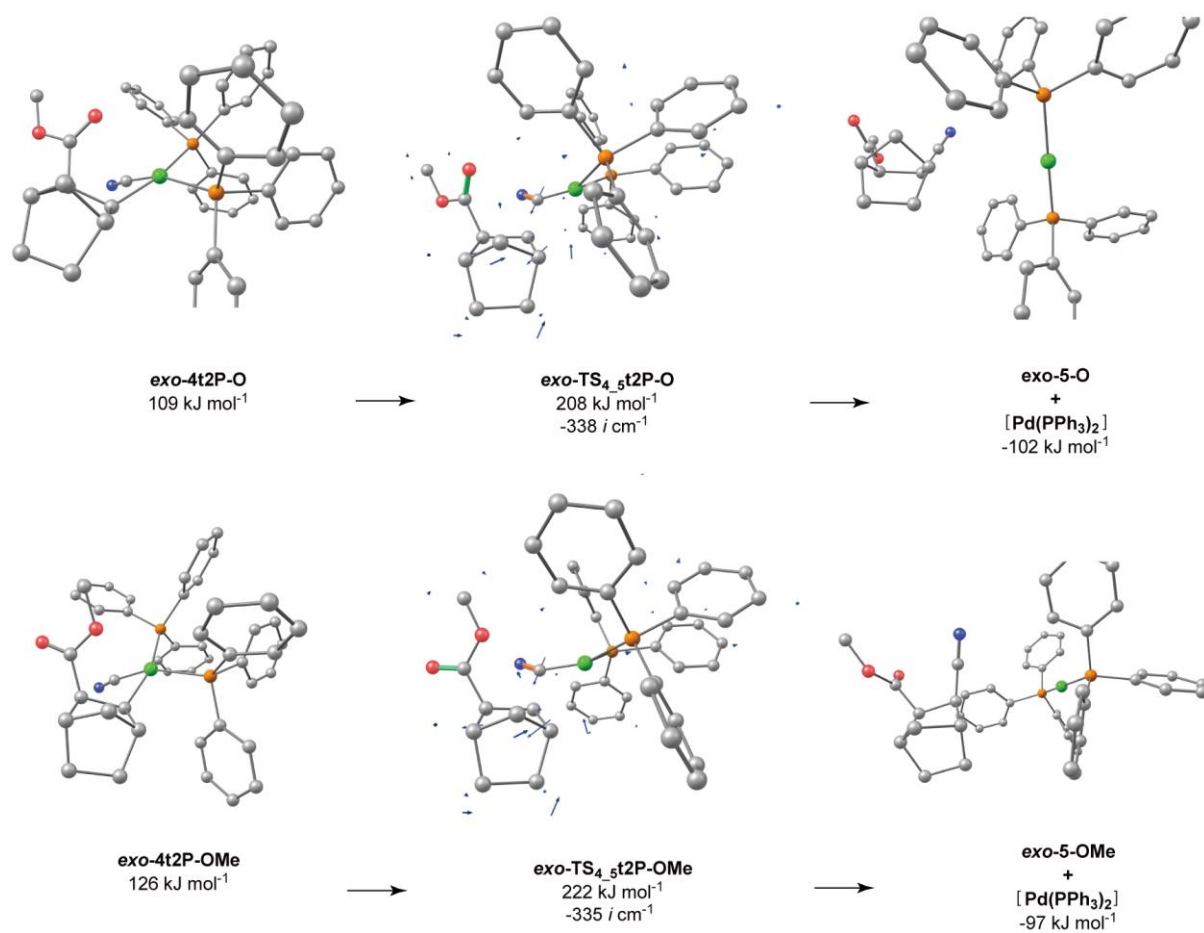
**Figure S6.** Continued



**Figure S7.** The 3D structures for the selected transition states with displacement vectors for normal mode displacements with imaginary frequencies.



**Figure S8.** Comparison of associative mechanism and dissociative mechanism for reductive elimination calculated at the BHandHLYP(PCM)def2-TZVP//BHandHLYP/def2-SVP and M05-2X(PCM)def2-TZVP//BHandHLYP/def2-SVP levels; dissociative mechanism.



**Figure S8.** Continued; associative mechanism.

### Cartesian coordinates for optimized structures

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NBE

|   |              |              |              |
|---|--------------|--------------|--------------|
| 6 | -1.268571000 | 0.661435000  | -0.499823000 |
| 6 | -0.084714000 | 1.117344000  | 0.320211000  |
| 6 | 1.176850000  | 0.773553000  | -0.514539000 |
| 6 | 1.176907000  | -0.773497000 | -0.514513000 |
| 6 | -0.084649000 | -1.117344000 | 0.320223000  |
| 6 | -1.268514000 | -0.661510000 | -0.499843000 |
| 1 | -1.910972000 | 1.309541000  | -1.066056000 |
| 1 | -0.118193000 | 2.135368000  | 0.681710000  |
| 1 | 1.129988000  | 1.194499000  | -1.510522000 |
| 1 | 2.066495000  | 1.165494000  | -0.034437000 |
| 1 | 1.130087000  | -1.194479000 | -1.510482000 |
| 1 | 2.066570000  | -1.165362000 | -0.034382000 |
| 1 | -1.910866000 | -1.309654000 | -1.066087000 |
| 6 | -0.034428000 | 0.000008000  | 1.367879000  |
| 1 | -0.118076000 | -2.135366000 | 0.681733000  |
| 1 | -0.892204000 | -0.000014000 | 2.028305000  |
| 1 | 0.879888000  | 0.000039000  | 1.952643000  |

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toluene

|   |              |              |              |
|---|--------------|--------------|--------------|
| 6 | -1.885297000 | -0.000035000 | 0.008331000  |
| 6 | -1.188651000 | 1.191954000  | 0.001967000  |
| 6 | -1.188557000 | -1.192005000 | 0.001968000  |
| 1 | -1.720331000 | 2.126561000  | 0.001720000  |
| 1 | -1.720186000 | -2.126642000 | 0.001722000  |
| 6 | 0.192033000  | 1.189080000  | -0.008713000 |
| 6 | 0.192093000  | -1.189043000 | -0.008714000 |
| 1 | 0.725133000  | 2.124041000  | -0.017655000 |
| 1 | 0.725259000  | -2.123972000 | -0.017660000 |
| 6 | 0.903785000  | 0.000055000  | -0.011132000 |
| 1 | -2.960101000 | -0.000075000 | 0.013863000  |
| 6 | 2.402304000  | 0.000021000  | 0.009191000  |
| 1 | 2.803416000  | 0.878642000  | -0.481517000 |
| 1 | 2.777106000  | -0.002956000 | 1.028711000  |
| 1 | 2.803450000  | -0.875756000 | -0.486581000 |

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Pd(PPh<sub>3</sub>)

|    |              |              |              |
|----|--------------|--------------|--------------|
| 46 | 0.000468000  | 0.000757000  | 2.569302000  |
| 15 | 0.000538000  | 0.000179000  | 0.355623000  |
| 6  | 1.644857000  | 0.172494000  | -0.430145000 |
| 6  | 2.714564000  | -0.493390000 | 0.153981000  |
| 6  | 3.976639000  | -0.423611000 | -0.396748000 |
| 6  | 4.195349000  | 0.331978000  | -1.533172000 |
| 6  | 3.144044000  | 1.010507000  | -2.114125000 |
| 6  | 1.876361000  | 0.928544000  | -1.568995000 |
| 6  | -0.971439000 | 1.337559000  | -0.430266000 |
| 6  | -0.929250000 | 2.597271000  | 0.153027000  |
| 6  | -1.621299000 | 3.654927000  | -0.397806000 |
| 6  | -2.385932000 | 3.465748000  | -1.533494000 |
| 6  | -2.448176000 | 2.215682000  | -2.113649000 |
| 6  | -1.742798000 | 1.159238000  | -1.568401000 |
| 6  | -0.672778000 | -1.510435000 | -0.428978000 |
| 6  | -0.130351000 | -2.093840000 | -1.563665000 |
| 6  | -0.693970000 | -3.232787000 | -2.107881000 |
| 6  | -1.811393000 | -3.799131000 | -1.530245000 |
| 6  | -2.359849000 | -3.226986000 | -0.397925000 |
| 6  | -1.788527000 | -2.099128000 | 0.151985000  |
| 1  | 2.552183000  | -1.060579000 | 1.053388000  |
| 1  | 4.791911000  | -0.948557000 | 0.067614000  |
| 1  | 5.181043000  | 0.396953000  | -1.957424000 |
| 1  | 3.306933000  | 1.606565000  | -2.994048000 |
| 1  | 1.069033000  | 1.462583000  | -2.034161000 |
| 1  | -0.356186000 | 2.740862000  | 1.051910000  |
| 1  | -1.574066000 | 4.623742000  | 0.065911000  |
| 1  | -2.935486000 | 4.286572000  | -1.957809000 |
| 1  | -3.046447000 | 2.058105000  | -2.993038000 |
| 1  | -1.801826000 | 0.192756000  | -2.032938000 |
| 1  | 0.738999000  | -1.665517000 | -2.026402000 |
| 1  | -0.256535000 | -3.675672000 | -2.984573000 |
| 1  | -2.248596000 | -4.685260000 | -1.953834000 |
| 1  | -3.225426000 | -3.666726000 | 0.063885000  |
| 1  | -2.201427000 | -1.671162000 | 1.048296000  |

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Pd(PPh<sub>3</sub>)<sub>2</sub>

|    |              |              |              |
|----|--------------|--------------|--------------|
| 46 | 0.000028000  | -0.000156000 | 0.001297000  |
| 15 | 2.308363000  | 0.000645000  | 0.000392000  |
| 15 | -2.308279000 | -0.000618000 | 0.000070000  |
| 6  | 3.087346000  | 1.646224000  | 0.178942000  |
| 6  | 2.476292000  | 2.718038000  | -0.458996000 |
| 6  | 3.016056000  | 3.984972000  | -0.384081000 |
| 6  | 4.167550000  | 4.204831000  | 0.347505000  |
| 6  | 4.774656000  | 3.150845000  | 0.999116000  |
| 6  | 4.240084000  | 1.879223000  | 0.913147000  |
| 6  | 3.087053000  | -0.667263000 | -1.514191000 |
| 6  | 4.239737000  | -0.147913000 | -2.083115000 |
| 6  | 4.774260000  | -0.709298000 | -3.227354000 |
| 6  | 4.167159000  | -1.800679000 | -3.814248000 |
| 6  | 3.015766000  | -2.324404000 | -3.257949000 |
| 6  | 2.476075000  | -1.755818000 | -2.123230000 |
| 6  | 3.088780000  | -0.977189000 | 1.335071000  |
| 6  | 4.241418000  | -1.729311000 | 1.167995000  |
| 6  | 4.776993000  | -2.440539000 | 2.225118000  |
| 6  | 4.170927000  | -2.404510000 | 3.464252000  |
| 6  | 3.019624000  | -1.661129000 | 3.641435000  |
| 6  | 2.478905000  | -0.961681000 | 2.582881000  |
| 6  | -3.087535000 | 0.985381000  | -1.329260000 |
| 6  | -2.477153000 | 0.976662000  | -2.576874000 |
| 6  | -3.017016000 | 1.682474000  | -3.631624000 |
| 6  | -4.167992000 | 2.425465000  | -3.450681000 |
| 6  | -4.774565000 | 2.454706000  | -2.211626000 |
| 6  | -4.239830000 | 1.737127000  | -1.158381000 |
| 6  | -3.088003000 | 0.658007000  | 1.518163000  |
| 6  | -2.477545000 | 1.742849000  | 2.134221000  |
| 6  | -3.018056000 | 2.304458000  | 3.272004000  |
| 6  | -4.169736000 | 1.777201000  | 3.824383000  |
| 6  | -4.776353000 | 0.689369000  | 3.230435000  |
| 6  | -4.241044000 | 0.135094000  | 2.083096000  |
| 6  | -3.087506000 | -1.644886000 | -0.188999000 |
| 6  | -4.239703000 | -1.873145000 | -0.925541000 |
| 6  | -4.774483000 | -3.144108000 | -1.019677000 |
| 6  | -4.168109000 | -4.202200000 | -0.374051000 |
| 6  | -3.017152000 | -3.987073000 | 0.359791000  |

|      |              |              |              |
|------|--------------|--------------|--------------|
| 6    | -2.477202000 | -2.720716000 | 0.442922000  |
| 1    | 1.564802000  | 2.554606000  | -1.006259000 |
| 1    | 2.531128000  | 4.802442000  | -0.886493000 |
| 1    | 4.583725000  | 5.193798000  | 0.415570000  |
| 1    | 5.666194000  | 3.315385000  | 1.577216000  |
| 1    | 4.723214000  | 1.069584000  | 1.427714000  |
| 1    | 4.722888000  | 0.702440000  | -1.639088000 |
| 1    | 5.665782000  | -0.290946000 | -3.658950000 |
| 1    | 4.583323000  | -2.236233000 | -4.704741000 |
| 1    | 2.530872000  | -3.168319000 | -3.714592000 |
| 1    | 1.564708000  | -2.148119000 | -1.707790000 |
| 1    | 4.723680000  | -1.769006000 | 0.209057000  |
| 1    | 5.668409000  | -3.023301000 | 2.077207000  |
| 1    | 4.587775000  | -2.958828000 | 4.285747000  |
| 1    | 2.535527000  | -1.635754000 | 4.601039000  |
| 1    | 1.567512000  | -0.406122000 | 2.716297000  |
| 1    | -1.566069000 | 0.421288000  | -2.713115000 |
| 1    | -2.532555000 | 1.662276000  | -4.591172000 |
| 1    | -4.584211000 | 2.984673000  | -4.269180000 |
| 1    | -5.665757000 | 3.037052000  | -2.060756000 |
| 1    | -4.722547000 | 1.771516000  | -0.199481000 |
| 1    | -1.565984000 | 2.137758000  | 1.721769000  |
| 1    | -2.533574000 | 3.145643000  | 3.734081000  |
| 1    | -4.586507000 | 2.207253000  | 4.717277000  |
| 1    | -5.668097000 | 0.268267000  | 3.658913000  |
| 1    | -4.723801000 | -0.712587000 | 1.633540000  |
| 1    | -4.722269000 | -1.060268000 | -1.435501000 |
| 1    | -5.665612000 | -3.304915000 | -1.599456000 |
| 1    | -4.584437000 | -5.190642000 | -0.448511000 |
| 1    | -2.532785000 | -4.807715000 | 0.857564000  |
| 1    | -1.566081000 | -2.560836000 | 0.991894000  |
| 78   |              |              |              |
| 2t2P |              |              |              |
| 46   | -0.002969000 | -0.151090000 | -0.206452000 |
| 15   | 2.373561000  | -0.112046000 | -0.109358000 |
| 15   | -2.368784000 | -0.145040000 | -0.063221000 |
| 8    | 0.019118000  | 2.406036000  | -1.565150000 |
| 8    | -0.165578000 | 2.544958000  | 0.635696000  |



|   |              |              |              |
|---|--------------|--------------|--------------|
| 7 | 0.032456000  | -3.323631000 | 0.247438000  |
| 6 | 0.017318000  | -2.187492000 | 0.099138000  |
| 6 | -0.041791000 | 1.844583000  | -0.509723000 |
| 6 | -0.224028000 | 3.959908000  | 0.519270000  |
| 6 | 3.193243000  | 1.512556000  | 0.022572000  |
| 6 | 3.097181000  | 2.410349000  | -1.034299000 |
| 6 | 3.695300000  | 3.649121000  | -0.957080000 |
| 6 | 4.388331000  | 4.018050000  | 0.180895000  |
| 6 | 4.479154000  | 3.139334000  | 1.239047000  |
| 6 | 3.887769000  | 1.892257000  | 1.160163000  |
| 6 | 3.184583000  | -0.901810000 | -1.540125000 |
| 6 | 4.378934000  | -0.428691000 | -2.066299000 |
| 6 | 4.983130000  | -1.073293000 | -3.127286000 |
| 6 | 4.405060000  | -2.200881000 | -3.673542000 |
| 6 | 3.220842000  | -2.682688000 | -3.152492000 |
| 6 | 2.611139000  | -2.038313000 | -2.095885000 |
| 6 | 2.980635000  | -1.026437000 | 1.339915000  |
| 6 | 4.222860000  | -1.642778000 | 1.345609000  |
| 6 | 4.672230000  | -2.297136000 | 2.473922000  |
| 6 | 3.886829000  | -2.339791000 | 3.609073000  |
| 6 | 2.647535000  | -1.732582000 | 3.610275000  |
| 6 | 2.194456000  | -1.084701000 | 2.479490000  |
| 6 | -3.264499000 | 1.421027000  | -0.336333000 |
| 6 | -3.119812000 | 2.045207000  | -1.568600000 |
| 6 | -3.807934000 | 3.204944000  | -1.850883000 |
| 6 | -4.645979000 | 3.763383000  | -0.904102000 |
| 6 | -4.791474000 | 3.154097000  | 0.324369000  |
| 6 | -4.106295000 | 1.987180000  | 0.607191000  |
| 6 | -2.756323000 | -0.612115000 | 1.649782000  |
| 6 | -2.182378000 | 0.136261000  | 2.671720000  |
| 6 | -2.413966000 | -0.191255000 | 3.989804000  |
| 6 | -3.205739000 | -1.280434000 | 4.304965000  |
| 6 | -3.763077000 | -2.036615000 | 3.296256000  |
| 6 | -3.541686000 | -1.704207000 | 1.972726000  |
| 6 | -3.292020000 | -1.288092000 | -1.139746000 |
| 6 | -4.670587000 | -1.157810000 | -1.272551000 |
| 6 | -5.381404000 | -2.015552000 | -2.082940000 |
| 6 | -4.724344000 | -3.012186000 | -2.780395000 |

|   |              |              |              |
|---|--------------|--------------|--------------|
| 6 | -3.357789000 | -3.145285000 | -2.660168000 |
| 6 | -2.642941000 | -2.288434000 | -1.844596000 |
| 1 | 0.679635000  | 4.343497000  | 0.064785000  |
| 1 | -0.323312000 | 4.337239000  | 1.526399000  |
| 1 | -1.075246000 | 4.258657000  | -0.078315000 |
| 1 | 2.541626000  | 2.150108000  | -1.915344000 |
| 1 | 3.612225000  | 4.329841000  | -1.784757000 |
| 1 | 4.851830000  | 4.986250000  | 0.240653000  |
| 1 | 5.013368000  | 3.417371000  | 2.129453000  |
| 1 | 3.974244000  | 1.218204000  | 1.990569000  |
| 1 | 4.843437000  | 0.446399000  | -1.654197000 |
| 1 | 5.906100000  | -0.691349000 | -3.524586000 |
| 1 | 4.875020000  | -2.701640000 | -4.500695000 |
| 1 | 2.765520000  | -3.563312000 | -3.567547000 |
| 1 | 1.697971000  | -2.432860000 | -1.693378000 |
| 1 | 4.839333000  | -1.623612000 | 0.466288000  |
| 1 | 5.632951000  | -2.779073000 | 2.463203000  |
| 1 | 4.235058000  | -2.855639000 | 4.485610000  |
| 1 | 2.023656000  | -1.777578000 | 4.484058000  |
| 1 | 1.216518000  | -0.639702000 | 2.478857000  |
| 1 | -2.454869000 | 1.635224000  | -2.305937000 |
| 1 | -3.681791000 | 3.677197000  | -2.807977000 |
| 1 | -5.179780000 | 4.670319000  | -1.123852000 |
| 1 | -5.440469000 | 3.581825000  | 1.067024000  |
| 1 | -4.235923000 | 1.521793000  | 1.565509000  |
| 1 | -1.553183000 | 0.976107000  | 2.432548000  |
| 1 | -1.969985000 | 0.398062000  | 4.771654000  |
| 1 | -3.378857000 | -1.541296000 | 5.333345000  |
| 1 | -4.367954000 | -2.892623000 | 3.533925000  |
| 1 | -3.972570000 | -2.308361000 | 1.197426000  |
| 1 | -5.192018000 | -0.378917000 | -0.747824000 |
| 1 | -6.446449000 | -1.902680000 | -2.174483000 |
| 1 | -5.278195000 | -3.679217000 | -3.416176000 |
| 1 | -2.839355000 | -3.918537000 | -3.196887000 |
| 1 | -1.583890000 | -2.415854000 | -1.745106000 |

61

endo-3cP-N\_CN

|    |          |           |           |
|----|----------|-----------|-----------|
| Pd | 0.802380 | -1.159532 | -0.142784 |
|----|----------|-----------|-----------|

|   |           |           |           |
|---|-----------|-----------|-----------|
| O | -0.882389 | -3.011262 | -1.417190 |
| O | -0.909194 | -3.105532 | 0.798150  |
| N | 2.782168  | -3.628122 | -0.212865 |
| C | 2.085794  | -2.718991 | -0.195156 |
| C | -0.510506 | -2.609881 | -0.364523 |
| C | -1.792291 | -4.227898 | 0.739871  |
| H | -1.995868 | -4.490629 | 1.765984  |
| H | -2.706138 | -3.962084 | 0.227168  |
| H | -1.314568 | -5.050493 | 0.226780  |
| C | 4.244299  | 0.858190  | -1.080687 |
| C | 2.800430  | 0.868269  | -0.630866 |
| C | 2.796918  | 0.739511  | 0.693463  |
| C | 4.238822  | 0.650482  | 1.145348  |
| H | 1.959745  | 0.992746  | -1.287216 |
| H | 1.952875  | 0.726458  | 1.358602  |
| P | -0.977013 | 0.467802  | 0.003226  |
| C | -2.404109 | 0.094533  | -1.062026 |
| C | -3.716961 | 0.288803  | -0.658416 |
| C | -2.159398 | -0.389644 | -2.339976 |
| H | -3.935643 | 0.640362  | 0.331340  |
| H | -1.152954 | -0.591147 | -2.656164 |
| C | -4.760463 | 0.019803  | -1.521573 |
| C | -3.202028 | -0.644943 | -3.205839 |
| H | -5.772982 | 0.169001  | -1.193273 |
| H | -2.995143 | -1.021632 | -4.190624 |
| C | -4.505196 | -0.440042 | -2.798117 |
| H | -5.318913 | -0.649578 | -3.468454 |
| C | -1.629279 | 0.651534  | 1.690587  |
| C | -2.368730 | 1.765073  | 2.074649  |
| C | -1.394378 | -0.350546 | 2.620412  |
| H | -2.551806 | 2.559785  | 1.375475  |
| H | -0.829291 | -1.219598 | 2.341796  |
| C | -2.866006 | 1.867626  | 3.355989  |
| C | -1.893696 | -0.245634 | 3.905060  |
| H | -3.435588 | 2.734000  | 3.639046  |
| H | -1.701701 | -1.029309 | 4.614863  |
| C | -2.629197 | 0.861038  | 4.274162  |
| H | -3.014126 | 0.943954  | 5.274353  |

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | -0.509195 | 2.172086  | -0.468213 |
| C | -0.756721 | 2.664101  | -1.741485 |
| C | 0.169164  | 2.979246  | 0.436115  |
| H | -1.286193 | 2.068372  | -2.460022 |
| H | 0.371767  | 2.627926  | 1.430508  |
| C | -0.340258 | 3.931662  | -2.099233 |
| C | 0.578330  | 4.247092  | 0.080143  |
| H | -0.545998 | 4.297045  | -3.088837 |
| H | 1.095638  | 4.858668  | 0.796695  |
| C | 0.326520  | 4.727119  | -1.190086 |
| H | 0.645697  | 5.715182  | -1.467515 |
| C | 4.800173  | -0.570583 | -0.863982 |
| C | 4.882709  | 1.586336  | 0.111441  |
| H | 4.407650  | 0.871421  | 2.189499  |
| H | 5.966373  | 1.538995  | 0.110363  |
| H | 4.559873  | 2.615886  | 0.205271  |
| H | 4.421981  | 1.265512  | -2.065424 |
| C | 4.806262  | -0.709420 | 0.675074  |
| H | 4.196958  | -1.327398 | -1.343208 |
| H | 5.803018  | -0.639398 | -1.268841 |
| H | 5.814314  | -0.833957 | 1.053176  |
| H | 4.218157  | -1.546975 | 1.017901  |

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endo-3cP-N\_Pd LP(O)

|    |              |              |              |
|----|--------------|--------------|--------------|
| Pd | 0.802380000  | -1.159532000 | -0.142784000 |
| O  | -0.238397057 | -3.758414679 | -0.375277372 |
| O  | -1.741824993 | -2.196169387 | 0.089943804  |
| N  | 0.884153050  | -1.975593367 | 2.914300473  |
| C  | 0.878922768  | -1.669748187 | 1.810579085  |
| C  | -0.514697620 | -2.622677846 | -0.172123904 |
| C  | -2.755310629 | -3.199554764 | 0.184953498  |
| H  | -3.668159050 | -2.669897772 | 0.407552450  |
| H  | -2.844720987 | -3.734527701 | -0.750165496 |
| H  | -2.517940888 | -3.893640936 | 0.978706712  |
| C  | 4.244299000  | 0.858190000  | -1.080687000 |
| C  | 2.800430000  | 0.868269000  | -0.630866000 |
| C  | 2.796918000  | 0.739511000  | 0.693463000  |
| C  | 4.238822000  | 0.650482000  | 1.145348000  |

|   |              |              |              |
|---|--------------|--------------|--------------|
| H | 1.959745000  | 0.992746000  | -1.287216000 |
| H | 1.952875000  | 0.726458000  | 1.358602000  |
| P | 0.399414706  | -0.711312395 | -2.482119904 |
| C | 0.065095695  | -2.202548271 | -3.469612144 |
| C | -0.893625780 | -2.243740069 | -4.471300023 |
| C | 0.818878492  | -3.340225835 | -3.214723345 |
| H | -1.505791119 | -1.386361451 | -4.674248268 |
| H | 1.533778070  | -3.344401044 | -2.413219136 |
| C | -1.081360989 | -3.393689730 | -5.212021765 |
| C | 0.639808419  | -4.483842022 | -3.964422989 |
| H | -1.832145926 | -3.413329002 | -5.980898826 |
| H | 1.229968576  | -5.356336939 | -3.752382638 |
| C | -0.310842910 | -4.512462322 | -4.965378240 |
| H | -0.458921825 | -5.407034989 | -5.542617154 |
| C | -1.005096007 | 0.411007081  | -2.754414190 |
| C | -1.179651600 | 1.090706902  | -3.955163542 |
| C | -1.936895701 | 0.587864348  | -1.742293558 |
| H | -0.463664374 | 0.979628018  | -4.748228508 |
| H | -1.821620840 | 0.068778801  | -0.809843306 |
| C | -2.264590787 | 1.920652592  | -4.138820408 |
| C | -3.024114722 | 1.420918050  | -1.928362921 |
| H | -2.386698132 | 2.439886193  | -5.071898697 |
| H | -3.736547240 | 1.549328349  | -1.134146586 |
| C | -3.189754741 | 2.086971046  | -3.124547569 |
| H | -4.033367047 | 2.737601159  | -3.267467715 |
| C | 1.780333227  | 0.101031947  | -3.364646432 |
| C | 2.690849512  | -0.630941337 | -4.112807293 |
| C | 1.973167437  | 1.470741431  | -3.237374174 |
| H | 2.564568317  | -1.689280086 | -4.237311159 |
| H | 1.282975716  | 2.064865881  | -2.668214545 |
| C | 3.763578663  | -0.008430850 | -4.720975701 |
| C | 3.040502305  | 2.092214566  | -3.850671639 |
| H | 4.455319688  | -0.591884636 | -5.300825505 |
| H | 3.168171557  | 3.154191527  | -3.745862118 |
| C | 3.940888253  | 1.353985227  | -4.593395341 |
| H | 4.772877614  | 1.838410373  | -5.071135102 |
| C | 4.800173000  | -0.570583000 | -0.863982000 |
| C | 4.882709000  | 1.586336000  | 0.111441000  |

|   |             |              |              |
|---|-------------|--------------|--------------|
| H | 4.407650000 | 0.871421000  | 2.189499000  |
| H | 5.966373000 | 1.538995000  | 0.110363000  |
| H | 4.559873000 | 2.615886000  | 0.205271000  |
| H | 4.421981000 | 1.265512000  | -2.065424000 |
| C | 4.806262000 | -0.709420000 | 0.675074000  |
| H | 4.196958000 | -1.327398000 | -1.343208000 |
| H | 5.803018000 | -0.639398000 | -1.268841000 |
| H | 5.814314000 | -0.833957000 | 1.053176000  |
| H | 4.218157000 | -1.546975000 | 1.017901000  |

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endo-3cP-N\_Pd LP(OR)

|    |              |              |              |
|----|--------------|--------------|--------------|
| Pd | 0.802380000  | -1.159532000 | -0.142784000 |
| O  | -1.764880126 | -2.182242224 | -0.647462584 |
| O  | -0.210879741 | -3.720196595 | -0.277171059 |
| N  | 1.088730339  | -1.636277450 | -3.258731002 |
| C  | 0.997020973  | -1.440080092 | -2.134068599 |
| C  | -0.642768166 | -2.472745573 | -0.394511918 |
| C  | -1.167672748 | -4.749764944 | -0.536975500 |
| H  | -0.637659880 | -5.679378511 | -0.401757022 |
| H  | -1.994417671 | -4.679407928 | 0.155975083  |
| H  | -1.535488431 | -4.668339271 | -1.550003464 |
| C  | 4.244299000  | 0.858190000  | -1.080687000 |
| C  | 2.800430000  | 0.868269000  | -0.630866000 |
| C  | 2.796918000  | 0.739511000  | 0.693463000  |
| C  | 4.238822000  | 0.650482000  | 1.145348000  |
| H  | 1.959745000  | 0.992746000  | -1.287216000 |
| H  | 1.952875000  | 0.726458000  | 1.358602000  |
| P  | 0.401787841  | -1.132343996 | 2.239349718  |
| C  | -1.351674177 | -1.308382357 | 2.692202906  |
| C  | -1.779142860 | -2.073843649 | 3.767173498  |
| C  | -2.295958892 | -0.629719672 | 1.933776653  |
| H  | -1.073320310 | -2.626751742 | 4.356359085  |
| H  | -1.991231280 | -0.069189570 | 1.069800425  |
| C  | -3.120865622 | -2.144352200 | 4.085145204  |
| C  | -3.634407299 | -0.690005597 | 2.260724815  |
| H  | -3.438449201 | -2.746369312 | 4.916981561  |
| H  | -4.352336781 | -0.160601122 | 1.661720923  |
| C  | -4.049448099 | -1.447463229 | 3.337974812  |

|                 |              |              |              |
|-----------------|--------------|--------------|--------------|
| H               | -5.093649624 | -1.504135317 | 3.586618800  |
| C               | 1.294881681  | -2.448383439 | 3.120723137  |
| C               | 1.512638175  | -2.395725500 | 4.493337343  |
| C               | 1.763684481  | -3.542738327 | 2.409014874  |
| H               | 1.170430989  | -1.551712796 | 5.062955693  |
| H               | 1.601823859  | -3.603445967 | 1.349620097  |
| C               | 2.176949424  | -3.417648067 | 5.136763768  |
| C               | 2.429976589  | -4.566426227 | 3.056134171  |
| H               | 2.338410086  | -3.363548626 | 6.197967110  |
| H               | 2.789007141  | -5.406879042 | 2.490833354  |
| C               | 2.636916834  | -4.506020273 | 4.418282393  |
| H               | 3.158388759  | -5.300530825 | 4.920524813  |
| C               | 0.926750051  | 0.396077354  | 3.096108271  |
| C               | 0.026627956  | 1.413898510  | 3.376090012  |
| C               | 2.264574584  | 0.584277979  | 3.419053116  |
| H               | -1.014968553 | 1.295492391  | 3.146774152  |
| H               | 2.984430839  | -0.187009778 | 3.218520514  |
| C               | 0.452956670  | 2.587291366  | 3.967299775  |
| C               | 2.687916147  | 1.753261185  | 4.015565098  |
| H               | -0.260480095 | 3.362172594  | 4.181114710  |
| H               | 3.726239648  | 1.876597591  | 4.264064551  |
| C               | 1.783309024  | 2.760050086  | 4.290115585  |
| H               | 2.113403144  | 3.671216089  | 4.754791480  |
| C               | 4.800173000  | -0.570583000 | -0.863982000 |
| C               | 4.882709000  | 1.586336000  | 0.111441000  |
| H               | 4.407650000  | 0.871421000  | 2.189499000  |
| H               | 5.966373000  | 1.538995000  | 0.110363000  |
| H               | 4.559873000  | 2.615886000  | 0.205271000  |
| H               | 4.421981000  | 1.265512000  | -2.065424000 |
| C               | 4.806262000  | -0.709420000 | 0.675074000  |
| H               | 4.196958000  | -1.327398000 | -1.343208000 |
| H               | 5.803018000  | -0.639398000 | -1.268841000 |
| H               | 5.814314000  | -0.833957000 | 1.053176000  |
| H               | 4.218157000  | -1.546975000 | 1.017901000  |
| 61              |              |              |              |
| endo-3cP-N_PPh3 |              |              |              |
| Pd              | 0.802380000  | -1.159532000 | -0.142784000 |
| O               | -1.248354889 | -2.835237938 | 0.794209731  |

|   |              |              |              |
|---|--------------|--------------|--------------|
| O | -1.000779654 | -2.816689385 | -1.409355360 |
| N | -1.617828805 | 0.862907716  | -0.408745262 |
| C | -0.727275728 | 0.150654681  | -0.302066479 |
| C | -0.684186896 | -2.450028631 | -0.175759212 |
| C | -2.131748047 | -3.680275807 | -1.543858808 |
| H | -2.236348558 | -3.858806790 | -2.602425992 |
| H | -1.961674509 | -4.608711741 | -1.016867825 |
| H | -3.016336977 | -3.197921334 | -1.152731258 |
| C | 3.601625621  | 1.659612863  | -1.149916913 |
| C | 2.204450352  | 1.305157130  | -0.692248247 |
| C | 2.233340169  | 1.213542268  | 0.634857760  |
| C | 3.648328988  | 1.514145769  | 1.080567912  |
| H | 1.360938195  | 1.189978670  | -1.346665758 |
| H | 1.421151519  | 0.998249898  | 1.304923165  |
| P | 2.043829935  | -3.231065328 | -0.085112113 |
| C | 1.230301764  | -4.549567014 | 0.869047089  |
| C | 1.219440646  | -5.876128318 | 0.463659150  |
| C | 0.609968663  | -4.207455493 | 2.063037706  |
| H | 1.671397083  | -6.164921834 | -0.465515845 |
| H | 0.566382260  | -3.179874604 | 2.372368562  |
| C | 0.615146093  | -6.840703392 | 1.245145203  |
| C | 0.018673786  | -5.173929216 | 2.849340791  |
| H | 0.608836539  | -7.863732284 | 0.915588328  |
| H | -0.459161810 | -4.891641312 | 3.769386543  |
| C | 0.020675169  | -6.493164749 | 2.441809092  |
| H | -0.449897082 | -7.245391397 | 3.048529136  |
| C | 2.356559428  | -3.913305461 | -1.741356114 |
| C | 3.346222879  | -4.863551558 | -1.969082077 |
| C | 1.580507065  | -3.484644291 | -2.808084602 |
| H | 3.968334800  | -5.200500937 | -1.160768932 |
| H | 0.809054762  | -2.754876433 | -2.651554125 |
| C | 3.547555874  | -5.376093969 | -3.232568538 |
| C | 1.784233859  | -3.999674848 | -4.074530178 |
| H | 4.316218635  | -6.109741074 | -3.394025382 |
| H | 1.176248993  | -3.656255291 | -4.891381630 |
| C | 2.765692591  | -4.944611249 | -4.288434075 |
| H | 2.926266637  | -5.342101167 | -5.274154713 |
| C | 3.711446015  | -3.114770958 | 0.657332898  |



|   |             |              |              |
|---|-------------|--------------|--------------|
| C | 3.937664435 | -3.451652398 | 1.983947231  |
| C | 4.769769299 | -2.616512137 | -0.091784785 |
| H | 3.142776410 | -3.847416865 | 2.586485674  |
| H | 4.626803768 | -2.350956504 | -1.122479803 |
| C | 5.190520823 | -3.298016565 | 2.545091466  |
| C | 6.021723170 | -2.470087478 | 0.467444760  |
| H | 5.347213890 | -3.569498567 | 3.573145242  |
| H | 6.829196121 | -2.089425219 | -0.131022630 |
| C | 6.235970173 | -2.808758849 | 1.789078534  |
| H | 7.211706984 | -2.694348726 | 2.224919443  |
| C | 4.509904928 | 0.430595704  | -0.901130321 |
| C | 4.027492871 | 2.558746581  | 0.020180834  |
| H | 3.752893904 | 1.797798765  | 2.117956654  |
| H | 5.086151154 | 2.794914985  | 0.014088004  |
| H | 3.447812288 | 3.470911237  | 0.090369270  |
| H | 3.668114689 | 2.074026727  | -2.145421517 |
| C | 4.550489605 | 0.337194532  | 0.640827936  |
| H | 4.124822789 | -0.468978139 | -1.358047696 |
| H | 5.496487269 | 0.614774502  | -1.309881912 |
| H | 5.555876245 | 0.488796320  | 1.016133178  |
| H | 4.200247055 | -0.615537415 | 1.007608815  |

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endo-3cP-O\_COOR

|    |           |           |           |
|----|-----------|-----------|-----------|
| Pd | 1.042937  | -0.806534 | -0.068837 |
| O  | 3.350748  | -1.887266 | -1.333701 |
| O  | 3.250419  | -2.302149 | 0.840396  |
| N  | -0.060204 | -3.711427 | -0.225471 |
| C  | 0.361944  | -2.648365 | -0.179956 |
| C  | 2.781438  | -1.776801 | -0.290627 |
| C  | 4.450694  | -3.064779 | 0.743444  |
| H  | 4.318017  | -3.888694 | 0.055967  |
| H  | 4.645666  | -3.433262 | 1.738638  |
| H  | 5.271003  | -2.446045 | 0.404134  |
| C  | 3.183013  | 2.334577  | -0.991854 |
| C  | 1.896091  | 1.693501  | -0.518442 |
| C  | 2.029235  | 1.452672  | 0.789755  |
| C  | 3.407227  | 1.937224  | 1.196965  |
| H  | 1.019977  | 1.587975  | -1.128555 |

|   |           |           |           |
|---|-----------|-----------|-----------|
| H | 1.283710  | 1.117589  | 1.488167  |
| P | -1.319077 | 0.041435  | 0.032299  |
| C | -2.288571 | -0.645949 | -1.344599 |
| C | -3.662041 | -0.827463 | -1.271916 |
| C | -1.628566 | -0.974320 | -2.519086 |
| H | -4.192393 | -0.598550 | -0.366905 |
| H | -0.560930 | -0.869385 | -2.582765 |
| C | -4.359700 | -1.318294 | -2.356132 |
| C | -2.328077 | -1.456352 | -3.607276 |
| H | -5.422279 | -1.463068 | -2.284139 |
| H | -1.801576 | -1.711073 | -4.508686 |
| C | -3.694854 | -1.629405 | -3.526753 |
| H | -4.239545 | -2.016383 | -4.368743 |
| C | -2.219060 | -0.396851 | 1.553459  |
| C | -3.319801 | 0.328612  | 1.994510  |
| C | -1.810910 | -1.503707 | 2.284790  |
| H | -3.650322 | 1.194027  | 1.451243  |
| H | -0.970339 | -2.085017 | 1.958116  |
| C | -3.995636 | -0.045765 | 3.136898  |
| C | -2.490901 | -1.878515 | 3.427269  |
| H | -4.844886 | 0.525750  | 3.464824  |
| H | -2.163608 | -2.740477 | 3.979198  |
| C | -3.582108 | -1.151057 | 3.855949  |
| H | -4.108552 | -1.442178 | 4.746811  |
| C | -1.565482 | 1.844671  | -0.112881 |
| C | -1.953666 | 2.432681  | -1.307258 |
| C | -1.271454 | 2.666677  | 0.968829  |
| H | -2.190952 | 1.821458  | -2.157547 |
| H | -0.972525 | 2.237155  | 1.907860  |
| C | -2.050317 | 3.807529  | -1.416101 |
| C | -1.375845 | 4.036736  | 0.862189  |
| H | -2.357300 | 4.245116  | -2.348615 |
| H | -1.153378 | 4.655475  | 1.712502  |
| C | -1.764140 | 4.612410  | -0.333217 |
| H | -1.844764 | 5.680887  | -0.416834 |
| C | 4.315192  | 1.284487  | -0.947474 |
| C | 3.517921  | 3.155512  | 0.264978  |
| H | 3.530811  | 2.107533  | 2.256388  |

|   |          |           |           |
|---|----------|-----------|-----------|
| H | 4.512308 | 3.587547  | 0.241391  |
| H | 2.788520 | 3.926408  | 0.479343  |
| H | 3.102233 | 2.867333  | -1.927842 |
| C | 4.474918 | 1.016227  | 0.566919  |
| H | 4.076897 | 0.395295  | -1.509790 |
| H | 5.219457 | 1.710955  | -1.364952 |
| H | 5.457846 | 1.310716  | 0.915037  |
| H | 4.330744 | -0.018079 | 0.838221  |

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endo-3cP-O\_Pd LP(O)

|    |              |              |              |
|----|--------------|--------------|--------------|
| Pd | 1.043076000  | -0.806225000 | -0.067002000 |
| O  | 3.350171000  | -1.887959000 | -1.331961000 |
| O  | 3.251115000  | -2.301013000 | 0.842544000  |
| N  | -0.059586000 | -3.711810000 | -0.217880000 |
| C  | 0.362164000  | -2.648475000 | -0.174706000 |
| C  | 2.781498000  | -1.776630000 | -0.288632000 |
| C  | 4.451277000  | -3.063727000 | 0.745561000  |
| H  | 4.318264000  | -3.888156000 | 0.058758000  |
| H  | 4.646736000  | -3.431496000 | 1.740926000  |
| H  | 5.271471000  | -2.445277000 | 0.405417000  |
| C  | 1.232700502  | 3.057508174  | -0.640366536 |
| C  | 1.357682872  | 1.835809352  | 0.244603754  |
| C  | 2.567825128  | 1.310311648  | 0.028912246  |
| C  | 3.259055783  | 2.183688197  | -1.000099128 |
| H  | 0.633061962  | 1.555881308  | 0.984541378  |
| H  | 3.056036707  | 0.513216392  | 0.560076631  |
| P  | -1.319114000 | 0.041530000  | 0.032235000  |
| C  | -2.284945000 | -0.646558000 | -1.346845000 |
| C  | -3.656889000 | -0.838943000 | -1.274361000 |
| C  | -1.622994000 | -0.964935000 | -2.523077000 |
| H  | -4.188544000 | -0.618225000 | -0.368081000 |
| H  | -0.556154000 | -0.851753000 | -2.586677000 |
| C  | -4.351249000 | -1.330531000 | -2.360444000 |
| C  | -2.319231000 | -1.447453000 | -3.613059000 |
| H  | -5.412618000 | -1.483972000 | -2.288507000 |
| H  | -1.791211000 | -1.694231000 | -4.515786000 |
| C  | -3.684659000 | -1.631355000 | -3.532695000 |
| H  | -4.226743000 | -2.018885000 | -4.376108000 |

|                      |              |              |              |
|----------------------|--------------|--------------|--------------|
| C                    | -2.222091000 | -0.396764000 | 1.551540000  |
| C                    | -3.324337000 | 0.328386000  | 1.989403000  |
| C                    | -1.814821000 | -1.502613000 | 2.284871000  |
| H                    | -3.654152000 | 1.193071000  | 1.444531000  |
| H                    | -0.973140000 | -2.083684000 | 1.960637000  |
| C                    | -4.002525000 | -0.045347000 | 3.130588000  |
| C                    | -2.497157000 | -1.876770000 | 3.426179000  |
| H                    | -4.852897000 | 0.525913000  | 3.456039000  |
| H                    | -2.170497000 | -2.737950000 | 3.979698000  |
| C                    | -3.589849000 | -1.149662000 | 3.851654000  |
| H                    | -4.118101000 | -1.440273000 | 4.741613000  |
| C                    | -1.566379000 | 1.844652000  | -0.113018000 |
| C                    | -1.956846000 | 2.432904000  | -1.306492000 |
| C                    | -1.271391000 | 2.666388000  | 0.968660000  |
| H                    | -2.195047000 | 1.821910000  | -2.156680000 |
| H                    | -0.970898000 | 2.236620000  | 1.907087000  |
| C                    | -2.054697000 | 3.807755000  | -1.414539000 |
| C                    | -1.376892000 | 4.036396000  | 0.862828000  |
| H                    | -2.363497000 | 4.245530000  | -2.346370000 |
| H                    | -1.153596000 | 4.654905000  | 1.713093000  |
| C                    | -1.767422000 | 4.612352000  | -0.331749000 |
| H                    | -1.848931000 | 5.680814000  | -0.414753000 |
| C                    | 1.155018648  | 2.605498279  | -2.115527285 |
| C                    | 2.689081376  | 3.548253824  | -0.577935596 |
| H                    | 4.333804897  | 2.080515853  | -1.030598752 |
| H                    | 2.904522402  | 4.340086432  | -1.286879779 |
| H                    | 2.995983449  | 3.851944980  | 0.414958722  |
| H                    | 0.460201800  | 3.751156612  | -0.342830076 |
| C                    | 2.559247245  | 2.008462680  | -2.365646732 |
| H                    | 0.359497763  | 1.898159712  | -2.290063465 |
| H                    | 0.979936217  | 3.467381372  | -2.748275471 |
| H                    | 3.094652267  | 2.570711363  | -3.121477231 |
| H                    | 2.538187718  | 0.977171766  | -2.682178785 |
| 61                   |              |              |              |
| endo-3cP-O_Pd LP(OR) |              |              |              |
| Pd                   | 1.043076000  | -0.806225000 | -0.067002000 |
| O                    | 3.350171000  | -1.887959000 | -1.331961000 |
| O                    | 3.251115000  | -2.301013000 | 0.842544000  |

|   |              |              |              |
|---|--------------|--------------|--------------|
| N | -0.059586000 | -3.711810000 | -0.217880000 |
| C | 0.362164000  | -2.648475000 | -0.174706000 |
| C | 2.781498000  | -1.776630000 | -0.288632000 |
| C | 4.451277000  | -3.063727000 | 0.745561000  |
| H | 4.318264000  | -3.888156000 | 0.058758000  |
| H | 4.646736000  | -3.431496000 | 1.740926000  |
| H | 5.271471000  | -2.445277000 | 0.405417000  |
| C | 3.451817014  | 2.052235241  | 1.082045500  |
| C | 2.593290174  | 1.376191895  | 0.034554175  |
| C | 1.332217826  | 1.769929105  | 0.238961825  |
| C | 1.344348718  | 2.716208924  | 1.423807033  |
| H | 2.985990400  | 0.797412793  | -0.778922404 |
| H | 0.467813799  | 1.593782380  | -0.375550181 |
| P | -1.319114000 | 0.041530000  | 0.032235000  |
| C | -2.284945000 | -0.646558000 | -1.346845000 |
| C | -3.656889000 | -0.838943000 | -1.274361000 |
| C | -1.622994000 | -0.964935000 | -2.523077000 |
| H | -4.188544000 | -0.618225000 | -0.368081000 |
| H | -0.556154000 | -0.851753000 | -2.586677000 |
| C | -4.351249000 | -1.330531000 | -2.360444000 |
| C | -2.319231000 | -1.447453000 | -3.613059000 |
| H | -5.412618000 | -1.483972000 | -2.288507000 |
| H | -1.791211000 | -1.694231000 | -4.515786000 |
| C | -3.684659000 | -1.631355000 | -3.532695000 |
| H | -4.226743000 | -2.018885000 | -4.376108000 |
| C | -2.222091000 | -0.396764000 | 1.551540000  |
| C | -3.324337000 | 0.328386000  | 1.989403000  |
| C | -1.814821000 | -1.502613000 | 2.284871000  |
| H | -3.654152000 | 1.193071000  | 1.444531000  |
| H | -0.973140000 | -2.083684000 | 1.960637000  |
| C | -4.002525000 | -0.045347000 | 3.130588000  |
| C | -2.497157000 | -1.876770000 | 3.426179000  |
| H | -4.852897000 | 0.525913000  | 3.456039000  |
| H | -2.170497000 | -2.737950000 | 3.979698000  |
| C | -3.589849000 | -1.149662000 | 3.851654000  |
| H | -4.118101000 | -1.440273000 | 4.741613000  |
| C | -1.566379000 | 1.844652000  | -0.113018000 |
| C | -1.956846000 | 2.432904000  | -1.306492000 |

|   |              |             |              |
|---|--------------|-------------|--------------|
| C | -1.271391000 | 2.666388000 | 0.968660000  |
| H | -2.195047000 | 1.821910000 | -2.156680000 |
| H | -0.970898000 | 2.236620000 | 1.907087000  |
| C | -2.054697000 | 3.807755000 | -1.414539000 |
| C | -1.376892000 | 4.036396000 | 0.862828000  |
| H | -2.363497000 | 4.245530000 | -2.346370000 |
| H | -1.153596000 | 4.654905000 | 1.713093000  |
| C | -1.767422000 | 4.612352000 | -0.331749000 |
| H | -1.848931000 | 5.680814000 | -0.414753000 |
| C | 3.122916433  | 1.452381665 | 2.467125551  |
| C | 2.703206517  | 3.392551981 | 1.176425197  |
| H | 0.476539923  | 3.354753541 | 1.500155486  |
| H | 3.032038882  | 4.008801102 | 2.005956309  |
| H | 2.735374958  | 3.966065191 | 0.258653919  |
| H | 4.505363566  | 2.085681584 | 0.846776823  |
| C | 1.668115267  | 1.918581712 | 2.706040352  |
| H | 3.230216695  | 0.379234726 | 2.489182456  |
| H | 3.792566034  | 1.869986065 | 3.209447965  |
| H | 1.603521077  | 2.574360846 | 3.566181724  |
| H | 0.976389503  | 1.105836227 | 2.864650685  |

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endo-3cP-O\_PPh3

|    |              |              |              |
|----|--------------|--------------|--------------|
| Pd | 1.043076000  | -0.806225000 | -0.067002000 |
| O  | 3.350171000  | -1.887959000 | -1.331961000 |
| O  | 3.251115000  | -2.301013000 | 0.842544000  |
| N  | -0.059586000 | -3.711810000 | -0.217880000 |
| C  | 0.362164000  | -2.648475000 | -0.174706000 |
| C  | 2.781498000  | -1.776630000 | -0.288632000 |
| C  | 4.451277000  | -3.063727000 | 0.745561000  |
| H  | 4.318264000  | -3.888156000 | 0.058758000  |
| H  | 4.646736000  | -3.431496000 | 1.740926000  |
| H  | 5.271471000  | -2.445277000 | 0.405417000  |
| C  | 2.659667795  | 2.471936154  | 1.323475902  |
| C  | 2.765768522  | 1.095324014  | 0.702973952  |
| C  | 2.574542259  | 1.236007133  | -0.612607942 |
| C  | 2.343879221  | 2.711250374  | -0.876999251 |
| H  | 3.066296019  | 0.217451295  | 1.241458468  |
| H  | 2.694512204  | 0.501991416  | -1.388929484 |

|   |              |              |              |
|---|--------------|--------------|--------------|
| P | -1.428032185 | -0.362939675 | 0.007835002  |
| C | -2.251488032 | -1.196360957 | -1.383382342 |
| C | -3.573106230 | -1.614204132 | -1.326560877 |
| C | -1.533427600 | -1.395688151 | -2.552879090 |
| H | -4.143607081 | -1.488463070 | -0.425764076 |
| H | -0.499595510 | -1.106652289 | -2.604378510 |
| C | -4.164621085 | -2.209941206 | -2.421356917 |
| C | -2.128258557 | -1.982777405 | -3.651574990 |
| H | -5.186459532 | -2.537801380 | -2.361547876 |
| H | -1.557050911 | -2.134834230 | -4.548916110 |
| C | -3.444944189 | -2.391204768 | -3.586783191 |
| H | -3.906162163 | -2.860009338 | -4.437006873 |
| C | -2.261702735 | -0.951166873 | 1.516058776  |
| C | -3.473663159 | -0.420892589 | 1.943228399  |
| C | -1.684192956 | -1.976941079 | 2.251459995  |
| H | -3.936735712 | 0.379179467  | 1.396609614  |
| H | -0.754298863 | -2.408864410 | 1.935331362  |
| C | -4.092399221 | -0.906615511 | 3.075993799  |
| C | -2.306950030 | -2.463771469 | 3.384301390  |
| H | -5.029246306 | -0.485815053 | 3.393221465  |
| H | -1.847662259 | -3.260945694 | 3.939539204  |
| C | -3.509683746 | -1.929930295 | 3.799194191  |
| H | -3.991721348 | -2.307783286 | 4.682596034  |
| C | -1.969819057 | 1.374644653  | -0.136231122 |
| C | -2.439910395 | 1.894640561  | -1.332685664 |
| C | -1.826898289 | 2.229635411  | 0.950442577  |
| H | -2.564293746 | 1.255970522  | -2.186794781 |
| H | -1.469149602 | 1.851997144  | 1.891211958  |
| C | -2.763623119 | 3.234569552  | -1.438820564 |
| C | -2.157373313 | 3.563509399  | 0.846427022  |
| H | -3.130962808 | 3.618697678  | -2.373069213 |
| H | -2.048936155 | 4.207114405  | 1.700463927  |
| C | -2.625472650 | 4.071374093  | -0.351157909 |
| H | -2.882443515 | 5.111785216  | -0.432736683 |
| C | 1.193961851  | 2.952209888  | 1.236931813  |
| C | 3.288126234  | 3.295870502  | 0.186837724  |
| H | 2.498545357  | 3.015547766  | -1.901763566 |
| H | 3.173000617  | 4.365945249  | 0.319885452  |

|   |             |             |              |
|---|-------------|-------------|--------------|
| H | 4.329872961 | 3.058414121 | 0.011810439  |
| H | 3.102417558 | 2.558191812 | 2.304782660  |
| C | 0.978947516 | 3.124879419 | -0.284522514 |
| H | 0.502993322 | 2.254418479 | 1.683355206  |
| H | 1.093260443 | 3.898772446 | 1.754372766  |
| H | 0.773594426 | 4.158646234 | -0.535954695 |
| H | 0.168892706 | 2.528613852 | -0.675003719 |

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endo-3tP-N\_CN

|    |           |           |           |
|----|-----------|-----------|-----------|
| Pd | -1.073035 | 0.067919  | -0.128225 |
| O  | -0.852033 | 2.608239  | -1.466599 |
| O  | -0.603828 | 2.730012  | 0.729419  |
| N  | -1.381472 | -3.107840 | 0.272218  |
| C  | -1.301046 | -1.973509 | 0.129173  |
| C  | -0.787603 | 2.046317  | -0.409936 |
| C  | -0.461019 | 4.142897  | 0.622730  |
| H  | -0.332084 | 4.504462  | 1.631493  |
| H  | 0.404230  | 4.390087  | 0.022758  |
| H  | -1.341736 | 4.583927  | 0.175515  |
| C  | -4.762248 | 0.216199  | 0.965327  |
| C  | -3.539700 | 0.916418  | 0.409398  |
| C  | -3.541488 | 0.727084  | -0.916696 |
| C  | -4.767192 | -0.097466 | -1.248519 |
| H  | -2.891352 | 1.547608  | 0.988373  |
| H  | -2.889698 | 1.169405  | -1.646566 |
| P  | 1.203824  | -0.219226 | -0.003868 |
| C  | 2.274985  | 1.255174  | 0.018562  |
| C  | 3.012169  | 1.620207  | 1.132678  |
| C  | 2.358687  | 2.033282  | -1.129758 |
| H  | 2.968359  | 1.032047  | 2.028798  |
| H  | 1.787626  | 1.773418  | -2.001809 |
| C  | 3.819458  | 2.742620  | 1.100463  |
| C  | 3.166676  | 3.148261  | -1.161184 |
| H  | 4.387139  | 3.012438  | 1.972336  |
| H  | 3.222099  | 3.739219  | -2.057089 |
| C  | 3.899838  | 3.506618  | -0.044237 |
| H  | 4.529899  | 4.377156  | -0.069595 |
| C  | 1.588420  | -1.102706 | 1.533547  |



|   |           |           |           |
|---|-----------|-----------|-----------|
| C | 2.445163  | -2.189085 | 1.575572  |
| C | 0.984463  | -0.670264 | 2.706958  |
| H | 2.903003  | -2.555457 | 0.677115  |
| H | 0.298931  | 0.158280  | 2.685341  |
| C | 2.701653  | -2.826752 | 2.774296  |
| C | 1.249724  | -1.300970 | 3.902918  |
| H | 3.359256  | -3.676531 | 2.792670  |
| H | 0.775325  | -0.957572 | 4.803977  |
| C | 2.109468  | -2.382811 | 3.938125  |
| H | 2.306834  | -2.883646 | 4.868417  |
| C | 1.888797  | -1.184301 | -1.382088 |
| C | 3.261923  | -1.198131 | -1.604512 |
| C | 1.064230  | -1.908992 | -2.227699 |
| H | 3.918426  | -0.630858 | -0.971087 |
| H | 0.004141  | -1.915281 | -2.070156 |
| C | 3.795358  | -1.930779 | -2.642626 |
| C | 1.600942  | -2.638117 | -3.271185 |
| H | 4.858310  | -1.934179 | -2.801197 |
| H | 0.948615  | -3.194947 | -3.918411 |
| C | 2.964111  | -2.651834 | -3.479455 |
| H | 3.379725  | -3.219040 | -4.292484 |
| C | -4.567184 | -1.310523 | 0.832784  |
| H | -5.064516 | 0.546964  | 1.948388  |
| H | -5.073954 | -0.052849 | -2.283345 |
| C | -5.735697 | 0.471069  | -0.197696 |
| C | -4.572683 | -1.527468 | -0.697090 |
| H | -6.658108 | -0.093530 | -0.115795 |
| H | -5.960486 | 1.520068  | -0.346013 |
| H | -3.655547 | -1.655314 | 1.296359  |
| H | -5.395129 | -1.825530 | 1.305358  |
| H | -5.405441 | -2.150073 | -1.002043 |
| H | -3.665653 | -1.991940 | -1.052160 |

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endo-3tP-N\_COOR

|    |              |              |              |
|----|--------------|--------------|--------------|
| Pd | -1.071083000 | 0.067216000  | -0.135698000 |
| O  | -0.851531000 | 2.608833000  | -1.471189000 |
| O  | -0.607395000 | 2.729473000  | 0.725362000  |
| N  | -1.382050000 | -3.108873000 | 0.261127000  |

|   |              |              |              |
|---|--------------|--------------|--------------|
| C | -1.300409000 | -1.974578000 | 0.118555000  |
| C | -0.788353000 | 2.046520000  | -0.414819000 |
| C | -0.467643000 | 4.142768000  | 0.620241000  |
| H | -0.340443000 | 4.503689000  | 1.629454000  |
| H | 0.397583000  | 4.392542000  | 0.021317000  |
| H | -1.348948000 | 4.582295000  | 0.172679000  |
| C | -4.387063023 | 1.546859234  | -1.431497669 |
| C | -3.618644619 | 0.369702952  | -0.867981853 |
| C | -3.647027809 | 0.478280984  | 0.466775586  |
| C | -4.437055887 | 1.726901114  | 0.796688328  |
| H | -3.248808093 | -0.447604412 | -1.458899853 |
| H | -3.299714326 | -0.232432132 | 1.193041496  |
| P | 1.205260000  | -0.217485000 | -0.003820000 |
| C | 2.274869000  | 1.257761000  | 0.016350000  |
| C | 3.015245000  | 1.623129000  | 1.128305000  |
| C | 2.356427000  | 2.034738000  | -1.132860000 |
| H | 2.973156000  | 1.035607000  | 2.024927000  |
| H | 1.783062000  | 1.774423000  | -2.003280000 |
| C | 3.823110000  | 2.745027000  | 1.093209000  |
| C | 3.165014000  | 3.149198000  | -1.167202000 |
| H | 4.393168000  | 3.015285000  | 1.963394000  |
| H | 3.218662000  | 3.739385000  | -2.063715000 |
| C | 3.901087000  | 3.508027000  | -0.052341000 |
| H | 4.531630000  | 4.378150000  | -0.079968000 |
| C | 1.581921000  | -1.094678000 | 1.538907000  |
| C | 2.429633000  | -2.187824000 | 1.587289000  |
| C | 0.979092000  | -0.652412000 | 2.709363000  |
| H | 2.886466000  | -2.561151000 | 0.691165000  |
| H | 0.300544000  | 0.181731000  | 2.682814000  |
| C | 2.678458000  | -2.822654000 | 2.789123000  |
| C | 1.236736000  | -1.280301000 | 3.908398000  |
| H | 3.329196000  | -3.677571000 | 2.812425000  |
| H | 0.763425000  | -0.929283000 | 4.807101000  |
| C | 2.087476000  | -2.369085000 | 3.949830000  |
| H | 2.278928000  | -2.867583000 | 4.882617000  |
| C | 1.898087000  | -1.188567000 | -1.373563000 |
| C | 3.272762000  | -1.205534000 | -1.586020000 |
| C | 1.078428000  | -1.915793000 | -2.221874000 |

|   |              |              |              |
|---|--------------|--------------|--------------|
| H | 3.925762000  | -0.637047000 | -0.950088000 |
| H | 0.017211000  | -1.919600000 | -2.071944000 |
| C | 3.812369000  | -1.943521000 | -2.617145000 |
| C | 1.621426000  | -2.650209000 | -3.258363000 |
| H | 4.876442000  | -1.949346000 | -2.767980000 |
| H | 0.972823000  | -3.208777000 | -3.907830000 |
| C | 2.986037000  | -2.666887000 | -3.456829000 |
| H | 3.406600000  | -3.238264000 | -4.264375000 |
| C | -3.581983954 | 2.839505598  | -1.171667563 |
| H | -4.720474265 | 1.422571252  | -2.451590115 |
| H | -4.815903945 | 1.767013890  | 1.807549147  |
| C | -5.467288959 | 1.672538611  | -0.344015359 |
| C | -3.618116000 | 2.964829532  | 0.367979682  |
| H | -6.058724541 | 2.577579695  | -0.430281111 |
| H | -6.121752811 | 0.811388306  | -0.288933091 |
| H | -2.575995658 | 2.788139303  | -1.559238998 |
| H | -4.077735289 | 3.678351022  | -1.645642670 |
| H | -4.134899711 | 3.865958817  | 0.676253980  |
| H | -2.631457820 | 2.984186542  | 0.804645076  |

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endo-3tP-N\_Pd LP(O)

|    |              |              |              |
|----|--------------|--------------|--------------|
| Pd | -1.071083000 | 0.067216000  | -0.135698000 |
| O  | -0.851531000 | 2.608833000  | -1.471189000 |
| O  | -0.607395000 | 2.729473000  | 0.725362000  |
| N  | -1.382050000 | -3.108873000 | 0.261127000  |
| C  | -1.300409000 | -1.974578000 | 0.118555000  |
| C  | -0.788353000 | 2.046520000  | -0.414819000 |
| C  | -0.467643000 | 4.142768000  | 0.620241000  |
| H  | -0.340443000 | 4.503689000  | 1.629454000  |
| H  | 0.397583000  | 4.392542000  | 0.021317000  |
| H  | -1.348948000 | 4.582295000  | 0.172679000  |
| C  | -4.655931854 | 0.164512742  | -1.551168394 |
| C  | -3.727416279 | 0.184159384  | -0.354846252 |
| C  | -3.359265721 | 1.456881616  | -0.157829748 |
| C  | -4.043821016 | 2.289587135  | -1.220855890 |
| H  | -3.531624837 | -0.666986968 | 0.270589649  |
| H  | -2.794922330 | 1.860009246  | 0.662052324  |
| P  | 1.205260000  | -0.217485000 | -0.003820000 |

|   |              |              |              |
|---|--------------|--------------|--------------|
| C | 2.274869000  | 1.257761000  | 0.016350000  |
| C | 3.015245000  | 1.623129000  | 1.128305000  |
| C | 2.356427000  | 2.034738000  | -1.132860000 |
| H | 2.973156000  | 1.035607000  | 2.024927000  |
| H | 1.783062000  | 1.774423000  | -2.003280000 |
| C | 3.823110000  | 2.745027000  | 1.093209000  |
| C | 3.165014000  | 3.149198000  | -1.167202000 |
| H | 4.393168000  | 3.015285000  | 1.963394000  |
| H | 3.218662000  | 3.739385000  | -2.063715000 |
| C | 3.901087000  | 3.508027000  | -0.052341000 |
| H | 4.531630000  | 4.378150000  | -0.079968000 |
| C | 1.581921000  | -1.094678000 | 1.538907000  |
| C | 2.429633000  | -2.187824000 | 1.587289000  |
| C | 0.979092000  | -0.652412000 | 2.709363000  |
| H | 2.886466000  | -2.561151000 | 0.691165000  |
| H | 0.300544000  | 0.181731000  | 2.682814000  |
| C | 2.678458000  | -2.822654000 | 2.789123000  |
| C | 1.236736000  | -1.280301000 | 3.908398000  |
| H | 3.329196000  | -3.677571000 | 2.812425000  |
| H | 0.763425000  | -0.929283000 | 4.807101000  |
| C | 2.087476000  | -2.369085000 | 3.949830000  |
| H | 2.278928000  | -2.867583000 | 4.882617000  |
| C | 1.898087000  | -1.188567000 | -1.373563000 |
| C | 3.272762000  | -1.205534000 | -1.586020000 |
| C | 1.078428000  | -1.915793000 | -2.221874000 |
| H | 3.925762000  | -0.637047000 | -0.950088000 |
| H | 0.017211000  | -1.919600000 | -2.071944000 |
| C | 3.812369000  | -1.943521000 | -2.617145000 |
| C | 1.621426000  | -2.650209000 | -3.258363000 |
| H | 4.876442000  | -1.949346000 | -2.767980000 |
| H | 0.972823000  | -3.208777000 | -3.907830000 |
| C | 2.986037000  | -2.666887000 | -3.456829000 |
| H | 3.406600000  | -3.238264000 | -4.264375000 |
| C | -3.840205869 | 0.490106263  | -2.822065159 |
| H | -5.275203718 | -0.717380578 | -1.628406259 |
| H | -4.105046382 | 3.344697096  | -0.997318631 |
| C | -5.365622923 | 1.510510395  | -1.327718045 |
| C | -3.418781653 | 1.959177531  | -2.594564628 |

|   |              |              |              |
|---|--------------|--------------|--------------|
| H | -5.976716610 | 1.817518414  | -2.169530240 |
| H | -5.953782761 | 1.538833225  | -0.418761137 |
| H | -2.994510435 | -0.167454788 | -2.953500553 |
| H | -4.473990761 | 0.394212900  | -3.695680983 |
| H | -3.840973563 | 2.610098692  | -3.350995767 |
| H | -2.347552372 | 2.088947030  | -2.607733884 |

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endo-3tP-N\_Pd LP(OR)

|    |              |              |              |
|----|--------------|--------------|--------------|
| Pd | -1.071083000 | 0.067216000  | -0.135698000 |
| O  | -0.851531000 | 2.608833000  | -1.471189000 |
| O  | -0.607395000 | 2.729473000  | 0.725362000  |
| N  | -1.382050000 | -3.108873000 | 0.261127000  |
| C  | -1.300409000 | -1.974578000 | 0.118555000  |
| C  | -0.788353000 | 2.046520000  | -0.414819000 |
| C  | -0.467643000 | 4.142768000  | 0.620241000  |
| H  | -0.340443000 | 4.503689000  | 1.629454000  |
| H  | 0.397583000  | 4.392542000  | 0.021317000  |
| H  | -1.348948000 | 4.582295000  | 0.172679000  |
| C  | -4.212827194 | 2.019532531  | 0.951531496  |
| C  | -3.350100621 | 1.454088982  | -0.157382514 |
| C  | -3.736581379 | 0.186952018  | -0.355293486 |
| C  | -4.860158813 | -0.094809983 | 0.619500307  |
| H  | -2.659027791 | 2.035005105  | -0.739541659 |
| H  | -3.421621768 | -0.484101900 | -1.132267773 |
| P  | 1.205260000  | -0.217485000 | -0.003820000 |
| C  | 2.274869000  | 1.257761000  | 0.016350000  |
| C  | 3.015245000  | 1.623129000  | 1.128305000  |
| C  | 2.356427000  | 2.034738000  | -1.132860000 |
| H  | 2.973156000  | 1.035607000  | 2.024927000  |
| H  | 1.783062000  | 1.774423000  | -2.003280000 |
| C  | 3.823110000  | 2.745027000  | 1.093209000  |
| C  | 3.165014000  | 3.149198000  | -1.167202000 |
| H  | 4.393168000  | 3.015285000  | 1.963394000  |
| H  | 3.218662000  | 3.739385000  | -2.063715000 |
| C  | 3.901087000  | 3.508027000  | -0.052341000 |
| H  | 4.531630000  | 4.378150000  | -0.079968000 |
| C  | 1.581921000  | -1.094678000 | 1.538907000  |
| C  | 2.429633000  | -2.187824000 | 1.587289000  |

|   |              |              |              |
|---|--------------|--------------|--------------|
| C | 0.979092000  | -0.652412000 | 2.709363000  |
| H | 2.886466000  | -2.561151000 | 0.691165000  |
| H | 0.300544000  | 0.181731000  | 2.682814000  |
| C | 2.678458000  | -2.822654000 | 2.789123000  |
| C | 1.236736000  | -1.280301000 | 3.908398000  |
| H | 3.329196000  | -3.677571000 | 2.812425000  |
| H | 0.763425000  | -0.929283000 | 4.807101000  |
| C | 2.087476000  | -2.369085000 | 3.949830000  |
| H | 2.278928000  | -2.867583000 | 4.882617000  |
| C | 1.898087000  | -1.188567000 | -1.373563000 |
| C | 3.272762000  | -1.205534000 | -1.586020000 |
| C | 1.078428000  | -1.915793000 | -2.221874000 |
| H | 3.925762000  | -0.637047000 | -0.950088000 |
| H | 0.017211000  | -1.919600000 | -2.071944000 |
| C | 3.812369000  | -1.943521000 | -2.617145000 |
| C | 1.621426000  | -2.650209000 | -3.258363000 |
| H | 4.876442000  | -1.949346000 | -2.767980000 |
| H | 0.972823000  | -3.208777000 | -3.907830000 |
| C | 2.986037000  | -2.666887000 | -3.456829000 |
| H | 3.406600000  | -3.238264000 | -4.264375000 |
| C | -3.833364985 | 1.329761548  | 2.280750453  |
| H | -4.240591822 | 3.098579830  | 0.997195601  |
| H | -5.477903455 | -0.943035725 | 0.362831011  |
| C | -5.528138622 | 1.290559272  | 0.629266096  |
| C | -4.282372192 | -0.130905099 | 2.051903940  |
| H | -6.278807491 | 1.398484428  | 1.404627688  |
| H | -5.948785199 | 1.569622812  | -0.328918039 |
| H | -2.780560230 | 1.408843842  | 2.504827902  |
| H | -4.381430546 | 1.785768323  | 3.096694934  |
| H | -5.060739848 | -0.416012124 | 2.749750779  |
| H | -3.470800456 | -0.834369770 | 2.156949171  |

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endo-3tP-O\_CN

|    |              |              |              |
|----|--------------|--------------|--------------|
| Pd | -0.997436000 | -0.487439000 | -0.086252000 |
| O  | -1.521110000 | 2.027852000  | -1.374684000 |
| O  | -1.232068000 | 2.178346000  | 0.815500000  |
| N  | -0.537624000 | -3.656827000 | 0.306109000  |
| C  | -0.672381000 | -2.527902000 | 0.160690000  |

|   |              |              |              |
|---|--------------|--------------|--------------|
| C | -1.285067000 | 1.485311000  | -0.333860000 |
| C | -1.443820000 | 3.583672000  | 0.734404000  |
| H | -1.358828000 | 3.955470000  | 1.744158000  |
| H | -2.426504000 | 3.801255000  | 0.337383000  |
| H | -0.696491000 | 4.042217000  | 0.101072000  |
| H | -3.115856185 | -0.177498364 | -1.483694984 |
| C | -3.577539713 | -0.785548331 | -0.727744636 |
| C | -3.629465420 | -0.551222038 | 0.588542232  |
| H | -3.205032802 | 0.277849682  | 1.121727238  |
| C | -4.475423512 | -1.972977812 | -1.006929473 |
| C | -4.560944847 | -1.579219021 | 1.193082413  |
| P | 1.262000000  | -0.095766000 | -0.015323000 |
| C | 1.884190000  | 1.612829000  | -0.127539000 |
| C | 2.553603000  | 2.234022000  | 0.913772000  |
| C | 1.700877000  | 2.303575000  | -1.319174000 |
| H | 2.713296000  | 1.718222000  | 1.840782000  |
| H | 1.176218000  | 1.842906000  | -2.135609000 |
| C | 3.031709000  | 3.523338000  | 0.767242000  |
| C | 2.181449000  | 3.586084000  | -1.464334000 |
| H | 3.550737000  | 3.992251000  | 1.583287000  |
| H | 2.032238000  | 4.107685000  | -2.391963000 |
| C | 2.848323000  | 4.200287000  | -0.419770000 |
| H | 3.222262000  | 5.201582000  | -0.533857000 |
| C | 1.860781000  | -0.720488000 | 1.578706000  |
| C | 2.919445000  | -1.605358000 | 1.687193000  |
| C | 1.201442000  | -0.305732000 | 2.729516000  |
| H | 3.425717000  | -1.957819000 | 0.809244000  |
| H | 0.363084000  | 0.364588000  | 2.656472000  |
| C | 3.321385000  | -2.059239000 | 2.929245000  |
| C | 1.610787000  | -0.752035000 | 3.966975000  |
| H | 4.138275000  | -2.753763000 | 3.000983000  |
| H | 1.094122000  | -0.423973000 | 4.850367000  |
| C | 2.672964000  | -1.631431000 | 4.068609000  |
| H | 2.985221000  | -1.989106000 | 5.032872000  |
| C | 2.197570000  | -0.932402000 | -1.328556000 |
| C | 3.533987000  | -0.606065000 | -1.536681000 |
| C | 1.604444000  | -1.884205000 | -2.141527000 |
| H | 4.009392000  | 0.142299000  | -0.930026000 |

|   |              |              |              |
|---|--------------|--------------|--------------|
| H | 0.577479000  | -2.151939000 | -1.993994000 |
| C | 4.260417000  | -1.230691000 | -2.526799000 |
| C | 2.333130000  | -2.504545000 | -3.138212000 |
| H | 5.292817000  | -0.971121000 | -2.674376000 |
| H | 1.858885000  | -3.241239000 | -3.760158000 |
| C | 3.659635000  | -2.181629000 | -3.330979000 |
| H | 4.225266000  | -2.664898000 | -4.106864000 |
| H | -4.785696929 | -2.075271276 | -2.036544516 |
| C | -3.829984262 | -3.239997394 | -0.402412068 |
| C | -3.887063675 | -2.967582231 | 1.118876266  |
| H | -4.948532548 | -1.321314339 | 2.167717768  |
| C | -5.569917053 | -1.700779230 | 0.038740276  |
| H | -6.119065449 | -0.786457452 | -0.147050031 |
| H | -6.262774828 | -2.526684412 | 0.159890316  |
| H | -4.418094983 | -4.110982511 | -0.666786192 |
| H | -2.827878596 | -3.399713914 | -0.770833711 |
| H | -2.914477464 | -2.981130178 | 1.585939867  |
| H | -4.508195651 | -3.699298126 | 1.621943877  |

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endo-3tP-O\_COOR

|    |           |           |           |
|----|-----------|-----------|-----------|
| Pd | -0.997436 | -0.487439 | -0.086252 |
| O  | -1.521110 | 2.027852  | -1.374684 |
| O  | -1.232068 | 2.178346  | 0.815500  |
| N  | -0.537624 | -3.656827 | 0.306109  |
| C  | -0.672381 | -2.527902 | 0.160690  |
| C  | -1.285067 | 1.485311  | -0.333860 |
| C  | -1.443820 | 3.583672  | 0.734404  |
| H  | -1.358828 | 3.955470  | 1.744158  |
| H  | -2.426504 | 3.801255  | 0.337383  |
| H  | -0.696491 | 4.042217  | 0.101072  |
| H  | -2.804676 | -1.529556 | 1.391750  |
| C  | -3.484028 | -1.134321 | 0.659215  |
| C  | -3.500172 | -1.381343 | -0.655675 |
| H  | -2.827005 | -2.005701 | -1.211384 |
| C  | -4.737641 | -0.348168 | 0.982551  |
| C  | -4.762683 | -0.762548 | -1.215192 |
| P  | 1.262000  | -0.095766 | -0.015323 |
| C  | 1.884190  | 1.612829  | -0.127539 |



|   |           |           |           |
|---|-----------|-----------|-----------|
| C | 2.553603  | 2.234022  | 0.913772  |
| C | 1.700877  | 2.303575  | -1.319174 |
| H | 2.713296  | 1.718222  | 1.840782  |
| H | 1.176218  | 1.842906  | -2.135609 |
| C | 3.031709  | 3.523338  | 0.767242  |
| C | 2.181449  | 3.586084  | -1.464334 |
| H | 3.550737  | 3.992251  | 1.583287  |
| H | 2.032238  | 4.107685  | -2.391963 |
| C | 2.848323  | 4.200287  | -0.419770 |
| H | 3.222262  | 5.201582  | -0.533857 |
| C | 1.860781  | -0.720488 | 1.578706  |
| C | 2.919445  | -1.605358 | 1.687193  |
| C | 1.201442  | -0.305732 | 2.729516  |
| H | 3.425717  | -1.957819 | 0.809244  |
| H | 0.363084  | 0.364588  | 2.656472  |
| C | 3.321385  | -2.059239 | 2.929245  |
| C | 1.610787  | -0.752035 | 3.966975  |
| H | 4.138275  | -2.753763 | 3.000983  |
| H | 1.094122  | -0.423973 | 4.850367  |
| C | 2.672964  | -1.631431 | 4.068609  |
| H | 2.985221  | -1.989106 | 5.032872  |
| C | 2.197570  | -0.932402 | -1.328556 |
| C | 3.533987  | -0.606065 | -1.536681 |
| C | 1.604444  | -1.884205 | -2.141527 |
| H | 4.009392  | 0.142299  | -0.930026 |
| H | 0.577479  | -2.151939 | -1.993994 |
| C | 4.260417  | -1.230691 | -2.526799 |
| C | 2.333130  | -2.504545 | -3.138212 |
| H | 5.292817  | -0.971121 | -2.674376 |
| H | 1.858885  | -3.241239 | -3.760158 |
| C | 3.659635  | -2.181629 | -3.330979 |
| H | 4.225266  | -2.664898 | -4.106864 |
| H | -5.022849 | -0.356938 | 2.024386  |
| C | -4.616622 | 1.061804  | 0.362305  |
| C | -4.631972 | 0.775880  | -1.157497 |
| H | -5.069616 | -1.149988 | -2.175575 |
| C | -5.701062 | -1.004189 | -0.020888 |
| H | -5.876030 | -2.053566 | 0.179762  |

|   |           |           |           |
|---|-----------|-----------|-----------|
| H | -6.649197 | -0.484346 | -0.108363 |
| H | -5.468094 | 1.664292  | 0.656221  |
| H | -3.725624 | 1.574604  | 0.691878  |
| H | -3.748940 | 1.135520  | -1.662640 |
| H | -5.494462 | 1.230885  | -1.630119 |

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endo-3tP-O\_Pd LP(O)

|    |              |              |              |
|----|--------------|--------------|--------------|
| Pd | -0.997436000 | -0.487439000 | -0.086252000 |
| O  | -1.521110000 | 2.027852000  | -1.374684000 |
| O  | -1.232068000 | 2.178346000  | 0.815500000  |
| N  | -0.537624000 | -3.656827000 | 0.306109000  |
| C  | -0.672381000 | -2.527902000 | 0.160690000  |
| C  | -1.285067000 | 1.485311000  | -0.333860000 |
| C  | -1.443820000 | 3.583672000  | 0.734404000  |
| H  | -1.358828000 | 3.955470000  | 1.744158000  |
| H  | -2.426504000 | 3.801255000  | 0.337383000  |
| H  | -0.696491000 | 4.042217000  | 0.101072000  |
| H  | -3.381322218 | 0.234706440  | 0.490121695  |
| C  | -3.669460583 | -0.619895555 | -0.093803887 |
| C  | -3.314739417 | -1.895768445 | 0.097343887  |
| H  | -2.667175741 | -2.286741398 | 0.858652399  |
| C  | -4.733521071 | -0.607639418 | -1.171650503 |
| C  | -4.139213390 | -2.739746742 | -0.850202340 |
| P  | 1.262000000  | -0.095766000 | -0.015323000 |
| C  | 1.884190000  | 1.612829000  | -0.127539000 |
| C  | 2.553603000  | 2.234022000  | 0.913772000  |
| C  | 1.700877000  | 2.303575000  | -1.319174000 |
| H  | 2.713296000  | 1.718222000  | 1.840782000  |
| H  | 1.176218000  | 1.842906000  | -2.135609000 |
| C  | 3.031709000  | 3.523338000  | 0.767242000  |
| C  | 2.181449000  | 3.586084000  | -1.464334000 |
| H  | 3.550737000  | 3.992251000  | 1.583287000  |
| H  | 2.032238000  | 4.107685000  | -2.391963000 |
| C  | 2.848323000  | 4.200287000  | -0.419770000 |
| H  | 3.222262000  | 5.201582000  | -0.533857000 |
| C  | 1.860781000  | -0.720488000 | 1.578706000  |
| C  | 2.919445000  | -1.605358000 | 1.687193000  |
| C  | 1.201442000  | -0.305732000 | 2.729516000  |

|   |              |              |              |
|---|--------------|--------------|--------------|
| H | 3.425717000  | -1.957819000 | 0.809244000  |
| H | 0.363084000  | 0.364588000  | 2.656472000  |
| C | 3.321385000  | -2.059239000 | 2.929245000  |
| C | 1.610787000  | -0.752035000 | 3.966975000  |
| H | 4.138275000  | -2.753763000 | 3.000983000  |
| H | 1.094122000  | -0.423973000 | 4.850367000  |
| C | 2.672964000  | -1.631431000 | 4.068609000  |
| H | 2.985221000  | -1.989106000 | 5.032872000  |
| C | 2.197570000  | -0.932402000 | -1.328556000 |
| C | 3.533987000  | -0.606065000 | -1.536681000 |
| C | 1.604444000  | -1.884205000 | -2.141527000 |
| H | 4.009392000  | 0.142299000  | -0.930026000 |
| H | 0.577479000  | -2.151939000 | -1.993994000 |
| C | 4.260417000  | -1.230691000 | -2.526799000 |
| C | 2.333130000  | -2.504545000 | -3.138212000 |
| H | 5.292817000  | -0.971121000 | -2.674376000 |
| H | 1.858885000  | -3.241239000 | -3.760158000 |
| C | 3.659635000  | -2.181629000 | -3.330979000 |
| H | 4.225266000  | -2.664898000 | -4.106864000 |
| H | -5.336041486 | 0.288312907  | -1.204502650 |
| C | -4.083574172 | -0.993530871 | -2.519251540 |
| C | -3.670643061 | -2.467268039 | -2.297051328 |
| H | -4.199579641 | -3.786016022 | -0.588802958 |
| C | -5.444536192 | -1.926824582 | -0.825758317 |
| H | -5.920860912 | -1.912214960 | 0.146336139  |
| H | -6.158966344 | -2.239904864 | -1.579693920 |
| H | -4.814133055 | -0.907079211 | -3.314985667 |
| H | -3.253418652 | -0.349796501 | -2.768063741 |
| H | -2.612342755 | -2.632358876 | -2.427440630 |
| H | -4.196711907 | -3.125503119 | -2.978423659 |

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endo-3tP-O\_Pd LP(OR)

|    |              |              |              |
|----|--------------|--------------|--------------|
| Pd | -0.997436000 | -0.487439000 | -0.086252000 |
| O  | -1.521110000 | 2.027852000  | -1.374684000 |
| O  | -1.232068000 | 2.178346000  | 0.815500000  |
| N  | -0.537624000 | -3.656827000 | 0.306109000  |
| C  | -0.672381000 | -2.527902000 | 0.160690000  |
| C  | -1.285067000 | 1.485311000  | -0.333860000 |

|   |              |              |              |
|---|--------------|--------------|--------------|
| C | -1.443820000 | 3.583672000  | 0.734404000  |
| H | -1.358828000 | 3.955470000  | 1.744158000  |
| H | -2.426504000 | 3.801255000  | 0.337383000  |
| H | -0.696491000 | 4.042217000  | 0.101072000  |
| H | -2.591641849 | -2.438084262 | -0.522262255 |
| C | -3.272761320 | -1.882804923 | 0.095862727  |
| C | -3.711438680 | -0.632859077 | -0.092322727 |
| H | -3.447171153 | 0.039702248  | -0.885804392 |
| C | -4.073069028 | -2.470808418 | 1.239491917  |
| C | -4.805007654 | -0.381203779 | 0.922899939  |
| P | 1.262000000  | -0.095766000 | -0.015323000 |
| C | 1.884190000  | 1.612829000  | -0.127539000 |
| C | 2.553603000  | 2.234022000  | 0.913772000  |
| C | 1.700877000  | 2.303575000  | -1.319174000 |
| H | 2.713296000  | 1.718222000  | 1.840782000  |
| H | 1.176218000  | 1.842906000  | -2.135609000 |
| C | 3.031709000  | 3.523338000  | 0.767242000  |
| C | 2.181449000  | 3.586084000  | -1.464334000 |
| H | 3.550737000  | 3.992251000  | 1.583287000  |
| H | 2.032238000  | 4.107685000  | -2.391963000 |
| C | 2.848323000  | 4.200287000  | -0.419770000 |
| H | 3.222262000  | 5.201582000  | -0.533857000 |
| C | 1.860781000  | -0.720488000 | 1.578706000  |
| C | 2.919445000  | -1.605358000 | 1.687193000  |
| C | 1.201442000  | -0.305732000 | 2.729516000  |
| H | 3.425717000  | -1.957819000 | 0.809244000  |
| H | 0.363084000  | 0.364588000  | 2.656472000  |
| C | 3.321385000  | -2.059239000 | 2.929245000  |
| C | 1.610787000  | -0.752035000 | 3.966975000  |
| H | 4.138275000  | -2.753763000 | 3.000983000  |
| H | 1.094122000  | -0.423973000 | 4.850367000  |
| C | 2.672964000  | -1.631431000 | 4.068609000  |
| H | 2.985221000  | -1.989106000 | 5.032872000  |
| C | 2.197570000  | -0.932402000 | -1.328556000 |
| C | 3.533987000  | -0.606065000 | -1.536681000 |
| C | 1.604444000  | -1.884205000 | -2.141527000 |
| H | 4.009392000  | 0.142299000  | -0.930026000 |
| H | 0.577479000  | -2.151939000 | -1.993994000 |

|   |              |              |              |
|---|--------------|--------------|--------------|
| C | 4.260417000  | -1.230691000 | -2.526799000 |
| C | 2.333130000  | -2.504545000 | -3.138212000 |
| H | 5.292817000  | -0.971121000 | -2.674376000 |
| H | 1.858885000  | -3.241239000 | -3.760158000 |
| C | 3.659635000  | -2.181629000 | -3.330979000 |
| H | 4.225266000  | -2.664898000 | -4.106864000 |
| H | -4.062693133 | -3.549624645 | 1.293237356  |
| C | -3.668265561 | -1.759192820 | 2.549877025  |
| C | -4.172428790 | -0.313629621 | 2.330895857  |
| H | -5.460837038 | 0.443892588  | 0.686770883  |
| C | -5.424050376 | -1.788401452 | 0.966355442  |
| H | -5.870772802 | -2.088063113 | 0.026829883  |
| H | -6.140412800 | -1.917173292 | 1.770775288  |
| H | -4.170201160 | -2.226258912 | 3.389098623  |
| H | -2.605810284 | -1.818458055 | 2.731910137  |
| H | -3.385194361 | 0.421392495  | 2.396167108  |
| H | -4.932686658 | -0.052633245 | 3.057655082  |

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exo-3cP-N\_CN

|    |           |           |           |
|----|-----------|-----------|-----------|
| Pd | 0.812141  | -1.185608 | -0.012707 |
| O  | -0.810143 | -2.886073 | -1.540596 |
| O  | -1.154096 | -3.089967 | 0.637033  |
| N  | 2.553750  | -3.785785 | 0.466678  |
| C  | 1.937177  | -2.843375 | 0.256207  |
| C  | -0.565502 | -2.553506 | -0.424559 |
| C  | -2.077622 | -4.148392 | 0.386764  |
| H  | -2.438556 | -4.455699 | 1.355925  |
| H  | -2.895609 | -3.800069 | -0.228800 |
| H  | -1.579331 | -4.970637 | -0.107538 |
| C  | 3.926627  | 0.493112  | -1.229622 |
| C  | 2.661640  | 0.723465  | -0.444669 |
| C  | 2.827302  | 0.165104  | 0.762411  |
| C  | 4.210009  | -0.441910 | 0.784632  |
| H  | 1.914355  | 1.436441  | -0.726487 |
| H  | 2.245776  | 0.366551  | 1.644572  |
| P  | -0.926946 | 0.491197  | 0.002360  |
| C  | -2.156363 | 0.269817  | -1.317909 |
| C  | -3.521309 | 0.414848  | -1.121617 |

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | -1.690885 | -0.062296 | -2.583241 |
| H | -3.909473 | 0.646097  | -0.148553 |
| H | -0.640586 | -0.223626 | -2.744966 |
| C | -4.399754 | 0.248591  | -2.174203 |
| C | -2.567603 | -0.213680 | -3.636551 |
| H | -5.455907 | 0.356710  | -2.006558 |
| H | -2.191585 | -0.473390 | -4.609015 |
| C | -3.924853 | -0.058166 | -3.433596 |
| H | -4.610392 | -0.188675 | -4.251134 |
| C | -1.835220 | 0.527494  | 1.580013  |
| C | -2.656329 | 1.600654  | 1.912250  |
| C | -1.698252 | -0.514792 | 2.483762  |
| H | -2.759889 | 2.430793  | 1.237937  |
| H | -1.070880 | -1.351730 | 2.246896  |
| C | -3.333368 | 1.621167  | 3.111982  |
| C | -2.374993 | -0.490528 | 3.689418  |
| H | -3.964821 | 2.456609  | 3.353833  |
| H | -2.255582 | -1.304769 | 4.380552  |
| C | -3.193671 | 0.573297  | 4.004083  |
| H | -3.717829 | 0.592080  | 4.942398  |
| C | -0.395518 | 2.232716  | -0.166989 |
| C | -0.542136 | 2.941122  | -1.348927 |
| C | 0.238779  | 2.847918  | 0.906221  |
| H | -1.033490 | 2.492976  | -2.191297 |
| H | 0.359933  | 2.321508  | 1.835595  |
| C | -0.067004 | 4.235304  | -1.455517 |
| C | 0.708760  | 4.139261  | 0.800115  |
| H | -0.193486 | 4.771633  | -2.378309 |
| H | 1.191662  | 4.600806  | 1.642088  |
| C | 0.558372  | 4.837317  | -0.383719 |
| H | 0.924185  | 5.844443  | -0.466833 |
| C | 4.960638  | 1.437071  | -0.552198 |
| H | 3.852047  | 0.601727  | -2.301414 |
| C | 5.160949  | 0.785088  | 0.837406  |
| C | 4.385597  | -0.854326 | -0.678646 |
| H | 4.389064  | -1.193935 | 1.536587  |
| H | 3.758457  | -1.681349 | -0.968833 |
| H | 5.416931  | -1.077514 | -0.925795 |

|   |          |          |           |
|---|----------|----------|-----------|
| H | 5.881632 | 1.440069 | -1.122808 |
| H | 4.607565 | 2.458950 | -0.493425 |
| H | 4.922671 | 1.454297 | 1.654518  |
| H | 6.183662 | 0.454258 | 0.971914  |

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exo-3cP-N\_Pd LP(O)

|    |              |              |              |
|----|--------------|--------------|--------------|
| Pd | 0.812141000  | -1.185608000 | -0.012707000 |
| O  | -0.810143000 | -2.886073000 | -1.540596000 |
| O  | -1.154096000 | -3.089967000 | 0.637033000  |
| N  | 2.553750000  | -3.785785000 | 0.466678000  |
| C  | 1.937177000  | -2.843375000 | 0.256207000  |
| C  | -0.565502000 | -2.553506000 | -0.424559000 |
| C  | -2.077622000 | -4.148392000 | 0.386764000  |
| H  | -2.438556000 | -4.455699000 | 1.355925000  |
| H  | -2.895609000 | -3.800069000 | -0.228800000 |
| H  | -1.579331000 | -4.970637000 | -0.107538000 |
| C  | 2.724504958  | 1.889318441  | -0.954353151 |
| C  | 2.371436723  | 0.998782767  | 0.208270976  |
| C  | 3.117505277  | -0.110213767 | 0.109471024  |
| C  | 3.973634213  | 0.039418813  | -1.125636969 |
| H  | 1.836571127  | 1.339452704  | 1.070856521  |
| H  | 3.313428583  | -0.820138689 | 0.893423877  |
| P  | -0.926946000 | 0.491197000  | 0.002360000  |
| C  | -2.156363000 | 0.269817000  | -1.317909000 |
| C  | -3.521309000 | 0.414848000  | -1.121617000 |
| C  | -1.690885000 | -0.062296000 | -2.583241000 |
| H  | -3.909473000 | 0.646097000  | -0.148553000 |
| H  | -0.640586000 | -0.223626000 | -2.744966000 |
| C  | -4.399754000 | 0.248591000  | -2.174203000 |
| C  | -2.567603000 | -0.213680000 | -3.636551000 |
| H  | -5.455907000 | 0.356710000  | -2.006558000 |
| H  | -2.191585000 | -0.473390000 | -4.609015000 |
| C  | -3.924853000 | -0.058166000 | -3.433596000 |
| H  | -4.610392000 | -0.188675000 | -4.251134000 |
| C  | -1.835220000 | 0.527494000  | 1.580013000  |
| C  | -2.656329000 | 1.600654000  | 1.912250000  |
| C  | -1.698252000 | -0.514792000 | 2.483762000  |
| H  | -2.759889000 | 2.430793000  | 1.237937000  |

|   |              |              |              |
|---|--------------|--------------|--------------|
| H | -1.070880000 | -1.351730000 | 2.246896000  |
| C | -3.333368000 | 1.621167000  | 3.111982000  |
| C | -2.374993000 | -0.490528000 | 3.689418000  |
| H | -3.964821000 | 2.456609000  | 3.353833000  |
| H | -2.255582000 | -1.304769000 | 4.380552000  |
| C | -3.193671000 | 0.573297000  | 4.004083000  |
| H | -3.717829000 | 0.592080000  | 4.942398000  |
| C | -0.395518000 | 2.232716000  | -0.166989000 |
| C | -0.542136000 | 2.941122000  | -1.348927000 |
| C | 0.238779000  | 2.847918000  | 0.906221000  |
| H | -1.033490000 | 2.492976000  | -2.191297000 |
| H | 0.359933000  | 2.321508000  | 1.835595000  |
| C | -0.067004000 | 4.235304000  | -1.455517000 |
| C | 0.708760000  | 4.139261000  | 0.800115000  |
| H | -0.193486000 | 4.771633000  | -2.378309000 |
| H | 1.191662000  | 4.600806000  | 1.642088000  |
| C | 0.558372000  | 4.837317000  | -0.383719000 |
| H | 0.924185000  | 5.844443000  | -0.466833000 |
| C | 4.151665165  | 2.402114541  | -0.608818027 |
| H | 2.013577099  | 2.665076445  | -1.197002247 |
| C | 5.015094830  | 1.123522263  | -0.734899765 |
| C | 3.057521005  | 0.862842733  | -2.033827612 |
| H | 4.387900337  | -0.869508225 | -1.532175815 |
| H | 2.202746556  | 0.312860828  | -2.392102175 |
| H | 3.587315206  | 1.296671273  | -2.873861084 |
| H | 4.453792173  | 3.154409438  | -1.327571370 |
| H | 4.200247453  | 2.850367172  | 0.375590851  |
| H | 5.539651528  | 0.878062746  | 0.179911149  |
| H | 5.754620686  | 1.225223925  | -1.519909989 |

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exo-3cP-N\_Pd LP(OR)

|    |              |              |              |
|----|--------------|--------------|--------------|
| Pd | 0.812141000  | -1.185608000 | -0.012707000 |
| O  | -0.810143000 | -2.886073000 | -1.540596000 |
| O  | -1.154096000 | -3.089967000 | 0.637033000  |
| N  | 2.553750000  | -3.785785000 | 0.466678000  |
| C  | 1.937177000  | -2.843375000 | 0.256207000  |
| C  | -0.565502000 | -2.553506000 | -0.424559000 |
| C  | -2.077622000 | -4.148392000 | 0.386764000  |



|   |              |              |              |
|---|--------------|--------------|--------------|
| H | -2.438556000 | -4.455699000 | 1.355925000  |
| H | -2.895609000 | -3.800069000 | -0.228800000 |
| H | -1.579331000 | -4.970637000 | -0.107538000 |
| C | 4.044049672  | 0.078585367  | 1.385716208  |
| C | 3.232738685  | -0.013016049 | 0.119702981  |
| C | 2.256203315  | 0.901585049  | 0.198039019  |
| C | 2.415192195  | 1.608189714  | 1.523282695  |
| H | 3.568781050  | -0.521390515 | -0.760536739 |
| H | 1.672601026  | 1.284508337  | -0.620337139 |
| P | -0.926946000 | 0.491197000  | 0.002360000  |
| C | -2.156363000 | 0.269817000  | -1.317909000 |
| C | -3.521309000 | 0.414848000  | -1.121617000 |
| C | -1.690885000 | -0.062296000 | -2.583241000 |
| H | -3.909473000 | 0.646097000  | -0.148553000 |
| H | -0.640586000 | -0.223626000 | -2.744966000 |
| C | -4.399754000 | 0.248591000  | -2.174203000 |
| C | -2.567603000 | -0.213680000 | -3.636551000 |
| H | -5.455907000 | 0.356710000  | -2.006558000 |
| H | -2.191585000 | -0.473390000 | -4.609015000 |
| C | -3.924853000 | -0.058166000 | -3.433596000 |
| H | -4.610392000 | -0.188675000 | -4.251134000 |
| C | -1.835220000 | 0.527494000  | 1.580013000  |
| C | -2.656329000 | 1.600654000  | 1.912250000  |
| C | -1.698252000 | -0.514792000 | 2.483762000  |
| H | -2.759889000 | 2.430793000  | 1.237937000  |
| H | -1.070880000 | -1.351730000 | 2.246896000  |
| C | -3.333368000 | 1.621167000  | 3.111982000  |
| C | -2.374993000 | -0.490528000 | 3.689418000  |
| H | -3.964821000 | 2.456609000  | 3.353833000  |
| H | -2.255582000 | -1.304769000 | 4.380552000  |
| C | -3.193671000 | 0.573297000  | 4.004083000  |
| H | -3.717829000 | 0.592080000  | 4.942398000  |
| C | -0.395518000 | 2.232716000  | -0.166989000 |
| C | -0.542136000 | 2.941122000  | -1.348927000 |
| C | 0.238779000  | 2.847918000  | 0.906221000  |
| H | -1.033490000 | 2.492976000  | -2.191297000 |
| H | 0.359933000  | 2.321508000  | 1.835595000  |
| C | -0.067004000 | 4.235304000  | -1.455517000 |

|   |              |              |              |
|---|--------------|--------------|--------------|
| C | 0.708760000  | 4.139261000  | 0.800115000  |
| H | -0.193486000 | 4.771633000  | -2.378309000 |
| H | 1.191662000  | 4.600806000  | 1.642088000  |
| C | 0.558372000  | 4.837317000  | -0.383719000 |
| H | 0.924185000  | 5.844443000  | -0.466833000 |
| C | 4.815831081  | 1.420564821  | 1.235432415  |
| H | 4.664091224  | -0.773833927 | 1.620295206  |
| C | 3.689232870  | 2.477178225  | 1.338146543  |
| C | 2.979768042  | 0.488249096  | 2.400259168  |
| H | 1.549013231  | 2.135934786  | 1.889694699  |
| H | 2.263615187  | -0.286823534 | 2.619045877  |
| H | 3.405139356  | 0.860088899  | 3.325104959  |
| H | 5.529035800  | 1.524687600  | 2.044340434  |
| H | 5.365248272  | 1.476716130  | 0.304121897  |
| H | 3.628506954  | 3.113872320  | 0.464520705  |
| H | 3.828649773  | 3.116852109  | 2.201201014  |

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exo-3cP-N\_PPh3

|    |              |              |              |
|----|--------------|--------------|--------------|
| Pd | 0.812141000  | -1.185608000 | -0.012707000 |
| O  | -0.810143000 | -2.886073000 | -1.540596000 |
| O  | -1.154096000 | -3.089967000 | 0.637033000  |
| N  | 2.553750000  | -3.785785000 | 0.466678000  |
| C  | 1.937177000  | -2.843375000 | 0.256207000  |
| C  | -0.565502000 | -2.553506000 | -0.424559000 |
| C  | -2.077622000 | -4.148392000 | 0.386764000  |
| H  | -2.438556000 | -4.455699000 | 1.355925000  |
| H  | -2.895609000 | -3.800069000 | -0.228800000 |
| H  | -1.579331000 | -4.970637000 | -0.107538000 |
| C  | 3.077123413  | 1.487705511  | 1.299640340  |
| C  | 3.049539894  | 0.059462051  | 0.821345874  |
| C  | 2.962777155  | 0.082333157  | -0.515890892 |
| C  | 2.931944826  | 1.533252862  | -0.933885861 |
| H  | 3.329558555  | -0.772954228 | 1.433607027  |
| H  | 3.185147068  | -0.730475740 | -1.184362830 |
| P  | -1.033399526 | 0.373223803  | -0.031393730 |
| C  | -2.231499153 | 0.059501058  | -1.361702272 |
| C  | -3.605035451 | 0.116194047  | -1.180522623 |
| C  | -1.731771372 | -0.252711832 | -2.619012553 |

|   |              |              |              |
|---|--------------|--------------|--------------|
| H | -4.017884691 | 0.330205874  | -0.213695140 |
| H | -0.671481804 | -0.346054409 | -2.768623815 |
| C | -4.459410647 | -0.117014834 | -2.240192826 |
| C | -2.585392688 | -0.470973484 | -3.679534134 |
| H | -5.522108846 | -0.077097322 | -2.084202913 |
| H | -2.182799327 | -0.714177097 | -4.645606409 |
| C | -3.952009571 | -0.403254021 | -3.491717025 |
| H | -4.618755941 | -0.585975313 | -4.314776506 |
| C | -1.835220000 | 0.527494000  | 1.580013000  |
| C | -2.656329000 | 1.600654000  | 1.912250000  |
| C | -1.698252000 | -0.514792000 | 2.483762000  |
| H | -2.759889000 | 2.430793000  | 1.237937000  |
| H | -1.070880000 | -1.351730000 | 2.246896000  |
| C | -3.333368000 | 1.621167000  | 3.111982000  |
| C | -2.374993000 | -0.490528000 | 3.689418000  |
| H | -3.964821000 | 2.456609000  | 3.353833000  |
| H | -2.255582000 | -1.304769000 | 4.380552000  |
| C | -3.193671000 | 0.573297000  | 4.004083000  |
| H | -3.717829000 | 0.592080000  | 4.942398000  |
| C | -0.615746430 | 2.144326299  | -0.212349718 |
| C | -0.795996245 | 2.830822991  | -1.402536944 |
| C | -0.034688391 | 2.809614291  | 0.861125634  |
| H | -1.247858454 | 2.343715764  | -2.245387999 |
| H | 0.110886401  | 2.300750213  | 1.796746894  |
| C | -0.405796989 | 4.152440560  | -1.516950385 |
| C | 0.350552624  | 4.128064643  | 0.747172146  |
| H | -0.557409587 | 4.670910821  | -2.446140235 |
| H | 0.793105622  | 4.627981673  | 1.589411108  |
| C | 0.167241226  | 4.803969001  | -0.444847945 |
| H | 0.466970472  | 5.832185024  | -0.534089509 |
| C | 4.483696700  | 1.995141398  | 0.871620451  |
| H | 2.837256752  | 1.649405291  | 2.340031926  |
| C | 4.379144020  | 2.033060976  | -0.672347310 |
| C | 2.207950030  | 2.176681571  | 0.250990352  |
| H | 2.547108876  | 1.737651896  | -1.920375062 |
| H | 1.164073244  | 1.914980293  | 0.308556084  |
| H | 2.312373175  | 3.255315175  | 0.264799269  |
| H | 4.655346281  | 2.984032092  | 1.279623302  |

|   |             |             |              |
|---|-------------|-------------|--------------|
| H | 5.278525501 | 1.351150008 | 1.226407382  |
| H | 5.121677255 | 1.413889459 | -1.159748724 |
| H | 4.495112910 | 3.042154244 | -1.048863930 |

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exo-3cP-O\_COOR

|    |           |           |           |
|----|-----------|-----------|-----------|
| Pd | 1.039795  | -0.875443 | -0.117989 |
| O  | 3.235441  | -2.223079 | -1.356974 |
| O  | 3.251721  | -2.292104 | 0.857059  |
| N  | -0.218328 | -3.740025 | -0.201671 |
| C  | 0.256367  | -2.698270 | -0.185225 |
| C  | 2.729485  | -1.931262 | -0.315947 |
| C  | 4.424082  | -3.101240 | 0.814672  |
| H  | 4.230208  | -4.017952 | 0.275126  |
| H  | 4.670829  | -3.315780 | 1.843089  |
| H  | 5.237469  | -2.571871 | 0.336057  |
| C  | 3.229532  | 1.802693  | -1.180069 |
| C  | 1.912071  | 1.419017  | -0.557098 |
| C  | 2.154136  | 1.099524  | 0.729318  |
| C  | 3.635506  | 1.273732  | 0.958605  |
| H  | 0.968554  | 1.711566  | -0.972465 |
| H  | 1.436985  | 1.094987  | 1.529601  |
| P  | -1.290321 | 0.052903  | 0.033648  |
| C  | -2.315625 | -0.591281 | -1.323169 |
| C  | -3.693112 | -0.721499 | -1.223429 |
| C  | -1.691455 | -0.943156 | -2.510452 |
| H  | -4.196438 | -0.474736 | -0.307792 |
| H  | -0.622032 | -0.878581 | -2.594829 |
| C  | -4.429837 | -1.185243 | -2.293680 |
| C  | -2.429703 | -1.398544 | -3.584419 |
| H  | -5.495431 | -1.290552 | -2.200701 |
| H  | -1.930831 | -1.672855 | -4.495753 |
| C  | -3.800177 | -1.520479 | -3.477018 |
| H  | -4.375285 | -1.886875 | -4.307924 |
| C  | -2.171526 | -0.350880 | 1.575831  |
| C  | -3.241007 | 0.410984  | 2.032938  |
| C  | -1.780945 | -1.462383 | 2.309459  |
| H  | -3.557057 | 1.281366  | 1.488798  |
| H  | -0.965571 | -2.071763 | 1.971036  |

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | -3.903891 | 0.067135  | 3.192249  |
| C | -2.447765 | -1.806268 | 3.469440  |
| H | -4.729088 | 0.666419  | 3.531834  |
| H | -2.134428 | -2.672514 | 4.022775  |
| C | -3.508085 | -1.043386 | 3.913355  |
| H | -4.024392 | -1.310903 | 4.817471  |
| C | -1.473409 | 1.865499  | -0.096147 |
| C | -1.871714 | 2.477193  | -1.275259 |
| C | -1.111458 | 2.667936  | 0.980191  |
| H | -2.159372 | 1.881577  | -2.121072 |
| H | -0.806581 | 2.219758  | 1.908690  |
| C | -1.911773 | 3.855739  | -1.374615 |
| C | -1.157491 | 4.042054  | 0.882536  |
| H | -2.228105 | 4.311758  | -2.295094 |
| H | -0.883049 | 4.645696  | 1.728523  |
| C | -1.556603 | 4.641171  | -0.297916 |
| H | -1.592783 | 5.712592  | -0.374263 |
| H | 3.275176  | 1.786530  | -2.258065 |
| C | 3.532735  | 3.184954  | -0.533057 |
| C | 3.818108  | 2.818127  | 0.943437  |
| C | 4.217163  | 0.928755  | -0.412144 |
| H | 4.048844  | 0.774994  | 1.821474  |
| H | 4.165494  | -0.112657 | -0.677034 |
| H | 5.239449  | 1.271340  | -0.521210 |
| H | 4.402227  | 3.625576  | -1.005144 |
| H | 2.710706  | 3.880470  | -0.643628 |
| H | 3.154126  | 3.317475  | 1.637492  |
| H | 4.833957  | 3.069674  | 1.222508  |

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exo-3cP-O\_Pd LP(O)

|    |              |              |              |
|----|--------------|--------------|--------------|
| Pd | 1.039391000  | -0.875556000 | -0.116786000 |
| O  | 3.233950000  | -2.222653000 | -1.357449000 |
| O  | 3.252092000  | -2.293194000 | 0.856511000  |
| N  | -0.217091000 | -3.741011000 | -0.199235000 |
| C  | 0.256657000  | -2.698837000 | -0.183251000 |
| C  | 2.728625000  | -1.931905000 | -0.315750000 |
| C  | 4.424890000  | -3.101728000 | 0.812452000  |
| H  | 4.230975000  | -4.018134000 | 0.272436000  |

|   |              |              |              |
|---|--------------|--------------|--------------|
| H | 4.672665000  | -3.316759000 | 1.840504000  |
| H | 5.237453000  | -2.571495000 | 0.333413000  |
| C | 1.329875081  | 2.654182252  | -0.859175120 |
| C | 1.441180932  | 1.567724727  | 0.179092814  |
| C | 2.624427068  | 0.951560273  | -0.009959814 |
| C | 3.298487757  | 1.633114718  | -1.175523284 |
| H | 0.860960704  | 1.566401994  | 1.080089036  |
| H | 3.162762631  | 0.371221467  | 0.716721825  |
| P | -1.289812000 | 0.053722000  | 0.033875000  |
| C | -2.316268000 | -0.594987000 | -1.319908000 |
| C | -3.693560000 | -0.725280000 | -1.217867000 |
| C | -1.693451000 | -0.950393000 | -2.506832000 |
| H | -4.195636000 | -0.475477000 | -0.302348000 |
| H | -0.624207000 | -0.885554000 | -2.592849000 |
| C | -4.431533000 | -1.192564000 | -2.285710000 |
| C | -2.432992000 | -1.409215000 | -3.578442000 |
| H | -5.496998000 | -1.297846000 | -2.191137000 |
| H | -1.935285000 | -1.686045000 | -4.489649000 |
| C | -3.803277000 | -1.531253000 | -3.468811000 |
| H | -4.379401000 | -1.900402000 | -4.297797000 |
| C | -2.170382000 | -0.345441000 | 1.577791000  |
| C | -3.238828000 | 0.418283000  | 2.033943000  |
| C | -1.780492000 | -1.456061000 | 2.313204000  |
| H | -3.554519000 | 1.287629000  | 1.487976000  |
| H | -0.965794000 | -2.066781000 | 1.975635000  |
| C | -3.901465000 | 0.077232000  | 3.194256000  |
| C | -2.447063000 | -1.797104000 | 3.474152000  |
| H | -4.725920000 | 0.677908000  | 3.533190000  |
| H | -2.134407000 | -2.662694000 | 4.028909000  |
| C | -3.506388000 | -1.032294000 | 3.917194000  |
| H | -4.022510000 | -1.297578000 | 4.822079000  |
| C | -1.472946000 | 1.865742000  | -0.102148000 |
| C | -1.871726000 | 2.473260000  | -1.283214000 |
| C | -1.110636000 | 2.671840000  | 0.971294000  |
| H | -2.159710000 | 1.874591000  | -2.126744000 |
| H | -0.805736000 | 2.226941000  | 1.901331000  |
| C | -1.911833000 | 3.851433000  | -1.387330000 |
| C | -1.156831000 | 4.045653000  | 0.868921000  |

|   |              |             |              |
|---|--------------|-------------|--------------|
| H | -2.228485000 | 4.304342000 | -2.309242000 |
| H | -0.882256000 | 4.652243000 | 1.712761000  |
| C | -1.556313000 | 4.640605000 | -0.313474000 |
| H | -1.592559000 | 5.711754000 | -0.393601000 |
| H | 0.339101742  | 3.035207537 | -1.053004284 |
| C | 2.354062454  | 3.716242430 | -0.364935383 |
| C | 3.714248389  | 3.012072123 | -0.588758452 |
| C | 2.107435042  | 2.062721114 | -2.031597601 |
| H | 4.093369829  | 1.084947099 | -1.656979347 |
| H | 1.592249900  | 1.258642127 | -2.526965312 |
| H | 2.379424830  | 2.813331755 | -2.764398941 |
| H | 2.269732966  | 4.612129119 | -0.967674390 |
| H | 2.189532644  | 3.997588731 | 0.667268200  |
| H | 4.292577030  | 2.914048100 | 0.321096509  |
| H | 4.321697266  | 3.548114124 | -1.307618755 |

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exo-3cP-O\_Pd LP(OR)

|    |              |              |              |
|----|--------------|--------------|--------------|
| Pd | 1.039391000  | -0.875556000 | -0.116786000 |
| O  | 3.233950000  | -2.222653000 | -1.357449000 |
| O  | 3.252092000  | -2.293194000 | 0.856511000  |
| N  | -0.217091000 | -3.741011000 | -0.199235000 |
| C  | 0.256657000  | -2.698837000 | -0.183251000 |
| C  | 2.728625000  | -1.931905000 | -0.315750000 |
| C  | 4.424890000  | -3.101728000 | 0.812452000  |
| H  | 4.230975000  | -4.018134000 | 0.272436000  |
| H  | 4.672665000  | -3.316759000 | 1.840504000  |
| H  | 5.237453000  | -2.571495000 | 0.333413000  |
| C  | 3.478788200  | 1.462193305  | 1.178916214  |
| C  | 2.656123821  | 1.019687888  | -0.003535275 |
| C  | 1.409484179  | 1.499597112  | 0.172668275  |
| C  | 1.407665503  | 2.262930278  | 1.474486867  |
| H  | 3.094865303  | 0.716922388  | -0.933207485 |
| H  | 0.672686038  | 1.653369123  | -0.594239268 |
| P  | -1.289812000 | 0.053722000  | 0.033875000  |
| C  | -2.316268000 | -0.594987000 | -1.319908000 |
| C  | -3.693560000 | -0.725280000 | -1.217867000 |
| C  | -1.693451000 | -0.950393000 | -2.506832000 |
| H  | -4.195636000 | -0.475477000 | -0.302348000 |

|   |              |              |              |
|---|--------------|--------------|--------------|
| H | -0.624207000 | -0.885554000 | -2.592849000 |
| C | -4.431533000 | -1.192564000 | -2.285710000 |
| C | -2.432992000 | -1.409215000 | -3.578442000 |
| H | -5.496998000 | -1.297846000 | -2.191137000 |
| H | -1.935285000 | -1.686045000 | -4.489649000 |
| C | -3.803277000 | -1.531253000 | -3.468811000 |
| H | -4.379401000 | -1.900402000 | -4.297797000 |
| C | -2.170382000 | -0.345441000 | 1.577791000  |
| C | -3.238828000 | 0.418283000  | 2.033943000  |
| C | -1.780492000 | -1.456061000 | 2.313204000  |
| H | -3.554519000 | 1.287629000  | 1.487976000  |
| H | -0.965794000 | -2.066781000 | 1.975635000  |
| C | -3.901465000 | 0.077232000  | 3.194256000  |
| C | -2.447063000 | -1.797104000 | 3.474152000  |
| H | -4.725920000 | 0.677908000  | 3.533190000  |
| H | -2.134407000 | -2.662694000 | 4.028909000  |
| C | -3.506388000 | -1.032294000 | 3.917194000  |
| H | -4.022510000 | -1.297578000 | 4.822079000  |
| C | -1.472946000 | 1.865742000  | -0.102148000 |
| C | -1.871726000 | 2.473260000  | -1.283214000 |
| C | -1.110636000 | 2.671840000  | 0.971294000  |
| H | -2.159710000 | 1.874591000  | -2.126744000 |
| H | -0.805736000 | 2.226941000  | 1.901331000  |
| C | -1.911833000 | 3.851433000  | -1.387330000 |
| C | -1.156831000 | 4.045653000  | 0.868921000  |
| H | -2.228485000 | 4.304342000  | -2.309242000 |
| H | -0.882256000 | 4.652243000  | 1.712761000  |
| C | -1.556313000 | 4.640605000  | -0.313474000 |
| H | -1.592559000 | 5.711754000  | -0.393601000 |
| H | 4.394978280  | 0.920862022  | 1.357628275  |
| C | 3.658353113  | 2.987425698  | 0.928662142  |
| C | 2.227967702  | 3.540712317  | 1.138256648  |
| C | 2.442842725  | 1.498291909  | 2.298967155  |
| H | 0.442874805  | 2.445903719  | 1.921504559  |
| H | 2.129934259  | 0.522502674  | 2.626490557  |
| H | 2.784471229  | 2.066565615  | 3.156141315  |
| H | 4.350044810  | 3.396976806  | 1.654505940  |
| H | 4.052319331  | 3.199219988  | -0.057037524 |



|                |              |              |              |
|----------------|--------------|--------------|--------------|
| H              | 1.844683918  | 4.057957235  | 0.267934862  |
| H              | 2.190715913  | 4.230227026  | 1.972688832  |
| 61             |              |              |              |
| exo-3cP-O_PPh3 |              |              |              |
| Pd             | 1.039391000  | -0.875556000 | -0.116786000 |
| O              | 3.233950000  | -2.222653000 | -1.357449000 |
| O              | 3.252092000  | -2.293194000 | 0.856511000  |
| N              | -0.217091000 | -3.741011000 | -0.199235000 |
| C              | 0.256657000  | -2.698837000 | -0.183251000 |
| C              | 2.728625000  | -1.931905000 | -0.315750000 |
| C              | 4.424890000  | -3.101728000 | 0.812452000  |
| H              | 4.230975000  | -4.018134000 | 0.272436000  |
| H              | 4.672665000  | -3.316759000 | 1.840504000  |
| H              | 5.237453000  | -2.571495000 | 0.333413000  |
| C              | 2.365421854  | 2.193919092  | 1.266882880  |
| C              | 2.664714266  | 0.829536185  | 0.701495772  |
| C              | 2.574550175  | 0.922212961  | -0.639679982 |
| C              | 2.216072899  | 2.352109775  | -0.962637591 |
| H              | 3.194319594  | 0.078119762  | 1.252261612  |
| H              | 3.024205693  | 0.258208942  | -1.354923361 |
| P              | -1.289812000 | 0.053722000  | 0.033875000  |
| C              | -2.316268000 | -0.594987000 | -1.319908000 |
| C              | -3.693560000 | -0.725280000 | -1.217867000 |
| C              | -1.693451000 | -0.950393000 | -2.506832000 |
| H              | -4.195636000 | -0.475477000 | -0.302348000 |
| H              | -0.624207000 | -0.885554000 | -2.592849000 |
| C              | -4.431533000 | -1.192564000 | -2.285710000 |
| C              | -2.432992000 | -1.409215000 | -3.578442000 |
| H              | -5.496998000 | -1.297846000 | -2.191137000 |
| H              | -1.935285000 | -1.686045000 | -4.489649000 |
| C              | -3.803277000 | -1.531253000 | -3.468811000 |
| H              | -4.379401000 | -1.900402000 | -4.297797000 |
| C              | -2.170382000 | -0.345441000 | 1.577791000  |
| C              | -3.238828000 | 0.418283000  | 2.033943000  |
| C              | -1.780492000 | -1.456061000 | 2.313204000  |
| H              | -3.554519000 | 1.287629000  | 1.487976000  |
| H              | -0.965794000 | -2.066781000 | 1.975635000  |
| C              | -3.901465000 | 0.077232000  | 3.194256000  |

|   |              |              |              |
|---|--------------|--------------|--------------|
| C | -2.447063000 | -1.797104000 | 3.474152000  |
| H | -4.725920000 | 0.677908000  | 3.533190000  |
| H | -2.134407000 | -2.662694000 | 4.028909000  |
| C | -3.506388000 | -1.032294000 | 3.917194000  |
| H | -4.022510000 | -1.297578000 | 4.822079000  |
| C | -1.472946000 | 1.865742000  | -0.102148000 |
| C | -1.871726000 | 2.473260000  | -1.283214000 |
| C | -1.110636000 | 2.671840000  | 0.971294000  |
| H | -2.159710000 | 1.874591000  | -2.126744000 |
| H | -0.805736000 | 2.226941000  | 1.901331000  |
| C | -1.911833000 | 3.851433000  | -1.387330000 |
| C | -1.156831000 | 4.045653000  | 0.868921000  |
| H | -2.228485000 | 4.304342000  | -2.309242000 |
| H | -0.882256000 | 4.652243000  | 1.712761000  |
| C | -1.556313000 | 4.640605000  | -0.313474000 |
| H | -1.592559000 | 5.711754000  | -0.393601000 |
| H | 2.091508025  | 2.233371652  | 2.309857728  |
| C | 3.633950535  | 3.013486893  | 0.892252238  |
| C | 3.527274823  | 3.126907268  | -0.647817395 |
| C | 1.377130141  | 2.756615673  | 0.249212849  |
| H | 1.804590657  | 2.533308476  | -1.943440621 |
| H | 0.403649625  | 2.301361591  | 0.298480721  |
| H | 1.269581745  | 3.831752086  | 0.332324917  |
| H | 3.590851109  | 3.987700033  | 1.363495200  |
| H | 4.546654708  | 2.530908353  | 1.217458451  |
| H | 4.384322160  | 2.710053235  | -1.161248358 |
| H | 3.427221225  | 4.158970540  | -0.960755054 |

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exo-3tP-N\_CN

|    |           |           |           |
|----|-----------|-----------|-----------|
| Pd | -1.088291 | 0.016025  | -0.019826 |
| O  | -0.997475 | 2.590815  | -1.397606 |
| O  | -0.577607 | 2.656443  | 0.772914  |
| N  | -1.273921 | -3.083152 | 0.805709  |
| C  | -1.224226 | -1.985686 | 0.478470  |
| C  | -0.859442 | 1.997478  | -0.365558 |
| C  | -0.419514 | 4.068153  | 0.683326  |
| H  | -0.199665 | 4.406459  | 1.684564  |
| H  | 0.395435  | 4.315855  | 0.016655  |

|   |           |           |           |
|---|-----------|-----------|-----------|
| H | -1.326726 | 4.533760  | 0.322114  |
| C | -4.398029 | -0.679637 | 0.878606  |
| C | -3.412572 | 0.422105  | 0.570352  |
| C | -3.466151 | 0.636327  | -0.759957 |
| C | -4.475571 | -0.321497 | -1.331281 |
| H | -3.044636 | 1.117997  | 1.304025  |
| H | -3.104312 | 1.496473  | -1.286846 |
| P | 1.219383  | -0.210674 | -0.023192 |
| C | 2.250347  | 1.263405  | -0.318889 |
| C | 3.124316  | 1.769701  | 0.628868  |
| C | 2.165780  | 1.886060  | -1.557953 |
| H | 3.210597  | 1.303238  | 1.591193  |
| H | 1.485566  | 1.516023  | -2.302771 |
| C | 3.900488  | 2.878105  | 0.343231  |
| C | 2.942703  | 2.987273  | -1.842298 |
| H | 4.575064  | 3.259130  | 1.088293  |
| H | 2.865158  | 3.458360  | -2.805059 |
| C | 3.812933  | 3.487231  | -0.890630 |
| H | 4.417823  | 4.347711  | -1.112354 |
| C | 1.723617  | -0.817395 | 1.610526  |
| C | 2.535658  | -1.924160 | 1.784948  |
| C | 1.241794  | -0.145780 | 2.727303  |
| H | 2.897915  | -2.471781 | 0.936239  |
| H | 0.593539  | 0.703979  | 2.604339  |
| C | 2.870632  | -2.346922 | 3.057547  |
| C | 1.585188  | -0.563488 | 3.994573  |
| H | 3.493209  | -3.214080 | 3.181486  |
| H | 1.206702  | -0.036149 | 4.851147  |
| C | 2.400995  | -1.667201 | 4.161780  |
| H | 2.659489  | -2.000800 | 5.150318  |
| C | 1.852475  | -1.375978 | -1.265880 |
| C | 3.214978  | -1.420688 | -1.542926 |
| C | 0.998678  | -2.217546 | -1.960111 |
| H | 3.893364  | -0.764524 | -1.029648 |
| H | -0.053717 | -2.200277 | -1.758268 |
| C | 3.709793  | -2.298793 | -2.482452 |
| C | 1.496226  | -3.093141 | -2.906287 |
| H | 4.765193  | -2.324638 | -2.683819 |

|   |           |           |           |
|---|-----------|-----------|-----------|
| H | 0.821303  | -3.740249 | -3.435709 |
| C | 2.849538  | -3.137288 | -3.167036 |
| H | 3.235274  | -3.818888 | -3.903342 |
| H | -4.265925 | -1.191905 | 1.818726  |
| C | -5.781742 | 0.001581  | 0.688273  |
| C | -5.832739 | 0.258091  | -0.837031 |
| C | -4.336779 | -1.520453 | -0.397882 |
| H | -4.421262 | -0.497017 | -2.395031 |
| H | -3.412261 | -2.060852 | -0.512157 |
| H | -5.170101 | -2.208498 | -0.478807 |
| H | -6.569761 | -0.673160 | 0.999556  |
| H | -5.877363 | 0.908962  | 1.271032  |
| H | -5.948823 | 1.305117  | -1.086777 |
| H | -6.648559 | -0.282453 | -1.301429 |

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exo-3tP-N\_COOR

|    |              |              |              |
|----|--------------|--------------|--------------|
| Pd | -1.085531000 | -0.003232000 | -0.049790000 |
| O  | -1.014967000 | 2.571178000  | -1.419967000 |
| O  | -0.607283000 | 2.645472000  | 0.752551000  |
| N  | -1.234448000 | -3.116559000 | 0.728907000  |
| C  | -1.201199000 | -2.012827000 | 0.421166000  |
| C  | -0.875073000 | 1.981447000  | -0.386082000 |
| C  | -0.465645000 | 4.058706000  | 0.661291000  |
| H  | -0.255045000 | 4.401323000  | 1.663049000  |
| H  | 0.349767000  | 4.315095000  | -0.001508000 |
| H  | -1.376477000 | 4.512815000  | 0.294533000  |
| C  | -4.141056488 | 1.013559206  | -1.452726942 |
| C  | -3.428435688 | -0.093186994 | -0.713764031 |
| C  | -3.555016707 | 0.167403706  | 0.603291692  |
| C  | -4.344194364 | 1.441445566  | 0.736420077  |
| H  | -3.207123739 | -1.052922400 | -1.146383896 |
| H  | -3.402622054 | -0.521799834 | 1.410122267  |
| P  | 1.223343000  | -0.207305000 | -0.020800000 |
| C  | 2.243462000  | 1.279168000  | -0.290965000 |
| C  | 3.101632000  | 1.785555000  | 0.671098000  |
| C  | 2.168139000  | 1.911130000  | -1.525917000 |
| H  | 3.181022000  | 1.312117000  | 1.630586000  |
| H  | 1.500290000  | 1.541228000  | -2.281912000 |

|   |              |              |              |
|---|--------------|--------------|--------------|
| C | 3.870913000  | 2.903277000  | 0.403725000  |
| C | 2.938347000  | 3.021587000  | -1.792072000 |
| H | 4.533021000  | 3.284266000  | 1.159901000  |
| H | 2.868050000  | 3.499635000  | -2.751959000 |
| C | 3.792561000  | 3.521688000  | -0.826110000 |
| H | 4.392195000  | 4.389347000  | -1.033652000 |
| C | 1.705539000  | -0.817499000 | 1.618253000  |
| C | 2.513810000  | -1.925610000 | 1.801061000  |
| C | 1.208887000  | -0.148623000 | 2.730225000  |
| H | 2.887163000  | -2.471335000 | 0.955988000  |
| H | 0.563480000  | 0.702401000  | 2.601117000  |
| C | 2.830572000  | -2.352346000 | 3.076982000  |
| C | 1.534105000  | -0.570247000 | 4.000933000  |
| H | 3.450404000  | -3.220567000 | 3.207025000  |
| H | 1.144305000  | -0.044778000 | 4.853575000  |
| C | 2.346434000  | -1.675247000 | 4.176481000  |
| H | 2.590784000  | -2.011816000 | 5.167599000  |
| C | 1.889889000  | -1.358012000 | -1.259198000 |
| C | 3.257941000  | -1.389225000 | -1.509161000 |
| C | 1.056942000  | -2.200051000 | -1.977833000 |
| H | 3.920447000  | -0.732052000 | -0.976827000 |
| H | 0.000545000  | -2.193083000 | -1.797024000 |
| C | 3.778655000  | -2.254980000 | -2.446016000 |
| C | 1.580573000  | -3.063070000 | -2.921470000 |
| H | 4.838068000  | -2.270628000 | -2.626274000 |
| H | 0.921722000  | -3.710775000 | -3.470052000 |
| C | 2.939187000  | -3.094160000 | -3.155161000 |
| H | 3.345229000  | -3.766089000 | -3.889430000 |
| H | -3.880144503 | 1.142123739  | -2.491678910 |
| C | -5.644185931 | 0.724614709  | -1.183170392 |
| C | -5.783602014 | 1.010806543  | 0.331179619  |
| C | -3.926672605 | 2.204831419  | -0.517465157 |
| H | -4.276699028 | 1.950285940  | 1.686059834  |
| H | -2.909973465 | 2.558876933  | -0.496775656 |
| H | -4.592626633 | 3.029793359  | -0.741936572 |
| H | -6.258539815 | 1.397809468  | -1.768468273 |
| H | -5.922594406 | -0.287625181 | -1.447670746 |
| H | -6.130815388 | 0.153444946  | 0.893727839  |

|                    |              |              |              |
|--------------------|--------------|--------------|--------------|
| H                  | -6.471930375 | 1.826245498  | 0.517260623  |
| 61                 |              |              |              |
| exo-3tP-N_Pd LP(O) |              |              |              |
| Pd                 | -1.085531000 | -0.003232000 | -0.049790000 |
| O                  | -1.014967000 | 2.571178000  | -1.419967000 |
| O                  | -0.607283000 | 2.645472000  | 0.752551000  |
| N                  | -1.234448000 | -3.116559000 | 0.728907000  |
| C                  | -1.201199000 | -2.012827000 | 0.421166000  |
| C                  | -0.875073000 | 1.981447000  | -0.386082000 |
| C                  | -0.465645000 | 4.058706000  | 0.661291000  |
| H                  | -0.255045000 | 4.401323000  | 1.663049000  |
| H                  | 0.349767000  | 4.315095000  | -0.001508000 |
| H                  | -1.376477000 | 4.512815000  | 0.294533000  |
| C                  | -4.279550309 | -0.440919011 | -1.444423701 |
| C                  | -3.514138596 | -0.160077341 | -0.173969213 |
| C                  | -3.356847404 | 1.177003341  | -0.096246787 |
| C                  | -4.011385882 | 1.778706910  | -1.310017521 |
| H                  | -3.452053438 | -0.849392223 | 0.649572772  |
| H                  | -3.095878682 | 1.741546112  | 0.776901546  |
| P                  | 1.223343000  | -0.207305000 | -0.020800000 |
| C                  | 2.243462000  | 1.279168000  | -0.290965000 |
| C                  | 3.101632000  | 1.785555000  | 0.671098000  |
| C                  | 2.168139000  | 1.911130000  | -1.525917000 |
| H                  | 3.181022000  | 1.312117000  | 1.630586000  |
| H                  | 1.500290000  | 1.541228000  | -2.281912000 |
| C                  | 3.870913000  | 2.903277000  | 0.403725000  |
| C                  | 2.938347000  | 3.021587000  | -1.792072000 |
| H                  | 4.533021000  | 3.284266000  | 1.159901000  |
| H                  | 2.868050000  | 3.499635000  | -2.751959000 |
| C                  | 3.792561000  | 3.521688000  | -0.826110000 |
| H                  | 4.392195000  | 4.389347000  | -1.033652000 |
| C                  | 1.705539000  | -0.817499000 | 1.618253000  |
| C                  | 2.513810000  | -1.925610000 | 1.801061000  |
| C                  | 1.208887000  | -0.148623000 | 2.730225000  |
| H                  | 2.887163000  | -2.471335000 | 0.955988000  |
| H                  | 0.563480000  | 0.702401000  | 2.601117000  |
| C                  | 2.830572000  | -2.352346000 | 3.076982000  |
| C                  | 1.534105000  | -0.570247000 | 4.000933000  |

|   |              |              |              |
|---|--------------|--------------|--------------|
| H | 3.450404000  | -3.220567000 | 3.207025000  |
| H | 1.144305000  | -0.044778000 | 4.853575000  |
| C | 2.346434000  | -1.675247000 | 4.176481000  |
| H | 2.590784000  | -2.011816000 | 5.167599000  |
| C | 1.889889000  | -1.358012000 | -1.259198000 |
| C | 3.257941000  | -1.389225000 | -1.509161000 |
| C | 1.056942000  | -2.200051000 | -1.977833000 |
| H | 3.920447000  | -0.732052000 | -0.976827000 |
| H | 0.000545000  | -2.193083000 | -1.797024000 |
| C | 3.778655000  | -2.254980000 | -2.446016000 |
| C | 1.580573000  | -3.063070000 | -2.921470000 |
| H | 4.838068000  | -2.270628000 | -2.626274000 |
| H | 0.921722000  | -3.710775000 | -3.470052000 |
| C | 2.939187000  | -3.094160000 | -3.155161000 |
| H | 3.345229000  | -3.766089000 | -3.889430000 |
| H | -4.222548816 | -1.448480227 | -1.825994558 |
| C | -5.715388469 | 0.060925168  | -1.124941339 |
| C | -5.529498693 | 1.593746691  | -1.022463366 |
| C | -3.799202034 | 0.688756358  | -2.357059245 |
| H | -3.720070863 | 2.787255152  | -1.561524611 |
| H | -2.776313924 | 0.580061385  | -2.675396710 |
| H | -4.436399671 | 0.816840515  | -3.224248962 |
| H | -6.384832665 | -0.200384208 | -1.935347019 |
| H | -6.111917939 | -0.376637648 | -0.217524966 |
| H | -5.817437021 | 1.991429142  | -0.057566107 |
| H | -6.107396708 | 2.112990152  | -1.777303001 |

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exo-3tP-N\_Pd LP(OR)

|    |              |              |              |
|----|--------------|--------------|--------------|
| Pd | -1.085531000 | -0.003232000 | -0.049790000 |
| O  | -1.014967000 | 2.571178000  | -1.419967000 |
| O  | -0.607283000 | 2.645472000  | 0.752551000  |
| N  | -1.234448000 | -3.116559000 | 0.728907000  |
| C  | -1.201199000 | -2.012827000 | 0.421166000  |
| C  | -0.875073000 | 1.981447000  | -0.386082000 |
| C  | -0.465645000 | 4.058706000  | 0.661291000  |
| H  | -0.255045000 | 4.401323000  | 1.663049000  |
| H  | 0.349767000  | 4.315095000  | -0.001508000 |
| H  | -1.376477000 | 4.512815000  | 0.294533000  |

|   |              |              |              |
|---|--------------|--------------|--------------|
| C | -3.897526494 | 1.742241155  | 1.126788613  |
| C | -3.231904958 | 1.149797614  | -0.091710611 |
| C | -3.639081042 | -0.132871614 | -0.178505389 |
| C | -4.566690871 | -0.390068600 | 0.977823681  |
| H | -2.832326889 | 1.738587141  | -0.898491397 |
| H | -3.576339874 | -0.767900943 | -1.039901072 |
| P | 1.223343000  | -0.207305000 | -0.020800000 |
| C | 2.243462000  | 1.279168000  | -0.290965000 |
| C | 3.101632000  | 1.785555000  | 0.671098000  |
| C | 2.168139000  | 1.911130000  | -1.525917000 |
| H | 3.181022000  | 1.312117000  | 1.630586000  |
| H | 1.500290000  | 1.541228000  | -2.281912000 |
| C | 3.870913000  | 2.903277000  | 0.403725000  |
| C | 2.938347000  | 3.021587000  | -1.792072000 |
| H | 4.533021000  | 3.284266000  | 1.159901000  |
| H | 2.868050000  | 3.499635000  | -2.751959000 |
| C | 3.792561000  | 3.521688000  | -0.826110000 |
| H | 4.392195000  | 4.389347000  | -1.033652000 |
| C | 1.705539000  | -0.817499000 | 1.618253000  |
| C | 2.513810000  | -1.925610000 | 1.801061000  |
| C | 1.208887000  | -0.148623000 | 2.730225000  |
| H | 2.887163000  | -2.471335000 | 0.955988000  |
| H | 0.563480000  | 0.702401000  | 2.601117000  |
| C | 2.830572000  | -2.352346000 | 3.076982000  |
| C | 1.534105000  | -0.570247000 | 4.000933000  |
| H | 3.450404000  | -3.220567000 | 3.207025000  |
| H | 1.144305000  | -0.044778000 | 4.853575000  |
| C | 2.346434000  | -1.675247000 | 4.176481000  |
| H | 2.590784000  | -2.011816000 | 5.167599000  |
| C | 1.889889000  | -1.358012000 | -1.259198000 |
| C | 3.257941000  | -1.389225000 | -1.509161000 |
| C | 1.056942000  | -2.200051000 | -1.977833000 |
| H | 3.920447000  | -0.732052000 | -0.976827000 |
| H | 0.000545000  | -2.193083000 | -1.797024000 |
| C | 3.778655000  | -2.254980000 | -2.446016000 |
| C | 1.580573000  | -3.063070000 | -2.921470000 |
| H | 4.838068000  | -2.270628000 | -2.626274000 |
| H | 0.921722000  | -3.710775000 | -3.470052000 |



|   |              |              |              |
|---|--------------|--------------|--------------|
| C | 2.939187000  | -3.094160000 | -3.155161000 |
| H | 3.345229000  | -3.766089000 | -3.889430000 |
| H | -3.453845708 | 2.640780771  | 1.526537301  |
| C | -5.386199734 | 1.877197853  | 0.701128592  |
| C | -5.847003571 | 0.404237788  | 0.588669556  |
| C | -3.994112774 | 0.529003119  | 2.053357066  |
| H | -4.738668665 | -1.424602054 | 1.233663443  |
| H | -3.043190755 | 0.207908685  | 2.443355916  |
| H | -4.685323335 | 0.690174632  | 2.872317436  |
| H | -5.941030386 | 2.405088271  | 1.467085604  |
| H | -5.501349604 | 2.426176837  | -0.224864872 |
| H | -6.206514948 | 0.147534968  | -0.399734089 |
| H | -6.639077844 | 0.183300414  | 1.293770815  |

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exo-3tP-O\_CN

|    |              |              |              |
|----|--------------|--------------|--------------|
| Pd | -1.049911000 | -0.246590000 | -0.542245000 |
| O  | -0.807075210 | 2.408065566  | -1.693797193 |
| O  | -0.958192032 | 2.376714460  | 0.513497919  |
| N  | -0.952463000 | -3.437829000 | -0.209471000 |
| C  | -0.977029000 | -2.298692000 | -0.333575000 |
| C  | -0.913433889 | 1.771395205  | -0.684933802 |
| C  | -0.856255659 | 3.796316024  | 0.525040428  |
| H  | -0.917211830 | 4.089641954  | 1.562138682  |
| H  | -1.664855150 | 4.243149255  | -0.038123641 |
| H  | 0.087099358  | 4.112951572  | 0.101094150  |
| H  | -2.859978358 | 0.863142924  | -2.339040161 |
| C  | -3.131125305 | 0.011365067  | -1.746550173 |
| C  | -3.473471524 | 0.039048277  | -0.437844699 |
| H  | -3.521228132 | 0.919580107  | 0.172035246  |
| C  | -3.677262518 | -1.268741263 | -2.326095081 |
| C  | -4.248444459 | -1.225930176 | -0.156717858 |
| P  | 1.200540000  | -0.156047000 | 0.016710000  |
| C  | 2.047393000  | 1.458969000  | 0.068258000  |
| C  | 2.598348000  | 1.984529000  | 1.225236000  |
| C  | 2.171870000  | 2.169136000  | -1.119485000 |
| H  | 2.522226000  | 1.451967000  | 2.153446000  |
| H  | 1.743193000  | 1.784130000  | -2.026227000 |
| C  | 3.260904000  | 3.198161000  | 1.196350000  |

|   |              |              |              |
|---|--------------|--------------|--------------|
| C | 2.835799000  | 3.375731000  | -1.147259000 |
| H | 3.684667000  | 3.592486000  | 2.102070000  |
| H | 2.922939000  | 3.913112000  | -2.073830000 |
| C | 3.382293000  | 3.894493000  | 0.012434000  |
| H | 3.899627000  | 4.836503000  | -0.009875000 |
| C | 1.356790000  | -0.826762000 | 1.696145000  |
| C | 2.189118000  | -1.886384000 | 2.011332000  |
| C | 0.563300000  | -0.268435000 | 2.691730000  |
| H | 2.789870000  | -2.349895000 | 1.252715000  |
| H | -0.104184000 | 0.541602000  | 2.455085000  |
| C | 2.239094000  | -2.371278000 | 3.304943000  |
| C | 0.622260000  | -0.747478000 | 3.982197000  |
| H | 2.882699000  | -3.200470000 | 3.535437000  |
| H | 0.005714000  | -0.306105000 | 4.743916000  |
| C | 1.462025000  | -1.801689000 | 4.291409000  |
| H | 1.501140000  | -2.182337000 | 5.295834000  |
| C | 2.301951000  | -1.112775000 | -1.067352000 |
| C | 3.680946000  | -0.997597000 | -0.922744000 |
| C | 1.798139000  | -1.935610000 | -2.060884000 |
| H | 4.093803000  | -0.349294000 | -0.171879000 |
| H | 0.739126000  | -2.041172000 | -2.186257000 |
| C | 4.532450000  | -1.703319000 | -1.743893000 |
| C | 2.654118000  | -2.636671000 | -2.889335000 |
| H | 5.595548000  | -1.607795000 | -1.618255000 |
| H | 2.247959000  | -3.271343000 | -3.655365000 |
| C | 4.018993000  | -2.524636000 | -2.731148000 |
| H | 4.683485000  | -3.071294000 | -3.375496000 |
| C | -5.210792502 | -1.034705864 | -2.373267945 |
| H | -3.232768203 | -1.593856179 | -3.252844230 |
| H | -4.325156667 | -1.517760187 | 0.879170228  |
| C | -5.605400076 | -1.006026682 | -0.876719563 |
| C | -3.583495396 | -2.207676166 | -1.122533316 |
| H | -4.156874560 | -3.117351780 | -1.255755592 |
| H | -2.566430011 | -2.459251635 | -0.850998260 |
| H | -5.469763887 | -0.122475574 | -2.895415649 |
| H | -5.691483632 | -1.855374542 | -2.891674126 |
| H | -6.286897847 | -1.812199111 | -0.633177001 |
| H | -6.078877804 | -0.077891493 | -0.582593593 |

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exo-3tP-O\_COOR

|    |           |           |           |
|----|-----------|-----------|-----------|
| Pd | -1.021625 | -0.436313 | -0.170379 |
| O  | -1.483816 | 2.122150  | -1.413143 |
| O  | -1.149051 | 2.230785  | 0.771921  |
| N  | -0.635352 | -3.623900 | 0.099737  |
| C  | -0.737008 | -2.485916 | 0.004553  |
| C  | -1.251829 | 1.552284  | -0.385572 |
| C  | -1.312450 | 3.642456  | 0.711542  |
| H  | -1.197839 | 3.998546  | 1.724189  |
| H  | -2.293538 | 3.899641  | 0.333961  |
| H  | -0.560343 | 4.084130  | 0.071911  |
| H  | -3.093347 | -2.199671 | 0.613051  |
| C  | -3.448534 | -1.238354 | 0.300856  |
| C  | -3.314498 | -0.702116 | -0.927972 |
| H  | -2.879866 | -1.194298 | -1.780323 |
| C  | -4.519171 | -0.463571 | 1.018540  |
| C  | -4.309990 | 0.428057  | -1.027605 |
| P  | 1.266553  | -0.116741 | -0.009180 |
| C  | 1.941306  | 1.576480  | -0.045483 |
| C  | 2.606816  | 2.142018  | 1.029152  |
| C  | 1.800791  | 2.314006  | -1.214632 |
| H  | 2.733575  | 1.590046  | 1.940422  |
| H  | 1.280880  | 1.897473  | -2.057682 |
| C  | 3.122313  | 3.422213  | 0.937746  |
| C  | 2.318588  | 3.587205  | -1.305257 |
| H  | 3.637413  | 3.847485  | 1.779855  |
| H  | 2.201809  | 4.144713  | -2.216575 |
| C  | 2.980984  | 4.145861  | -0.227223 |
| H  | 3.383965  | 5.139853  | -0.298129 |
| C  | 1.796276  | -0.805049 | 1.584470  |
| C  | 2.823555  | -1.724984 | 1.702817  |
| C  | 1.109576  | -0.404986 | 2.724587  |
| H  | 3.350279  | -2.066847 | 0.832712  |
| H  | 0.294715  | 0.292808  | 2.643792  |
| C  | 3.167685  | -2.228027 | 2.943400  |
| C  | 1.461447  | -0.900291 | 3.961251  |
| H  | 3.960680  | -2.949112 | 3.021582  |

|   |           |           |           |
|---|-----------|-----------|-----------|
| H | 0.923792  | -0.582587 | 4.835911  |
| C | 2.492740  | -1.814537 | 4.072619  |
| H | 2.760091  | -2.209982 | 5.035648  |
| C | 2.234103  | -0.935420 | -1.311660 |
| C | 3.587084  | -0.644236 | -1.453841 |
| C | 1.646884  | -1.837063 | -2.183916 |
| H | 4.058927  | 0.065924  | -0.800209 |
| H | 0.607006  | -2.077768 | -2.088152 |
| C | 4.334820  | -1.253858 | -2.437358 |
| C | 2.397095  | -2.442697 | -3.173928 |
| H | 5.379724  | -1.021456 | -2.533523 |
| H | 1.926994  | -3.140546 | -3.842162 |
| C | 3.739491  | -2.154878 | -3.301058 |
| H | 4.321836  | -2.626538 | -4.071722 |
| C | -5.826075 | -0.916062 | 0.305264  |
| H | -4.538314 | -0.553277 | 2.094062  |
| H | -4.127600 | 1.154259  | -1.803210 |
| C | -5.684154 | -0.291477 | -1.103218 |
| C | -4.352508 | 0.930044  | 0.417879  |
| H | -5.205214 | 1.570704  | 0.609918  |
| H | -3.451693 | 1.426667  | 0.741659  |
| H | -5.928619 | -1.993291 | 0.282001  |
| H | -6.684440 | -0.515853 | 0.831101  |
| H | -6.469072 | 0.430335  | -1.293939 |
| H | -5.716978 | -1.028609 | -1.895125 |

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exo-3tP-O\_Pd LP(O)

|    |              |              |              |
|----|--------------|--------------|--------------|
| Pd | -1.049911000 | -0.246590000 | -0.542245000 |
| O  | -0.807075210 | 2.408065566  | -1.693797193 |
| O  | -0.958192032 | 2.376714460  | 0.513497919  |
| N  | -0.952463000 | -3.437829000 | -0.209471000 |
| C  | -0.977029000 | -2.298692000 | -0.333575000 |
| C  | -0.913433889 | 1.771395205  | -0.684933802 |
| C  | -0.856255659 | 3.796316024  | 0.525040428  |
| H  | -0.917211830 | 4.089641954  | 1.562138682  |
| H  | -1.664855150 | 4.243149255  | -0.038123641 |
| H  | 0.087099358  | 4.112951572  | 0.101094150  |
| H  | -3.371035561 | 1.212454304  | -0.073316069 |

|   |              |              |              |
|---|--------------|--------------|--------------|
| C | -3.231235282 | 0.691673189  | -1.000318487 |
| C | -3.373361548 | -0.641259845 | -1.184076386 |
| H | -3.648969612 | -1.345942489 | -0.424449430 |
| C | -3.355210280 | 1.346636229  | -2.352525566 |
| C | -3.593101994 | -0.862959121 | -2.661354087 |
| P | 1.200540000  | -0.156047000 | 0.016710000  |
| C | 2.047393000  | 1.458969000  | 0.068258000  |
| C | 2.598348000  | 1.984529000  | 1.225236000  |
| C | 2.171870000  | 2.169136000  | -1.119485000 |
| H | 2.522226000  | 1.451967000  | 2.153446000  |
| H | 1.743193000  | 1.784130000  | -2.026227000 |
| C | 3.260904000  | 3.198161000  | 1.196350000  |
| C | 2.835799000  | 3.375731000  | -1.147259000 |
| H | 3.684667000  | 3.592486000  | 2.102070000  |
| H | 2.922939000  | 3.913112000  | -2.073830000 |
| C | 3.382293000  | 3.894493000  | 0.012434000  |
| H | 3.899627000  | 4.836503000  | -0.009875000 |
| C | 1.356790000  | -0.826762000 | 1.696145000  |
| C | 2.189118000  | -1.886384000 | 2.011332000  |
| C | 0.563300000  | -0.268435000 | 2.691730000  |
| H | 2.789870000  | -2.349895000 | 1.252715000  |
| H | -0.104184000 | 0.541602000  | 2.455085000  |
| C | 2.239094000  | -2.371278000 | 3.304943000  |
| C | 0.622260000  | -0.747478000 | 3.982197000  |
| H | 2.882699000  | -3.200470000 | 3.535437000  |
| H | 0.005714000  | -0.306105000 | 4.743916000  |
| C | 1.462025000  | -1.801689000 | 4.291409000  |
| H | 1.501140000  | -2.182337000 | 5.295834000  |
| C | 2.301951000  | -1.112775000 | -1.067352000 |
| C | 3.680946000  | -0.997597000 | -0.922744000 |
| C | 1.798139000  | -1.935610000 | -2.060884000 |
| H | 4.093803000  | -0.349294000 | -0.171879000 |
| H | 0.739126000  | -2.041172000 | -2.186257000 |
| C | 4.532450000  | -1.703319000 | -1.743893000 |
| C | 2.654118000  | -2.636671000 | -2.889335000 |
| H | 5.595548000  | -1.607795000 | -1.618255000 |
| H | 2.247959000  | -3.271343000 | -3.655365000 |
| C | 4.018993000  | -2.524636000 | -2.731148000 |

|   |              |              |              |
|---|--------------|--------------|--------------|
| H | 4.683485000  | -3.071294000 | -3.375496000 |
| C | -4.860473045 | 1.202925769  | -2.702158760 |
| H | -2.958174942 | 2.345855314  | -2.430391162 |
| H | -3.413437390 | -1.862641477 | -3.025317633 |
| C | -5.024807392 | -0.321335028 | -2.916210014 |
| C | -2.761742912 | 0.270799407  | -3.263197605 |
| H | -2.981640315 | 0.441045455  | -4.310423931 |
| H | -1.695019622 | 0.139324519  | -3.135685736 |
| H | -5.501099939 | 1.590660193  | -1.920412187 |
| H | -5.080974260 | 1.753925562  | -3.608295865 |
| H | -5.328844570 | -0.546370768 | -3.931388070 |
| H | -5.754491923 | -0.764940471 | -2.250702035 |

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exo-3tP-O\_Pd LP(OR)

|    |           |           |           |
|----|-----------|-----------|-----------|
| Pd | -1.050596 | -0.247138 | -0.539481 |
| O  | -0.983837 | 2.399861  | -1.733630 |
| O  | -1.122254 | 2.392052  | 0.474626  |
| N  | -0.953653 | -3.438371 | -0.203877 |
| C  | -0.977691 | -2.299296 | -0.328515 |
| C  | -1.044328 | 1.772906  | -0.715056 |
| C  | -1.112181 | 3.815015  | 0.464971  |
| H  | -1.186552 | 4.119320  | 1.498045  |
| H  | -1.950888 | 4.200504  | -0.099582 |
| H  | -0.193496 | 4.185711  | 0.030727  |
| H  | -3.087242 | -1.587879 | -1.878366 |
| C  | -3.309192 | -0.946731 | -1.047859 |
| C  | -3.340530 | 0.405460  | -1.083099 |
| H  | -3.151451 | 1.007533  | -1.949911 |
| C  | -4.110700 | -1.382906 | 0.152194  |
| C  | -4.166673 | 0.859404  | 0.096393  |
| P  | 1.200530  | -0.155254 | 0.015587  |
| C  | 2.044632  | 1.460951  | 0.072157  |
| C  | 2.594362  | 1.983472  | 1.231110  |
| C  | 2.168013  | 2.175651  | -1.112974 |
| H  | 2.518989  | 1.447431  | 2.157391  |
| H  | 1.740347  | 1.793082  | -2.021219 |
| C  | 3.254542  | 3.198456  | 1.206762  |
| C  | 2.829705  | 3.383538  | -1.136260 |

|   |           |           |           |
|---|-----------|-----------|-----------|
| H | 3.677282  | 3.590318  | 2.114024  |
| H | 2.916107  | 3.924316  | -2.060910 |
| C | 3.374923  | 3.899218  | 0.025384  |
| H | 3.890530  | 4.842238  | 0.006554  |
| C | 1.362842  | -0.832520 | 1.691830  |
| C | 2.204026  | -1.886819 | 2.001215  |
| C | 0.567108  | -0.284358 | 2.691167  |
| H | 2.807202  | -2.342243 | 1.239607  |
| H | -0.106698 | 0.521766  | 2.459227  |
| C | 2.259955  | -2.376867 | 3.292603  |
| C | 0.631994  | -0.768335 | 3.979470  |
| H | 2.910313  | -3.202050 | 3.518462  |
| H | 0.013516  | -0.334833 | 4.744123  |
| C | 1.480190  | -1.817495 | 4.282753  |
| H | 1.523804  | -2.202192 | 5.285445  |
| C | 2.301056  | -1.106220 | -1.074581 |
| C | 3.680184  | -0.980974 | -0.940295 |
| C | 1.796152  | -1.936698 | -2.061321 |
| H | 4.093880  | -0.327154 | -0.194748 |
| H | 0.737100  | -2.050383 | -2.178770 |
| C | 4.530836  | -1.683773 | -1.764903 |
| C | 2.651117  | -2.635009 | -2.892964 |
| H | 5.594073  | -1.580080 | -1.647196 |
| H | 2.243918  | -3.275614 | -3.653467 |
| C | 4.016315  | -2.512587 | -2.745187 |
| H | 4.680055  | -3.056930 | -3.392251 |
| C | -5.579345 | -1.080041 | -0.247807 |
| H | -3.926790 | -2.385631 | 0.502699  |
| H | -4.038261 | 1.886328  | 0.401412  |
| C | -5.618626 | 0.466926  | -0.285414 |
| C | -3.850851 | -0.229694 | 1.122467  |
| H | -4.536442 | -0.226081 | 1.961502  |
| H | -2.832897 | -0.196315 | 1.488688  |
| H | -5.847253 | -1.531983 | -1.194295 |
| H | -6.252958 | -1.472988 | 0.503956  |
| H | -6.312059 | 0.861601  | 0.447427  |
| H | -5.907402 | 0.858611  | -1.252531 |

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exo-3tP-O

|    |              |              |              |
|----|--------------|--------------|--------------|
| 46 | -1.120069000 | -0.169607000 | -0.255174000 |
| 15 | 1.181608000  | -0.166388000 | 0.038967000  |
| 6  | 2.024807000  | 1.414120000  | 0.384191000  |
| 6  | 1.739569000  | 2.067051000  | 1.577032000  |
| 6  | 2.950025000  | 1.973246000  | -0.481684000 |
| 6  | 2.371920000  | 3.248251000  | 1.896394000  |
| 1  | 1.012496000  | 1.660302000  | 2.254967000  |
| 6  | 3.579702000  | 3.162013000  | -0.161648000 |
| 1  | 3.190061000  | 1.485043000  | -1.406497000 |
| 6  | 3.294515000  | 3.799903000  | 1.026668000  |
| 1  | 2.138839000  | 3.741362000  | 2.822416000  |
| 1  | 4.295994000  | 3.583014000  | -0.843669000 |
| 1  | 3.786351000  | 4.722681000  | 1.276223000  |
| 6  | 1.804143000  | -1.230071000 | 1.378384000  |
| 6  | 3.099090000  | -1.057621000 | 1.856289000  |
| 6  | 1.011438000  | -2.221640000 | 1.934414000  |
| 6  | 3.589505000  | -1.864163000 | 2.860177000  |
| 1  | 3.726841000  | -0.286988000 | 1.449422000  |
| 6  | 1.504682000  | -3.026210000 | 2.943423000  |
| 1  | 0.016599000  | -2.383229000 | 1.570754000  |
| 6  | 2.791015000  | -2.850631000 | 3.407280000  |
| 1  | 4.592600000  | -1.718871000 | 3.217938000  |
| 1  | 0.877847000  | -3.792466000 | 3.361260000  |
| 1  | 3.171857000  | -3.477320000 | 4.193407000  |
| 6  | 1.926231000  | -0.761892000 | -1.505768000 |
| 6  | 1.494427000  | -0.193816000 | -2.697629000 |
| 6  | 2.876944000  | -1.766446000 | -1.541648000 |
| 6  | 2.022185000  | -0.609989000 | -3.900191000 |
| 1  | 0.739937000  | 0.573115000  | -2.683551000 |
| 6  | 3.396871000  | -2.189560000 | -2.750052000 |
| 1  | 3.204288000  | -2.235193000 | -0.633497000 |
| 6  | 2.975219000  | -1.610885000 | -3.928216000 |
| 1  | 1.680439000  | -0.163367000 | -4.816117000 |
| 1  | 4.126278000  | -2.978680000 | -2.766565000 |
| 1  | 3.377925000  | -1.944795000 | -4.867231000 |
| 6  | -3.401946000 | 0.585476000  | -0.608452000 |
| 6  | -4.196700000 | 0.769891000  | 0.662029000  |



|   |              |              |              |
|---|--------------|--------------|--------------|
| 6 | -4.133103000 | -1.433057000 | 0.232962000  |
| 6 | -3.367153000 | -0.743140000 | -0.867304000 |
| 6 | -3.848704000 | -0.511656000 | 1.420473000  |
| 1 | -4.510311000 | -0.693168000 | 2.259331000  |
| 1 | -2.821653000 | -0.542227000 | 1.761145000  |
| 6 | -5.657169000 | 0.454249000  | 0.244306000  |
| 1 | -5.976720000 | 1.040383000  | -0.608418000 |
| 6 | -5.613328000 | -1.065054000 | -0.051618000 |
| 1 | -5.907913000 | -1.306441000 | -1.065182000 |
| 1 | -4.052253000 | 1.705615000  | 1.177448000  |
| 1 | -3.933199000 | -2.486061000 | 0.350420000  |
| 1 | -3.166666000 | -1.193132000 | -1.819519000 |
| 1 | -3.242825000 | 1.359984000  | -1.333931000 |
| 6 | -1.147180000 | 1.818654000  | 0.144536000  |
| 8 | -1.390711000 | 2.328247000  | 1.197653000  |
| 8 | -0.853909000 | 2.566821000  | -0.937555000 |
| 6 | -0.820529000 | 3.975631000  | -0.751813000 |
| 1 | -0.583077000 | 4.397059000  | -1.717270000 |
| 1 | -1.779503000 | 4.341654000  | -0.408593000 |
| 1 | -0.062908000 | 4.246268000  | -0.028582000 |
| 6 | -1.027356000 | -2.191464000 | -0.630766000 |
| 7 | -0.997644000 | -3.318008000 | -0.836043000 |
| 1 | -6.331331000 | 0.677453000  | 1.062561000  |
| 1 | -6.265171000 | -1.615862000 | 0.615734000  |

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exo-3tP-OMe

|    |              |              |              |
|----|--------------|--------------|--------------|
| 46 | 1.094328000  | -0.264676000 | 0.216679000  |
| 15 | -1.205585000 | -0.155851000 | -0.022929000 |
| 6  | -1.983164000 | 1.481347000  | -0.229670000 |
| 6  | -1.704775000 | 2.184957000  | -1.394631000 |
| 6  | -2.852833000 | 2.032753000  | 0.694790000  |
| 6  | -2.289448000 | 3.409145000  | -1.630526000 |
| 1  | -1.026474000 | 1.774885000  | -2.120804000 |
| 6  | -3.434553000 | 3.264980000  | 0.459538000  |
| 1  | -3.084797000 | 1.507594000  | 1.601104000  |
| 6  | -3.156673000 | 3.954046000  | -0.701170000 |
| 1  | -2.067676000 | 3.939702000  | -2.538704000 |
| 1  | -4.106714000 | 3.681257000  | 1.187713000  |

|   |              |              |              |
|---|--------------|--------------|--------------|
| 1 | -3.611556000 | 4.910750000  | -0.883830000 |
| 6 | -1.966149000 | -1.075027000 | -1.396393000 |
| 6 | -3.330766000 | -0.933839000 | -1.631298000 |
| 6 | -1.221784000 | -1.884701000 | -2.236658000 |
| 6 | -3.935544000 | -1.601201000 | -2.672617000 |
| 1 | -3.923414000 | -0.294636000 | -1.002824000 |
| 6 | -1.829915000 | -2.547620000 | -3.286563000 |
| 1 | -0.173279000 | -2.019612000 | -2.065481000 |
| 6 | -3.183306000 | -2.410353000 | -3.504746000 |
| 1 | -4.991186000 | -1.485769000 | -2.838865000 |
| 1 | -1.238725000 | -3.176593000 | -3.926427000 |
| 1 | -3.654198000 | -2.928896000 | -4.320343000 |
| 6 | -1.874346000 | -0.826272000 | 1.524520000  |
| 6 | -1.452059000 | -0.247100000 | 2.716892000  |
| 6 | -2.721916000 | -1.919584000 | 1.563435000  |
| 6 | -1.898555000 | -0.741810000 | 3.922928000  |
| 1 | -0.770943000 | 0.586491000  | 2.700791000  |
| 6 | -3.158430000 | -2.417588000 | 2.776440000  |
| 1 | -3.032009000 | -2.398198000 | 0.654507000  |
| 6 | -2.753436000 | -1.828019000 | 3.954972000  |
| 1 | -1.569413000 | -0.285710000 | 4.838825000  |
| 1 | -3.809320000 | -3.272585000 | 2.795248000  |
| 1 | -3.092739000 | -2.218599000 | 4.897246000  |
| 6 | 3.393848000  | 0.361288000  | 0.732894000  |
| 6 | 4.209767000  | 0.798093000  | -0.460471000 |
| 6 | 4.108528000  | -1.443054000 | -0.513163000 |
| 6 | 3.337221000  | -0.990490000 | 0.700453000  |
| 6 | 3.853420000  | -0.284984000 | -1.479527000 |
| 1 | 4.522933000  | -0.295062000 | -2.331681000 |
| 1 | 2.829414000  | -0.228462000 | -1.826708000 |
| 6 | 5.660022000  | 0.376838000  | -0.104641000 |
| 1 | 5.974425000  | 0.761929000  | 0.857321000  |
| 6 | 5.589796000  | -1.169381000 | -0.141325000 |
| 1 | 5.866860000  | -1.626676000 | 0.800061000  |
| 1 | 4.092383000  | 1.826094000  | -0.764636000 |
| 1 | 3.894135000  | -2.442467000 | -0.855618000 |
| 1 | 3.113482000  | -1.630281000 | 1.531352000  |
| 1 | 3.235527000  | 0.965670000  | 1.604959000  |

|   |             |              |              |
|---|-------------|--------------|--------------|
| 6 | 1.072611000 | 1.740768000  | 0.528352000  |
| 8 | 0.835421000 | 2.249548000  | 1.586701000  |
| 8 | 1.363448000 | 2.488024000  | -0.547807000 |
| 6 | 1.358731000 | 3.897705000  | -0.364564000 |
| 1 | 1.610529000 | 4.322305000  | -1.325131000 |
| 1 | 0.382293000 | 4.238426000  | -0.047881000 |
| 1 | 2.089541000 | 4.190586000  | 0.378057000  |
| 6 | 1.015072000 | -2.312620000 | 0.036278000  |
| 7 | 0.999199000 | -3.454582000 | -0.051558000 |
| 1 | 6.349294000 | 0.758203000  | -0.848633000 |
| 1 | 6.242772000 | -1.575618000 | -0.904338000 |

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exo-3cP-O

|    |              |              |              |
|----|--------------|--------------|--------------|
| 46 | 1.167071000  | -0.719176000 | -0.059039000 |
| 15 | -1.206089000 | -0.015575000 | -0.042467000 |
| 6  | -2.209464000 | -0.792223000 | -1.352554000 |
| 6  | -1.787008000 | -1.991027000 | -1.909788000 |
| 6  | -3.403558000 | -0.233509000 | -1.794717000 |
| 6  | -2.542890000 | -2.615832000 | -2.882412000 |
| 1  | -0.878929000 | -2.451741000 | -1.573101000 |
| 6  | -4.154990000 | -0.858356000 | -2.767399000 |
| 1  | -3.749029000 | 0.697439000  | -1.385785000 |
| 6  | -3.725183000 | -2.052187000 | -3.314049000 |
| 1  | -2.202587000 | -3.546495000 | -3.298093000 |
| 1  | -5.075708000 | -0.412371000 | -3.097549000 |
| 1  | -4.310706000 | -2.539165000 | -4.072827000 |
| 6  | -1.986351000 | -0.483340000 | 1.533497000  |
| 6  | -3.347722000 | -0.723548000 | 1.644853000  |
| 6  | -1.193479000 | -0.575718000 | 2.666563000  |
| 6  | -3.903962000 | -1.038651000 | 2.866877000  |
| 1  | -3.978204000 | -0.680896000 | 0.776953000  |
| 6  | -1.751483000 | -0.882080000 | 3.891219000  |
| 1  | -0.131435000 | -0.431694000 | 2.592060000  |
| 6  | -3.107535000 | -1.113895000 | 3.993001000  |
| 1  | -4.958728000 | -1.233075000 | 2.937598000  |
| 1  | -1.121889000 | -0.958655000 | 4.758614000  |
| 1  | -3.541441000 | -1.366102000 | 4.943598000  |
| 6  | -1.613325000 | 1.759699000  | -0.203066000 |

|   |              |              |              |
|---|--------------|--------------|--------------|
| 6 | -1.514572000 | 2.382638000  | -1.442002000 |
| 6 | -1.940662000 | 2.532757000  | 0.900189000  |
| 6 | -1.737988000 | 3.736350000  | -1.573141000 |
| 1 | -1.279463000 | 1.804359000  | -2.317776000 |
| 6 | -2.161278000 | 3.891261000  | 0.769426000  |
| 1 | -2.031456000 | 2.077286000  | 1.868114000  |
| 6 | -2.059970000 | 4.497209000  | -0.464882000 |
| 1 | -1.664102000 | 4.197130000  | -2.541565000 |
| 1 | -2.417817000 | 4.472077000  | 1.636805000  |
| 1 | -2.235416000 | 5.552707000  | -0.566436000 |
| 6 | 2.876472000  | 0.757667000  | -0.881667000 |
| 6 | 3.808377000  | 1.345203000  | 0.148628000  |
| 6 | 1.877867000  | 2.479599000  | 0.282916000  |
| 6 | 1.705493000  | 1.436254000  | -0.799005000 |
| 6 | 2.825357000  | 1.758860000  | 1.243374000  |
| 1 | 3.270691000  | 2.426899000  | 1.971099000  |
| 1 | 2.384861000  | 0.913405000  | 1.754217000  |
| 6 | 4.176917000  | 2.735255000  | -0.435134000 |
| 1 | 4.553970000  | 2.669503000  | -1.448141000 |
| 6 | 2.846381000  | 3.519434000  | -0.336504000 |
| 1 | 2.497690000  | 3.882407000  | -1.295235000 |
| 1 | 4.643302000  | 0.730529000  | 0.442080000  |
| 1 | 0.970684000  | 2.897337000  | 0.690192000  |
| 1 | 1.005623000  | 1.537119000  | -1.604530000 |
| 1 | 3.209706000  | 0.196191000  | -1.733414000 |
| 6 | 2.942053000  | -1.668345000 | 0.167873000  |
| 8 | 3.595038000  | -1.634855000 | 1.161238000  |
| 8 | 3.292599000  | -2.377737000 | -0.905836000 |
| 6 | 4.443441000  | -3.203927000 | -0.768095000 |
| 1 | 4.552407000  | -3.715479000 | -1.712288000 |
| 1 | 5.322159000  | -2.608175000 | -0.557803000 |
| 1 | 4.299657000  | -3.917303000 | 0.031822000  |
| 6 | 0.531480000  | -2.516814000 | 0.498610000  |
| 7 | 0.132034000  | -3.548780000 | 0.789287000  |
| 1 | 4.950457000  | 3.192566000  | 0.169810000  |
| 1 | 2.941921000  | 4.375728000  | 0.320500000  |

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exo-3cP-OMe

|    |              |              |              |
|----|--------------|--------------|--------------|
| 46 | 1.137458000  | -0.725599000 | -0.314539000 |
| 15 | -1.213166000 | -0.010977000 | -0.018127000 |
| 6  | -2.324677000 | -0.671363000 | -1.303970000 |
| 6  | -1.950374000 | -1.804557000 | -2.012144000 |
| 6  | -3.553669000 | -0.083605000 | -1.583622000 |
| 6  | -2.787391000 | -2.338202000 | -2.972669000 |
| 1  | -1.014407000 | -2.285621000 | -1.805792000 |
| 6  | -4.386537000 | -0.617622000 | -2.543755000 |
| 1  | -3.862704000 | 0.799968000  | -1.057126000 |
| 6  | -4.004124000 | -1.747493000 | -3.241151000 |
| 1  | -2.482111000 | -3.218659000 | -3.507673000 |
| 1  | -5.333178000 | -0.150600000 | -2.747190000 |
| 1  | -4.652862000 | -2.163258000 | -3.990820000 |
| 6  | -1.864615000 | -0.608257000 | 1.572272000  |
| 6  | -3.208105000 | -0.889002000 | 1.769053000  |
| 6  | -0.984586000 | -0.763087000 | 2.631891000  |
| 6  | -3.661597000 | -1.304369000 | 3.003792000  |
| 1  | -3.904643000 | -0.800519000 | 0.957025000  |
| 6  | -1.439518000 | -1.169217000 | 3.869775000  |
| 1  | 0.065532000  | -0.588838000 | 2.486089000  |
| 6  | -2.779221000 | -1.440330000 | 4.057508000  |
| 1  | -4.703782000 | -1.529348000 | 3.139974000  |
| 1  | -0.743465000 | -1.292446000 | 4.679149000  |
| 1  | -3.133207000 | -1.770230000 | 5.017386000  |
| 6  | -1.621145000 | 1.771598000  | 0.001543000  |
| 6  | -1.604670000 | 2.494189000  | -1.186147000 |
| 6  | -1.872850000 | 2.450193000  | 1.183776000  |
| 6  | -1.834249000 | 3.853145000  | -1.190691000 |
| 1  | -1.429772000 | 1.990061000  | -2.120059000 |
| 6  | -2.099699000 | 3.814092000  | 1.179779000  |
| 1  | -1.900434000 | 1.916458000  | 2.114883000  |
| 6  | -2.080224000 | 4.519434000  | -0.004666000 |
| 1  | -1.824851000 | 4.391880000  | -2.120903000 |
| 1  | -2.297429000 | 4.320889000  | 2.106937000  |
| 1  | -2.260754000 | 5.578957000  | -0.007485000 |
| 6  | 2.804400000  | 0.839510000  | -1.053952000 |
| 6  | 3.812522000  | 1.272761000  | -0.018996000 |
| 6  | 1.918013000  | 2.397913000  | 0.396231000  |

|   |             |              |              |
|---|-------------|--------------|--------------|
| 6 | 1.655929000 | 1.512671000  | -0.802260000 |
| 6 | 2.912664000 | 1.545151000  | 1.186156000  |
| 1 | 3.416622000 | 2.104893000  | 1.965375000  |
| 1 | 2.485818000 | 0.644391000  | 1.607188000  |
| 6 | 4.170819000 | 2.724852000  | -0.433391000 |
| 1 | 4.479259000 | 2.790972000  | -1.469082000 |
| 6 | 2.864519000 | 3.501833000  | -0.141360000 |
| 1 | 2.461254000 | 3.994108000  | -1.017243000 |
| 1 | 4.657460000 | 0.618876000  | 0.127503000  |
| 1 | 1.048081000 | 2.766418000  | 0.916739000  |
| 1 | 0.904116000 | 1.726284000  | -1.535463000 |
| 1 | 3.070970000 | 0.385950000  | -1.988739000 |
| 6 | 2.870389000 | -1.753140000 | -0.547119000 |
| 8 | 3.275093000 | -2.175283000 | -1.582834000 |
| 8 | 3.505656000 | -1.944781000 | 0.609755000  |
| 6 | 4.656929000 | -2.780371000 | 0.565532000  |
| 1 | 5.020194000 | -2.834489000 | 1.580542000  |
| 1 | 4.391671000 | -3.765834000 | 0.207887000  |
| 1 | 5.412820000 | -2.359997000 | -0.085175000 |
| 6 | 0.523355000 | -2.552790000 | 0.160466000  |
| 7 | 0.136348000 | -3.594393000 | 0.432835000  |
| 1 | 4.990768000 | 3.089009000  | 0.173774000  |
| 1 | 3.019302000 | 4.260617000  | 0.616480000  |

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exo-3cP-N

|    |              |              |              |
|----|--------------|--------------|--------------|
| 46 | -0.861533000 | -1.142180000 | -0.439367000 |
| 15 | 0.895232000  | 0.462009000  | -0.015361000 |
| 6  | 1.201447000  | 0.688624000  | 1.765211000  |
| 6  | 0.697598000  | -0.243378000 | 2.659986000  |
| 6  | 1.930951000  | 1.765176000  | 2.259048000  |
| 6  | 0.922740000  | -0.106003000 | 4.016900000  |
| 1  | 0.140243000  | -1.086410000 | 2.298450000  |
| 6  | 2.154769000  | 1.900288000  | 3.611966000  |
| 1  | 2.318294000  | 2.508108000  | 1.586654000  |
| 6  | 1.650107000  | 0.963171000  | 4.494540000  |
| 1  | 0.524577000  | -0.836868000 | 4.696783000  |
| 1  | 2.720077000  | 2.738041000  | 3.978046000  |
| 1  | 1.822078000  | 1.070947000  | 5.550221000  |

|   |              |              |              |
|---|--------------|--------------|--------------|
| 6 | 2.491870000  | -0.006929000 | -0.756478000 |
| 6 | 2.481249000  | -0.561812000 | -2.028524000 |
| 6 | 3.708958000  | 0.183997000  | -0.119264000 |
| 6 | 3.661841000  | -0.887999000 | -2.662295000 |
| 1 | 1.547818000  | -0.771629000 | -2.516357000 |
| 6 | 4.889153000  | -0.155107000 | -0.749297000 |
| 1 | 3.745107000  | 0.585323000  | 0.874940000  |
| 6 | 4.868396000  | -0.683923000 | -2.024359000 |
| 1 | 3.634368000  | -1.324040000 | -3.643906000 |
| 1 | 5.824453000  | -0.007825000 | -0.240426000 |
| 1 | 5.788363000  | -0.949834000 | -2.512743000 |
| 6 | 0.657018000  | 2.176563000  | -0.620444000 |
| 6 | -0.081450000 | 3.086468000  | 0.125635000  |
| 6 | 1.136977000  | 2.574569000  | -1.859133000 |
| 6 | -0.326916000 | 4.357284000  | -0.349844000 |
| 1 | -0.463050000 | 2.807281000  | 1.089702000  |
| 6 | 0.886291000  | 3.846189000  | -2.337967000 |
| 1 | 1.720088000  | 1.899245000  | -2.455429000 |
| 6 | 0.155179000  | 4.741595000  | -1.585997000 |
| 1 | -0.895005000 | 5.047480000  | 0.247171000  |
| 1 | 1.270728000  | 4.134927000  | -3.299277000 |
| 1 | -0.035634000 | 5.732026000  | -1.957151000 |
| 6 | -2.469861000 | 0.811984000  | -0.637411000 |
| 6 | -3.197480000 | 1.192278000  | 0.634464000  |
| 6 | -4.287947000 | -0.550355000 | -0.258640000 |
| 6 | -3.134856000 | -0.226348000 | -1.170135000 |
| 6 | -3.703837000 | -0.172616000 | 1.103292000  |
| 1 | -4.459356000 | -0.097197000 | 1.876784000  |
| 1 | -2.920551000 | -0.843940000 | 1.428028000  |
| 6 | -4.525582000 | 1.831651000  | 0.151654000  |
| 1 | -4.358814000 | 2.635566000  | -0.554325000 |
| 6 | -5.276349000 | 0.629063000  | -0.469648000 |
| 1 | -5.520302000 | 0.778315000  | -1.513793000 |
| 1 | -2.646225000 | 1.788450000  | 1.346275000  |
| 1 | -4.707427000 | -1.536854000 | -0.366475000 |
| 1 | -3.047447000 | -0.591417000 | -2.175359000 |
| 1 | -1.806185000 | 1.463271000  | -1.169514000 |
| 6 | 0.483128000  | -2.603007000 | -0.288802000 |

|   |              |              |              |
|---|--------------|--------------|--------------|
| 8 | 1.088202000  | -3.056354000 | -1.203417000 |
| 8 | 0.608944000  | -3.054683000 | 0.959366000  |
| 6 | 1.444039000  | -4.195717000 | 1.132232000  |
| 1 | 1.416593000  | -4.422128000 | 2.187231000  |
| 1 | 1.061129000  | -5.028256000 | 0.558218000  |
| 1 | 2.455845000  | -3.979492000 | 0.816904000  |
| 6 | -2.060002000 | -2.750824000 | -0.642776000 |
| 7 | -2.768100000 | -3.645157000 | -0.735620000 |
| 1 | -5.070104000 | 2.243052000  | 0.993694000  |
| 1 | -6.202648000 | 0.429130000  | 0.055223000  |

27

exo-3t-O

|    |              |              |              |
|----|--------------|--------------|--------------|
| 46 | -0.538658000 | 0.878192000  | -0.072971000 |
| 6  | 0.578769000  | -0.991450000 | -0.648922000 |
| 6  | 1.174502000  | -1.766413000 | 0.501787000  |
| 6  | 2.509231000  | 0.007246000  | 0.151390000  |
| 6  | 1.395035000  | 0.092894000  | -0.859717000 |
| 6  | 1.805963000  | -0.652576000 | 1.338367000  |
| 1  | 2.503432000  | -1.031815000 | 2.075139000  |
| 1  | 1.088165000  | -0.005970000 | 1.826664000  |
| 6  | 2.447632000  | -2.405998000 | -0.112128000 |
| 1  | 2.234174000  | -2.959984000 | -1.017820000 |
| 6  | 3.366430000  | -1.182955000 | -0.354761000 |
| 1  | 3.654182000  | -1.071519000 | -1.392494000 |
| 1  | 0.513113000  | -2.458888000 | 0.999488000  |
| 1  | 3.045068000  | 0.924285000  | 0.332280000  |
| 1  | 1.492306000  | 0.625191000  | -1.786488000 |
| 1  | -0.043098000 | -1.447653000 | -1.393718000 |
| 6  | -2.072881000 | -0.303610000 | 0.023101000  |
| 8  | -2.836690000 | 0.537987000  | 0.415634000  |
| 8  | -2.360312000 | -1.549320000 | -0.217552000 |
| 6  | -3.720222000 | -1.949954000 | 0.005968000  |
| 1  | -3.759045000 | -2.997212000 | -0.246210000 |
| 1  | -3.984445000 | -1.794698000 | 1.042248000  |
| 1  | -4.381998000 | -1.377790000 | -0.628407000 |
| 6  | 0.578348000  | 2.605508000  | 0.033164000  |
| 7  | 1.207239000  | 3.560408000  | 0.095580000  |
| 1  | 2.888356000  | -3.097980000 | 0.594962000  |



|            |              |              |              |
|------------|--------------|--------------|--------------|
| 1          | 4.276540000  | -1.251135000 | 0.227812000  |
| 27         |              |              |              |
| exo-3t-OMe |              |              |              |
| 46         | 0.536748000  | 1.040940000  | 0.059791000  |
| 6          | -0.516944000 | -0.862630000 | 0.870874000  |
| 6          | -0.919808000 | -1.895190000 | -0.153021000 |
| 6          | -2.339925000 | -0.168272000 | -0.386482000 |
| 6          | -1.395889000 | 0.191399000  | 0.729662000  |
| 6          | -1.446111000 | -1.018838000 | -1.289971000 |
| 1          | -2.011381000 | -1.583110000 | -2.021308000 |
| 1          | -0.673001000 | -0.453108000 | -1.794680000 |
| 6          | -2.253718000 | -2.460791000 | 0.403110000  |
| 1          | -2.163861000 | -2.795352000 | 1.428961000  |
| 6          | -3.232362000 | -1.272756000 | 0.239087000  |
| 1          | -3.678795000 | -0.960836000 | 1.174644000  |
| 1          | -0.177560000 | -2.637812000 | -0.396971000 |
| 1          | -2.869967000 | 0.657330000  | -0.832563000 |
| 1          | -1.660207000 | 0.876747000  | 1.512019000  |
| 1          | -0.018796000 | -1.105894000 | 1.789999000  |
| 6          | 1.885203000  | -0.395065000 | 0.328923000  |
| 8          | 2.589250000  | -0.381782000 | 1.287726000  |
| 8          | 2.103412000  | -1.136663000 | -0.748711000 |
| 6          | 3.289751000  | -1.933751000 | -0.744666000 |
| 1          | 3.289783000  | -2.463106000 | -1.684333000 |
| 1          | 4.164824000  | -1.304165000 | -0.663552000 |
| 1          | 3.271257000  | -2.626843000 | 0.085345000  |
| 6          | -0.559244000 | 2.749461000  | -0.274679000 |
| 7          | -1.166719000 | 3.698338000  | -0.481138000 |
| 1          | -2.562795000 | -3.312986000 | -0.189317000 |
| 1          | -4.039906000 | -1.516293000 | -0.439789000 |
| 27         |              |              |              |
| exo-3c-O   |              |              |              |
| 46         | 0.690843000  | -0.850018000 | -0.175842000 |
| 6          | -1.276965000 | 0.360114000  | -0.907735000 |
| 6          | -2.017820000 | 1.186379000  | 0.113840000  |
| 6          | -2.565176000 | -0.956601000 | 0.479124000  |
| 6          | -1.598630000 | -0.929492000 | -0.680346000 |
| 6          | -2.065685000 | 0.228673000  | 1.306571000  |

|   |              |              |              |
|---|--------------|--------------|--------------|
| 1 | -2.779631000 | 0.540120000  | 2.059303000  |
| 1 | -1.101778000 | 0.072072000  | 1.769288000  |
| 6 | -3.497927000 | 1.118263000  | -0.355920000 |
| 1 | -3.615416000 | 1.412803000  | -1.390896000 |
| 6 | -3.875492000 | -0.360309000 | -0.102907000 |
| 1 | -4.197794000 | -0.873393000 | -0.999968000 |
| 1 | -1.640295000 | 2.181308000  | 0.290326000  |
| 1 | -2.682086000 | -1.905008000 | 0.981213000  |
| 1 | -1.480556000 | -1.734953000 | -1.387805000 |
| 1 | -0.845982000 | 0.754873000  | -1.809368000 |
| 6 | 1.336411000  | 0.922669000  | 0.334729000  |
| 8 | 1.111741000  | 1.398406000  | 1.391520000  |
| 8 | 1.982272000  | 1.493038000  | -0.655831000 |
| 6 | 2.555900000  | 2.774939000  | -0.377110000 |
| 1 | 3.054288000  | 3.069366000  | -1.286573000 |
| 1 | 1.782877000  | 3.484263000  | -0.115638000 |
| 1 | 3.263653000  | 2.691330000  | 0.435201000  |
| 6 | 2.547495000  | -1.416133000 | 0.194195000  |
| 7 | 3.604752000  | -1.805348000 | 0.394535000  |
| 1 | -4.101718000 | 1.787458000  | 0.244193000  |
| 1 | -4.672394000 | -0.444559000 | 0.625539000  |

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exo-3c-OMe

|    |              |              |              |
|----|--------------|--------------|--------------|
| 46 | 0.460003000  | -0.571896000 | -0.020606000 |
| 6  | -1.224214000 | 0.892201000  | 0.541975000  |
| 6  | -2.335802000 | 0.119238000  | 1.215163000  |
| 6  | -2.496354000 | -0.273305000 | -0.989420000 |
| 6  | -1.322970000 | 0.656283000  | -0.789075000 |
| 6  | -2.436593000 | -1.101868000 | 0.296896000  |
| 1  | -3.329213000 | -1.691351000 | 0.465807000  |
| 1  | -1.583527000 | -1.779624000 | 0.357238000  |
| 6  | -3.635914000 | 0.867262000  | 0.822050000  |
| 1  | -3.584823000 | 1.921526000  | 1.060972000  |
| 6  | -3.746096000 | 0.598044000  | -0.697316000 |
| 1  | -3.754200000 | 1.505007000  | -1.287492000 |
| 1  | -2.216394000 | -0.061713000 | 2.272448000  |
| 1  | -2.523455000 | -0.808005000 | -1.926472000 |
| 1  | -0.870127000 | 1.239258000  | -1.568975000 |

|   |              |              |              |
|---|--------------|--------------|--------------|
| 1 | -0.706525000 | 1.714521000  | 0.999727000  |
| 6 | 1.785401000  | 0.816294000  | -0.350869000 |
| 8 | 1.806695000  | 1.415686000  | -1.370944000 |
| 8 | 2.553879000  | 1.026883000  | 0.689386000  |
| 6 | 3.571552000  | 2.021040000  | 0.532671000  |
| 1 | 4.097855000  | 2.042206000  | 1.473190000  |
| 1 | 4.238228000  | 1.740860000  | -0.270408000 |
| 1 | 3.127366000  | 2.983277000  | 0.318401000  |
| 6 | 1.963191000  | -1.884086000 | 0.030394000  |
| 7 | 2.778974000  | -2.686029000 | 0.058338000  |
| 1 | -4.479773000 | 0.451305000  | 1.358651000  |
| 1 | -4.646159000 | 0.044977000  | -0.935929000 |

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exo-3c-N

|    |              |              |              |
|----|--------------|--------------|--------------|
| 46 | -0.548889000 | 0.199627000  | -0.000057000 |
| 6  | 1.745495000  | 0.714620000  | -0.672387000 |
| 6  | 2.503536000  | -0.511687000 | -1.120695000 |
| 6  | 2.503598000  | -0.511144000 | 1.120853000  |
| 6  | 1.745535000  | 0.714946000  | 0.671996000  |
| 6  | 2.161223000  | -1.496730000 | 0.000327000  |
| 1  | 2.795895000  | -2.374693000 | 0.000522000  |
| 1  | 1.125302000  | -1.824418000 | 0.000434000  |
| 6  | 3.985545000  | -0.205333000 | -0.773340000 |
| 1  | 4.315571000  | 0.734689000  | -1.195517000 |
| 6  | 3.985588000  | -0.204957000 | 0.773266000  |
| 1  | 4.315636000  | 0.735269000  | 1.194969000  |
| 1  | 2.334582000  | -0.832795000 | -2.137419000 |
| 1  | 2.334702000  | -0.831759000 | 2.137743000  |
| 1  | 1.501720000  | 1.549850000  | 1.302240000  |
| 1  | 1.501658000  | 1.549226000  | -1.303019000 |
| 6  | -2.260276000 | -0.666099000 | 0.000083000  |
| 8  | -1.939125000 | -1.824816000 | 0.000189000  |
| 8  | -3.465086000 | -0.193281000 | -0.000067000 |
| 6  | -4.533126000 | -1.146711000 | 0.000016000  |
| 1  | -5.439198000 | -0.563146000 | -0.000133000 |
| 1  | -4.476971000 | -1.766850000 | -0.883662000 |
| 1  | -4.477082000 | -1.766576000 | 0.883893000  |
| 6  | -1.195390000 | 2.036215000  | 0.000020000  |

|   |              |              |              |
|---|--------------|--------------|--------------|
| 7 | -1.493255000 | 3.140404000  | 0.000071000  |
| 1 | 4.626559000  | -0.984483000 | -1.167369000 |
| 1 | 4.626625000  | -0.983915000 | 1.167638000  |

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exo-3c-N'

|    |              |              |              |
|----|--------------|--------------|--------------|
| 46 | -0.600215000 | -0.096745000 | -0.238134000 |
| 6  | 1.655547000  | -0.959532000 | -0.641129000 |
| 6  | 2.475547000  | -1.221247000 | 0.601971000  |
| 6  | 2.622139000  | 0.971312000  | 0.152216000  |
| 6  | 1.755612000  | 0.353024000  | -0.912928000 |
| 6  | 2.284957000  | 0.094650000  | 1.360389000  |
| 1  | 2.989695000  | 0.214391000  | 2.174528000  |
| 1  | 1.279906000  | 0.247906000  | 1.731278000  |
| 6  | 3.948858000  | -1.061774000 | 0.139337000  |
| 1  | 4.178877000  | -1.685397000 | -0.715088000 |
| 6  | 4.049830000  | 0.450579000  | -0.172407000 |
| 1  | 4.336620000  | 0.652037000  | -1.196445000 |
| 1  | 2.263975000  | -2.139303000 | 1.129664000  |
| 1  | 2.533239000  | 2.039579000  | 0.268866000  |
| 1  | 1.500274000  | 0.837661000  | -1.836419000 |
| 1  | 1.332860000  | -1.722878000 | -1.328762000 |
| 6  | -2.450182000 | -0.462391000 | 0.032690000  |
| 8  | -2.440952000 | -1.659315000 | -0.081230000 |
| 8  | -3.466401000 | 0.296913000  | 0.272143000  |
| 6  | -4.736088000 | -0.350701000 | 0.420009000  |
| 1  | -5.441378000 | 0.441554000  | 0.610080000  |
| 1  | -4.989182000 | -0.879873000 | -0.487893000 |
| 1  | -4.703774000 | -1.042673000 | 1.249765000  |
| 6  | -0.722773000 | 1.842286000  | -0.024526000 |
| 7  | -0.729472000 | 2.979425000  | 0.097516000  |
| 1  | 4.620739000  | -1.344701000 | 0.940631000  |
| 1  | 4.772475000  | 0.937971000  | 0.470293000  |

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exo-3t2N-O

|    |              |              |              |
|----|--------------|--------------|--------------|
| 46 | 0.000031000  | -0.212767000 | -0.509743000 |
| 6  | -2.256101000 | 0.543963000  | -0.441762000 |
| 6  | -2.861429000 | 0.649030000  | 0.937489000  |
| 6  | -2.859574000 | -1.527909000 | 0.382806000  |

|   |              |              |              |
|---|--------------|--------------|--------------|
| 6 | -2.258744000 | -0.775416000 | -0.776371000 |
| 6 | -2.412756000 | -0.670061000 | 1.567076000  |
| 1 | -2.952603000 | -0.901445000 | 2.477367000  |
| 1 | -1.349396000 | -0.715150000 | 1.760963000  |
| 6 | -4.365521000 | 0.347100000  | 0.706888000  |
| 1 | -4.799497000 | 0.977436000  | -0.059392000 |
| 6 | -4.363997000 | -1.153041000 | 0.323677000  |
| 1 | -4.796053000 | -1.340199000 | -0.651353000 |
| 1 | -2.648593000 | 1.555976000  | 1.479961000  |
| 1 | -2.645660000 | -2.583766000 | 0.413358000  |
| 1 | -2.232951000 | -1.162231000 | -1.775956000 |
| 1 | -2.240646000 | 1.350230000  | -1.149001000 |
| 6 | -0.000488000 | 1.762861000  | 0.002497000  |
| 8 | -0.000178000 | 2.171651000  | 1.122981000  |
| 8 | -0.001067000 | 2.599010000  | -1.050820000 |
| 6 | -0.001207000 | 3.991280000  | -0.759816000 |
| 1 | -0.001433000 | 4.493566000  | -1.715398000 |
| 1 | -0.880439000 | 4.264738000  | -0.191322000 |
| 1 | 0.878112000  | 4.264988000  | -0.191584000 |
| 6 | 0.000647000  | -2.227151000 | -0.905723000 |
| 7 | 0.000946000  | -3.353955000 | -1.109603000 |
| 1 | -4.919346000 | 0.520695000  | 1.621543000  |
| 1 | -4.917641000 | -1.744824000 | 1.042256000  |
| 6 | 4.365195000  | 0.348406000  | 0.707861000  |
| 6 | 2.860867000  | 0.648960000  | 0.938579000  |
| 6 | 2.860620000  | -1.527348000 | 0.381414000  |
| 6 | 4.364801000  | -1.151291000 | 0.322898000  |
| 1 | 4.798817000  | 0.979943000  | -0.057634000 |
| 1 | 4.918793000  | 0.521326000  | 1.622780000  |
| 1 | 4.797113000  | -1.337008000 | -0.652293000 |
| 1 | 4.918763000  | -1.743528000 | 1.040857000  |
| 6 | 2.413060000  | -0.671167000 | 1.566600000  |
| 1 | 1.349704000  | -0.717338000 | 1.760272000  |
| 1 | 2.952944000  | -0.903234000 | 2.476696000  |
| 6 | 2.255834000  | 0.544994000  | -0.440913000 |
| 1 | 2.240025000  | 1.352148000  | -1.147097000 |
| 6 | 2.259390000  | -0.773982000 | -0.776974000 |
| 1 | 2.233633000  | -1.159797000 | -1.776955000 |

|              |              |              |              |
|--------------|--------------|--------------|--------------|
| 1            | 2.647211000  | 1.555187000  | 1.481936000  |
| 1            | 2.647481000  | -2.583390000 | 0.410736000  |
| 44           |              |              |              |
| exo-3t2N-OMe |              |              |              |
| 46           | -0.000009000 | -0.310971000 | -0.540172000 |
| 6            | -2.267262000 | 0.425793000  | -0.666518000 |
| 6            | -2.900877000 | 0.835412000  | 0.641512000  |
| 6            | -2.875590000 | -1.409274000 | 0.599584000  |
| 6            | -2.257363000 | -0.934808000 | -0.689967000 |
| 6            | -2.455761000 | -0.299478000 | 1.564152000  |
| 1            | -3.010442000 | -0.323055000 | 2.494529000  |
| 1            | -1.395076000 | -0.290782000 | 1.778557000  |
| 6            | -4.398758000 | 0.474487000  | 0.459846000  |
| 1            | -4.819928000 | 0.908891000  | -0.438167000 |
| 6            | -4.380711000 | -1.073113000 | 0.430628000  |
| 1            | -4.792852000 | -1.482776000 | -0.482882000 |
| 1            | -2.711367000 | 1.846086000  | 0.966294000  |
| 1            | -2.655408000 | -2.427625000 | 0.874743000  |
| 1            | -2.210501000 | -1.539165000 | -1.574407000 |
| 1            | -2.239960000 | 1.051198000  | -1.537274000 |
| 6            | 0.000010000  | 1.726653000  | -0.669276000 |
| 8            | -0.000726000 | 2.365034000  | -1.677769000 |
| 8            | 0.000459000  | 2.316652000  | 0.535930000  |
| 6            | 0.000293000  | 3.738851000  | 0.548291000  |
| 1            | 0.000708000  | 4.026435000  | 1.588906000  |
| 1            | 0.878952000  | 4.126938000  | 0.049923000  |
| 1            | -0.878890000 | 4.126724000  | 0.050681000  |
| 6            | -0.000009000 | -2.359237000 | -0.392489000 |
| 7            | 0.000003000  | -3.498939000 | -0.281185000 |
| 1            | -4.971747000 | 0.847182000  | 1.300359000  |
| 1            | -4.944459000 | -1.490221000 | 1.256044000  |
| 6            | 4.398757000  | 0.474464000  | 0.459742000  |
| 6            | 2.900878000  | 0.835378000  | 0.641443000  |
| 6            | 2.875599000  | -1.409309000 | 0.599504000  |
| 6            | 4.380714000  | -1.073137000 | 0.430512000  |
| 1            | 4.819903000  | 0.908877000  | -0.438278000 |
| 1            | 4.971763000  | 0.847155000  | 1.300245000  |
| 1            | 4.792834000  | -1.482790000 | -0.483012000 |

|   |             |              |              |
|---|-------------|--------------|--------------|
| 1 | 4.944486000 | -1.490248000 | 1.255910000  |
| 6 | 2.455791000 | -0.299519000 | 1.564088000  |
| 1 | 1.395113000 | -0.290829000 | 1.778522000  |
| 1 | 3.010497000 | -0.323098000 | 2.494451000  |
| 6 | 2.267240000 | 0.425761000  | -0.666576000 |
| 1 | 2.239913000 | 1.051174000  | -1.537323000 |
| 6 | 2.257340000 | -0.934839000 | -0.690030000 |
| 1 | 2.210458000 | -1.539193000 | -1.574471000 |
| 1 | 2.711370000 | 1.846052000  | 0.966235000  |
| 1 | 2.655428000 | -2.427661000 | 0.874665000  |

44

exo-3c2N-O

|    |              |              |              |
|----|--------------|--------------|--------------|
| 46 | 0.119085000  | -0.604239000 | -0.274993000 |
| 6  | 2.047434000  | 0.866027000  | -0.639579000 |
| 6  | 2.596868000  | 1.531917000  | 0.595772000  |
| 6  | 0.768899000  | 2.675938000  | -0.018252000 |
| 6  | 0.935282000  | 1.539881000  | -1.002194000 |
| 6  | 1.315926000  | 2.037690000  | 1.260167000  |
| 1  | 1.509923000  | 2.763403000  | 2.040850000  |
| 1  | 0.700094000  | 1.240290000  | 1.654875000  |
| 6  | 3.182179000  | 2.868682000  | 0.066203000  |
| 1  | 3.877999000  | 2.718953000  | -0.749619000 |
| 6  | 1.920343000  | 3.658693000  | -0.355285000 |
| 1  | 1.927377000  | 3.937999000  | -1.401406000 |
| 1  | 3.265505000  | 0.938391000  | 1.197461000  |
| 1  | -0.208754000 | 3.130561000  | 0.028919000  |
| 1  | 0.521017000  | 1.534156000  | -1.993047000 |
| 1  | 2.620058000  | 0.223658000  | -1.280326000 |
| 6  | 1.735857000  | -1.580253000 | 0.355921000  |
| 8  | 2.136949000  | -1.517462000 | 1.470462000  |
| 8  | 2.307755000  | -2.300487000 | -0.599839000 |
| 6  | 3.391199000  | -3.134849000 | -0.196000000 |
| 1  | 3.703071000  | -3.658242000 | -1.086389000 |
| 1  | 4.204359000  | -2.541213000 | 0.200315000  |
| 1  | 3.059975000  | -3.835800000 | 0.557474000  |
| 6  | -0.637680000 | -2.402430000 | 0.110882000  |
| 7  | -1.106793000 | -3.426056000 | 0.312864000  |
| 1  | 3.717137000  | 3.374317000  | 0.860660000  |

|   |              |              |              |
|---|--------------|--------------|--------------|
| 1 | 1.813207000  | 4.568023000  | 0.223817000  |
| 6 | -4.635098000 | -0.018370000 | -0.158296000 |
| 6 | -3.330573000 | -0.784247000 | 0.193019000  |
| 6 | -2.747498000 | 1.362831000  | 0.466352000  |
| 6 | -4.235183000 | 1.463945000  | 0.035367000  |
| 1 | -4.980508000 | -0.234172000 | -1.161305000 |
| 1 | -5.423902000 | -0.305862000 | 0.526046000  |
| 1 | -4.362654000 | 2.056804000  | -0.861830000 |
| 1 | -4.818149000 | 1.930771000  | 0.820509000  |
| 6 | -2.796248000 | 0.096790000  | 1.323382000  |
| 1 | -1.830943000 | -0.223971000 | 1.690889000  |
| 1 | -3.488231000 | 0.178982000  | 2.153198000  |
| 6 | -2.384156000 | -0.430409000 | -0.925078000 |
| 1 | -2.256343000 | -1.021215000 | -1.812034000 |
| 6 | -2.031458000 | 0.853888000  | -0.763254000 |
| 1 | -1.619086000 | 1.488321000  | -1.521559000 |
| 1 | -3.446385000 | -1.836351000 | 0.392771000  |
| 1 | -2.349332000 | 2.258820000  | 0.919634000  |

44

exo-3c2N-OMe

|    |              |              |              |
|----|--------------|--------------|--------------|
| 46 | 0.108044000  | -0.608555000 | -0.435305000 |
| 6  | 2.055754000  | 0.861938000  | -0.721541000 |
| 6  | 2.639173000  | 1.408970000  | 0.555970000  |
| 6  | 0.825229000  | 2.634511000  | 0.077242000  |
| 6  | 0.951001000  | 1.583723000  | -1.002942000 |
| 6  | 1.381079000  | 1.879792000  | 1.286595000  |
| 1  | 1.602295000  | 2.532436000  | 2.122711000  |
| 1  | 0.752484000  | 1.064421000  | 1.620807000  |
| 6  | 3.243971000  | 2.774519000  | 0.132781000  |
| 1  | 3.922273000  | 2.680394000  | -0.705543000 |
| 6  | 1.991035000  | 3.620190000  | -0.196704000 |
| 1  | 1.985890000  | 3.986637000  | -1.215405000 |
| 1  | 3.311542000  | 0.756696000  | 1.090493000  |
| 1  | -0.140812000 | 3.103246000  | 0.183174000  |
| 1  | 0.516161000  | 1.668210000  | -1.981525000 |
| 1  | 2.603717000  | 0.265780000  | -1.424242000 |
| 6  | 1.728985000  | -1.753944000 | -0.258740000 |
| 8  | 2.313885000  | -2.223295000 | -1.177646000 |



|   |              |              |              |
|---|--------------|--------------|--------------|
| 8 | 2.079792000  | -1.922157000 | 1.008908000  |
| 6 | 3.158470000  | -2.823670000 | 1.247919000  |
| 1 | 3.285732000  | -2.848210000 | 2.319030000  |
| 1 | 2.910292000  | -3.807409000 | 0.874493000  |
| 1 | 4.061892000  | -2.475618000 | 0.764932000  |
| 6 | -0.698613000 | -2.385573000 | -0.060391000 |
| 7 | -1.198694000 | -3.389732000 | 0.163611000  |
| 1 | 3.802363000  | 3.201121000  | 0.957025000  |
| 1 | 1.912375000  | 4.479024000  | 0.458980000  |
| 6 | -4.625545000 | 0.122144000  | 0.008789000  |
| 6 | -3.335311000 | -0.713108000 | 0.231556000  |
| 6 | -2.660775000 | 1.383573000  | 0.647719000  |
| 6 | -4.162205000 | 1.569309000  | 0.301176000  |
| 1 | -5.025739000 | 0.001306000  | -0.989766000 |
| 1 | -5.391257000 | -0.194591000 | 0.706337000  |
| 1 | -4.309399000 | 2.237857000  | -0.537899000 |
| 1 | -4.690100000 | 1.989072000  | 1.149368000  |
| 6 | -2.715641000 | 0.053583000  | 1.400978000  |
| 1 | -1.746614000 | -0.329199000 | 1.690667000  |
| 1 | -3.363617000 | 0.089436000  | 2.268822000  |
| 6 | -2.430179000 | -0.299916000 | -0.899872000 |
| 1 | -2.364835000 | -0.820016000 | -1.836670000 |
| 6 | -2.021698000 | 0.953789000  | -0.652725000 |
| 1 | -1.621968000 | 1.633568000  | -1.377837000 |
| 1 | -3.480325000 | -1.773528000 | 0.352235000  |
| 1 | -2.209307000 | 2.225666000  | 1.151622000  |

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exo-3c2N-N

|    |              |              |              |
|----|--------------|--------------|--------------|
| 46 | -0.119040000 | -0.604355000 | -0.275095000 |
| 6  | 2.384583000  | -0.430380000 | -0.924962000 |
| 6  | 3.330673000  | -0.783992000 | 0.193478000  |
| 6  | 2.747840000  | 1.363244000  | 0.465977000  |
| 6  | 2.031967000  | 0.853971000  | -0.763603000 |
| 6  | 2.796201000  | 0.097488000  | 1.323432000  |
| 1  | 3.487980000  | 0.179826000  | 2.153398000  |
| 1  | 1.830763000  | -0.223024000 | 1.690792000  |
| 6  | 4.635422000  | -0.018418000 | -0.157688000 |
| 1  | 4.981101000  | -0.234643000 | -1.160503000 |

|             |              |              |              |
|-------------|--------------|--------------|--------------|
| 6           | 4.235626000  | 1.464017000  | 0.035290000  |
| 1           | 4.363375000  | 2.056502000  | -0.862105000 |
| 1           | 3.446308000  | -1.836040000 | 0.393594000  |
| 1           | 2.349663000  | 2.259440000  | 0.918829000  |
| 1           | 1.619473000  | 1.488227000  | -1.521980000 |
| 1           | 2.256607000  | -1.021569000 | -1.811627000 |
| 6           | -1.735761000 | -1.580269000 | 0.355966000  |
| 8           | -2.136917000 | -1.517138000 | 1.470460000  |
| 8           | -2.307602000 | -2.300738000 | -0.599619000 |
| 6           | -3.390955000 | -3.135144000 | -0.195590000 |
| 1           | -3.702277000 | -3.659331000 | -1.085694000 |
| 1           | -3.059830000 | -3.835373000 | 0.558581000  |
| 1           | -4.204467000 | -2.541444000 | 0.199891000  |
| 6           | 0.637574000  | -2.402630000 | 0.110667000  |
| 7           | 1.106591000  | -3.426317000 | 0.312532000  |
| 1           | 5.423962000  | -0.305771000 | 0.527004000  |
| 1           | 4.818473000  | 1.931083000  | 0.820366000  |
| 6           | -3.182558000 | 2.868613000  | 0.066101000  |
| 6           | -2.597278000 | 1.531793000  | 0.595539000  |
| 6           | -0.769290000 | 2.675972000  | -0.018082000 |
| 6           | -1.920704000 | 3.658776000  | -0.355041000 |
| 1           | -3.878247000 | 2.719011000  | -0.749847000 |
| 1           | -3.717664000 | 3.374085000  | 0.860552000  |
| 1           | -1.927617000 | 3.938314000  | -1.401094000 |
| 1           | -1.813684000 | 4.567983000  | 0.224263000  |
| 6           | -1.316414000 | 2.037468000  | 1.260157000  |
| 1           | -0.700593000 | 1.240004000  | 1.654738000  |
| 1           | -1.510500000 | 2.762984000  | 2.040987000  |
| 6           | -2.047665000 | 0.866071000  | -0.639848000 |
| 1           | -2.620141000 | 0.223659000  | -1.280665000 |
| 6           | -0.935614000 | 1.540115000  | -1.002267000 |
| 1           | -0.521108000 | 1.534755000  | -1.993012000 |
| 1           | -3.265973000 | 0.938169000  | 1.197054000  |
| 1           | 0.208369000  | 3.130561000  | 0.029228000  |
| 44          |              |              |              |
| exo-3c2N-N' |              |              |              |
| 46          | -0.107401000 | -0.608285000 | -0.435676000 |
| 6           | 2.430464000  | -0.297893000 | -0.900006000 |

|   |              |              |              |
|---|--------------|--------------|--------------|
| 6 | 3.335278000  | -0.711272000 | 0.231581000  |
| 6 | 2.659108000  | 1.384659000  | 0.648896000  |
| 6 | 2.021050000  | 0.955378000  | -0.652232000 |
| 6 | 2.714462000  | 0.054169000  | 1.401213000  |
| 1 | 3.361969000  | 0.089818000  | 2.269412000  |
| 1 | 1.745538000  | -0.329463000 | 1.690116000  |
| 6 | 4.625066000  | 0.125049000  | 0.010094000  |
| 1 | 5.025848000  | 0.005225000  | -0.988343000 |
| 6 | 4.160586000  | 1.571687000  | 0.303323000  |
| 1 | 4.307771000  | 2.240945000  | -0.535184000 |
| 1 | 3.480981000  | -1.771677000 | 0.351580000  |
| 1 | 2.206713000  | 2.226065000  | 1.153126000  |
| 1 | 1.621458000  | 1.635598000  | -1.377016000 |
| 1 | 2.365686000  | -0.817532000 | -1.837091000 |
| 6 | -1.727583000 | -1.754683000 | -0.257692000 |
| 8 | -2.313560000 | -2.224439000 | -1.175645000 |
| 8 | -2.076338000 | -1.923087000 | 1.010554000  |
| 6 | -3.153978000 | -2.825473000 | 1.251202000  |
| 1 | -3.278788000 | -2.851066000 | 2.322574000  |
| 1 | -4.058692000 | -2.477450000 | 0.770610000  |
| 1 | -2.906103000 | -3.808702000 | 0.876269000  |
| 6 | 0.700285000  | -2.385612000 | -0.064111000 |
| 7 | 1.201010000  | -3.389940000 | 0.157675000  |
| 1 | 5.390628000  | -0.191685000 | 0.707804000  |
| 1 | 4.687766000  | 1.991170000  | 1.152097000  |
| 6 | -3.246328000 | 2.772098000  | 0.132032000  |
| 6 | -2.640434000 | 1.407104000  | 0.555419000  |
| 6 | -0.827478000 | 2.634157000  | 0.076876000  |
| 6 | -1.994062000 | 3.618806000  | -0.197357000 |
| 1 | -3.924414000 | 2.677310000  | -0.706389000 |
| 1 | -3.805209000 | 3.198310000  | 0.956146000  |
| 1 | -1.989081000 | 3.985152000  | -1.216094000 |
| 1 | -1.916239000 | 4.477773000  | 0.458252000  |
| 6 | -1.382857000 | 1.879037000  | 1.286178000  |
| 1 | -0.753623000 | 1.064215000  | 1.620523000  |
| 1 | -1.604770000 | 2.531529000  | 2.122227000  |
| 6 | -2.056347000 | 0.860453000  | -0.721965000 |
| 1 | -2.603705000 | 0.263781000  | -1.424695000 |

|   |              |             |              |
|---|--------------|-------------|--------------|
| 6 | -0.952197000 | 1.583220000 | -1.003274000 |
| 1 | -0.517276000 | 1.668320000 | -1.981764000 |
| 1 | -3.312314000 | 0.754312000 | 1.089923000  |
| 1 | 0.138186000  | 3.103660000 | 0.182940000  |

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exo-3tT-O

|    |              |              |              |
|----|--------------|--------------|--------------|
| 46 | -0.194636000 | -0.595940000 | -0.426908000 |
| 6  | -1.977070000 | 0.936102000  | -0.528264000 |
| 6  | -2.427062000 | 1.476629000  | 0.807608000  |
| 6  | -3.237732000 | -0.612162000 | 0.637942000  |
| 6  | -2.472833000 | -0.332291000 | -0.630179000 |
| 6  | -2.448857000 | 0.207427000  | 1.660058000  |
| 1  | -2.986865000 | 0.341489000  | 2.590727000  |
| 1  | -1.463688000 | -0.188203000 | 1.870253000  |
| 6  | -3.949203000 | 1.708195000  | 0.618226000  |
| 1  | -4.168600000 | 2.317760000  | -0.249595000 |
| 6  | -4.507616000 | 0.268715000  | 0.500320000  |
| 1  | -5.030365000 | 0.093671000  | -0.431576000 |
| 1  | -1.874031000 | 2.320909000  | 1.186866000  |
| 1  | -3.417172000 | -1.652643000 | 0.854172000  |
| 1  | -2.655101000 | -0.853278000 | -1.549596000 |
| 1  | -1.726275000 | 1.556580000  | -1.366150000 |
| 6  | 0.564726000  | 1.271521000  | -0.323693000 |
| 8  | 0.867237000  | 1.833157000  | 0.684074000  |
| 8  | 0.780216000  | 1.819010000  | -1.530739000 |
| 6  | 1.410125000  | 3.092819000  | -1.548715000 |
| 1  | 1.486609000  | 3.372089000  | -2.588770000 |
| 1  | 0.820395000  | 3.820163000  | -1.006022000 |
| 1  | 2.393894000  | 3.038680000  | -1.101383000 |
| 6  | -0.884343000 | -2.542430000 | -0.492195000 |
| 7  | -1.219659000 | -3.637350000 | -0.518708000 |
| 1  | -4.353236000 | 2.219201000  | 1.483644000  |
| 1  | -5.197018000 | 0.045325000  | 1.305168000  |
| 6  | 3.515213000  | -0.017626000 | 1.084931000  |
| 6  | 3.688397000  | 0.129665000  | -0.293170000 |
| 6  | 2.616715000  | -0.955889000 | 1.539881000  |
| 1  | 4.400846000  | 0.849078000  | -0.657424000 |
| 1  | 2.482260000  | -1.096200000 | 2.597239000  |

|   |             |              |              |
|---|-------------|--------------|--------------|
| 6 | 2.963708000 | -0.615991000 | -1.182335000 |
| 6 | 1.887328000 | -1.735511000 | 0.652169000  |
| 1 | 3.111008000 | -0.491684000 | -2.239361000 |
| 1 | 1.259201000 | -2.525129000 | 1.018521000  |
| 6 | 2.041016000 | -1.560887000 | -0.721382000 |
| 1 | 1.592468000 | -2.256539000 | -1.406452000 |
| 6 | 4.264840000 | 0.858942000  | 2.034900000  |
| 1 | 3.763189000 | 1.818217000  | 2.122081000  |
| 1 | 4.314322000 | 0.420656000  | 3.023404000  |
| 1 | 5.275305000 | 1.043838000  | 1.689656000  |

42

exo-3tT-OMe

|    |              |              |              |
|----|--------------|--------------|--------------|
| 46 | -0.224839000 | -0.666487000 | -0.409745000 |
| 6  | -2.044162000 | 0.803453000  | -0.730090000 |
| 6  | -2.458222000 | 1.591407000  | 0.489307000  |
| 6  | -3.233559000 | -0.498160000 | 0.766299000  |
| 6  | -2.519175000 | -0.464878000 | -0.560158000 |
| 6  | -2.424750000 | 0.516340000  | 1.575929000  |
| 1  | -2.931272000 | 0.824467000  | 2.482695000  |
| 1  | -1.425507000 | 0.178760000  | 1.819739000  |
| 6  | -3.990256000 | 1.763734000  | 0.316445000  |
| 1  | -4.250366000 | 2.186541000  | -0.645878000 |
| 6  | -4.524190000 | 0.322978000  | 0.506719000  |
| 1  | -5.075931000 | -0.039220000 | -0.351475000 |
| 1  | -1.913449000 | 2.503954000  | 0.672782000  |
| 1  | -3.384456000 | -1.477175000 | 1.190577000  |
| 1  | -2.721562000 | -1.160504000 | -1.350926000 |
| 1  | -1.831824000 | 1.249119000  | -1.681962000 |
| 6  | 0.511035000  | 1.143626000  | -0.905164000 |
| 8  | 0.704441000  | 1.504474000  | -2.026070000 |
| 8  | 0.838633000  | 1.898053000  | 0.150389000  |
| 6  | 1.445185000  | 3.152376000  | -0.132170000 |
| 1  | 1.626656000  | 3.617419000  | 0.825213000  |
| 1  | 2.374620000  | 3.014569000  | -0.668645000 |
| 1  | 0.787512000  | 3.768915000  | -0.730947000 |
| 6  | -0.893504000 | -2.577601000 | 0.013710000  |
| 7  | -1.216622000 | -3.646536000 | 0.268700000  |
| 1  | -4.373787000 | 2.431212000  | 1.078588000  |

|   |              |              |              |
|---|--------------|--------------|--------------|
| 1 | -5.180265000 | 0.255231000  | 1.365743000  |
| 6 | 3.629079000  | 0.110303000  | 0.870518000  |
| 6 | 3.707753000  | 0.043802000  | -0.522289000 |
| 6 | 2.733319000  | -0.707926000 | 1.521432000  |
| 1 | 4.405649000  | 0.677570000  | -1.040971000 |
| 1 | 2.666448000  | -0.679567000 | 2.594149000  |
| 6 | 2.912830000  | -0.811146000 | -1.236013000 |
| 6 | 1.934599000  | -1.596928000 | 0.814054000  |
| 1 | 2.986008000  | -0.848825000 | -2.306926000 |
| 1 | 1.312593000  | -2.296858000 | 1.338594000  |
| 6 | 2.011183000  | -1.651444000 | -0.574977000 |
| 1 | 1.517657000  | -2.441419000 | -1.111797000 |
| 6 | 4.496666000  | 1.066230000  | 1.626414000  |
| 1 | 4.158106000  | 2.087693000  | 1.481404000  |
| 1 | 4.480311000  | 0.859508000  | 2.688520000  |
| 1 | 5.524252000  | 1.015533000  | 1.284545000  |

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exo-3tTr-O

|    |              |              |              |
|----|--------------|--------------|--------------|
| 46 | 0.051761000  | 0.072417000  | -0.117426000 |
| 6  | -2.234116000 | 0.012127000  | -0.687990000 |
| 6  | -3.180660000 | -0.105430000 | 0.482300000  |
| 6  | -2.285594000 | -2.140188000 | 0.155225000  |
| 6  | -1.692886000 | -1.225834000 | -0.886111000 |
| 6  | -2.491676000 | -1.178478000 | 1.326133000  |
| 1  | -3.141797000 | -1.585943000 | 2.090906000  |
| 1  | -1.569581000 | -0.842606000 | 1.782481000  |
| 6  | -4.370639000 | -0.922465000 | -0.085981000 |
| 1  | -4.773503000 | -0.488112000 | -0.992582000 |
| 6  | -3.753461000 | -2.324452000 | -0.311817000 |
| 1  | -3.819044000 | -2.653774000 | -1.341202000 |
| 1  | -3.445465000 | 0.817749000  | 0.972162000  |
| 1  | -1.739799000 | -3.051147000 | 0.338665000  |
| 1  | -1.284967000 | -1.582008000 | -1.811482000 |
| 1  | -2.318877000 | 0.764821000  | -1.447596000 |
| 6  | -0.734342000 | 1.910512000  | 0.189415000  |
| 8  | -1.107814000 | 2.317425000  | 1.247486000  |
| 8  | -0.693479000 | 2.702002000  | -0.894669000 |
| 6  | -1.115785000 | 4.050195000  | -0.717848000 |

|   |              |              |              |
|---|--------------|--------------|--------------|
| 1 | -1.015962000 | 4.520559000  | -1.684218000 |
| 1 | -2.144608000 | 4.086935000  | -0.384939000 |
| 1 | -0.495280000 | 4.553079000  | 0.011828000  |
| 6 | 0.896186000  | -1.792815000 | -0.355852000 |
| 7 | 1.355836000  | -2.830420000 | -0.511620000 |
| 1 | -5.172682000 | -0.955995000 | 0.641278000  |
| 1 | -4.241139000 | -3.073725000 | 0.299552000  |
| 6 | 2.676148000  | -0.003296000 | 1.835014000  |
| 6 | 1.977890000  | 1.005877000  | 1.168513000  |
| 6 | 3.615208000  | -0.742216000 | 1.171911000  |
| 1 | 1.334883000  | 1.663326000  | 1.722095000  |
| 1 | 4.137573000  | -1.526533000 | 1.690098000  |
| 6 | 2.262267000  | 1.250705000  | -0.173714000 |
| 6 | 3.893259000  | -0.522758000 | -0.179696000 |
| 1 | 1.831474000  | 2.097619000  | -0.674483000 |
| 6 | 3.218072000  | 0.479171000  | -0.833585000 |
| 1 | 3.424639000  | 0.674235000  | -1.870551000 |
| 1 | 2.475920000  | -0.188334000 | 2.874283000  |
| 6 | 4.855785000  | -1.410282000 | -0.897909000 |
| 1 | 4.370553000  | -2.355669000 | -1.121883000 |
| 1 | 5.183292000  | -0.969618000 | -1.830964000 |
| 1 | 5.728917000  | -1.620768000 | -0.291100000 |

42

exo-3tTr-OMe

|    |              |              |              |
|----|--------------|--------------|--------------|
| 46 | 0.074675000  | 0.062824000  | -0.209606000 |
| 6  | -2.192730000 | -0.172809000 | -0.831716000 |
| 6  | -3.189764000 | -0.098737000 | 0.299650000  |
| 6  | -2.234560000 | -2.128638000 | 0.401832000  |
| 6  | -1.616589000 | -1.408641000 | -0.768883000 |
| 6  | -2.515630000 | -0.970180000 | 1.359694000  |
| 1  | -3.189364000 | -1.246392000 | 2.161905000  |
| 1  | -1.620884000 | -0.527403000 | 1.778456000  |
| 6  | -4.333684000 | -1.044787000 | -0.151535000 |
| 1  | -4.702487000 | -0.801605000 | -1.140176000 |
| 6  | -3.674848000 | -2.443893000 | -0.080301000 |
| 1  | -3.685613000 | -2.964240000 | -1.029659000 |
| 1  | -3.503898000 | 0.890275000  | 0.592619000  |
| 1  | -1.676283000 | -2.970308000 | 0.777391000  |

|   |              |              |              |
|---|--------------|--------------|--------------|
| 1 | -1.157959000 | -1.919921000 | -1.592240000 |
| 1 | -2.259075000 | 0.421884000  | -1.722061000 |
| 6 | -0.699905000 | 1.913084000  | -0.456176000 |
| 8 | -0.641273000 | 2.541911000  | -1.469579000 |
| 8 | -1.193291000 | 2.441965000  | 0.673257000  |
| 6 | -1.649362000 | 3.788700000  | 0.601249000  |
| 1 | -2.010729000 | 4.032013000  | 1.588841000  |
| 1 | -0.841690000 | 4.451992000  | 0.321650000  |
| 1 | -2.444759000 | 3.883467000  | -0.126126000 |
| 6 | 0.942507000  | -1.795330000 | 0.009180000  |
| 7 | 1.414092000  | -2.833640000 | 0.117534000  |
| 1 | -5.168228000 | -0.965371000 | 0.534567000  |
| 1 | -4.172826000 | -3.078344000 | 0.642541000  |
| 6 | 2.643721000  | 0.519452000  | 1.690168000  |
| 6 | 1.971949000  | 1.312900000  | 0.755499000  |
| 6 | 3.605533000  | -0.359459000 | 1.279282000  |
| 1 | 1.330948000  | 2.102477000  | 1.098359000  |
| 1 | 4.106535000  | -0.977186000 | 2.002971000  |
| 6 | 2.306487000  | 1.200803000  | -0.593288000 |
| 6 | 3.934451000  | -0.496178000 | -0.071686000 |
| 1 | 1.876643000  | 1.871871000  | -1.313517000 |
| 6 | 3.284995000  | 0.293679000  | -0.990672000 |
| 1 | 3.529755000  | 0.210213000  | -2.034199000 |
| 1 | 2.406205000  | 0.613702000  | 2.733888000  |
| 6 | 4.922059000  | -1.531554000 | -0.497921000 |
| 1 | 4.440195000  | -2.504893000 | -0.495132000 |
| 1 | 5.292458000  | -1.341050000 | -1.497129000 |
| 1 | 5.766119000  | -1.577097000 | 0.180500000  |

42

exo-3cT-O

|    |              |              |              |
|----|--------------|--------------|--------------|
| 46 | 0.049105000  | 0.304415000  | -0.155254000 |
| 6  | -2.237914000 | -0.320742000 | -0.771870000 |
| 6  | -3.247169000 | -0.362000000 | 0.348677000  |
| 6  | -2.035398000 | -2.241489000 | 0.483096000  |
| 6  | -1.501566000 | -1.446791000 | -0.686764000 |
| 6  | -2.472384000 | -1.120821000 | 1.427122000  |
| 1  | -3.112388000 | -1.474909000 | 2.226311000  |
| 1  | -1.657318000 | -0.547352000 | 1.845700000  |



|             |              |              |              |
|-------------|--------------|--------------|--------------|
| 6           | -4.252171000 | -1.459263000 | -0.097066000 |
| 1           | -4.642079000 | -1.281773000 | -1.091329000 |
| 6           | -3.416405000 | -2.757551000 | -0.000547000 |
| 1           | -3.349834000 | -3.288067000 | -0.942056000 |
| 1           | -3.689586000 | 0.579807000  | 0.629696000  |
| 1           | -1.385762000 | -3.006713000 | 0.881755000  |
| 1           | -0.937815000 | -1.875717000 | -1.493609000 |
| 1           | -2.320095000 | 0.313336000  | -1.634541000 |
| 6           | -1.004805000 | 1.914296000  | 0.289621000  |
| 8           | -1.490413000 | 2.109870000  | 1.352132000  |
| 8           | -1.117090000 | 2.728752000  | -0.747874000 |
| 6           | -1.767653000 | 3.974537000  | -0.500786000 |
| 1           | -1.739414000 | 4.507323000  | -1.438346000 |
| 1           | -2.789722000 | 3.815140000  | -0.184210000 |
| 1           | -1.236982000 | 4.525082000  | 0.263333000  |
| 6           | 1.523820000  | 1.561797000  | 0.260912000  |
| 7           | 2.392335000  | 2.263992000  | 0.509420000  |
| 1           | -5.094214000 | -1.481076000 | 0.583641000  |
| 1           | -3.832397000 | -3.440604000 | 0.730076000  |
| 6           | 1.899176000  | -1.529981000 | -1.398144000 |
| 6           | 3.042691000  | -0.849360000 | -1.786073000 |
| 6           | 1.733695000  | -1.876515000 | -0.066227000 |
| 1           | 3.183508000  | -0.582100000 | -2.817272000 |
| 1           | 0.899068000  | -2.479826000 | 0.239705000  |
| 6           | 3.991433000  | -0.511440000 | -0.852432000 |
| 6           | 2.701252000  | -1.527777000 | 0.866600000  |
| 1           | 4.864781000  | 0.036225000  | -1.158774000 |
| 1           | 2.560609000  | -1.796041000 | 1.898496000  |
| 6           | 3.831642000  | -0.832535000 | 0.491141000  |
| 1           | 1.184952000  | -1.837080000 | -2.139557000 |
| 6           | 4.829274000  | -0.369411000 | 1.502596000  |
| 1           | 4.758857000  | -0.939625000 | 2.420478000  |
| 1           | 5.842135000  | -0.449998000 | 1.125579000  |
| 1           | 4.643441000  | 0.674261000  | 1.737477000  |
| 42          |              |              |              |
| exo-3cT-OMe |              |              |              |
| 46          | 0.065200000  | 0.275989000  | -0.321019000 |
| 6           | -2.193428000 | -0.498108000 | -0.872368000 |

|   |              |              |              |
|---|--------------|--------------|--------------|
| 6 | -3.234731000 | -0.308016000 | 0.202365000  |
| 6 | -2.032920000 | -2.113024000 | 0.761614000  |
| 6 | -1.463871000 | -1.578164000 | -0.532739000 |
| 6 | -2.494826000 | -0.821875000 | 1.438763000  |
| 1 | -3.158062000 | -1.004403000 | 2.275903000  |
| 1 | -1.685866000 | -0.175892000 | 1.751752000  |
| 6 | -4.230790000 | -1.476457000 | -0.031765000 |
| 1 | -4.590396000 | -1.510284000 | -1.052089000 |
| 6 | -3.401332000 | -2.722928000 | 0.357581000  |
| 1 | -3.309126000 | -3.437679000 | -0.450228000 |
| 1 | -3.688116000 | 0.669110000  | 0.260013000  |
| 1 | -1.397257000 | -2.775144000 | 1.330766000  |
| 1 | -0.872085000 | -2.161434000 | -1.212364000 |
| 1 | -2.243002000 | -0.044198000 | -1.843579000 |
| 6 | -0.993546000 | 1.941329000  | -0.425152000 |
| 8 | -1.317795000 | 2.448126000  | -1.445903000 |
| 8 | -1.311696000 | 2.401405000  | 0.773944000  |
| 6 | -1.996478000 | 3.652706000  | 0.804686000  |
| 1 | -2.152676000 | 3.872590000  | 1.849148000  |
| 1 | -1.389510000 | 4.418988000  | 0.343235000  |
| 1 | -2.942204000 | 3.583098000  | 0.283955000  |
| 6 | 1.508906000  | 1.599330000  | -0.023533000 |
| 7 | 2.358223000  | 2.339051000  | 0.177837000  |
| 1 | -5.092500000 | -1.359089000 | 0.613712000  |
| 1 | -3.840087000 | -3.239938000 | 1.202322000  |
| 6 | 1.954168000  | -1.717217000 | -1.137845000 |
| 6 | 3.101243000  | -1.095482000 | -1.606746000 |
| 6 | 1.759182000  | -1.841438000 | 0.228907000  |
| 1 | 3.264430000  | -0.999635000 | -2.664430000 |
| 1 | 0.921989000  | -2.395578000 | 0.611326000  |
| 6 | 4.024003000  | -0.597013000 | -0.720427000 |
| 6 | 2.701051000  | -1.332600000 | 1.113020000  |
| 1 | 4.899996000  | -0.096713000 | -1.093014000 |
| 1 | 2.537899000  | -1.429379000 | 2.171606000  |
| 6 | 3.834176000  | -0.694660000 | 0.653832000  |
| 1 | 1.261598000  | -2.151403000 | -1.834959000 |
| 6 | 4.802858000  | -0.058998000 | 1.597377000  |
| 1 | 4.717194000  | -0.473403000 | 2.594172000  |

|           |              |              |              |
|-----------|--------------|--------------|--------------|
| 1         | 5.825052000  | -0.185098000 | 1.260261000  |
| 1         | 4.599893000  | 1.006106000  | 1.654773000  |
| 42        |              |              |              |
| exo-3cT-N |              |              |              |
| 46        | 0.090972000  | 0.458166000  | -0.185109000 |
| 6         | 2.271581000  | -0.912011000 | -0.810217000 |
| 6         | 2.977883000  | -1.567878000 | 0.354954000  |
| 6         | 3.561288000  | 0.595703000  | 0.348105000  |
| 6         | 2.632067000  | 0.377072000  | -0.817016000 |
| 6         | 3.010536000  | -0.413225000 | 1.358401000  |
| 1         | 3.688876000  | -0.593132000 | 2.184117000  |
| 1         | 2.037864000  | -0.138626000 | 1.744408000  |
| 6         | 4.471887000  | -1.617236000 | -0.062277000 |
| 1         | 4.612709000  | -2.097539000 | -1.022358000 |
| 6         | 4.873326000  | -0.122739000 | -0.069880000 |
| 1         | 5.234829000  | 0.211458000  | -1.033900000 |
| 1         | 2.577473000  | -2.513583000 | 0.692348000  |
| 1         | 3.671318000  | 1.617255000  | 0.673010000  |
| 1         | 2.496358000  | 1.078603000  | -1.617733000 |
| 1         | 1.832879000  | -1.446893000 | -1.631735000 |
| 6         | -1.628541000 | 1.273781000  | 0.326148000  |
| 8         | -2.194840000 | 1.024894000  | 1.339020000  |
| 8         | -2.095319000 | 2.093436000  | -0.604295000 |
| 6         | -3.312314000 | 2.766169000  | -0.296825000 |
| 1         | -3.510671000 | 3.410668000  | -1.139089000 |
| 1         | -4.118190000 | 2.056125000  | -0.164795000 |
| 1         | -3.199092000 | 3.349603000  | 0.606483000  |
| 6         | 0.752637000  | 2.223881000  | 0.403492000  |
| 7         | 1.197885000  | 3.224531000  | 0.734007000  |
| 1         | 5.043836000  | -2.175414000 | 0.669473000  |
| 1         | 5.650158000  | 0.079812000  | 0.657205000  |
| 6         | -0.774621000 | -2.018812000 | -0.190250000 |
| 6         | -1.066936000 | -1.432142000 | -1.414418000 |
| 6         | -1.785597000 | -2.239474000 | 0.736278000  |
| 1         | -0.321536000 | -1.353061000 | -2.184002000 |
| 1         | -1.542631000 | -2.682608000 | 1.685031000  |
| 6         | -2.389885000 | -1.099609000 | -1.706714000 |
| 6         | -3.089435000 | -1.898037000 | 0.456752000  |

|   |              |              |              |
|---|--------------|--------------|--------------|
| 1 | -2.630195000 | -0.662955000 | -2.658419000 |
| 6 | -3.377512000 | -1.338803000 | -0.788547000 |
| 1 | -4.394799000 | -1.079254000 | -1.023517000 |
| 1 | 0.215250000  | -2.376334000 | 0.019210000  |
| 6 | -4.168868000 | -2.071058000 | 1.475244000  |
| 1 | -3.908053000 | -2.826821000 | 2.205064000  |
| 1 | -4.321144000 | -1.135958000 | 2.005658000  |
| 1 | -5.108825000 | -2.348837000 | 1.013327000  |

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exo-3cT-N'

|    |              |              |              |
|----|--------------|--------------|--------------|
| 46 | 0.112255000  | 0.338870000  | -0.336396000 |
| 6  | 2.249523000  | -1.246729000 | -0.285055000 |
| 6  | 2.976611000  | -1.311073000 | 1.038275000  |
| 6  | 3.605263000  | 0.581930000  | 0.016403000  |
| 6  | 2.632874000  | -0.119438000 | -0.896409000 |
| 6  | 3.068246000  | 0.174855000  | 1.390318000  |
| 1  | 3.771431000  | 0.373865000  | 2.190501000  |
| 1  | 2.116408000  | 0.631173000  | 1.625110000  |
| 6  | 4.454644000  | -1.599787000 | 0.661940000  |
| 1  | 4.553345000  | -2.475031000 | 0.032184000  |
| 6  | 4.886904000  | -0.293675000 | -0.046765000 |
| 1  | 5.222844000  | -0.457055000 | -1.062739000 |
| 1  | 2.564560000  | -1.978650000 | 1.781885000  |
| 1  | 3.748047000  | 1.633542000  | -0.169888000 |
| 1  | 2.485562000  | 0.134327000  | -1.929214000 |
| 1  | 1.776845000  | -2.089306000 | -0.752532000 |
| 6  | -1.573000000 | 1.355452000  | -0.229591000 |
| 8  | -2.325751000 | 1.494598000  | -1.134664000 |
| 8  | -1.779417000 | 1.833759000  | 0.990704000  |
| 6  | -2.933513000 | 2.651295000  | 1.157874000  |
| 1  | -2.915966000 | 2.975000000  | 2.187001000  |
| 1  | -2.886806000 | 3.503037000  | 0.493342000  |
| 1  | -3.834630000 | 2.088652000  | 0.952922000  |
| 6  | 0.842392000  | 2.168838000  | -0.478601000 |
| 7  | 1.325607000  | 3.202357000  | -0.562854000 |
| 1  | 5.038633000  | -1.774288000 | 1.557853000  |
| 1  | 5.691860000  | 0.195905000  | 0.487580000  |
| 6  | -0.966829000 | -1.843280000 | 0.362254000  |

|   |              |              |              |
|---|--------------|--------------|--------------|
| 6 | -1.030244000 | -1.914013000 | -1.021848000 |
| 6 | -2.131808000 | -1.624544000 | 1.098495000  |
| 1 | -0.164544000 | -2.165596000 | -1.604365000 |
| 1 | -2.071292000 | -1.571551000 | 2.170546000  |
| 6 | -2.259144000 | -1.769195000 | -1.657480000 |
| 6 | -3.350003000 | -1.493433000 | 0.474736000  |
| 1 | -2.314492000 | -1.815837000 | -2.728992000 |
| 6 | -3.393791000 | -1.570271000 | -0.918284000 |
| 1 | -4.338608000 | -1.455866000 | -1.419654000 |
| 1 | -0.054876000 | -2.069450000 | 0.883650000  |
| 6 | -4.607310000 | -1.264133000 | 1.253688000  |
| 1 | -4.411890000 | -1.226022000 | 2.317363000  |
| 1 | -5.075884000 | -0.329918000 | 0.962670000  |
| 1 | -5.327060000 | -2.055104000 | 1.070976000  |

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exo-TS3\_4tP-O

|    |              |              |              |
|----|--------------|--------------|--------------|
| 46 | 1.173680000  | -0.468008000 | 0.362810000  |
| 15 | -1.211173000 | -0.114735000 | -0.059699000 |
| 6  | -1.813705000 | 1.572669000  | -0.413128000 |
| 6  | -1.382573000 | 2.202094000  | -1.574886000 |
| 6  | -2.663769000 | 2.258448000  | 0.440123000  |
| 6  | -1.806161000 | 3.476514000  | -1.882592000 |
| 1  | -0.705288000 | 1.699049000  | -2.239801000 |
| 6  | -3.079392000 | 3.542049000  | 0.136278000  |
| 1  | -3.010695000 | 1.793807000  | 1.343423000  |
| 6  | -2.656495000 | 4.151632000  | -1.026229000 |
| 1  | -1.464155000 | 3.946293000  | -2.786737000 |
| 1  | -3.739873000 | 4.059114000  | 0.808641000  |
| 1  | -2.984486000 | 5.147168000  | -1.265014000 |
| 6  | -1.909625000 | -1.091027000 | -1.436473000 |
| 6  | -2.980526000 | -0.632825000 | -2.193726000 |
| 6  | -1.380819000 | -2.344183000 | -1.716831000 |
| 6  | -3.506951000 | -1.406307000 | -3.208228000 |
| 1  | -3.407815000 | 0.332291000  | -1.998814000 |
| 6  | -1.913156000 | -3.116996000 | -2.729413000 |
| 1  | -0.564443000 | -2.729465000 | -1.137136000 |
| 6  | -2.973650000 | -2.650528000 | -3.479127000 |
| 1  | -4.334038000 | -1.034324000 | -3.785538000 |

|   |              |              |              |
|---|--------------|--------------|--------------|
| 1 | -1.493120000 | -4.085975000 | -2.928643000 |
| 1 | -3.382943000 | -3.252532000 | -4.270287000 |
| 6 | -2.161498000 | -0.622174000 | 1.406671000  |
| 6 | -1.594019000 | -0.434007000 | 2.658006000  |
| 6 | -3.430130000 | -1.174545000 | 1.320706000  |
| 6 | -2.287196000 | -0.772825000 | 3.801743000  |
| 1 | -0.599867000 | -0.032642000 | 2.738611000  |
| 6 | -4.119935000 | -1.521886000 | 2.464543000  |
| 1 | -3.879555000 | -1.346716000 | 0.360696000  |
| 6 | -3.551779000 | -1.318186000 | 3.706340000  |
| 1 | -1.832752000 | -0.626140000 | 4.764556000  |
| 1 | -5.099028000 | -1.958095000 | 2.383993000  |
| 1 | -4.087902000 | -1.594870000 | 4.596055000  |
| 6 | 3.266677000  | 0.633098000  | 0.489126000  |
| 6 | 4.167688000  | 0.708765000  | -0.734567000 |
| 6 | 3.976408000  | -1.484624000 | -0.289357000 |
| 6 | 3.158216000  | -0.780535000 | 0.773358000  |
| 6 | 3.778055000  | -0.559408000 | -1.491460000 |
| 1 | 4.456646000  | -0.777274000 | -2.307645000 |
| 1 | 2.764415000  | -0.539492000 | -1.870536000 |
| 6 | 5.569655000  | 0.324979000  | -0.215070000 |
| 1 | 5.853363000  | 0.893121000  | 0.663125000  |
| 6 | 5.448961000  | -1.192809000 | 0.060315000  |
| 1 | 5.686596000  | -1.456052000 | 1.083636000  |
| 1 | 4.122371000  | 1.639536000  | -1.276435000 |
| 1 | 3.739089000  | -2.528707000 | -0.421585000 |
| 1 | 3.236353000  | -1.124686000 | 1.790274000  |
| 1 | 3.471034000  | 1.288259000  | 1.317998000  |
| 6 | 1.744261000  | 1.650346000  | 0.035701000  |
| 8 | 1.689594000  | 2.114250000  | -1.058053000 |
| 8 | 1.389160000  | 2.317905000  | 1.136144000  |
| 6 | 0.956708000  | 3.663910000  | 0.960714000  |
| 1 | 0.765852000  | 4.040431000  | 1.953674000  |
| 1 | 1.732861000  | 4.245083000  | 0.479582000  |
| 1 | 0.058335000  | 3.703761000  | 0.363302000  |
| 6 | 0.895145000  | -2.412443000 | 0.772174000  |
| 7 | 0.761063000  | -3.527496000 | 0.996822000  |
| 1 | 6.307780000  | 0.530897000  | -0.980811000 |

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| 1               | 6.109727000  | -1.762376000 | -0.583081000 |
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| exo-TS3_4tP-OMe |              |              |              |
| 46              | 1.145104000  | -0.651642000 | 0.154263000  |
| 15              | -1.240262000 | -0.116476000 | -0.023045000 |
| 6               | -1.717900000 | 1.611554000  | -0.388495000 |
| 6               | -1.494545000 | 2.082484000  | -1.677247000 |
| 6               | -2.289221000 | 2.463182000  | 0.540909000  |
| 6               | -1.852672000 | 3.364434000  | -2.031254000 |
| 1               | -1.049830000 | 1.437135000  | -2.413959000 |
| 6               | -2.638167000 | 3.755025000  | 0.188508000  |
| 1               | -2.473416000 | 2.124135000  | 1.542360000  |
| 6               | -2.426963000 | 4.207026000  | -1.096628000 |
| 1               | -1.684059000 | 3.707198000  | -3.036200000 |
| 1               | -3.083338000 | 4.402227000  | 0.922363000  |
| 1               | -2.707369000 | 5.207773000  | -1.371249000 |
| 6               | -2.279629000 | -1.014765000 | -1.225247000 |
| 6               | -3.559370000 | -0.557261000 | -1.526415000 |
| 6               | -1.818667000 | -2.164274000 | -1.846253000 |
| 6               | -4.356332000 | -1.235606000 | -2.421803000 |
| 1               | -3.935615000 | 0.336241000  | -1.063675000 |
| 6               | -2.620660000 | -2.842836000 | -2.746040000 |
| 1               | -0.844165000 | -2.548880000 | -1.621371000 |
| 6               | -3.886432000 | -2.382250000 | -3.035904000 |
| 1               | -5.342360000 | -0.868523000 | -2.642384000 |
| 1               | -2.246808000 | -3.734980000 | -3.214201000 |
| 1               | -4.507185000 | -2.910851000 | -3.736788000 |
| 6               | -1.963972000 | -0.473092000 | 1.610643000  |
| 6               | -1.313765000 | 0.021466000  | 2.736291000  |
| 6               | -3.095390000 | -1.254703000 | 1.779116000  |
| 6               | -1.804436000 | -0.240525000 | 3.997914000  |
| 1               | -0.421879000 | 0.612619000  | 2.629121000  |
| 6               | -3.577026000 | -1.525265000 | 3.045637000  |
| 1               | -3.599573000 | -1.667678000 | 0.926819000  |
| 6               | -2.937297000 | -1.015730000 | 4.155867000  |
| 1               | -1.293304000 | 0.151627000  | 4.858373000  |
| 1               | -4.451003000 | -2.140399000 | 3.160295000  |
| 1               | -3.312483000 | -1.228881000 | 5.140454000  |

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| 6 | 3.241334000 | 0.350895000  | 0.663722000  |
| 6 | 4.204914000 | 0.779372000  | -0.434264000 |
| 6 | 3.975985000 | -1.439009000 | -0.700437000 |
| 6 | 3.117341000 | -1.081270000 | 0.494977000  |
| 6 | 3.842417000 | -0.183211000 | -1.563618000 |
| 1 | 4.557008000 | -0.153309000 | -2.377680000 |
| 1 | 2.847130000 | -0.026666000 | -1.959317000 |
| 6 | 5.575769000 | 0.220823000  | 0.006274000  |
| 1 | 5.814118000 | 0.479433000  | 1.031186000  |
| 6 | 5.432373000 | -1.303189000 | -0.215370000 |
| 1 | 5.620227000 | -1.879790000 | 0.681725000  |
| 1 | 4.208126000 | 1.832702000  | -0.663378000 |
| 1 | 3.736703000 | -2.385047000 | -1.160256000 |
| 1 | 3.166185000 | -1.717351000 | 1.361737000  |
| 1 | 3.412156000 | 0.711296000  | 1.662886000  |
| 6 | 1.719017000 | 1.464578000  | 0.560959000  |
| 8 | 1.341569000 | 1.917367000  | 1.598827000  |
| 8 | 1.747479000 | 2.160774000  | -0.566984000 |
| 6 | 1.408275000 | 3.542081000  | -0.465511000 |
| 1 | 1.475018000 | 3.933768000  | -1.468087000 |
| 1 | 0.409052000 | 3.664521000  | -0.077328000 |
| 1 | 2.111009000 | 4.045924000  | 0.186073000  |
| 6 | 0.898972000 | -2.632193000 | -0.029189000 |
| 7 | 0.805062000 | -3.768433000 | -0.138479000 |
| 1 | 6.354753000 | 0.640565000  | -0.618787000 |
| 1 | 6.118512000 | -1.654711000 | -0.977372000 |

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exo-TS3\_4tP-N

|    |              |              |              |
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| 46 | 1.157407000  | 0.176073000  | 0.183236000  |
| 15 | -1.196519000 | -0.208919000 | -0.042750000 |
| 6  | -2.228221000 | 1.269766000  | -0.315462000 |
| 6  | -1.940614000 | 2.078452000  | -1.407921000 |
| 6  | -3.288942000 | 1.609092000  | 0.508424000  |
| 6  | -2.705222000 | 3.193773000  | -1.673721000 |
| 1  | -1.108068000 | 1.847959000  | -2.046777000 |
| 6  | -4.049659000 | 2.733058000  | 0.245081000  |
| 1  | -3.528688000 | 1.000005000  | 1.359112000  |
| 6  | -3.762276000 | 3.524886000  | -0.846588000 |



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| 1 | -2.468253000 | 3.809287000  | -2.522378000 |
| 1 | -4.867982000 | 2.984590000  | 0.895268000  |
| 1 | -4.354975000 | 4.398049000  | -1.051692000 |
| 6 | -1.742147000 | -1.331000000 | -1.374571000 |
| 6 | -2.969787000 | -1.174070000 | -2.004580000 |
| 6 | -0.921285000 | -2.380578000 | -1.762681000 |
| 6 | -3.366497000 | -2.046682000 | -2.997539000 |
| 1 | -3.619190000 | -0.365527000 | -1.727154000 |
| 6 | -1.322113000 | -3.254860000 | -2.752864000 |
| 1 | 0.026055000  | -2.528799000 | -1.282669000 |
| 6 | -2.543420000 | -3.089201000 | -3.374010000 |
| 1 | -4.318411000 | -1.908584000 | -3.477515000 |
| 1 | -0.675138000 | -4.064332000 | -3.038074000 |
| 1 | -2.851767000 | -3.767210000 | -4.149261000 |
| 6 | -1.846492000 | -0.934000000 | 1.494355000  |
| 6 | -1.403460000 | -0.401541000 | 2.698453000  |
| 6 | -2.744164000 | -1.987922000 | 1.515674000  |
| 6 | -1.863718000 | -0.902057000 | 3.897334000  |
| 1 | -0.694743000 | 0.408139000  | 2.695639000  |
| 6 | -3.196131000 | -2.496458000 | 2.718541000  |
| 1 | -3.087614000 | -2.422899000 | 0.596126000  |
| 6 | -2.760885000 | -1.953391000 | 3.909278000  |
| 1 | -1.514717000 | -0.479067000 | 4.821821000  |
| 1 | -3.886479000 | -3.320356000 | 2.721375000  |
| 1 | -3.112011000 | -2.351609000 | 4.844001000  |
| 6 | 3.200547000  | 0.489408000  | 0.515282000  |
| 6 | 4.079398000  | 0.666708000  | -0.713163000 |
| 6 | 4.190559000  | -1.521840000 | -0.211400000 |
| 6 | 3.272595000  | -0.918838000 | 0.833990000  |
| 6 | 3.870991000  | -0.666142000 | -1.436057000 |
| 1 | 4.576090000  | -0.823444000 | -2.243508000 |
| 1 | 2.865350000  | -0.805484000 | -1.812725000 |
| 6 | 5.532864000  | 0.505798000  | -0.232258000 |
| 1 | 5.766749000  | 1.167495000  | 0.592655000  |
| 6 | 5.592363000  | -0.988998000 | 0.164511000  |
| 1 | 5.821830000  | -1.141612000 | 1.212620000  |
| 1 | 3.880556000  | 1.560982000  | -1.283581000 |
| 1 | 4.124607000  | -2.594070000 | -0.309911000 |

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| 1 | 3.393711000  | -1.219139000 | 1.860026000  |
| 1 | 3.315025000  | 1.189299000  | 1.326312000  |
| 6 | 1.062391000  | 2.151425000  | -0.207958000 |
| 8 | 1.290974000  | 2.685740000  | -1.253296000 |
| 8 | 0.716959000  | 2.875191000  | 0.875562000  |
| 6 | 0.622865000  | 4.281300000  | 0.698937000  |
| 1 | 0.358921000  | 4.685079000  | 1.665318000  |
| 1 | 1.567108000  | 4.692226000  | 0.365924000  |
| 1 | -0.140242000 | 4.525833000  | -0.028304000 |
| 6 | 1.713796000  | -1.863001000 | 0.657286000  |
| 7 | 1.386381000  | -2.955703000 | 0.773370000  |
| 1 | 6.229596000  | 0.725175000  | -1.033796000 |
| 1 | 6.341598000  | -1.523593000 | -0.406450000 |

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|    |              |              |              |
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| 46 | 1.032405000  | -0.663501000 | -0.069662000 |
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| 6  | -1.959933000 | -2.004982000 | -1.771296000 |
| 6  | -3.336367000 | -0.051201000 | -1.876422000 |
| 6  | -2.755823000 | -2.609764000 | -2.723509000 |
| 1  | -1.130946000 | -2.545600000 | -1.356132000 |
| 6  | -4.126608000 | -0.657883000 | -2.830905000 |
| 1  | -3.574741000 | 0.946301000  | -1.558922000 |
| 6  | -3.837174000 | -1.938988000 | -3.257103000 |
| 1  | -2.525464000 | -3.608988000 | -3.044964000 |
| 1  | -4.968032000 | -0.128332000 | -3.239827000 |
| 1  | -4.452588000 | -2.411415000 | -4.001315000 |
| 6  | -2.021171000 | -0.404076000 | 1.533289000  |
| 6  | -3.404306000 | -0.449505000 | 1.642715000  |
| 6  | -1.248424000 | -0.671365000 | 2.651428000  |
| 6  | -3.999741000 | -0.745102000 | 2.850110000  |
| 1  | -4.021507000 | -0.265572000 | 0.783080000  |
| 6  | -1.845616000 | -0.962240000 | 3.862241000  |
| 1  | -0.177406000 | -0.677764000 | 2.573725000  |
| 6  | -3.220428000 | -0.998697000 | 3.963158000  |
| 1  | -5.071528000 | -0.785344000 | 2.920581000  |
| 1  | -1.233380000 | -1.176882000 | 4.718764000  |

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| 1 | -3.685684000 | -1.236129000 | 4.902718000  |
| 6 | -1.493267000 | 1.817539000  | -0.209056000 |
| 6 | -1.267195000 | 2.428792000  | -1.437057000 |
| 6 | -1.847034000 | 2.609759000  | 0.871073000  |
| 6 | -1.400681000 | 3.792201000  | -1.581194000 |
| 1 | -0.995485000 | 1.834526000  | -2.290929000 |
| 6 | -1.974268000 | 3.979471000  | 0.727678000  |
| 1 | -2.027579000 | 2.162922000  | 1.830340000  |
| 6 | -1.753150000 | 4.573752000  | -0.496057000 |
| 1 | -1.229063000 | 4.246267000  | -2.540317000 |
| 1 | -2.250650000 | 4.577718000  | 1.576870000  |
| 1 | -1.855558000 | 5.637841000  | -0.607661000 |
| 6 | 3.049397000  | 0.389678000  | -0.688508000 |
| 6 | 3.940001000  | 1.126909000  | 0.297233000  |
| 6 | 2.016645000  | 2.283733000  | 0.261747000  |
| 6 | 1.822539000  | 1.142119000  | -0.719298000 |
| 6 | 2.918622000  | 1.634484000  | 1.312527000  |
| 1 | 3.344947000  | 2.352010000  | 2.003769000  |
| 1 | 2.448507000  | 0.837511000  | 1.872770000  |
| 6 | 4.323306000  | 2.438099000  | -0.422518000 |
| 1 | 4.705373000  | 2.262338000  | -1.421130000 |
| 6 | 3.008351000  | 3.252308000  | -0.412878000 |
| 1 | 2.684898000  | 3.543150000  | -1.404887000 |
| 1 | 4.772597000  | 0.559725000  | 0.680109000  |
| 1 | 1.109663000  | 2.752167000  | 0.612665000  |
| 1 | 1.383021000  | 1.368064000  | -1.677069000 |
| 1 | 3.468248000  | 0.042580000  | -1.616007000 |
| 6 | 3.075214000  | -1.428248000 | 0.042346000  |
| 8 | 3.538399000  | -1.581750000 | 1.121632000  |
| 8 | 3.286359000  | -2.224931000 | -0.995145000 |
| 6 | 3.880661000  | -3.489029000 | -0.700946000 |
| 1 | 3.999835000  | -3.982677000 | -1.652677000 |
| 1 | 4.838764000  | -3.352228000 | -0.218554000 |
| 1 | 3.220908000  | -4.057024000 | -0.059184000 |
| 6 | 0.537921000  | -2.598462000 | 0.442556000  |
| 7 | 0.281447000  | -3.693559000 | 0.661768000  |
| 1 | 5.104153000  | 2.941414000  | 0.134897000  |
| 1 | 3.112418000  | 4.158147000  | 0.173789000  |

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exo-TS3\_4cP-OMe

|    |              |              |              |
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| 46 | 1.010079000  | -0.646583000 | -0.301969000 |
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| 6  | -2.065854000 | -1.861387000 | -1.875246000 |
| 6  | -3.462257000 | 0.074471000  | -1.713000000 |
| 6  | -2.918863000 | -2.390286000 | -2.823074000 |
| 1  | -1.204402000 | -2.423322000 | -1.568969000 |
| 6  | -4.310137000 | -0.456293000 | -2.663149000 |
| 1  | -3.685908000 | 1.036999000  | -1.293120000 |
| 6  | -4.039444000 | -1.690239000 | -3.220750000 |
| 1  | -2.701116000 | -3.352482000 | -3.249095000 |
| 1  | -5.181217000 | 0.095712000  | -2.966689000 |
| 1  | -4.699313000 | -2.103004000 | -3.962331000 |
| 6  | -1.916590000 | -0.548154000 | 1.557396000  |
| 6  | -3.288165000 | -0.638422000 | 1.750206000  |
| 6  | -1.067442000 | -0.878303000 | 2.600687000  |
| 6  | -3.797281000 | -1.039097000 | 2.966964000  |
| 1  | -3.963716000 | -0.407690000 | 0.947687000  |
| 6  | -1.577794000 | -1.274040000 | 3.821152000  |
| 1  | -0.004152000 | -0.851484000 | 2.453414000  |
| 6  | -2.942136000 | -1.354111000 | 4.005938000  |
| 1  | -4.861075000 | -1.113236000 | 3.101599000  |
| 1  | -0.907093000 | -1.536388000 | 4.618624000  |
| 1  | -3.340022000 | -1.673343000 | 4.952178000  |
| 6  | -1.522323000 | 1.817111000  | -0.023520000 |
| 6  | -1.361218000 | 2.531917000  | -1.205054000 |
| 6  | -1.835978000 | 2.510636000  | 1.134014000  |
| 6  | -1.518957000 | 3.900087000  | -1.228304000 |
| 1  | -1.122130000 | 2.014758000  | -2.117006000 |
| 6  | -1.987220000 | 3.885334000  | 1.111772000  |
| 1  | -1.967388000 | 1.982582000  | 2.059390000  |
| 6  | -1.830646000 | 4.582753000  | -0.066554000 |
| 1  | -1.398265000 | 4.435042000  | -2.152853000 |
| 1  | -2.232116000 | 4.406264000  | 2.019575000  |
| 1  | -1.952011000 | 5.650561000  | -0.083970000 |
| 6  | 2.992499000  | 0.498697000  | -0.894006000 |

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| 6 | 3.940422000 | 1.050564000  | 0.156648000  |
| 6 | 2.025937000 | 2.191435000  | 0.430057000  |
| 6 | 1.767472000 | 1.236339000  | -0.722036000 |
| 6 | 2.982331000 | 1.374288000  | 1.301049000  |
| 1 | 3.451822000 | 1.964928000  | 2.079063000  |
| 1 | 2.535887000 | 0.493766000  | 1.744046000  |
| 6 | 4.292988000 | 2.468520000  | -0.345349000 |
| 1 | 4.617429000 | 2.468108000  | -1.378996000 |
| 6 | 2.985708000 | 3.264422000  | -0.121610000 |
| 1 | 2.609235000 | 3.720963000  | -1.028652000 |
| 1 | 4.793720000 | 0.432835000  | 0.385560000  |
| 1 | 1.144416000 | 2.590597000  | 0.908881000  |
| 1 | 1.280810000 | 1.627839000  | -1.599967000 |
| 1 | 3.357906000 | 0.342091000  | -1.892347000 |
| 6 | 3.019383000 | -1.447775000 | -0.673038000 |
| 8 | 3.224259000 | -2.037283000 | -1.680213000 |
| 8 | 3.520012000 | -1.767787000 | 0.508806000  |
| 6 | 4.147608000 | -3.047897000 | 0.594407000  |
| 1 | 4.525474000 | -3.119624000 | 1.602275000  |
| 1 | 3.414385000 | -3.820605000 | 0.407925000  |
| 1 | 4.952930000 | -3.121435000 | -0.123412000 |
| 6 | 0.562749000 | -2.612864000 | 0.130180000  |
| 7 | 0.342637000 | -3.705636000 | 0.395433000  |
| 1 | 5.106934000 | 2.870614000  | 0.245892000  |
| 1 | 3.128996000 | 4.055662000  | 0.605735000  |

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|    |              |              |              |
|----|--------------|--------------|--------------|
| 46 | -0.894502000 | -0.904441000 | -0.454374000 |
| 15 | 0.952674000  | 0.408632000  | -0.005672000 |
| 6  | 1.164720000  | 0.673774000  | 1.782074000  |
| 6  | 0.754857000  | -0.333082000 | 2.646140000  |
| 6  | 1.750683000  | 1.816786000  | 2.309446000  |
| 6  | 0.930291000  | -0.196465000 | 4.008769000  |
| 1  | 0.311281000  | -1.230259000 | 2.253385000  |
| 6  | 1.919316000  | 1.952073000  | 3.672401000  |
| 1  | 2.074006000  | 2.607942000  | 1.659163000  |
| 6  | 1.508991000  | 0.945606000  | 4.524433000  |
| 1  | 0.609930000  | -0.984176000 | 4.666019000  |

|   |              |              |              |
|---|--------------|--------------|--------------|
| 1 | 2.371510000  | 2.843809000  | 4.067181000  |
| 1 | 1.639171000  | 1.052555000  | 5.586178000  |
| 6 | 2.545899000  | -0.246306000 | -0.589678000 |
| 6 | 2.580804000  | -0.976937000 | -1.767770000 |
| 6 | 3.733262000  | 0.007070000  | 0.083199000  |
| 6 | 3.783270000  | -1.429459000 | -2.272822000 |
| 1 | 1.669444000  | -1.227303000 | -2.275643000 |
| 6 | 4.932304000  | -0.453560000 | -0.419026000 |
| 1 | 3.727478000  | 0.555522000  | 1.006022000  |
| 6 | 4.959585000  | -1.168103000 | -1.601104000 |
| 1 | 3.792775000  | -2.004237000 | -3.180550000 |
| 1 | 5.844085000  | -0.257166000 | 0.115326000  |
| 1 | 5.894271000  | -1.530361000 | -1.989611000 |
| 6 | 0.911503000  | 2.086337000  | -0.732297000 |
| 6 | 0.077063000  | 3.061005000  | -0.199204000 |
| 6 | 1.651843000  | 2.397258000  | -1.862619000 |
| 6 | -0.007604000 | 4.310779000  | -0.773733000 |
| 1 | -0.504846000 | 2.848958000  | 0.676980000  |
| 6 | 1.559657000  | 3.647689000  | -2.444400000 |
| 1 | 2.309870000  | 1.667898000  | -2.294377000 |
| 6 | 0.732597000  | 4.607967000  | -1.902389000 |
| 1 | -0.653158000 | 5.052868000  | -0.339943000 |
| 1 | 2.142438000  | 3.867815000  | -3.320320000 |
| 1 | 0.665218000  | 5.581786000  | -2.352313000 |
| 6 | -2.304906000 | 0.671512000  | -0.623105000 |
| 6 | -2.942451000 | 1.250203000  | 0.636119000  |
| 6 | -4.398746000 | -0.294432000 | -0.087559000 |
| 6 | -3.239527000 | -0.347546000 | -1.070202000 |
| 6 | -3.670731000 | 0.034040000  | 1.212656000  |
| 1 | -4.350657000 | 0.291251000  | 2.016149000  |
| 1 | -3.012351000 | -0.757799000 | 1.547298000  |
| 6 | -4.134972000 | 2.106510000  | 0.174252000  |
| 1 | -3.846943000 | 2.842566000  | -0.566124000 |
| 6 | -5.108754000 | 1.042995000  | -0.385816000 |
| 1 | -5.313222000 | 1.170511000  | -1.442239000 |
| 1 | -2.269503000 | 1.756825000  | 1.312253000  |
| 1 | -5.038128000 | -1.163026000 | -0.100766000 |
| 1 | -3.472221000 | -0.406588000 | -2.119939000 |

|   |              |              |              |
|---|--------------|--------------|--------------|
| 1 | -1.958992000 | 1.370230000  | -1.367776000 |
| 6 | 0.157840000  | -2.678064000 | -0.387419000 |
| 8 | 0.645372000  | -3.278431000 | -1.299518000 |
| 8 | 0.178996000  | -3.210882000 | 0.861164000  |
| 6 | 0.735751000  | -4.510192000 | 0.988519000  |
| 1 | 0.653395000  | -4.771283000 | 2.033876000  |
| 1 | 0.188917000  | -5.220649000 | 0.382607000  |
| 1 | 1.773804000  | -4.518109000 | 0.681627000  |
| 6 | -2.671609000 | -2.019919000 | -0.931116000 |
| 7 | -3.116120000 | -3.071343000 | -1.032500000 |
| 1 | -4.576645000 | 2.637663000  | 1.011042000  |
| 1 | -6.061685000 | 1.066232000  | 0.128599000  |

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exo-TS3\_4t-O

|    |              |              |              |
|----|--------------|--------------|--------------|
| 46 | 0.771417000  | -0.899459000 | 0.048133000  |
| 6  | -0.561221000 | 0.992723000  | -0.581999000 |
| 6  | -1.545260000 | 1.598796000  | 0.408637000  |
| 6  | -2.250417000 | -0.517537000 | 0.118237000  |
| 6  | -1.043612000 | -0.373534000 | -0.773944000 |
| 6  | -1.889344000 | 0.397424000  | 1.289274000  |
| 1  | -2.731970000 | 0.594631000  | 1.940458000  |
| 1  | -1.058140000 | 0.043660000  | 1.884192000  |
| 6  | -2.855578000 | 1.769323000  | -0.387514000 |
| 1  | -2.704656000 | 2.288233000  | -1.326581000 |
| 6  | -3.352315000 | 0.315776000  | -0.573934000 |
| 1  | -3.483311000 | 0.043767000  | -1.613887000 |
| 1  | -1.198290000 | 2.490243000  | 0.907007000  |
| 1  | -2.525555000 | -1.535735000 | 0.343917000  |
| 1  | -1.066612000 | -0.803697000 | -1.760389000 |
| 1  | -0.307071000 | 1.551638000  | -1.466896000 |
| 6  | 1.159363000  | 1.255119000  | 0.207252000  |
| 8  | 1.273895000  | 1.581273000  | 1.341532000  |
| 8  | 1.985154000  | 1.582801000  | -0.771327000 |
| 6  | 3.137097000  | 2.344783000  | -0.403074000 |
| 1  | 3.677642000  | 2.515218000  | -1.320001000 |
| 1  | 2.834188000  | 3.281431000  | 0.044280000  |
| 1  | 3.744222000  | 1.791031000  | 0.299419000  |
| 6  | 0.552039000  | -2.880107000 | -0.025696000 |

|   |              |              |              |
|---|--------------|--------------|--------------|
| 7 | 0.430879000  | -4.017961000 | -0.069606000 |
| 1 | -3.557865000 | 2.354946000  | 0.192467000  |
| 1 | -4.300829000 | 0.156289000  | -0.075927000 |

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exo-TS3\_4t-OMe

|    |              |              |              |
|----|--------------|--------------|--------------|
| 46 | -1.066513000 | 0.622152000  | -0.108559000 |
| 6  | 0.869106000  | -0.634275000 | -0.787202000 |
| 6  | 1.891405000  | -1.111706000 | 0.234657000  |
| 6  | 1.904703000  | 1.130309000  | 0.416778000  |
| 6  | 0.906113000  | 0.823588000  | -0.669728000 |
| 6  | 1.742658000  | -0.072785000 | 1.346509000  |
| 1  | 2.534755000  | -0.141616000 | 2.081980000  |
| 1  | 0.786328000  | -0.107867000 | 1.850875000  |
| 6  | 3.259329000  | -0.715559000 | -0.360798000 |
| 1  | 3.374757000  | -1.046998000 | -1.385695000 |
| 6  | 3.279781000  | 0.824651000  | -0.217729000 |
| 1  | 3.420899000  | 1.335411000  | -1.161980000 |
| 1  | 1.810508000  | -2.150119000 | 0.513568000  |
| 1  | 1.812451000  | 2.113851000  | 0.849689000  |
| 1  | 0.897034000  | 1.433919000  | -1.556455000 |
| 1  | 0.910887000  | -1.042091000 | -1.783798000 |
| 6  | -0.788350000 | -1.526895000 | -0.458199000 |
| 8  | -1.429906000 | -1.891259000 | -1.387727000 |
| 8  | -0.763751000 | -2.106391000 | 0.727069000  |
| 6  | -1.607923000 | -3.248603000 | 0.892100000  |
| 1  | -1.446606000 | -3.585077000 | 1.903449000  |
| 1  | -2.642601000 | -2.974051000 | 0.741884000  |
| 1  | -1.334056000 | -4.016924000 | 0.182301000  |
| 6  | -1.450296000 | 2.542804000  | 0.260869000  |
| 7  | -1.668287000 | 3.643174000  | 0.490998000  |
| 1  | 4.051910000  | -1.175949000 | 0.215796000  |
| 1  | 4.071437000  | 1.148349000  | 0.446839000  |

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exo-TS3\_4t-N

|    |              |              |              |
|----|--------------|--------------|--------------|
| 46 | -0.745385000 | 0.782985000  | -0.047013000 |
| 6  | 0.849572000  | -0.445194000 | -0.637672000 |
| 6  | 1.391436000  | -1.387890000 | 0.425236000  |
| 6  | 2.944204000  | 0.240969000  | 0.292338000  |



|   |              |              |              |
|---|--------------|--------------|--------------|
| 6 | 1.900191000  | 0.615034000  | -0.729946000 |
| 6 | 2.101412000  | -0.426029000 | 1.381670000  |
| 1 | 2.713809000  | -0.934930000 | 2.116191000  |
| 1 | 1.433447000  | 0.256679000  | 1.891411000  |
| 6 | 2.596528000  | -2.111030000 | -0.202959000 |
| 1 | 2.349417000  | -2.565600000 | -1.153940000 |
| 6 | 3.649729000  | -0.982740000 | -0.332235000 |
| 1 | 3.956410000  | -0.804065000 | -1.356496000 |
| 1 | 0.645427000  | -2.045489000 | 0.841332000  |
| 1 | 3.607476000  | 1.041966000  | 0.582829000  |
| 1 | 2.231834000  | 0.963085000  | -1.693548000 |
| 1 | 0.548824000  | -0.903913000 | -1.565383000 |
| 6 | -1.968247000 | -0.781287000 | -0.102639000 |
| 8 | -1.814155000 | -1.947028000 | -0.292360000 |
| 8 | -3.185688000 | -0.257389000 | 0.155088000  |
| 6 | -4.282610000 | -1.162427000 | 0.190804000  |
| 1 | -5.155856000 | -0.565643000 | 0.406626000  |
| 1 | -4.392824000 | -1.661579000 | -0.762782000 |
| 1 | -4.134610000 | -1.907160000 | 0.961621000  |
| 6 | 0.953387000  | 2.103350000  | -0.149631000 |
| 7 | 0.310740000  | 2.981942000  | 0.214011000  |
| 1 | 2.948735000  | -2.899435000 | 0.451979000  |
| 1 | 4.545548000  | -1.206026000 | 0.233084000  |

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exo-TS3\_4t-N'

|    |              |              |              |
|----|--------------|--------------|--------------|
| 46 | 0.730321000  | -0.960765000 | -0.021675000 |
| 6  | -0.701133000 | 0.461498000  | -0.595524000 |
| 6  | -1.204321000 | 1.405154000  | 0.491628000  |
| 6  | -2.902774000 | -0.046058000 | 0.203288000  |
| 6  | -1.851569000 | -0.476357000 | -0.788115000 |
| 6  | -2.052172000 | 0.475258000  | 1.363292000  |
| 1  | -2.645161000 | 1.007016000  | 2.097673000  |
| 1  | -1.481284000 | -0.297161000 | 1.862611000  |
| 6  | -2.297937000 | 2.279649000  | -0.146092000 |
| 1  | -1.961057000 | 2.753699000  | -1.059576000 |
| 6  | -3.450266000 | 1.272512000  | -0.384521000 |
| 1  | -3.720392000 | 1.177351000  | -1.429984000 |
| 1  | -0.424093000 | 1.961397000  | 0.986302000  |

|   |              |              |              |
|---|--------------|--------------|--------------|
| 1 | -3.656833000 | -0.787528000 | 0.421278000  |
| 1 | -2.169267000 | -0.742754000 | -1.781895000 |
| 1 | -0.339730000 | 0.940022000  | -1.491698000 |
| 6 | 2.215148000  | 0.311866000  | 0.045989000  |
| 8 | 3.251901000  | -0.213927000 | 0.339196000  |
| 8 | 2.113347000  | 1.612631000  | -0.203949000 |
| 6 | 3.315710000  | 2.370363000  | -0.108837000 |
| 1 | 3.042830000  | 3.387872000  | -0.344021000 |
| 1 | 3.724980000  | 2.310494000  | 0.890676000  |
| 1 | 4.051644000  | 2.004814000  | -0.812246000 |
| 6 | -1.096354000 | -2.081394000 | -0.238823000 |
| 7 | -0.547704000 | -3.024172000 | 0.119599000  |
| 1 | -2.603585000 | 3.066042000  | 0.534607000  |
| 1 | -4.346894000 | 1.558550000  | 0.150457000  |

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exo-TS3\_4c-O

|    |              |              |              |
|----|--------------|--------------|--------------|
| 46 | 0.690875000  | -0.951392000 | -0.194356000 |
| 6  | -0.982044000 | 0.734686000  | -0.530541000 |
| 6  | -1.975949000 | 1.059437000  | 0.577846000  |
| 6  | -2.321954000 | -1.105885000 | 0.095690000  |
| 6  | -1.239672000 | -0.642500000 | -0.843522000 |
| 6  | -2.022175000 | -0.262234000 | 1.339296000  |
| 1  | -2.821236000 | -0.296402000 | 2.069347000  |
| 1  | -1.087494000 | -0.502198000 | 1.830842000  |
| 6  | -3.359194000 | 1.063504000  | -0.107406000 |
| 1  | -3.377778000 | 1.685233000  | -0.994055000 |
| 6  | -3.616545000 | -0.429080000 | -0.412393000 |
| 1  | -3.797801000 | -0.622543000 | -1.462270000 |
| 1  | -1.745016000 | 1.944466000  | 1.147452000  |
| 1  | -2.399181000 | -2.176572000 | 0.222732000  |
| 1  | -1.224693000 | -0.989255000 | -1.867560000 |
| 1  | -0.864585000 | 1.419546000  | -1.353828000 |
| 6  | 0.691131000  | 1.233302000  | 0.188578000  |
| 8  | 0.717403000  | 1.574661000  | 1.316153000  |
| 8  | 1.404402000  | 1.720797000  | -0.804554000 |
| 6  | 2.535676000  | 2.517407000  | -0.425812000 |
| 1  | 2.978706000  | 2.842841000  | -1.352895000 |
| 1  | 2.213934000  | 3.361975000  | 0.166573000  |

|   |              |              |             |
|---|--------------|--------------|-------------|
| 1 | 3.229646000  | 1.906743000  | 0.135020000 |
| 6 | 2.668687000  | -1.224117000 | 0.345423000 |
| 7 | 3.777362000  | -1.356215000 | 0.603695000 |
| 1 | -4.099519000 | 1.458466000  | 0.576955000 |
| 1 | -4.468994000 | -0.805555000 | 0.140438000 |

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exo-TS3\_4c-OMe

|    |              |              |              |
|----|--------------|--------------|--------------|
| 46 | -0.724837000 | -0.988880000 | 0.160061000  |
| 6  | 1.045535000  | 0.525325000  | 0.772144000  |
| 6  | 1.893772000  | 1.138209000  | -0.336922000 |
| 6  | 2.203030000  | -1.078939000 | -0.518099000 |
| 6  | 1.273163000  | -0.889121000 | 0.651882000  |
| 6  | 1.786232000  | 0.079595000  | -1.430952000 |
| 1  | 2.486432000  | 0.243050000  | -2.240812000 |
| 1  | 0.788911000  | -0.011265000 | -1.842945000 |
| 6  | 3.354094000  | 0.942768000  | 0.128120000  |
| 1  | 3.513323000  | 1.294688000  | 1.139784000  |
| 6  | 3.581024000  | -0.577642000 | -0.024628000 |
| 1  | 3.886845000  | -1.055981000 | 0.897204000  |
| 1  | 1.638746000  | 2.150626000  | -0.603937000 |
| 1  | 2.217902000  | -2.071822000 | -0.945299000 |
| 1  | 1.381632000  | -1.504026000 | 1.534259000  |
| 1  | 1.098797000  | 0.948719000  | 1.760095000  |
| 6  | -0.717916000 | 1.181828000  | 0.615588000  |
| 8  | -1.230248000 | 1.493221000  | 1.632068000  |
| 8  | -0.877751000 | 1.749085000  | -0.557344000 |
| 6  | -1.984861000 | 2.655992000  | -0.665406000 |
| 1  | -1.934263000 | 3.050058000  | -1.667319000 |
| 1  | -2.905766000 | 2.109819000  | -0.516085000 |
| 1  | -1.891560000 | 3.444627000  | 0.067308000  |
| 6  | -2.721882000 | -1.046600000 | -0.383788000 |
| 7  | -3.814612000 | -1.050193000 | -0.729130000 |
| 1  | 4.017178000  | 1.506212000  | -0.516317000 |
| 1  | 4.337468000  | -0.791822000 | -0.770240000 |

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exo-TS3\_4c-N

|    |              |              |              |
|----|--------------|--------------|--------------|
| 46 | -0.624893000 | -0.016605000 | -0.255596000 |
| 6  | 1.304964000  | -0.679554000 | -0.751731000 |

|   |              |              |              |
|---|--------------|--------------|--------------|
| 6 | 2.061415000  | -1.419651000 | 0.335360000  |
| 6 | 2.669982000  | 0.734670000  | 0.513311000  |
| 6 | 1.683469000  | 0.681660000  | -0.635386000 |
| 6 | 2.129195000  | -0.355913000 | 1.435206000  |
| 1 | 2.824507000  | -0.611769000 | 2.225288000  |
| 1 | 1.170765000  | -0.109572000 | 1.875031000  |
| 6 | 3.534424000  | -1.449229000 | -0.121977000 |
| 1 | 3.646192000  | -1.867439000 | -1.114451000 |
| 6 | 3.935002000  | 0.042572000  | -0.050023000 |
| 1 | 4.231769000  | 0.449089000  | -1.009207000 |
| 1 | 1.655925000  | -2.382931000 | 0.609922000  |
| 1 | 2.831838000  | 1.715459000  | 0.929679000  |
| 1 | 1.854432000  | 1.274856000  | -1.514070000 |
| 1 | 1.196372000  | -1.125090000 | -1.728301000 |
| 6 | -2.565964000 | -0.115516000 | 0.063902000  |
| 8 | -2.401864000 | -1.309211000 | -0.164876000 |
| 8 | -3.709433000 | 0.418222000  | 0.352428000  |
| 6 | -4.848516000 | -0.449015000 | 0.404103000  |
| 1 | -5.684546000 | 0.183562000  | 0.655267000  |
| 1 | -5.001249000 | -0.919568000 | -0.557074000 |
| 1 | -4.703717000 | -1.208120000 | 1.160027000  |
| 6 | 0.356652000  | 1.888970000  | -0.088693000 |
| 7 | 0.451089000  | 3.009741000  | 0.130276000  |
| 1 | 4.131611000  | -2.049527000 | 0.555315000  |
| 1 | 4.760195000  | 0.200618000  | 0.633196000  |

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exo-TS3\_4c-N'

|    |              |              |              |
|----|--------------|--------------|--------------|
| 46 | -0.624893000 | -0.016604000 | -0.255595000 |
| 6  | 1.304963000  | -0.679554000 | -0.751731000 |
| 6  | 2.061415000  | -1.419652000 | 0.335359000  |
| 6  | 2.669983000  | 0.734669000  | 0.513310000  |
| 6  | 1.683470000  | 0.681660000  | -0.635386000 |
| 6  | 2.129196000  | -0.355913000 | 1.435206000  |
| 1  | 2.824507000  | -0.611770000 | 2.225288000  |
| 1  | 1.170766000  | -0.109572000 | 1.875031000  |
| 6  | 3.534423000  | -1.449231000 | -0.121978000 |
| 1  | 3.646190000  | -1.867440000 | -1.114452000 |
| 6  | 3.935002000  | 0.042570000  | -0.050024000 |

|   |              |              |              |
|---|--------------|--------------|--------------|
| 1 | 4.231769000  | 0.449088000  | -1.009208000 |
| 1 | 1.655923000  | -2.382931000 | 0.609921000  |
| 1 | 2.831839000  | 1.715458000  | 0.929679000  |
| 1 | 1.854432000  | 1.274857000  | -1.514070000 |
| 1 | 1.196371000  | -1.125090000 | -1.728301000 |
| 6 | -2.565964000 | -0.115515000 | 0.063902000  |
| 8 | -2.401863000 | -1.309210000 | -0.164875000 |
| 8 | -3.709434000 | 0.418221000  | 0.352427000  |
| 6 | -4.848516000 | -0.449016000 | 0.404102000  |
| 1 | -5.684547000 | 0.183560000  | 0.655263000  |
| 1 | -5.001248000 | -0.919571000 | -0.557076000 |
| 1 | -4.703718000 | -1.208121000 | 1.160027000  |
| 6 | 0.356652000  | 1.888970000  | -0.088693000 |
| 7 | 0.451091000  | 3.009742000  | 0.130277000  |
| 1 | 4.131610000  | -2.049529000 | 0.555314000  |
| 1 | 4.760196000  | 0.200616000  | 0.633196000  |

44

exo-TS3\_4t2N-O

|    |              |              |              |
|----|--------------|--------------|--------------|
| 46 | -0.033731000 | -0.419561000 | -0.528741000 |
| 6  | -2.146660000 | 0.675495000  | -0.388757000 |
| 6  | -2.909621000 | 0.783877000  | 0.925231000  |
| 6  | -2.729405000 | -1.423142000 | 0.542734000  |
| 6  | -2.054928000 | -0.751829000 | -0.633448000 |
| 6  | -2.413428000 | -0.449095000 | 1.678407000  |
| 1  | -2.991793000 | -0.644622000 | 2.573359000  |
| 1  | -1.364954000 | -0.398555000 | 1.939031000  |
| 6  | -4.353059000 | 0.362303000  | 0.579116000  |
| 1  | -4.742447000 | 0.892496000  | -0.282049000 |
| 6  | -4.236607000 | -1.163084000 | 0.347980000  |
| 1  | -4.582714000 | -1.469076000 | -0.631516000 |
| 1  | -2.822181000 | 1.734824000  | 1.426038000  |
| 1  | -2.460879000 | -2.458078000 | 0.684243000  |
| 1  | -2.255625000 | -1.131040000 | -1.620620000 |
| 1  | -2.446467000 | 1.300045000  | -1.212023000 |
| 6  | -0.580092000 | 1.683846000  | -0.085243000 |
| 8  | -0.323324000 | 2.052477000  | 1.015069000  |
| 8  | -0.404361000 | 2.437229000  | -1.172611000 |
| 6  | 0.134886000  | 3.736847000  | -0.961178000 |

|   |              |              |              |
|---|--------------|--------------|--------------|
| 1 | 0.191074000  | 4.194441000  | -1.936494000 |
| 1 | -0.510239000 | 4.310642000  | -0.309151000 |
| 1 | 1.118568000  | 3.676350000  | -0.514858000 |
| 6 | 0.189449000  | -2.391660000 | -0.838939000 |
| 7 | 0.315187000  | -3.517689000 | -1.004442000 |
| 1 | -5.004753000 | 0.587599000  | 1.414506000  |
| 1 | -4.810375000 | -1.716538000 | 1.081986000  |
| 6 | 4.290597000  | 0.757352000  | 0.799556000  |
| 6 | 2.750519000  | 0.825529000  | 0.974222000  |
| 6 | 3.091937000  | -1.311501000 | 0.380890000  |
| 6 | 4.526091000  | -0.716197000 | 0.386049000  |
| 1 | 4.651638000  | 1.463906000  | 0.062512000  |
| 1 | 4.781882000  | 0.986070000  | 1.737956000  |
| 1 | 5.012915000  | -0.811753000 | -0.576218000 |
| 1 | 5.138047000  | -1.236549000 | 1.112824000  |
| 6 | 2.484821000  | -0.559739000 | 1.566563000  |
| 1 | 1.435043000  | -0.774017000 | 1.717663000  |
| 1 | 3.023107000  | -0.730234000 | 2.491579000  |
| 6 | 2.200682000  | 0.652691000  | -0.423448000 |
| 1 | 2.014503000  | 1.458385000  | -1.107588000 |
| 6 | 2.416679000  | -0.627360000 | -0.778785000 |
| 1 | 2.398448000  | -1.024283000 | -1.775006000 |
| 1 | 2.386386000  | 1.678269000  | 1.525829000  |
| 1 | 3.036458000  | -2.388279000 | 0.385809000  |

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exo-TS3\_4t2N-OMe

|    |              |              |              |
|----|--------------|--------------|--------------|
| 46 | -0.030872000 | -0.488176000 | -0.504192000 |
| 6  | -2.199998000 | 0.514095000  | -0.650663000 |
| 6  | -2.993982000 | 0.898009000  | 0.590560000  |
| 6  | -2.700568000 | -1.323657000 | 0.759396000  |
| 6  | -2.034525000 | -0.924912000 | -0.539371000 |
| 6  | -2.457289000 | -0.088062000 | 1.627154000  |
| 1  | -3.045814000 | -0.091115000 | 2.536813000  |
| 1  | -1.417489000 | 0.073860000  | 1.878487000  |
| 6  | -4.408146000 | 0.330063000  | 0.342301000  |
| 1  | -4.800600000 | 0.613581000  | -0.626981000 |
| 6  | -4.213857000 | -1.197159000 | 0.493391000  |
| 1  | -4.523731000 | -1.750915000 | -0.384018000 |

|                |              |              |              |
|----------------|--------------|--------------|--------------|
| 1              | -2.974068000 | 1.945556000  | 0.845665000  |
| 1              | -2.385920000 | -2.277449000 | 1.152403000  |
| 1              | -2.204719000 | -1.539878000 | -1.406137000 |
| 1              | -2.522886000 | 0.897107000  | -1.603276000 |
| 6              | -0.674345000 | 1.623398000  | -0.720339000 |
| 8              | -0.448445000 | 2.143243000  | -1.766993000 |
| 8              | -0.480131000 | 2.217392000  | 0.452428000  |
| 6              | 0.007985000  | 3.554227000  | 0.412182000  |
| 1              | 0.064786000  | 3.877436000  | 1.439829000  |
| 1              | 0.985182000  | 3.590266000  | -0.049455000 |
| 1              | -0.669253000 | 4.184349000  | -0.148789000 |
| 6              | 0.286130000  | -2.461457000 | -0.313284000 |
| 7              | 0.463201000  | -3.585352000 | -0.184285000 |
| 1              | -5.089646000 | 0.718376000  | 1.089370000  |
| 1              | -4.776124000 | -1.582707000 | 1.335723000  |
| 6              | 4.332628000  | 0.920575000  | 0.570618000  |
| 6              | 2.802221000  | 0.948607000  | 0.825559000  |
| 6              | 3.183381000  | -1.204674000 | 0.331871000  |
| 6              | 4.594672000  | -0.565826000 | 0.226192000  |
| 1              | 4.627868000  | 1.595514000  | -0.222986000 |
| 1              | 4.865290000  | 1.217020000  | 1.466643000  |
| 1              | 5.033014000  | -0.699785000 | -0.754511000 |
| 1              | 5.261295000  | -1.025048000 | 0.945986000  |
| 6              | 2.614416000  | -0.407722000 | 1.506827000  |
| 1              | 1.582724000  | -0.649980000 | 1.723932000  |
| 1              | 3.206756000  | -0.510081000 | 2.408638000  |
| 6              | 2.185882000  | 0.683992000  | -0.529609000 |
| 1              | 1.931541000  | 1.444895000  | -1.242065000 |
| 6              | 2.423080000  | -0.607178000 | -0.823487000 |
| 1              | 2.361294000  | -1.059156000 | -1.795015000 |
| 1              | 2.448207000  | 1.822744000  | 1.351884000  |
| 1              | 3.162494000  | -2.280004000 | 0.401423000  |
| 44             |              |              |              |
| exo-TS3_4t2N-N |              |              |              |
| 46             | -0.007236000 | 0.025104000  | -0.465398000 |
| 6              | -2.066434000 | 0.432980000  | -0.407609000 |
| 6              | -2.727891000 | 0.531157000  | 0.957096000  |
| 6              | -3.004844000 | -1.603818000 | 0.307568000  |

|   |              |              |              |
|---|--------------|--------------|--------------|
| 6 | -2.241636000 | -0.938059000 | -0.817888000 |
| 6 | -2.466127000 | -0.863376000 | 1.530217000  |
| 1 | -3.045192000 | -1.066829000 | 2.422742000  |
| 1 | -1.422295000 | -1.065541000 | 1.732303000  |
| 6 | -4.243983000 | 0.452462000  | 0.697827000  |
| 1 | -4.575519000 | 1.187824000  | -0.024844000 |
| 6 | -4.425491000 | -1.001048000 | 0.199134000  |
| 1 | -4.820898000 | -1.058430000 | -0.808140000 |
| 1 | -2.407292000 | 1.368766000  | 1.556882000  |
| 1 | -2.966401000 | -2.681289000 | 0.308015000  |
| 1 | -2.509519000 | -1.158571000 | -1.835348000 |
| 1 | -2.261798000 | 1.205194000  | -1.132318000 |
| 6 | 0.200446000  | 1.952551000  | 0.119586000  |
| 8 | 0.247257000  | 2.335438000  | 1.250425000  |
| 8 | 0.278451000  | 2.819863000  | -0.909251000 |
| 6 | 0.413230000  | 4.193954000  | -0.573202000 |
| 1 | 0.453232000  | 4.726621000  | -1.511791000 |
| 1 | -0.430977000 | 4.531502000  | 0.013732000  |
| 1 | 1.318933000  | 4.365815000  | -0.006038000 |
| 6 | -0.684492000 | -1.963251000 | -0.942351000 |
| 7 | -0.466354000 | -3.069707000 | -1.147265000 |
| 1 | -4.797422000 | 0.623698000  | 1.614160000  |
| 1 | -5.097722000 | -1.561063000 | 0.837293000  |
| 6 | 4.446697000  | -0.240172000 | 0.563749000  |
| 6 | 3.033495000  | 0.345117000  | 0.826520000  |
| 6 | 2.606643000  | -1.804073000 | 0.343082000  |
| 6 | 4.152045000  | -1.724211000 | 0.233387000  |
| 1 | 4.961938000  | 0.275252000  | -0.237151000 |
| 1 | 5.056281000  | -0.148052000 | 1.454651000  |
| 1 | 4.508138000  | -2.016866000 | -0.746291000 |
| 1 | 4.610355000  | -2.387048000 | 0.957641000  |
| 6 | 2.370186000  | -0.848728000 | 1.514382000  |
| 1 | 1.325678000  | -0.680927000 | 1.742533000  |
| 1 | 2.889916000  | -1.153599000 | 2.415164000  |
| 6 | 2.365929000  | 0.317096000  | -0.527384000 |
| 1 | 2.427222000  | 1.117684000  | -1.239425000 |
| 6 | 2.108804000  | -0.978746000 | -0.818794000 |
| 1 | 1.938882000  | -1.380430000 | -1.798945000 |



|                 |              |              |              |
|-----------------|--------------|--------------|--------------|
| 1               | 3.013737000  | 1.289877000  | 1.346634000  |
| 1               | 2.202938000  | -2.801823000 | 0.416403000  |
| 44              |              |              |              |
| exo-TS3_4t2N-N' |              |              |              |
| 46              | -0.004730000 | -0.060401000 | -0.552184000 |
| 6               | -2.072821000 | 0.302441000  | -0.588820000 |
| 6               | -2.769038000 | 0.699169000  | 0.702605000  |
| 6               | -2.990567000 | -1.533307000 | 0.566194000  |
| 6               | -2.214292000 | -1.130621000 | -0.669958000 |
| 6               | -2.493516000 | -0.515432000 | 1.591144000  |
| 1               | -3.088377000 | -0.519384000 | 2.496470000  |
| 1               | -1.450365000 | -0.639975000 | 1.851352000  |
| 6               | -4.276862000 | 0.526506000  | 0.440396000  |
| 1               | -4.603437000 | 1.063887000  | -0.441213000 |
| 6               | -4.419437000 | -1.007126000 | 0.294475000  |
| 1               | -4.790790000 | -1.308621000 | -0.677765000 |
| 1               | -2.482654000 | 1.662098000  | 1.095820000  |
| 1               | -2.931038000 | -2.579491000 | 0.819589000  |
| 1               | -2.454881000 | -1.589043000 | -1.612072000 |
| 1               | -2.268096000 | 0.880032000  | -1.476530000 |
| 6               | 0.170553000  | 1.957676000  | -0.581193000 |
| 8               | 0.270229000  | 2.641898000  | -1.555198000 |
| 8               | 0.164637000  | 2.504169000  | 0.651239000  |
| 6               | 0.282214000  | 3.918551000  | 0.717933000  |
| 1               | 0.259316000  | 4.169688000  | 1.768106000  |
| 1               | 1.211725000  | 4.250037000  | 0.273423000  |
| 1               | -0.537696000 | 4.398102000  | 0.199224000  |
| 6               | -0.636561000 | -2.119284000 | -0.513379000 |
| 7               | -0.393613000 | -3.235448000 | -0.418776000 |
| 1               | -4.855561000 | 0.894988000  | 1.279916000  |
| 1               | -5.095108000 | -1.417416000 | 1.034684000  |
| 6               | 4.475171000  | -0.075275000 | 0.448266000  |
| 6               | 3.056930000  | 0.531068000  | 0.620757000  |
| 6               | 2.655326000  | -1.674720000 | 0.553783000  |
| 6               | 4.197594000  | -1.598059000 | 0.405240000  |
| 1               | 4.970014000  | 0.288517000  | -0.443376000 |
| 1               | 5.096385000  | 0.188584000  | 1.295857000  |
| 1               | 4.543776000  | -2.063725000 | -0.508724000 |

|   |             |              |              |
|---|-------------|--------------|--------------|
| 1 | 4.676217000 | -2.108734000 | 1.232318000  |
| 6 | 2.421017000 | -0.520835000 | 1.530554000  |
| 1 | 1.375954000 | -0.329314000 | 1.737944000  |
| 1 | 2.956805000 | -0.646609000 | 2.464252000  |
| 6 | 2.370103000 | 0.244353000  | -0.692796000 |
| 1 | 2.405687000 | 0.901159000  | -1.540511000 |
| 6 | 2.128331000 | -1.085702000 | -0.732080000 |
| 1 | 1.948569000 | -1.664788000 | -1.617347000 |
| 1 | 3.036032000 | 1.556948000  | 0.954668000  |
| 1 | 2.266581000 | -2.645328000 | 0.818761000  |

44

exo-TS3\_4c2N-O

|    |              |              |              |
|----|--------------|--------------|--------------|
| 46 | -0.071518000 | -0.467556000 | -0.335736000 |
| 6  | 2.117450000  | 0.442697000  | -0.491664000 |
| 6  | 2.808208000  | 1.267854000  | 0.590308000  |
| 6  | 0.976099000  | 2.446036000  | 0.057599000  |
| 6  | 0.927493000  | 1.220742000  | -0.836126000 |
| 6  | 1.615270000  | 1.876077000  | 1.324307000  |
| 1  | 1.911488000  | 2.643041000  | 2.030072000  |
| 1  | 1.011671000  | 1.137779000  | 1.834411000  |
| 6  | 3.379033000  | 2.498778000  | -0.138619000 |
| 1  | 3.958296000  | 2.227558000  | -1.013075000 |
| 6  | 2.119413000  | 3.327546000  | -0.481318000 |
| 1  | 2.020462000  | 3.524754000  | -1.541995000 |
| 1  | 3.522026000  | 0.722827000  | 1.187261000  |
| 1  | 0.038031000  | 2.968434000  | 0.174615000  |
| 1  | 0.746233000  | 1.396586000  | -1.886965000 |
| 1  | 2.716759000  | 0.080675000  | -1.309262000 |
| 6  | 1.912052000  | -1.221281000 | 0.309920000  |
| 8  | 1.981467000  | -1.319993000 | 1.488133000  |
| 8  | 2.325178000  | -2.113696000 | -0.567318000 |
| 6  | 2.648087000  | -3.406880000 | -0.047007000 |
| 1  | 3.013951000  | -3.971971000 | -0.889415000 |
| 1  | 3.407768000  | -3.320745000 | 0.717373000  |
| 1  | 1.755161000  | -3.861847000 | 0.358409000  |
| 6  | -0.671376000 | -2.425932000 | 0.037275000  |
| 7  | -0.977138000 | -3.517267000 | 0.205694000  |
| 1  | 4.039030000  | 3.041901000  | 0.526876000  |

|   |              |              |              |
|---|--------------|--------------|--------------|
| 1 | 2.129423000  | 4.284945000  | 0.027113000  |
| 6 | -4.530360000 | 0.169830000  | -0.103546000 |
| 6 | -3.260100000 | -0.644901000 | 0.256670000  |
| 6 | -2.585798000 | 1.480811000  | 0.502396000  |
| 6 | -4.066958000 | 1.637238000  | 0.069008000  |
| 1 | -4.886778000 | -0.044204000 | -1.103297000 |
| 1 | -5.330126000 | -0.074222000 | 0.584749000  |
| 1 | -4.170673000 | 2.222153000  | -0.836627000 |
| 1 | -4.628815000 | 2.140222000  | 0.846935000  |
| 6 | -2.686050000 | 0.227893000  | 1.372995000  |
| 1 | -1.735641000 | -0.128349000 | 1.747374000  |
| 1 | -3.374131000 | 0.351088000  | 2.200744000  |
| 6 | -2.309896000 | -0.349530000 | -0.876230000 |
| 1 | -2.298967000 | -0.910840000 | -1.791194000 |
| 6 | -1.899820000 | 0.940448000  | -0.731637000 |
| 1 | -1.554205000 | 1.567734000  | -1.529170000 |
| 1 | -3.419658000 | -1.688525000 | 0.471055000  |
| 1 | -2.151143000 | 2.364403000  | 0.945483000  |

44

exo-TS3\_4c2N-OMe

|    |              |              |              |
|----|--------------|--------------|--------------|
| 46 | -0.073443000 | -0.441327000 | -0.466707000 |
| 6  | 2.120431000  | 0.465808000  | -0.648414000 |
| 6  | 2.845936000  | 1.085753000  | 0.539635000  |
| 6  | 1.013060000  | 2.348915000  | 0.261242000  |
| 6  | 0.922158000  | 1.285788000  | -0.819721000 |
| 6  | 1.682904000  | 1.575859000  | 1.399146000  |
| 1  | 2.007827000  | 2.216427000  | 2.210457000  |
| 1  | 1.081101000  | 0.771810000  | 1.802366000  |
| 6  | 3.411526000  | 2.418151000  | 0.009169000  |
| 1  | 3.965919000  | 2.290687000  | -0.912675000 |
| 6  | 2.151713000  | 3.298522000  | -0.159281000 |
| 1  | 2.026127000  | 3.665588000  | -1.170655000 |
| 1  | 3.574201000  | 0.448071000  | 1.014561000  |
| 1  | 0.086679000  | 2.853137000  | 0.492460000  |
| 1  | 0.706415000  | 1.629901000  | -1.820650000 |
| 1  | 2.695838000  | 0.273937000  | -1.537419000 |
| 6  | 1.942265000  | -1.357794000 | -0.338124000 |
| 8  | 2.241038000  | -2.065075000 | -1.239519000 |

|   |              |              |              |
|---|--------------|--------------|--------------|
| 8 | 2.096010000  | -1.631546000 | 0.941916000  |
| 6 | 2.449164000  | -2.983064000 | 1.254789000  |
| 1 | 2.578054000  | -3.006032000 | 2.325243000  |
| 1 | 1.646859000  | -3.640973000 | 0.951410000  |
| 1 | 3.366472000  | -3.252983000 | 0.750353000  |
| 6 | -0.705970000 | -2.383652000 | -0.063113000 |
| 7 | -1.039554000 | -3.441532000 | 0.223917000  |
| 1 | 4.093135000  | 2.840615000  | 0.737393000  |
| 1 | 2.185572000  | 4.160703000  | 0.497033000  |
| 6 | -4.529641000 | 0.230249000  | -0.006938000 |
| 6 | -3.259482000 | -0.621121000 | 0.256431000  |
| 6 | -2.550604000 | 1.475215000  | 0.625024000  |
| 6 | -4.042416000 | 1.677052000  | 0.250566000  |
| 1 | -4.919742000 | 0.089141000  | -1.007050000 |
| 1 | -5.310577000 | -0.052228000 | 0.688233000  |
| 1 | -4.166215000 | 2.323925000  | -0.609211000 |
| 1 | -4.573347000 | 2.131518000  | 1.078491000  |
| 6 | -2.639394000 | 0.166765000  | 1.410401000  |
| 1 | -1.682318000 | -0.225855000 | 1.726028000  |
| 1 | -3.298742000 | 0.239396000  | 2.267027000  |
| 6 | -2.341787000 | -0.258112000 | -0.882981000 |
| 1 | -2.363781000 | -0.756439000 | -1.833806000 |
| 6 | -1.910138000 | 1.013495000  | -0.664206000 |
| 1 | -1.581389000 | 1.690020000  | -1.427864000 |
| 1 | -3.424784000 | -1.674995000 | 0.405128000  |
| 1 | -2.092777000 | 2.322382000  | 1.113331000  |

44

exo-TS3\_4c2N-N

|    |              |              |              |
|----|--------------|--------------|--------------|
| 46 | 0.024037000  | 0.417982000  | -0.295348000 |
| 6  | -2.401272000 | 0.676769000  | -0.584352000 |
| 6  | -3.379302000 | 0.436529000  | 0.545980000  |
| 6  | -2.384791000 | -1.540292000 | 0.174458000  |
| 6  | -1.754512000 | -0.576839000 | -0.821381000 |
| 6  | -2.644433000 | -0.618692000 | 1.369100000  |
| 1  | -3.278789000 | -1.071329000 | 2.121510000  |
| 1  | -1.746730000 | -0.242490000 | 1.843276000  |
| 6  | -4.494825000 | -0.415303000 | -0.103021000 |
| 1  | -4.862990000 | 0.022530000  | -1.023046000 |

|                 |              |              |              |
|-----------------|--------------|--------------|--------------|
| 6               | -3.824669000 | -1.792722000 | -0.312141000 |
| 1               | -3.855886000 | -2.122844000 | -1.343215000 |
| 1               | -3.718573000 | 1.326585000  | 1.050221000  |
| 1               | -1.821492000 | -2.439997000 | 0.371093000  |
| 1               | -1.656570000 | -0.895592000 | -1.846664000 |
| 1               | -2.697373000 | 1.291241000  | -1.414292000 |
| 6               | 1.493733000  | 1.717193000  | 0.321848000  |
| 8               | 1.909944000  | 1.797859000  | 1.437353000  |
| 8               | 1.906362000  | 2.549841000  | -0.646536000 |
| 6               | 2.785990000  | 3.595119000  | -0.253267000 |
| 1               | 2.988044000  | 4.165002000  | -1.147924000 |
| 1               | 2.318200000  | 4.222672000  | 0.493396000  |
| 1               | 3.705756000  | 3.193713000  | 0.152575000  |
| 6               | -1.329005000 | 2.049689000  | 0.087440000  |
| 7               | -1.605260000 | 3.106034000  | 0.434086000  |
| 1               | -5.334435000 | -0.480134000 | 0.577912000  |
| 1               | -4.304032000 | -2.556887000 | 0.289889000  |
| 6               | 3.557669000  | -2.357050000 | -0.065195000 |
| 6               | 2.830058000  | -1.084018000 | 0.438959000  |
| 6               | 1.163891000  | -2.570036000 | 0.229283000  |
| 6               | 2.408628000  | -3.384962000 | -0.204411000 |
| 1               | 4.086579000  | -2.188319000 | -0.994986000 |
| 1               | 4.286817000  | -2.678022000 | 0.668711000  |
| 1               | 2.312520000  | -3.776845000 | -1.209519000 |
| 1               | 2.551324000  | -4.228181000 | 0.460923000  |
| 6               | 1.768234000  | -1.711649000 | 1.341040000  |
| 1               | 1.089237000  | -0.983356000 | 1.763199000  |
| 1               | 2.199172000  | -2.305417000 | 2.138323000  |
| 6               | 2.001809000  | -0.648260000 | -0.745109000 |
| 1               | 2.397520000  | -0.049427000 | -1.543329000 |
| 6               | 0.981578000  | -1.552044000 | -0.875065000 |
| 1               | 0.503895000  | -1.791868000 | -1.805162000 |
| 1               | 3.464104000  | -0.331751000 | 0.877899000  |
| 1               | 0.301713000  | -3.170866000 | 0.475052000  |
| 44              |              |              |              |
| exo-TS3_4c2N-N' |              |              |              |
| 46              | 0.000538000  | 0.398604000  | -0.468087000 |
| 6               | -2.445612000 | 0.551256000  | -0.611607000 |

|   |              |              |              |
|---|--------------|--------------|--------------|
| 6 | -3.355679000 | 0.412212000  | 0.590510000  |
| 6 | -2.315860000 | -1.565448000 | 0.386611000  |
| 6 | -1.771178000 | -0.703630000 | -0.743258000 |
| 6 | -2.543568000 | -0.522428000 | 1.483723000  |
| 1 | -3.121716000 | -0.904292000 | 2.316419000  |
| 1 | -1.635112000 | -0.069956000 | 1.860656000  |
| 6 | -4.474027000 | -0.537824000 | 0.102973000  |
| 1 | -4.903874000 | -0.216828000 | -0.838199000 |
| 6 | -3.769691000 | -1.910960000 | 0.011499000  |
| 1 | -3.843053000 | -2.355909000 | -0.973212000 |
| 1 | -3.697813000 | 1.343816000  | 1.010615000  |
| 1 | -1.713515000 | -2.421726000 | 0.649984000  |
| 1 | -1.716685000 | -1.133800000 | -1.730512000 |
| 1 | -2.804190000 | 1.061293000  | -1.486587000 |
| 6 | 1.460084000  | 1.841704000  | -0.294127000 |
| 8 | 1.992125000  | 2.411284000  | -1.197999000 |
| 8 | 1.720128000  | 2.154173000  | 0.985153000  |
| 6 | 2.588605000  | 3.257595000  | 1.205307000  |
| 1 | 2.668100000  | 3.363706000  | 2.276968000  |
| 1 | 3.563374000  | 3.074534000  | 0.771292000  |
| 1 | 2.175357000  | 4.157178000  | 0.769285000  |
| 6 | -1.385463000 | 2.015297000  | -0.144018000 |
| 7 | -1.677600000 | 3.084856000  | 0.144037000  |
| 1 | -5.274520000 | -0.548538000 | 0.832330000  |
| 1 | -4.191126000 | -2.615482000 | 0.720191000  |
| 6 | 3.627656000  | -2.222675000 | -0.026782000 |
| 6 | 2.873313000  | -0.916173000 | 0.331198000  |
| 6 | 1.257814000  | -2.467986000 | 0.409479000  |
| 6 | 2.512812000  | -3.295221000 | 0.031670000  |
| 1 | 4.108145000  | -2.166246000 | -0.995346000 |
| 1 | 4.399757000  | -2.416410000 | 0.707864000  |
| 1 | 2.387839000  | -3.824675000 | -0.904701000 |
| 1 | 2.716220000  | -4.033558000 | 0.798166000  |
| 6 | 1.877802000  | -1.445868000 | 1.362881000  |
| 1 | 1.186405000  | -0.690837000 | 1.712946000  |
| 1 | 2.365047000  | -1.910253000 | 2.212081000  |
| 6 | 1.978790000  | -0.675806000 | -0.860053000 |
| 1 | 2.314317000  | -0.170642000 | -1.745432000 |

|   |             |              |              |
|---|-------------|--------------|--------------|
| 6 | 0.989023000 | -1.619030000 | -0.813819000 |
| 1 | 0.474320000 | -1.997254000 | -1.675614000 |
| 1 | 3.502766000 | -0.091796000 | 0.625804000  |
| 1 | 0.431470000 | -3.055863000 | 0.778391000  |

42

exo-TS3\_4tT-O

|    |              |              |              |
|----|--------------|--------------|--------------|
| 46 | -0.285348000 | -0.789629000 | -0.396726000 |
| 6  | -1.845358000 | 1.014407000  | -0.522552000 |
| 6  | -2.416582000 | 1.609268000  | 0.755214000  |
| 6  | -3.081482000 | -0.538435000 | 0.767287000  |
| 6  | -2.288632000 | -0.369391000 | -0.509659000 |
| 6  | -2.356690000 | 0.420494000  | 1.713413000  |
| 1  | -2.906971000 | 0.602359000  | 2.628699000  |
| 1  | -1.348078000 | 0.117147000  | 1.961115000  |
| 6  | -3.935260000 | 1.705477000  | 0.497355000  |
| 1  | -4.164750000 | 2.200682000  | -0.438766000 |
| 6  | -4.398386000 | 0.229189000  | 0.529058000  |
| 1  | -4.893247000 | -0.077459000 | -0.384149000 |
| 1  | -1.951436000 | 2.526794000  | 1.078777000  |
| 1  | -3.202762000 | -1.560409000 | 1.090023000  |
| 1  | -2.663739000 | -0.818214000 | -1.413190000 |
| 1  | -1.962865000 | 1.561736000  | -1.441796000 |
| 6  | 0.015300000  | 1.394592000  | -0.464153000 |
| 8  | 0.492592000  | 1.869407000  | 0.513633000  |
| 8  | 0.362169000  | 1.722131000  | -1.704523000 |
| 6  | 1.352431000  | 2.736865000  | -1.844031000 |
| 1  | 1.493587000  | 2.864059000  | -2.905899000 |
| 1  | 1.004162000  | 3.658317000  | -1.395519000 |
| 1  | 2.274205000  | 2.434169000  | -1.370916000 |
| 6  | -0.672277000 | -2.759344000 | -0.362173000 |
| 7  | -0.870421000 | -3.886990000 | -0.334192000 |
| 1  | -4.400435000 | 2.282824000  | 1.286891000  |
| 1  | -5.087232000 | 0.050656000  | 1.346100000  |
| 6  | 3.568632000  | 0.308312000  | 1.091686000  |
| 6  | 3.757023000  | 0.375393000  | -0.285459000 |
| 6  | 2.752576000  | -0.684840000 | 1.593691000  |
| 1  | 4.411603000  | 1.128651000  | -0.689383000 |
| 1  | 2.608647000  | -0.766912000 | 2.656400000  |

|   |             |              |              |
|---|-------------|--------------|--------------|
| 6 | 3.128101000 | -0.504746000 | -1.133280000 |
| 6 | 2.126641000 | -1.589863000 | 0.751129000  |
| 1 | 3.293642000 | -0.442826000 | -2.193836000 |
| 1 | 1.544548000 | -2.393951000 | 1.160423000  |
| 6 | 2.300377000 | -1.497768000 | -0.621978000 |
| 1 | 1.881465000 | -2.245617000 | -1.269797000 |
| 6 | 4.214298000 | 1.309213000  | 1.997299000  |
| 1 | 3.609422000 | 2.209397000  | 2.055563000  |
| 1 | 4.321591000 | 0.920601000  | 3.002161000  |
| 1 | 5.195246000 | 1.594611000  | 1.635894000  |

42

exo-TS3\_4tT-OMe

|    |              |              |              |
|----|--------------|--------------|--------------|
| 46 | 0.335712000  | 0.819436000  | -0.330628000 |
| 6  | 2.019998000  | -0.873863000 | -0.735830000 |
| 6  | 2.656960000  | -1.645899000 | 0.411187000  |
| 6  | 3.127859000  | 0.509505000  | 0.844173000  |
| 6  | 2.344863000  | 0.525410000  | -0.449661000 |
| 6  | 2.496399000  | -0.673333000 | 1.579631000  |
| 1  | 3.065096000  | -0.977872000 | 2.450042000  |
| 1  | 1.466787000  | -0.509266000 | 1.868504000  |
| 6  | 4.175846000  | -1.554719000 | 0.154605000  |
| 1  | 4.440192000  | -1.836604000 | -0.857623000 |
| 6  | 4.505804000  | -0.077787000 | 0.476697000  |
| 1  | 4.965962000  | 0.442798000  | -0.353914000 |
| 1  | 2.287964000  | -2.649984000 | 0.548730000  |
| 1  | 3.160937000  | 1.456149000  | 1.360006000  |
| 1  | 2.705930000  | 1.151157000  | -1.248367000 |
| 1  | 2.205984000  | -1.217651000 | -1.740106000 |
| 6  | 0.204788000  | -1.334785000 | -0.851484000 |
| 8  | -0.265580000 | -1.494944000 | -1.930797000 |
| 8  | -0.178057000 | -1.969342000 | 0.242538000  |
| 6  | -1.212197000 | -2.940582000 | 0.086098000  |
| 1  | -1.393695000 | -3.333966000 | 1.073707000  |
| 1  | -2.102368000 | -2.477969000 | -0.311625000 |
| 1  | -0.881816000 | -3.725276000 | -0.581819000 |
| 6  | 0.578652000  | 2.749691000  | 0.135196000  |
| 7  | 0.698890000  | 3.851530000  | 0.423364000  |
| 1  | 4.697344000  | -2.230398000 | 0.821408000  |



|   |              |              |              |
|---|--------------|--------------|--------------|
| 1 | 5.180747000  | -0.001134000 | 1.320784000  |
| 6 | -3.963237000 | -0.360700000 | 0.685215000  |
| 6 | -3.887772000 | -0.397187000 | -0.704546000 |
| 6 | -3.197808000 | 0.569244000  | 1.360523000  |
| 1 | -4.477529000 | -1.116450000 | -1.246737000 |
| 1 | -3.244860000 | 0.617386000  | 2.434095000  |
| 6 | -3.077199000 | 0.472794000  | -1.393736000 |
| 6 | -2.391483000 | 1.464477000  | 0.674342000  |
| 1 | -3.032444000 | 0.429531000  | -2.466439000 |
| 1 | -1.844141000 | 2.217801000  | 1.209398000  |
| 6 | -2.327321000 | 1.420267000  | -0.707796000 |
| 1 | -1.769432000 | 2.165342000  | -1.246291000 |
| 6 | -4.868696000 | -1.302269000 | 1.418778000  |
| 1 | -4.676047000 | -2.333335000 | 1.140671000  |
| 1 | -4.744287000 | -1.214261000 | 2.490351000  |
| 1 | -5.908955000 | -1.098069000 | 1.186295000  |

42

exo-TS3\_4tT-N

|    |              |              |              |
|----|--------------|--------------|--------------|
| 46 | -0.108781000 | -0.329149000 | -0.368915000 |
| 6  | -1.921330000 | 0.704872000  | -0.454311000 |
| 6  | -2.500874000 | 1.217562000  | 0.855149000  |
| 6  | -3.488537000 | -0.774745000 | 0.517166000  |
| 6  | -2.568812000 | -0.580082000 | -0.669063000 |
| 6  | -2.710298000 | -0.082118000 | 1.635206000  |
| 1  | -3.308419000 | 0.053723000  | 2.528090000  |
| 1  | -1.789112000 | -0.585952000 | 1.898508000  |
| 6  | -3.959238000 | 1.610291000  | 0.554907000  |
| 1  | -4.035707000 | 2.293789000  | -0.281632000 |
| 6  | -4.627280000 | 0.242850000  | 0.273655000  |
| 1  | -5.038954000 | 0.168705000  | -0.726009000 |
| 1  | -1.914536000 | 1.982923000  | 1.339841000  |
| 1  | -3.815222000 | -1.789795000 | 0.679647000  |
| 1  | -2.928618000 | -0.834428000 | -1.650760000 |
| 1  | -1.876238000 | 1.384415000  | -1.288812000 |
| 6  | 0.808088000  | 1.448170000  | -0.101212000 |
| 8  | 1.200179000  | 1.893251000  | 0.937023000  |
| 8  | 0.957422000  | 2.142227000  | -1.248030000 |
| 6  | 1.613468000  | 3.396904000  | -1.149605000 |

|   |              |              |              |
|---|--------------|--------------|--------------|
| 1 | 1.628800000  | 3.804466000  | -2.149798000 |
| 1 | 1.079531000  | 4.061108000  | -0.482247000 |
| 1 | 2.624024000  | 3.276474000  | -0.780560000 |
| 6 | -1.410538000 | -2.028224000 | -0.601258000 |
| 7 | -1.399428000 | -3.173105000 | -0.650301000 |
| 1 | -4.408909000 | 2.095192000  | 1.413901000  |
| 1 | -5.435529000 | 0.043856000  | 0.966250000  |
| 6 | 3.561874000  | -0.415252000 | 0.943085000  |
| 6 | 3.736192000  | -0.247792000 | -0.429155000 |
| 6 | 2.569498000  | -1.265796000 | 1.379468000  |
| 1 | 4.513156000  | 0.406891000  | -0.783248000 |
| 1 | 2.425608000  | -1.418026000 | 2.434118000  |
| 6 | 2.927487000  | -0.888930000 | -1.332846000 |
| 6 | 1.747778000  | -1.929294000 | 0.477743000  |
| 1 | 3.078334000  | -0.746482000 | -2.387217000 |
| 1 | 1.030159000  | -2.645736000 | 0.831270000  |
| 6 | 1.915089000  | -1.737357000 | -0.888754000 |
| 1 | 1.350958000  | -2.323671000 | -1.589996000 |
| 6 | 4.397885000  | 0.354826000  | 1.914108000  |
| 1 | 3.946494000  | 1.326041000  | 2.092929000  |
| 1 | 4.470839000  | -0.156294000 | 2.866007000  |
| 1 | 5.399772000  | 0.516233000  | 1.534271000  |

42

exo-TS3\_4tT-N'

|    |              |              |              |
|----|--------------|--------------|--------------|
| 46 | -0.095085000 | -0.426709000 | -0.245716000 |
| 6  | -1.955718000 | 0.477455000  | -0.749487000 |
| 6  | -2.612955000 | 1.376889000  | 0.282744000  |
| 6  | -3.526420000 | -0.652970000 | 0.601715000  |
| 6  | -2.546978000 | -0.831828000 | -0.539458000 |
| 6  | -2.828036000 | 0.410189000  | 1.448729000  |
| 1  | -3.476285000 | 0.813433000  | 2.217333000  |
| 1  | -1.908291000 | 0.065550000  | 1.903753000  |
| 6  | -4.063936000 | 1.581333000  | -0.192331000 |
| 1  | -4.114635000 | 1.938591000  | -1.213363000 |
| 6  | -4.677601000 | 0.171232000  | -0.020025000 |
| 1  | -5.032140000 | -0.254405000 | -0.951337000 |
| 1  | -2.071952000 | 2.284370000  | 0.499752000  |
| 1  | -3.833162000 | -1.566415000 | 1.086172000  |

|   |              |              |              |
|---|--------------|--------------|--------------|
| 1 | -2.843293000 | -1.421683000 | -1.389149000 |
| 1 | -1.872713000 | 0.833127000  | -1.762477000 |
| 6 | 0.798988000  | 1.339996000  | -0.622345000 |
| 8 | 1.358036000  | 1.650420000  | -1.630690000 |
| 8 | 0.716572000  | 2.201838000  | 0.414517000  |
| 6 | 1.324212000  | 3.471010000  | 0.231452000  |
| 1 | 1.151142000  | 4.019814000  | 1.145665000  |
| 1 | 2.387054000  | 3.369485000  | 0.053305000  |
| 1 | 0.883885000  | 3.992683000  | -0.608637000 |
| 6 | -1.372009000 | -2.130143000 | 0.082142000  |
| 7 | -1.364160000 | -3.214020000 | 0.454778000  |
| 1 | -4.571723000 | 2.307389000  | 0.432489000  |
| 1 | -5.516524000 | 0.182307000  | 0.664614000  |
| 6 | 3.726662000  | -0.118119000 | 0.560325000  |
| 6 | 3.772177000  | -0.575843000 | -0.756970000 |
| 6 | 2.752640000  | -0.616354000 | 1.394087000  |
| 1 | 4.520167000  | -0.183023000 | -1.422887000 |
| 1 | 2.699676000  | -0.280142000 | 2.414062000  |
| 6 | 2.875745000  | -1.501661000 | -1.219805000 |
| 6 | 1.835806000  | -1.564103000 | 0.941509000  |
| 1 | 2.929431000  | -1.841571000 | -2.237508000 |
| 1 | 1.151557000  | -2.019901000 | 1.633309000  |
| 6 | 1.896240000  | -2.012477000 | -0.371234000 |
| 1 | 1.259239000  | -2.812513000 | -0.697444000 |
| 6 | 4.712933000  | 0.903525000  | 1.033858000  |
| 1 | 4.606592000  | 1.828059000  | 0.475711000  |
| 1 | 4.576281000  | 1.127278000  | 2.083954000  |
| 1 | 5.731338000  | 0.557451000  | 0.892091000  |

42

exo-TS3\_4tTr-O

|    |              |              |              |
|----|--------------|--------------|--------------|
| 46 | 0.060652000  | -0.149478000 | -0.167539000 |
| 6  | -2.263933000 | 0.283023000  | -0.574273000 |
| 6  | -3.301007000 | 0.088176000  | 0.521853000  |
| 6  | -2.371222000 | -1.939126000 | 0.239926000  |
| 6  | -1.675761000 | -1.037580000 | -0.756948000 |
| 6  | -2.639385000 | -0.975816000 | 1.397047000  |
| 1  | -3.321420000 | -1.383289000 | 2.133597000  |
| 1  | -1.745443000 | -0.627535000 | 1.896608000  |

|                  |              |              |              |
|------------------|--------------|--------------|--------------|
| 6                | -4.427176000 | -0.730948000 | -0.142998000 |
| 1                | -4.754797000 | -0.297505000 | -1.080602000 |
| 6                | -3.797499000 | -2.134244000 | -0.313113000 |
| 1                | -3.796289000 | -2.474110000 | -1.341395000 |
| 1                | -3.626229000 | 0.994002000  | 1.008846000  |
| 1                | -1.841911000 | -2.851689000 | 0.464243000  |
| 1                | -1.520569000 | -1.409684000 | -1.755332000 |
| 1                | -2.544969000 | 0.828319000  | -1.459070000 |
| 6                | -1.158315000 | 1.689004000  | 0.064038000  |
| 8                | -1.250220000 | 2.066968000  | 1.186682000  |
| 8                | -0.905773000 | 2.486756000  | -0.969652000 |
| 6                | -0.712299000 | 3.867461000  | -0.673677000 |
| 1                | -0.552732000 | 4.351572000  | -1.624177000 |
| 1                | -1.587056000 | 4.271294000  | -0.182186000 |
| 1                | 0.147686000  | 4.002866000  | -0.031594000 |
| 6                | 1.024017000  | -1.892725000 | -0.389146000 |
| 7                | 1.560630000  | -2.893795000 | -0.535977000 |
| 1                | -5.288164000 | -0.760624000 | 0.513500000  |
| 1                | -4.327557000 | -2.875946000 | 0.272526000  |
| 6                | 2.693914000  | 0.239587000  | 1.847554000  |
| 6                | 1.983749000  | 1.172529000  | 1.099413000  |
| 6                | 3.673004000  | -0.517769000 | 1.256587000  |
| 1                | 1.267794000  | 1.812079000  | 1.580392000  |
| 1                | 4.202435000  | -1.250176000 | 1.839635000  |
| 6                | 2.290373000  | 1.332324000  | -0.244754000 |
| 6                | 3.976928000  | -0.379849000 | -0.094948000 |
| 1                | 1.804930000  | 2.094515000  | -0.826651000 |
| 6                | 3.284733000  | 0.558957000  | -0.829189000 |
| 1                | 3.506724000  | 0.686263000  | -1.873661000 |
| 1                | 2.472961000  | 0.115327000  | 2.891906000  |
| 6                | 4.978979000  | -1.281857000 | -0.739173000 |
| 1                | 4.509059000  | -2.233796000 | -0.967497000 |
| 1                | 5.355306000  | -0.861828000 | -1.663652000 |
| 1                | 5.819200000  | -1.474166000 | -0.082235000 |
| 42               |              |              |              |
| exo-TS3_4tTr-OMe |              |              |              |
| 46               | -0.096006000 | 0.179642000  | -0.208315000 |
| 6                | 2.221183000  | -0.093279000 | -0.783637000 |

|   |              |              |              |
|---|--------------|--------------|--------------|
| 6 | 3.308090000  | -0.128453000 | 0.280324000  |
| 6 | 2.332890000  | 1.882494000  | 0.521728000  |
| 6 | 1.605503000  | 1.219097000  | -0.627429000 |
| 6 | 2.675226000  | 0.684981000  | 1.409071000  |
| 1 | 3.386482000  | 0.929787000  | 2.188834000  |
| 1 | 1.810924000  | 0.209445000  | 1.853351000  |
| 6 | 4.385036000  | 0.854734000  | -0.227440000 |
| 1 | 4.667911000  | 0.660504000  | -1.255169000 |
| 6 | 3.726258000  | 2.240949000  | -0.032732000 |
| 1 | 3.668086000  | 2.813107000  | -0.950250000 |
| 1 | 3.682208000  | -1.109683000 | 0.525565000  |
| 1 | 1.799842000  | 2.702223000  | 0.976791000  |
| 1 | 1.403989000  | 1.809667000  | -1.504873000 |
| 1 | 2.474456000  | -0.401350000 | -1.784062000 |
| 6 | 1.131045000  | -1.633051000 | -0.566105000 |
| 8 | 0.818648000  | -2.232636000 | -1.544958000 |
| 8 | 1.377763000  | -2.206263000 | 0.604779000  |
| 6 | 1.275770000  | -3.627440000 | 0.648337000  |
| 1 | 1.527545000  | -3.908696000 | 1.658660000  |
| 1 | 0.271407000  | -3.946352000 | 0.404740000  |
| 1 | 1.965713000  | -4.073009000 | -0.055635000 |
| 6 | -1.076836000 | 1.904684000  | 0.062976000  |
| 7 | -1.621259000 | 2.901785000  | 0.207926000  |
| 1 | 5.279464000  | 0.753518000  | 0.375046000  |
| 1 | 4.273585000  | 2.837671000  | 0.687315000  |
| 6 | -2.692182000 | -0.734235000 | 1.636457000  |
| 6 | -1.980906000 | -1.439617000 | 0.670997000  |
| 6 | -3.692498000 | 0.125793000  | 1.262180000  |
| 1 | -1.258462000 | -2.174035000 | 0.972847000  |
| 1 | -4.222826000 | 0.683510000  | 2.013280000  |
| 6 | -2.306034000 | -1.274793000 | -0.668268000 |
| 6 | -4.015943000 | 0.316151000  | -0.078421000 |
| 1 | -1.808745000 | -1.858855000 | -1.420671000 |
| 6 | -3.321802000 | -0.400636000 | -1.030005000 |
| 1 | -3.560228000 | -0.272453000 | -2.070693000 |
| 1 | -2.456330000 | -0.866200000 | 2.676698000  |
| 6 | -5.043635000 | 1.328124000  | -0.468804000 |
| 1 | -4.596792000 | 2.317682000  | -0.451582000 |

|                |              |              |              |
|----------------|--------------|--------------|--------------|
| 1              | -5.421177000 | 1.146269000  | -1.467254000 |
| 1              | -5.880248000 | 1.329405000  | 0.220159000  |
| 42             |              |              |              |
| exo-TS3_4tTr-N |              |              |              |
| 46             | -0.023322000 | 0.314678000  | -0.110050000 |
| 6              | -1.988913000 | -0.145034000 | -0.663751000 |
| 6              | -3.003178000 | -0.209572000 | 0.464849000  |
| 6              | -2.291178000 | -2.324485000 | 0.174104000  |
| 6              | -1.535948000 | -1.503382000 | -0.846437000 |
| 6              | -2.433301000 | -1.335855000 | 1.330435000  |
| 1              | -3.131593000 | -1.681868000 | 2.082805000  |
| 1              | -1.492956000 | -1.088791000 | 1.806308000  |
| 6              | -4.244577000 | -0.904941000 | -0.125288000 |
| 1              | -4.594951000 | -0.422666000 | -1.029494000 |
| 6              | -3.739201000 | -2.346608000 | -0.373087000 |
| 1              | -3.781189000 | -2.638551000 | -1.415852000 |
| 1              | -3.188257000 | 0.733491000  | 0.954389000  |
| 1              | -1.869408000 | -3.294753000 | 0.382224000  |
| 1              | -1.396716000 | -1.893829000 | -1.838245000 |
| 1              | -2.232154000 | 0.428090000  | -1.542525000 |
| 6              | -0.637452000 | 2.221913000  | 0.166013000  |
| 8              | -1.317926000 | 2.628308000  | 1.061234000  |
| 8              | -0.158807000 | 3.071606000  | -0.770235000 |
| 6              | -0.517664000 | 4.439430000  | -0.631449000 |
| 1              | -0.060093000 | 4.953521000  | -1.463789000 |
| 1              | -1.592696000 | 4.559286000  | -0.662176000 |
| 1              | -0.151908000 | 4.841460000  | 0.304480000  |
| 6              | 0.275120000  | -1.796549000 | -0.415616000 |
| 7              | 0.963070000  | -2.713343000 | -0.401352000 |
| 1              | -5.061730000 | -0.894050000 | 0.586839000  |
| 1              | -4.316653000 | -3.073636000 | 0.184273000  |
| 6              | 2.623253000  | -0.158129000 | 1.823472000  |
| 6              | 2.115107000  | 0.928566000  | 1.113952000  |
| 6              | 3.409017000  | -1.085589000 | 1.192570000  |
| 1              | 1.589797000  | 1.707932000  | 1.633451000  |
| 1              | 3.787966000  | -1.926460000 | 1.746086000  |
| 6              | 2.422036000  | 1.059624000  | -0.235529000 |
| 6              | 3.717092000  | -0.972094000 | -0.163062000 |

|   |             |              |              |
|---|-------------|--------------|--------------|
| 1 | 2.108569000 | 1.933721000  | -0.775526000 |
| 6 | 3.222559000 | 0.107131000  | -0.859102000 |
| 1 | 3.456771000 | 0.220543000  | -1.902667000 |
| 1 | 2.404290000 | -0.258472000 | 2.870885000  |
| 6 | 4.523504000 | -2.032329000 | -0.841192000 |
| 1 | 3.901706000 | -2.903429000 | -1.023557000 |
| 1 | 4.909236000 | -1.689032000 | -1.792821000 |
| 1 | 5.359508000 | -2.346191000 | -0.226613000 |

42

exo-TS3\_4tTr-N'

|    |              |              |              |
|----|--------------|--------------|--------------|
| 46 | 0.016877000  | -0.368971000 | -0.139104000 |
| 6  | 1.902927000  | 0.399345000  | -0.622810000 |
| 6  | 2.894909000  | 0.560075000  | 0.516197000  |
| 6  | 1.932566000  | 2.578755000  | 0.275514000  |
| 6  | 1.293122000  | 1.697999000  | -0.772245000 |
| 6  | 2.187571000  | 1.583798000  | 1.407408000  |
| 1  | 2.833046000  | 1.992628000  | 2.175359000  |
| 1  | 1.279568000  | 1.213638000  | 1.866272000  |
| 6  | 4.044793000  | 1.417778000  | -0.046545000 |
| 1  | 4.452918000  | 1.005610000  | -0.960912000 |
| 6  | 3.369674000  | 2.793719000  | -0.257609000 |
| 1  | 3.381385000  | 3.118917000  | -1.291171000 |
| 1  | 3.204480000  | -0.365301000 | 0.974472000  |
| 1  | 1.392199000  | 3.483043000  | 0.504980000  |
| 1  | 1.098765000  | 2.097162000  | -1.751323000 |
| 1  | 2.217638000  | -0.129149000 | -1.505398000 |
| 6  | 0.721302000  | -2.278536000 | -0.035636000 |
| 8  | 0.033832000  | -3.211220000 | 0.274229000  |
| 8  | 2.015541000  | -2.479186000 | -0.350450000 |
| 6  | 2.482001000  | -3.818797000 | -0.291121000 |
| 1  | 3.524202000  | -3.783260000 | -0.573130000 |
| 1  | 2.377762000  | -4.219980000 | 0.708570000  |
| 1  | 1.930471000  | -4.450037000 | -0.975508000 |
| 6  | -0.535552000 | 1.705387000  | -0.316811000 |
| 7  | -1.331223000 | 2.528183000  | -0.252804000 |
| 1  | 4.854981000  | 1.485945000  | 0.670472000  |
| 1  | 3.851134000  | 3.568792000  | 0.325512000  |
| 6  | -2.768302000 | -0.165613000 | 1.769993000  |

|   |              |              |              |
|---|--------------|--------------|--------------|
| 6 | -2.129167000 | -1.181097000 | 1.063102000  |
| 6 | -3.633096000 | 0.681641000  | 1.128906000  |
| 1 | -1.527458000 | -1.913136000 | 1.565898000  |
| 1 | -4.114936000 | 1.469008000  | 1.681405000  |
| 6 | -2.389887000 | -1.327130000 | -0.293593000 |
| 6 | -3.892899000 | 0.555278000  | -0.235594000 |
| 1 | -1.981930000 | -2.169774000 | -0.818789000 |
| 6 | -3.270124000 | -0.456801000 | -0.929703000 |
| 1 | -3.470440000 | -0.583977000 | -1.978969000 |
| 1 | -2.589884000 | -0.056067000 | 2.824402000  |
| 6 | -4.794076000 | 1.531198000  | -0.921754000 |
| 1 | -4.274528000 | 2.473784000  | -1.064540000 |
| 1 | -5.104884000 | 1.167918000  | -1.893255000 |
| 1 | -5.681830000 | 1.730852000  | -0.332337000 |

42

exo-TS3\_4cT-O

|    |              |              |              |
|----|--------------|--------------|--------------|
| 46 | 0.108521000  | 0.096301000  | -0.226941000 |
| 6  | -2.260768000 | 0.195584000  | -0.480972000 |
| 6  | -3.232126000 | -0.174780000 | 0.632437000  |
| 6  | -2.038063000 | -2.037834000 | 0.265813000  |
| 6  | -1.493442000 | -1.016867000 | -0.714616000 |
| 6  | -2.397715000 | -1.150256000 | 1.459452000  |
| 1  | -2.986105000 | -1.667823000 | 2.207650000  |
| 1  | -1.549823000 | -0.679142000 | 1.938917000  |
| 6  | -4.252108000 | -1.127548000 | -0.022596000 |
| 1  | -4.665775000 | -0.721746000 | -0.937918000 |
| 6  | -3.439170000 | -2.422947000 | -0.249858000 |
| 1  | -3.422832000 | -2.734314000 | -1.287265000 |
| 1  | -3.663301000 | 0.663527000  | 1.155554000  |
| 1  | -1.394917000 | -2.885953000 | 0.456363000  |
| 1  | -1.358266000 | -1.336643000 | -1.738727000 |
| 1  | -2.644586000 | 0.715777000  | -1.342021000 |
| 6  | -1.362977000 | 1.702193000  | 0.191778000  |
| 8  | -1.479058000 | 1.970016000  | 1.337877000  |
| 8  | -1.259560000 | 2.563057000  | -0.801716000 |
| 6  | -0.985643000 | 3.918145000  | -0.429957000 |
| 1  | -0.974340000 | 4.472681000  | -1.354674000 |
| 1  | -1.758930000 | 4.286267000  | 0.229776000  |



|   |              |              |              |
|---|--------------|--------------|--------------|
| 1 | -0.021121000 | 3.966612000  | 0.056189000  |
| 6 | 1.557647000  | 1.554382000  | 0.171435000  |
| 7 | 2.328549000  | 2.379837000  | 0.368220000  |
| 1 | -5.079438000 | -1.295963000 | 0.655948000  |
| 1 | -3.840775000 | -3.245925000 | 0.330204000  |
| 6 | 1.579565000  | -1.719941000 | -1.003033000 |
| 6 | 2.658311000  | -1.131393000 | -1.666358000 |
| 6 | 1.626009000  | -1.844941000 | 0.383320000  |
| 1 | 2.641978000  | -1.046690000 | -2.737465000 |
| 1 | 0.855686000  | -2.383769000 | 0.902966000  |
| 6 | 3.733960000  | -0.673785000 | -0.955828000 |
| 6 | 2.729059000  | -1.375524000 | 1.087538000  |
| 1 | 4.550465000  | -0.202211000 | -1.472579000 |
| 1 | 2.748537000  | -1.468265000 | 2.158334000  |
| 6 | 3.782824000  | -0.777519000 | 0.435021000  |
| 1 | 0.806514000  | -2.205895000 | -1.566825000 |
| 6 | 4.920651000  | -0.176617000 | 1.191416000  |
| 1 | 5.006178000  | -0.598874000 | 2.184665000  |
| 1 | 5.861462000  | -0.318628000 | 0.672666000  |
| 1 | 4.750442000  | 0.891601000  | 1.290760000  |

42

exo-TS3\_4cT-OMe

|    |              |              |              |
|----|--------------|--------------|--------------|
| 46 | 0.111702000  | 0.051026000  | -0.332185000 |
| 6  | -2.258185000 | 0.043357000  | -0.652935000 |
| 6  | -3.199706000 | -0.078093000 | 0.537139000  |
| 6  | -1.974679000 | -1.957459000 | 0.571858000  |
| 6  | -1.458776000 | -1.171218000 | -0.620235000 |
| 6  | -2.338290000 | -0.833908000 | 1.546271000  |
| 1  | -2.908097000 | -1.184215000 | 2.398679000  |
| 1  | -1.491276000 | -0.259559000 | 1.899273000  |
| 6  | -4.211535000 | -1.169361000 | 0.129505000  |
| 1  | -4.647410000 | -0.981825000 | -0.844184000 |
| 6  | -3.374969000 | -2.468584000 | 0.177056000  |
| 1  | -3.365594000 | -2.999400000 | -0.767003000 |
| 1  | -3.645953000 | 0.846539000  | 0.866153000  |
| 1  | -1.316460000 | -2.732935000 | 0.937861000  |
| 1  | -1.328671000 | -1.709575000 | -1.548417000 |
| 1  | -2.681450000 | 0.323127000  | -1.602076000 |

|   |              |              |              |
|---|--------------|--------------|--------------|
| 6 | -1.363921000 | 1.692209000  | -0.552594000 |
| 8 | -1.291585000 | 2.300293000  | -1.565348000 |
| 8 | -1.483531000 | 2.204210000  | 0.654311000  |
| 6 | -1.261260000 | 3.615123000  | 0.760635000  |
| 1 | -1.453008000 | 3.858831000  | 1.793427000  |
| 1 | -0.234910000 | 3.833483000  | 0.500644000  |
| 1 | -1.937162000 | 4.147833000  | 0.106499000  |
| 6 | 1.502844000  | 1.580548000  | 0.008856000  |
| 7 | 2.226337000  | 2.432868000  | 0.262949000  |
| 1 | -5.024296000 | -1.197986000 | 0.844919000  |
| 1 | -3.752309000 | -3.150989000 | 0.930065000  |
| 6 | 1.650169000  | -1.797287000 | -0.838656000 |
| 6 | 2.725730000  | -1.255704000 | -1.545695000 |
| 6 | 1.668648000  | -1.757085000 | 0.553362000  |
| 1 | 2.730492000  | -1.295796000 | -2.619438000 |
| 1 | 0.904204000  | -2.257191000 | 1.117794000  |
| 6 | 3.772178000  | -0.686519000 | -0.872903000 |
| 6 | 2.743014000  | -1.176971000 | 1.218713000  |
| 1 | 4.586710000  | -0.254248000 | -1.425972000 |
| 1 | 2.741883000  | -1.145070000 | 2.293259000  |
| 6 | 3.793993000  | -0.627292000 | 0.521354000  |
| 1 | 0.904140000  | -2.368702000 | -1.356799000 |
| 6 | 4.897660000  | 0.090271000  | 1.224813000  |
| 1 | 4.986180000  | -0.228249000 | 2.255879000  |
| 1 | 5.850100000  | -0.064736000 | 0.731805000  |
| 1 | 4.683651000  | 1.155194000  | 1.216548000  |

42

exo-TS3\_4cT-N

|    |             |              |              |
|----|-------------|--------------|--------------|
| 46 | 0.120110000 | 0.216296000  | -0.236690000 |
| 6  | 1.998265000 | -0.582876000 | -0.750185000 |
| 6  | 2.708807000 | -1.501729000 | 0.233630000  |
| 6  | 3.526844000 | 0.547815000  | 0.632915000  |
| 6  | 2.531154000 | 0.718527000  | -0.496190000 |
| 6  | 2.883475000 | -0.576553000 | 1.441049000  |
| 1  | 3.551726000 | -0.982535000 | 2.190722000  |
| 1  | 1.954862000 | -0.284442000 | 1.915270000  |
| 6  | 4.166690000 | -1.623099000 | -0.250943000 |
| 1  | 4.228353000 | -1.936103000 | -1.285868000 |

|                |              |              |              |
|----------------|--------------|--------------|--------------|
| 6              | 4.713873000  | -0.195761000 | -0.021767000 |
| 1              | 5.044929000  | 0.284044000  | -0.934864000 |
| 1              | 2.231422000  | -2.454133000 | 0.418046000  |
| 1              | 3.785799000  | 1.457344000  | 1.150091000  |
| 1              | 2.778262000  | 1.367557000  | -1.316336000 |
| 1              | 1.916542000  | -0.898528000 | -1.779776000 |
| 6              | -1.544084000 | 1.288665000  | 0.304505000  |
| 8              | -2.153349000 | 1.197621000  | 1.331345000  |
| 8              | -1.906963000 | 2.186689000  | -0.632316000 |
| 6              | -2.985057000 | 3.048825000  | -0.306807000 |
| 1              | -3.101092000 | 3.713923000  | -1.150017000 |
| 1              | -3.897044000 | 2.486855000  | -0.146505000 |
| 1              | -2.764962000 | 3.615383000  | 0.588440000  |
| 6              | 1.331665000  | 1.945359000  | 0.190149000  |
| 7              | 1.495363000  | 3.011390000  | 0.577781000  |
| 1              | 4.708331000  | -2.350863000 | 0.343519000  |
| 1              | 5.554156000  | -0.196887000 | 0.661475000  |
| 6              | -0.879837000 | -2.045994000 | -0.059030000 |
| 6              | -1.086728000 | -1.572047000 | -1.352614000 |
| 6              | -1.931056000 | -2.067237000 | 0.852400000  |
| 1              | -0.325528000 | -1.679338000 | -2.102122000 |
| 1              | -1.754194000 | -2.422727000 | 1.851258000  |
| 6              | -2.366595000 | -1.147982000 | -1.720099000 |
| 6              | -3.186339000 | -1.635789000 | 0.494412000  |
| 1              | -2.543369000 | -0.797990000 | -2.720280000 |
| 6              | -3.390545000 | -1.192088000 | -0.814195000 |
| 1              | -4.371099000 | -0.859646000 | -1.105930000 |
| 1              | 0.057359000  | -2.495516000 | 0.206237000  |
| 6              | -4.296001000 | -1.578137000 | 1.491874000  |
| 1              | -4.141368000 | -2.282588000 | 2.299333000  |
| 1              | -4.335291000 | -0.581748000 | 1.921561000  |
| 1              | -5.255079000 | -1.785277000 | 1.032155000  |
| 42             |              |              |              |
| exo-TS3_4cT-N' |              |              |              |
| 46             | 0.137474000  | 0.111959000  | -0.357706000 |
| 6              | 2.003170000  | -0.848534000 | -0.520355000 |
| 6              | 2.653382000  | -1.363321000 | 0.755324000  |
| 6              | 3.520262000  | 0.678715000  | 0.420411000  |

|   |              |              |              |
|---|--------------|--------------|--------------|
| 6 | 2.566411000  | 0.446217000  | -0.733315000 |
| 6 | 2.819502000  | -0.066840000 | 1.554002000  |
| 1 | 3.452959000  | -0.186044000 | 2.424648000  |
| 1 | 1.886922000  | 0.393892000  | 1.855227000  |
| 6 | 4.121511000  | -1.676512000 | 0.406701000  |
| 1 | 4.206166000  | -2.343965000 | -0.441901000 |
| 6 | 4.703876000  | -0.272165000 | 0.126109000  |
| 1 | 5.076985000  | -0.161472000 | -0.884830000 |
| 1 | 2.137725000  | -2.176165000 | 1.248610000  |
| 1 | 3.791296000  | 1.708939000  | 0.585098000  |
| 1 | 2.859025000  | 0.748120000  | -1.722289000 |
| 1 | 1.939611000  | -1.510592000 | -1.370613000 |
| 6 | -1.510563000 | 1.332734000  | -0.306794000 |
| 8 | -2.312002000 | 1.501192000  | -1.178473000 |
| 8 | -1.608994000 | 2.006716000  | 0.858415000  |
| 6 | -2.638843000 | 2.977075000  | 0.949679000  |
| 1 | -2.530357000 | 3.438328000  | 1.920440000  |
| 1 | -2.534575000 | 3.719755000  | 0.169644000  |
| 1 | -3.616163000 | 2.518433000  | 0.862346000  |
| 6 | 1.379212000  | 1.855748000  | -0.596455000 |
| 7 | 1.560978000  | 2.986432000  | -0.642086000 |
| 1 | 4.622329000  | -2.148339000 | 1.245140000  |
| 1 | 5.522458000  | -0.040202000 | 0.796169000  |
| 6 | -1.035277000 | -1.788688000 | 0.664106000  |
| 6 | -0.971912000 | -2.054312000 | -0.700157000 |
| 6 | -2.247828000 | -1.403363000 | 1.240631000  |
| 1 | -0.091629000 | -2.491751000 | -1.128548000 |
| 1 | -2.285599000 | -1.202980000 | 2.295988000  |
| 6 | -2.125551000 | -1.918995000 | -1.474972000 |
| 6 | -3.384398000 | -1.283704000 | 0.480153000  |
| 1 | -2.085209000 | -2.119885000 | -2.529411000 |
| 6 | -3.302127000 | -1.544624000 | -0.890811000 |
| 1 | -4.183143000 | -1.432842000 | -1.497235000 |
| 1 | -0.195253000 | -2.003476000 | 1.298338000  |
| 6 | -4.682870000 | -0.844545000 | 1.077422000  |
| 1 | -4.621934000 | -0.780727000 | 2.155999000  |
| 1 | -4.958775000 | 0.133296000  | 0.695731000  |
| 1 | -5.483266000 | -1.530032000 | 0.820917000  |

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| 46 | -0.928795000 | -0.555210000 | -0.307180000 |
| 15 | 1.449219000  | -0.034353000 | 0.024872000  |
| 6  | 1.771971000  | 1.758386000  | 0.124544000  |
| 6  | 1.129311000  | 2.486386000  | 1.119213000  |
| 6  | 2.581865000  | 2.433488000  | -0.773833000 |
| 6  | 1.313647000  | 3.847096000  | 1.227541000  |
| 1  | 0.482301000  | 1.983689000  | 1.815630000  |
| 6  | 2.754799000  | 3.802314000  | -0.674769000 |
| 1  | 3.084324000  | 1.895107000  | -1.554925000 |
| 6  | 2.127252000  | 4.511021000  | 0.327198000  |
| 1  | 0.821335000  | 4.392100000  | 2.012974000  |
| 1  | 3.387548000  | 4.309616000  | -1.380423000 |
| 1  | 2.269168000  | 5.573521000  | 0.408900000  |
| 6  | 2.214706000  | -0.708812000 | 1.536089000  |
| 6  | 3.091363000  | 0.017475000  | 2.329291000  |
| 6  | 1.916165000  | -2.019894000 | 1.887944000  |
| 6  | 3.657896000  | -0.553199000 | 3.452252000  |
| 1  | 3.334973000  | 1.032381000  | 2.077212000  |
| 6  | 2.490356000  | -2.588259000 | 3.006362000  |
| 1  | 1.240668000  | -2.600753000 | 1.286864000  |
| 6  | 3.359266000  | -1.856924000 | 3.792343000  |
| 1  | 4.333590000  | 0.022852000  | 4.058474000  |
| 1  | 2.252112000  | -3.604258000 | 3.263520000  |
| 1  | 3.800383000  | -2.300793000 | 4.666575000  |
| 6  | 2.520764000  | -0.619085000 | -1.322221000 |
| 6  | 1.954689000  | -0.863895000 | -2.563455000 |
| 6  | 3.883517000  | -0.820199000 | -1.152398000 |
| 6  | 2.737436000  | -1.282434000 | -3.621176000 |
| 1  | 0.894857000  | -0.748617000 | -2.697691000 |
| 6  | 4.664335000  | -1.243083000 | -2.207486000 |
| 1  | 4.336293000  | -0.656726000 | -0.191790000 |
| 6  | 4.092582000  | -1.471361000 | -3.444763000 |
| 1  | 2.283949000  | -1.476490000 | -4.575961000 |
| 1  | 5.717560000  | -1.401553000 | -2.062141000 |
| 1  | 4.700982000  | -1.807847000 | -4.264733000 |
| 6  | -3.710675000 | 0.369178000  | -0.642139000 |

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| 6 | -4.758388000 | 0.172742000  | 0.477761000  |
| 6 | -3.627187000 | -1.769202000 | 0.466424000  |
| 6 | -2.918095000 | -0.968256000 | -0.632646000 |
| 6 | -3.982779000 | -0.682169000 | 1.481352000  |
| 1 | -4.609549000 | -1.036877000 | 2.292268000  |
| 1 | -3.114558000 | -0.187948000 | 1.903153000  |
| 6 | -5.795006000 | -0.828476000 | -0.040299000 |
| 1 | -6.171675000 | -0.555691000 | -1.019425000 |
| 6 | -5.021435000 | -2.169965000 | -0.038911000 |
| 1 | -4.977332000 | -2.630807000 | -1.017952000 |
| 1 | -5.183449000 | 1.099053000  | 0.841210000  |
| 1 | -3.048354000 | -2.600671000 | 0.837153000  |
| 1 | -2.991096000 | -1.469137000 | -1.588152000 |
| 1 | -4.210419000 | 0.567269000  | -1.586326000 |
| 6 | -2.830743000 | 1.541011000  | -0.385313000 |
| 8 | -1.636305000 | 1.447051000  | -0.163723000 |
| 8 | -3.420144000 | 2.706226000  | -0.415429000 |
| 6 | -2.618370000 | 3.861458000  | -0.183746000 |
| 1 | -3.284751000 | 4.702255000  | -0.291097000 |
| 1 | -2.200094000 | 3.832635000  | 0.812455000  |
| 1 | -1.815785000 | 3.913677000  | -0.905486000 |
| 6 | -0.566173000 | -2.459328000 | -0.509453000 |
| 7 | -0.337727000 | -3.577827000 | -0.604124000 |
| 1 | -6.644949000 | -0.864270000 | 0.631435000  |
| 1 | -5.484500000 | -2.884296000 | 0.633340000  |

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| 46 | -1.036902000 | -0.273942000 | -0.343177000 |
| 15 | 1.438182000  | -0.066059000 | 0.036596000  |
| 6  | 2.086352000  | 1.618610000  | 0.319105000  |
| 6  | 1.789666000  | 2.258458000  | 1.517915000  |
| 6  | 2.779475000  | 2.321416000  | -0.653421000 |
| 6  | 2.183964000  | 3.559420000  | 1.739978000  |
| 1  | 1.251266000  | 1.733407000  | 2.287195000  |
| 6  | 3.166493000  | 3.631453000  | -0.434191000 |
| 1  | 3.023753000  | 1.849548000  | -1.586596000 |
| 6  | 2.872096000  | 4.253025000  | 0.760710000  |
| 1  | 1.952853000  | 4.034502000  | 2.676237000  |

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| 1 | 3.704646000  | 4.160555000  | -1.199706000 |
| 1 | 3.177593000  | 5.269130000  | 0.932096000  |
| 6 | 2.113624000  | -0.997267000 | 1.455907000  |
| 6 | 3.259115000  | -0.586764000 | 2.128356000  |
| 6 | 1.488863000  | -2.169918000 | 1.857872000  |
| 6 | 3.764930000  | -1.328074000 | 3.175796000  |
| 1 | 3.760106000  | 0.318680000  | 1.841881000  |
| 6 | 2.000039000  | -2.911713000 | 2.904794000  |
| 1 | 0.613982000  | -2.519656000 | 1.345617000  |
| 6 | 3.135190000  | -2.493326000 | 3.567245000  |
| 1 | 4.650973000  | -0.994183000 | 3.684917000  |
| 1 | 1.504675000  | -3.819134000 | 3.198278000  |
| 1 | 3.528576000  | -3.070786000 | 4.384297000  |
| 6 | 2.370498000  | -0.660573000 | -1.409103000 |
| 6 | 1.734652000  | -0.687556000 | -2.640392000 |
| 6 | 3.693064000  | -1.073318000 | -1.327366000 |
| 6 | 2.410739000  | -1.098525000 | -3.772297000 |
| 1 | 0.699622000  | -0.407542000 | -2.712643000 |
| 6 | 4.366341000  | -1.489934000 | -2.456116000 |
| 1 | 4.198249000  | -1.082821000 | -0.379696000 |
| 6 | 3.727276000  | -1.499319000 | -3.681516000 |
| 1 | 1.902040000  | -1.120811000 | -4.718639000 |
| 1 | 5.388111000  | -1.814438000 | -2.378093000 |
| 1 | 4.251763000  | -1.830468000 | -4.559476000 |
| 6 | -3.860294000 | 0.666668000  | -0.556525000 |
| 6 | -4.911205000 | 0.392613000  | 0.536605000  |
| 6 | -3.703068000 | -1.499158000 | 0.480842000  |
| 6 | -3.038365000 | -0.643369000 | -0.608546000 |
| 6 | -4.102324000 | -0.452488000 | 1.520775000  |
| 1 | -4.708621000 | -0.854436000 | 2.324885000  |
| 1 | -3.256457000 | 0.072081000  | 1.953549000  |
| 6 | -5.904544000 | -0.635153000 | -0.010768000 |
| 1 | -6.283607000 | -0.355288000 | -0.987027000 |
| 6 | -5.080109000 | -1.944972000 | -0.033469000 |
| 1 | -5.018156000 | -2.389212000 | -1.019163000 |
| 1 | -5.366047000 | 1.296456000  | 0.916517000  |
| 1 | -3.092331000 | -2.316490000 | 0.828554000  |
| 1 | -3.127501000 | -1.114840000 | -1.576651000 |

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| 1         | -4.350149000 | 0.870567000  | -1.505976000 |
| 6         | -3.119561000 | 1.936281000  | -0.268051000 |
| 8         | -3.606721000 | 2.986961000  | -0.019578000 |
| 8         | -1.762389000 | 1.811039000  | -0.362320000 |
| 6         | -1.037550000 | 3.046418000  | -0.298205000 |
| 1         | -0.029318000 | 2.823462000  | -0.595686000 |
| 1         | -1.490842000 | 3.758983000  | -0.969883000 |
| 1         | -1.060726000 | 3.435296000  | 0.708684000  |
| 6         | -0.813399000 | -2.193222000 | -0.592892000 |
| 7         | -0.672693000 | -3.319267000 | -0.745579000 |
| 1         | -6.758326000 | -0.719314000 | 0.651511000  |
| 1         | -5.511404000 | -2.688416000 | 0.628171000  |
| 61        |              |              |              |
| exo-4tP-N |              |              |              |
| 46        | 1.118480000  | -0.000092000 | 0.154170000  |
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| 6         | -1.666917000 | 1.811378000  | -1.895119000 |
| 6         | -3.282128000 | 1.794786000  | -0.133678000 |
| 6         | -2.295728000 | 2.899610000  | -2.462794000 |
| 1         | -0.779030000 | 1.417392000  | -2.354327000 |
| 6         | -3.906177000 | 2.890287000  | -0.698643000 |
| 1         | -3.674104000 | 1.374735000  | 0.773466000  |
| 6         | -3.417161000 | 3.441901000  | -1.865343000 |
| 1         | -1.899998000 | 3.330957000  | -3.364070000 |
| 1         | -4.775051000 | 3.310336000  | -0.224959000 |
| 1         | -3.902998000 | 4.294733000  | -2.304057000 |
| 6         | -1.967617000 | -1.590217000 | -1.063463000 |
| 6         | -3.068671000 | -1.438506000 | -1.894038000 |
| 6         | -1.351266000 | -2.832982000 | -0.987799000 |
| 6         | -3.544889000 | -2.505612000 | -2.630556000 |
| 1         | -3.557769000 | -0.486439000 | -1.974109000 |
| 6         | -1.834375000 | -3.898938000 | -1.718785000 |
| 1         | -0.493503000 | -2.969622000 | -0.356665000 |
| 6         | -2.930540000 | -3.738064000 | -2.543495000 |
| 1         | -4.396723000 | -2.370152000 | -3.272226000 |
| 1         | -1.347090000 | -4.854473000 | -1.647708000 |
| 1         | -3.300978000 | -4.567770000 | -3.118125000 |



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|---|--------------|--------------|--------------|
| 6 | -2.036189000 | -0.457741000 | 1.591084000  |
| 6 | -1.522588000 | 0.294372000  | 2.640900000  |
| 6 | -3.066389000 | -1.349420000 | 1.843483000  |
| 6 | -2.041487000 | 0.165016000  | 3.912062000  |
| 1 | -0.716542000 | 0.983166000  | 2.458648000  |
| 6 | -3.577800000 | -1.484338000 | 3.120049000  |
| 1 | -3.469696000 | -1.946388000 | 1.047083000  |
| 6 | -3.069059000 | -0.726587000 | 4.154772000  |
| 1 | -1.636986000 | 0.754029000  | 4.715185000  |
| 1 | -4.373419000 | -2.183655000 | 3.303289000  |
| 1 | -3.466942000 | -0.833567000 | 5.147734000  |
| 6 | 3.187255000  | 0.250595000  | 0.437226000  |
| 6 | 4.022235000  | 0.491664000  | -0.822594000 |
| 6 | 4.723105000  | -1.541935000 | -0.161760000 |
| 6 | 3.682252000  | -1.151626000 | 0.900486000  |
| 6 | 4.131749000  | -0.911255000 | -1.422467000 |
| 1 | 4.811285000  | -0.964141000 | -2.265702000 |
| 1 | 3.177965000  | -1.332816000 | -1.716908000 |
| 6 | 5.478210000  | 0.741783000  | -0.400802000 |
| 1 | 5.552726000  | 1.497413000  | 0.371916000  |
| 6 | 5.948499000  | -0.654118000 | 0.081792000  |
| 1 | 6.257496000  | -0.660985000 | 1.121081000  |
| 1 | 3.613308000  | 1.253222000  | -1.468867000 |
| 1 | 4.938605000  | -2.602061000 | -0.195997000 |
| 1 | 4.089722000  | -1.176387000 | 1.904579000  |
| 1 | 3.370238000  | 0.993804000  | 1.200663000  |
| 6 | 1.127706000  | 1.940580000  | -0.176271000 |
| 8 | 1.444633000  | 2.500512000  | -1.180638000 |
| 8 | 0.693283000  | 2.626364000  | 0.897708000  |
| 6 | 0.614978000  | 4.038762000  | 0.755273000  |
| 1 | 0.266145000  | 4.412990000  | 1.706368000  |
| 1 | 1.585851000  | 4.455011000  | 0.521184000  |
| 1 | -0.080160000 | 4.304959000  | -0.030010000 |
| 6 | 2.486368000  | -1.990186000 | 0.873202000  |
| 7 | 1.472857000  | -2.514608000 | 0.798008000  |
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| 1 | 6.787737000  | -1.011488000 | -0.502940000 |

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| exo-4cP-O |              |              |              |
| 46        | 0.803319000  | -0.992786000 | 0.061633000  |
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| 6         | -2.181931000 | -2.049172000 | -1.730713000 |
| 6         | -3.357822000 | 0.025824000  | -1.891893000 |
| 6         | -3.030639000 | -2.595618000 | -2.673221000 |
| 1         | -1.414355000 | -2.659177000 | -1.297032000 |
| 6         | -4.202958000 | -0.523163000 | -2.833333000 |
| 1         | -3.495537000 | 1.050923000  | -1.604503000 |
| 6         | -4.040233000 | -1.836743000 | -3.227324000 |
| 1         | -2.898124000 | -3.620264000 | -2.968878000 |
| 1         | -4.986727000 | 0.077127000  | -3.258742000 |
| 1         | -4.697699000 | -2.264833000 | -3.962405000 |
| 6         | -2.146904000 | -0.198407000 | 1.525094000  |
| 6         | -3.531488000 | -0.139260000 | 1.584667000  |
| 6         | -1.430198000 | -0.365721000 | 2.699131000  |
| 6         | -4.183270000 | -0.234833000 | 2.796312000  |
| 1         | -4.108471000 | -0.032715000 | 0.685480000  |
| 6         | -2.082294000 | -0.453856000 | 3.912356000  |
| 1         | -0.360036000 | -0.450639000 | 2.662854000  |
| 6         | -3.459413000 | -0.388145000 | 3.962743000  |
| 1         | -5.257022000 | -0.197980000 | 2.827837000  |
| 1         | -1.513637000 | -0.592008000 | 4.813628000  |
| 1         | -3.968891000 | -0.469354000 | 4.905843000  |
| 6         | -1.306276000 | 1.760452000  | -0.397872000 |
| 6         | -0.964472000 | 2.212722000  | -1.666854000 |
| 6         | -1.643978000 | 2.691474000  | 0.570468000  |
| 6         | -0.972567000 | 3.558292000  | -1.960979000 |
| 1         | -0.703250000 | 1.507538000  | -2.435108000 |
| 6         | -1.644245000 | 4.042959000  | 0.277465000  |
| 1         | -1.914818000 | 2.368124000  | 1.557654000  |
| 6         | -1.311448000 | 4.479257000  | -0.986801000 |
| 1         | -0.713063000 | 3.889471000  | -2.950189000 |
| 1         | -1.910951000 | 4.751048000  | 1.040918000  |
| 1         | -1.316429000 | 5.529535000  | -1.215474000 |
| 6         | 3.361229000  | 0.320322000  | -0.707396000 |
| 6         | 4.150149000  | 1.216672000  | 0.271656000  |

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| 6 | 2.011220000  | 1.785064000  | 0.644063000  |
| 6 | 1.874445000  | 0.718078000  | -0.457954000 |
| 6 | 3.194780000  | 1.270016000  | 1.463718000  |
| 1 | 3.522527000  | 1.965687000  | 2.228681000  |
| 1 | 3.015766000  | 0.305135000  | 1.924724000  |
| 6 | 4.076385000  | 2.654033000  | -0.251433000 |
| 1 | 4.335701000  | 2.717289000  | -1.302018000 |
| 6 | 2.610476000  | 3.061215000  | 0.035442000  |
| 1 | 2.077753000  | 3.373084000  | -0.853897000 |
| 1 | 5.156686000  | 0.868963000  | 0.462244000  |
| 1 | 1.104159000  | 1.970112000  | 1.200434000  |
| 1 | 1.464561000  | 1.158080000  | -1.356895000 |
| 1 | 3.689843000  | 0.497950000  | -1.727110000 |
| 6 | 3.604393000  | -1.120923000 | -0.426230000 |
| 8 | 2.744272000  | -1.868622000 | -0.003837000 |
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| 6 | 5.091933000  | -2.922321000 | -0.390234000 |
| 1 | 6.127845000  | -3.066079000 | -0.652234000 |
| 1 | 4.927262000  | -3.142644000 | 0.654889000  |
| 1 | 4.452924000  | -3.552671000 | -0.991993000 |
| 6 | -0.052000000 | -2.775327000 | 0.653973000  |
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| 1 | 2.568614000  | 3.883276000  | 0.742603000  |

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|    |              |              |              |
|----|--------------|--------------|--------------|
| 46 | 0.809408000  | -1.034307000 | 0.015870000  |
| 15 | -1.180926000 | 0.049451000  | -0.045811000 |
| 6  | -2.324732000 | -0.578608000 | -1.320554000 |
| 6  | -2.222874000 | -1.886684000 | -1.771951000 |
| 6  | -3.335839000 | 0.228072000  | -1.831987000 |
| 6  | -3.111775000 | -2.374343000 | -2.709540000 |
| 1  | -1.462878000 | -2.534031000 | -1.381742000 |
| 6  | -4.221534000 | -0.262150000 | -2.768286000 |
| 1  | -3.432822000 | 1.246711000  | -1.507251000 |
| 6  | -4.110589000 | -1.565911000 | -3.210332000 |
| 1  | -3.018898000 | -3.391326000 | -3.043997000 |
| 1  | -4.996174000 | 0.376246000  | -3.152785000 |

|   |              |              |              |
|---|--------------|--------------|--------------|
| 1 | -4.799509000 | -1.947766000 | -3.941953000 |
| 6 | -2.053116000 | -0.115295000 | 1.540747000  |
| 6 | -3.435052000 | -0.039190000 | 1.630372000  |
| 6 | -1.313190000 | -0.295497000 | 2.698827000  |
| 6 | -4.061267000 | -0.131601000 | 2.855928000  |
| 1 | -4.030234000 | 0.077517000  | 0.744583000  |
| 6 | -1.939484000 | -0.379852000 | 3.925508000  |
| 1 | -0.244594000 | -0.390152000 | 2.640267000  |
| 6 | -3.314551000 | -0.297859000 | 4.005740000  |
| 1 | -5.133487000 | -0.081631000 | 2.910828000  |
| 1 | -1.353231000 | -0.526570000 | 4.814038000  |
| 1 | -3.804418000 | -0.375947000 | 4.959355000  |
| 6 | -1.163079000 | 1.843530000  | -0.363896000 |
| 6 | -0.843795000 | 2.304968000  | -1.635571000 |
| 6 | -1.420233000 | 2.768587000  | 0.634542000  |
| 6 | -0.795974000 | 3.655379000  | -1.902676000 |
| 1 | -0.644692000 | 1.604806000  | -2.426805000 |
| 6 | -1.364615000 | 4.124178000  | 0.367923000  |
| 1 | -1.672666000 | 2.437838000  | 1.624163000  |
| 6 | -1.055284000 | 4.570345000  | -0.898951000 |
| 1 | -0.554693000 | 3.994587000  | -2.893679000 |
| 1 | -1.569445000 | 4.828103000  | 1.153902000  |
| 1 | -1.016614000 | 5.624218000  | -1.106668000 |
| 6 | 3.377872000  | 0.232630000  | -0.814132000 |
| 6 | 4.241645000  | 1.036778000  | 0.184470000  |
| 6 | 2.144043000  | 1.608986000  | 0.733167000  |
| 6 | 1.925843000  | 0.643461000  | -0.447043000 |
| 6 | 3.362693000  | 1.008254000  | 1.434242000  |
| 1 | 3.749017000  | 1.634015000  | 2.231442000  |
| 1 | 3.193269000  | 0.011862000  | 1.826418000  |
| 6 | 4.169067000  | 2.513645000  | -0.213227000 |
| 1 | 4.366466000  | 2.659046000  | -1.268831000 |
| 6 | 2.732790000  | 2.921280000  | 0.195486000  |
| 1 | 2.154141000  | 3.316144000  | -0.629912000 |
| 1 | 5.248630000  | 0.653914000  | 0.279058000  |
| 1 | 1.273250000  | 1.762003000  | 1.354491000  |
| 1 | 1.481189000  | 1.163463000  | -1.282916000 |
| 1 | 3.637768000  | 0.504481000  | -1.831243000 |

|   |              |              |              |
|---|--------------|--------------|--------------|
| 6 | 3.735316000  | -1.221138000 | -0.713028000 |
| 8 | 2.774887000  | -1.971682000 | -0.110213000 |
| 8 | 4.748463000  | -1.713069000 | -1.081109000 |
| 6 | -0.109079000 | -2.808702000 | 0.577584000  |
| 7 | -0.513864000 | -3.834044000 | 0.892631000  |
| 1 | 4.910389000  | 3.085336000  | 0.332944000  |
| 1 | 2.750429000  | 3.680346000  | 0.970720000  |
| 6 | 3.078129000  | -3.367020000 | 0.070804000  |
| 1 | 2.228011000  | -3.791915000 | 0.574777000  |
| 1 | 3.226232000  | -3.828866000 | -0.893890000 |
| 1 | 3.978927000  | -3.457195000 | 0.658995000  |

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exo-4cP-N

|    |              |              |              |
|----|--------------|--------------|--------------|
| 46 | -0.634989000 | -1.169157000 | -0.457382000 |
| 15 | 0.842783000  | 0.481764000  | 0.004720000  |
| 6  | 1.066649000  | 0.734271000  | 1.793051000  |
| 6  | 0.840798000  | -0.335836000 | 2.647438000  |
| 6  | 1.489618000  | 1.944515000  | 2.329046000  |
| 6  | 1.035579000  | -0.196515000 | 4.007686000  |
| 1  | 0.527615000  | -1.282970000 | 2.248510000  |
| 6  | 1.679651000  | 2.081342000  | 3.688335000  |
| 1  | 1.666501000  | 2.787452000  | 1.687596000  |
| 6  | 1.452160000  | 1.010279000  | 4.530668000  |
| 1  | 0.857583000  | -1.034428000 | 4.656777000  |
| 1  | 2.004352000  | 3.024698000  | 4.088548000  |
| 1  | 1.598058000  | 1.118226000  | 5.590303000  |
| 6  | 2.514409000  | 0.231067000  | -0.671700000 |
| 6  | 2.653983000  | -0.428312000 | -1.883714000 |
| 6  | 3.647507000  | 0.720995000  | -0.037485000 |
| 6  | 3.899278000  | -0.575281000 | -2.460268000 |
| 1  | 1.797272000  | -0.861524000 | -2.362736000 |
| 6  | 4.892295000  | 0.564296000  | -0.610687000 |
| 1  | 3.567783000  | 1.216627000  | 0.911048000  |
| 6  | 5.019554000  | -0.078809000 | -1.826422000 |
| 1  | 3.991472000  | -1.098499000 | -3.394207000 |
| 1  | 5.762416000  | 0.941757000  | -0.104804000 |
| 1  | 5.990599000  | -0.203798000 | -2.270583000 |
| 6  | 0.393388000  | 2.130503000  | -0.646526000 |

|   |              |              |              |
|---|--------------|--------------|--------------|
| 6 | -0.525440000 | 2.933197000  | 0.016567000  |
| 6 | 0.907684000  | 2.576447000  | -1.855335000 |
| 6 | -0.910128000 | 4.149087000  | -0.507869000 |
| 1 | -0.941386000 | 2.615617000  | 0.952939000  |
| 6 | 0.516077000  | 3.790569000  | -2.384661000 |
| 1 | 1.624366000  | 1.982242000  | -2.389026000 |
| 6 | -0.391799000 | 4.581882000  | -1.712631000 |
| 1 | -1.617282000 | 4.757591000  | 0.026233000  |
| 1 | 0.929037000  | 4.117425000  | -3.321683000 |
| 1 | -0.692125000 | 5.529365000  | -2.121867000 |
| 6 | -2.345203000 | 0.131792000  | -0.591164000 |
| 6 | -2.997337000 | 0.579279000  | 0.726275000  |
| 6 | -4.580018000 | -0.752032000 | -0.151709000 |
| 6 | -3.443993000 | -0.800253000 | -1.181253000 |
| 6 | -3.795847000 | -0.652933000 | 1.155703000  |
| 1 | -4.437183000 | -0.466668000 | 2.009872000  |
| 1 | -3.183678000 | -1.522109000 | 1.364023000  |
| 6 | -4.134970000 | 1.559924000  | 0.403928000  |
| 1 | -3.810134000 | 2.356352000  | -0.254012000 |
| 6 | -5.202244000 | 0.645557000  | -0.249714000 |
| 1 | -5.421444000 | 0.921699000  | -1.274852000 |
| 1 | -2.304117000 | 0.947799000  | 1.469344000  |
| 1 | -5.289091000 | -1.565158000 | -0.237141000 |
| 1 | -3.772087000 | -0.552511000 | -2.183228000 |
| 1 | -2.150812000 | 0.961274000  | -1.256371000 |
| 6 | 0.811785000  | -2.643824000 | -0.370865000 |
| 8 | 1.429974000  | -3.115223000 | -1.279581000 |
| 8 | 0.907371000  | -3.194788000 | 0.867638000  |
| 6 | 1.713878000  | -4.355963000 | 0.986457000  |
| 1 | 1.665166000  | -4.651890000 | 2.024696000  |
| 1 | 1.337586000  | -5.149821000 | 0.354409000  |
| 1 | 2.737823000  | -4.145564000 | 0.705171000  |
| 6 | -2.761664000 | -2.094388000 | -1.207765000 |
| 7 | -2.083392000 | -3.015757000 | -1.124564000 |
| 1 | -4.522285000 | 2.019363000  | 1.308247000  |
| 1 | -6.137156000 | 0.677463000  | 0.296719000  |

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exo-4t-O

|    |              |              |              |
|----|--------------|--------------|--------------|
| 46 | -1.132517000 | -1.069147000 | 0.046408000  |
| 6  | 1.151727000  | 0.568082000  | -0.643271000 |
| 6  | 1.628616000  | 1.689835000  | 0.310060000  |
| 6  | -0.613483000 | 1.849170000  | 0.392109000  |
| 6  | -0.394975000 | 0.686033000  | -0.571686000 |
| 6  | 0.538010000  | 1.673328000  | 1.382481000  |
| 1  | 0.631887000  | 2.498574000  | 2.078591000  |
| 1  | 0.483665000  | 0.748484000  | 1.945393000  |
| 6  | 1.354886000  | 3.025263000  | -0.386136000 |
| 1  | 1.751848000  | 3.051289000  | -1.394133000 |
| 6  | -0.188325000 | 3.135264000  | -0.338179000 |
| 1  | -0.636940000 | 3.211301000  | -1.320810000 |
| 1  | 2.650114000  | 1.562846000  | 0.640949000  |
| 1  | -1.609412000 | 1.891192000  | 0.801620000  |
| 1  | -0.847927000 | 0.851219000  | -1.537715000 |
| 1  | 1.534265000  | 0.736082000  | -1.645555000 |
| 6  | 1.640253000  | -0.775636000 | -0.226838000 |
| 8  | 0.899830000  | -1.670904000 | 0.138050000  |
| 8  | 2.931142000  | -0.938240000 | -0.281828000 |
| 6  | 3.459768000  | -2.207873000 | 0.101313000  |
| 1  | 4.527221000  | -2.124131000 | -0.021524000 |
| 1  | 3.209339000  | -2.420567000 | 1.130815000  |
| 1  | 3.061712000  | -2.984598000 | -0.535924000 |
| 6  | -2.964643000 | -0.409145000 | -0.087717000 |
| 7  | -4.042897000 | -0.030360000 | -0.158381000 |
| 1  | 1.822992000  | 3.832785000  | 0.163894000  |
| 1  | -0.501461000 | 4.006022000  | 0.225693000  |

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exo-4t-N

|    |              |              |              |
|----|--------------|--------------|--------------|
| 46 | -0.779013000 | 0.814872000  | -0.016286000 |
| 6  | 0.789741000  | -0.329738000 | -0.600222000 |
| 6  | 1.279213000  | -1.369343000 | 0.398264000  |
| 6  | 2.988125000  | 0.096523000  | 0.338543000  |
| 6  | 1.970464000  | 0.681687000  | -0.658153000 |
| 6  | 2.074648000  | -0.525698000 | 1.396026000  |
| 1  | 2.627539000  | -1.121705000 | 2.112641000  |
| 1  | 1.471289000  | 0.195391000  | 1.934284000  |
| 6  | 2.407949000  | -2.163380000 | -0.282791000 |

|   |              |              |              |
|---|--------------|--------------|--------------|
| 1 | 2.118777000  | -2.518498000 | -1.263952000 |
| 6 | 3.578352000  | -1.149489000 | -0.329702000 |
| 1 | 3.925947000  | -0.949461000 | -1.336749000 |
| 1 | 0.488443000  | -1.987673000 | 0.791682000  |
| 1 | 3.721938000  | 0.813096000  | 0.681905000  |
| 1 | 2.388099000  | 0.816852000  | -1.648890000 |
| 1 | 0.525577000  | -0.743903000 | -1.561284000 |
| 6 | -2.019201000 | -0.706633000 | -0.116108000 |
| 8 | -1.882728000 | -1.863394000 | -0.356328000 |
| 8 | -3.221678000 | -0.168086000 | 0.171257000  |
| 6 | -4.338247000 | -1.050510000 | 0.173937000  |
| 1 | -5.196708000 | -0.445311000 | 0.422617000  |
| 1 | -4.464477000 | -1.502893000 | -0.800658000 |
| 1 | -4.200887000 | -1.831741000 | 0.909630000  |
| 6 | 1.388119000  | 1.952289000  | -0.227809000 |
| 7 | 0.778641000  | 2.852308000  | 0.126943000  |
| 1 | 2.668897000  | -3.032227000 | 0.310458000  |
| 1 | 4.429946000  | -1.504576000 | 0.237557000  |

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exo-4t-N'

|    |              |              |              |
|----|--------------|--------------|--------------|
| 46 | 0.757017000  | -1.000959000 | 0.008835000  |
| 6  | -0.659516000 | 0.343941000  | -0.568464000 |
| 6  | -1.090228000 | 1.382833000  | 0.462206000  |
| 6  | -2.932121000 | 0.104898000  | 0.261819000  |
| 6  | -1.935812000 | -0.535833000 | -0.720991000 |
| 6  | -2.008282000 | 0.579397000  | 1.384535000  |
| 1  | -2.528928000 | 1.194368000  | 2.109366000  |
| 1  | -1.503801000 | -0.224315000 | 1.907066000  |
| 6  | -2.102247000 | 2.321485000  | -0.217228000 |
| 1  | -1.737379000 | 2.692809000  | -1.166988000 |
| 6  | -3.364118000 | 1.434717000  | -0.364476000 |
| 1  | -3.682680000 | 1.319049000  | -1.394046000 |
| 1  | -0.264143000 | 1.896835000  | 0.927790000  |
| 1  | -3.749235000 | -0.546686000 | 0.540422000  |
| 1  | -2.322380000 | -0.583326000 | -1.732248000 |
| 1  | -0.334087000 | 0.779023000  | -1.501447000 |
| 6  | 2.258070000  | 0.225403000  | 0.049975000  |
| 8  | 3.285300000  | -0.312032000 | 0.353116000  |



|   |              |              |              |
|---|--------------|--------------|--------------|
| 8 | 2.170298000  | 1.517609000  | -0.233599000 |
| 6 | 3.382582000  | 2.263475000  | -0.164581000 |
| 1 | 3.120106000  | 3.277186000  | -0.425944000 |
| 1 | 3.795208000  | 2.225072000  | 0.834534000  |
| 1 | 4.109732000  | 1.869517000  | -0.861642000 |
| 6 | -1.508109000 | -1.878604000 | -0.329322000 |
| 7 | -1.015222000 | -2.854353000 | 0.006382000  |
| 1 | -2.303394000 | 3.182397000  | 0.410414000  |
| 1 | -4.201331000 | 1.847757000  | 0.184665000  |

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exo-4c-O

|    |              |              |              |
|----|--------------|--------------|--------------|
| 46 | -1.316003000 | -0.592762000 | 0.209245000  |
| 6  | 1.417727000  | 0.482197000  | 0.598887000  |
| 6  | 2.458051000  | 0.166196000  | -0.499741000 |
| 6  | 1.294550000  | -1.745744000 | -0.309252000 |
| 6  | 0.614969000  | -0.834062000 | 0.702581000  |
| 6  | 1.667385000  | -0.762132000 | -1.422282000 |
| 1  | 2.285174000  | -1.205636000 | -2.194180000 |
| 1  | 0.811445000  | -0.292538000 | -1.893591000 |
| 6  | 3.477859000  | -0.803233000 | 0.107221000  |
| 1  | 3.864296000  | -0.449656000 | 1.055579000  |
| 6  | 2.683119000  | -2.126338000 | 0.236100000  |
| 1  | 2.634255000  | -2.489378000 | 1.255178000  |
| 1  | 2.896316000  | 1.047345000  | -0.947383000 |
| 1  | 0.700638000  | -2.604612000 | -0.602824000 |
| 1  | 0.592001000  | -1.242726000 | 1.710973000  |
| 1  | 1.916302000  | 0.766389000  | 1.520176000  |
| 6  | 0.503502000  | 1.598445000  | 0.232812000  |
| 8  | -0.686383000 | 1.423991000  | 0.030710000  |
| 8  | 1.042975000  | 2.777536000  | 0.141345000  |
| 6  | 0.190600000  | 3.873233000  | -0.207317000 |
| 1  | 0.831424000  | 4.739368000  | -0.226699000 |
| 1  | -0.255415000 | 3.702228000  | -1.176303000 |
| 1  | -0.587898000 | 3.986731000  | 0.533073000  |
| 6  | -3.347232000 | -0.563316000 | -0.294140000 |
| 7  | -4.459542000 | -0.597719000 | -0.568179000 |
| 1  | 4.322461000  | -0.919549000 | -0.560866000 |
| 1  | 3.126039000  | -2.910577000 | -0.366830000 |

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exo-4c-OMe

|    |              |              |              |
|----|--------------|--------------|--------------|
| 46 | 1.106870000  | -0.715580000 | -0.216949000 |
| 6  | -1.430217000 | 0.784151000  | -0.591424000 |
| 6  | -2.522042000 | 0.612297000  | 0.486092000  |
| 6  | -1.605904000 | -1.431657000 | 0.334055000  |
| 6  | -0.826522000 | -0.623401000 | -0.689078000 |
| 6  | -1.862253000 | -0.392958000 | 1.430202000  |
| 1  | -2.532979000 | -0.747867000 | 2.203329000  |
| 1  | -0.958965000 | -0.023005000 | 1.903210000  |
| 6  | -3.648335000 | -0.230669000 | -0.121018000 |
| 1  | -3.973739000 | 0.152872000  | -1.080381000 |
| 6  | -3.028677000 | -1.645944000 | -0.218178000 |
| 1  | -3.019881000 | -2.034694000 | -1.228772000 |
| 1  | -2.844670000 | 1.550711000  | 0.913100000  |
| 1  | -1.122957000 | -2.355460000 | 0.637424000  |
| 1  | -0.845615000 | -1.038304000 | -1.695857000 |
| 1  | -1.866013000 | 1.116098000  | -1.528480000 |
| 6  | -0.461105000 | 1.874001000  | -0.212152000 |
| 8  | -0.729212000 | 3.002355000  | 0.009463000  |
| 8  | 0.823352000  | 1.426280000  | -0.148712000 |
| 6  | 1.842234000  | 2.386337000  | 0.197866000  |
| 1  | 2.766581000  | 1.834009000  | 0.212638000  |
| 1  | 1.857386000  | 3.167404000  | -0.547092000 |
| 1  | 1.622268000  | 2.804830000  | 1.168282000  |
| 6  | 3.138280000  | -0.926509000 | 0.276531000  |
| 7  | 4.250513000  | -0.969831000 | 0.549337000  |
| 1  | -4.509928000 | -0.227910000 | 0.535087000  |
| 1  | -3.566983000 | -2.356156000 | 0.398433000  |

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exo-4c-N

|    |              |              |              |
|----|--------------|--------------|--------------|
| 46 | -0.717553000 | 0.259005000  | -0.187903000 |
| 6  | 1.231518000  | -0.335160000 | -0.722682000 |
| 6  | 1.884046000  | -1.331302000 | 0.231320000  |
| 6  | 3.096027000  | 0.535653000  | 0.564832000  |
| 6  | 2.090173000  | 0.938082000  | -0.521574000 |
| 6  | 2.280458000  | -0.441567000 | 1.412488000  |
| 1  | 2.892128000  | -0.954179000 | 2.145915000  |

|   |              |              |              |
|---|--------------|--------------|--------------|
| 1 | 1.438317000  | 0.013606000  | 1.919695000  |
| 6 | 3.266182000  | -1.707646000 | -0.327898000 |
| 1 | 3.214666000  | -2.004537000 | -1.368209000 |
| 6 | 4.091104000  | -0.412008000 | -0.116933000 |
| 1 | 4.477106000  | -0.001930000 | -1.043090000 |
| 1 | 1.263089000  | -2.184347000 | 0.468965000  |
| 1 | 3.552182000  | 1.370276000  | 1.080153000  |
| 1 | 2.564998000  | 1.348798000  | -1.403892000 |
| 1 | 1.202638000  | -0.660097000 | -1.755367000 |
| 6 | -2.680366000 | -0.068544000 | 0.080634000  |
| 8 | -2.310085000 | -1.182391000 | -0.289884000 |
| 8 | -3.916626000 | 0.196468000  | 0.378458000  |
| 6 | -4.868767000 | -0.865928000 | 0.262083000  |
| 1 | -5.817523000 | -0.441553000 | 0.549640000  |
| 1 | -4.905560000 | -1.224177000 | -0.757371000 |
| 1 | -4.601325000 | -1.680735000 | 0.920576000  |
| 6 | 1.024778000  | 1.835983000  | -0.076329000 |
| 7 | 0.059193000  | 2.375799000  | 0.243441000  |
| 1 | 3.695751000  | -2.536263000 | 0.224975000  |
| 1 | 4.939393000  | -0.587670000 | 0.533203000  |

27

exo-4c-N'

|    |              |              |              |
|----|--------------|--------------|--------------|
| 46 | -0.717885000 | 0.258177000  | -0.188083000 |
| 6  | 1.232122000  | -0.335021000 | -0.722711000 |
| 6  | 1.884993000  | -1.330926000 | 0.231349000  |
| 6  | 3.096291000  | 0.536481000  | 0.565034000  |
| 6  | 2.090510000  | 0.938497000  | -0.521536000 |
| 6  | 2.280893000  | -0.440969000 | 1.412545000  |
| 1  | 2.892590000  | -0.953276000 | 2.146165000  |
| 1  | 1.438504000  | 0.013952000  | 1.919578000  |
| 6  | 3.267362000  | -1.706700000 | -0.327707000 |
| 1  | 3.216090000  | -2.003587000 | -1.368044000 |
| 6  | 4.091796000  | -0.410827000 | -0.116568000 |
| 1  | 4.477849000  | -0.000562000 | -1.042619000 |
| 1  | 1.264330000  | -2.184198000 | 0.468921000  |
| 1  | 3.552129000  | 1.371250000  | 1.080434000  |
| 1  | 2.565528000  | 1.349349000  | -1.403691000 |
| 1  | 1.203472000  | -0.659894000 | -1.755408000 |

|   |              |              |              |
|---|--------------|--------------|--------------|
| 6 | -2.680253000 | -0.069308000 | 0.080479000  |
| 8 | -2.311280000 | -1.183948000 | -0.289732000 |
| 8 | -3.916010000 | 0.197544000  | 0.378345000  |
| 6 | -4.869832000 | -0.863401000 | 0.262778000  |
| 1 | -5.817771000 | -0.437395000 | 0.550619000  |
| 1 | -4.907625000 | -1.221886000 | -0.756556000 |
| 1 | -4.603306000 | -1.678379000 | 0.921401000  |
| 6 | 1.024688000  | 1.835429000  | -0.076698000 |
| 7 | 0.058654000  | 2.374512000  | 0.243069000  |
| 1 | 3.697164000  | -2.535218000 | 0.225127000  |
| 1 | 4.940096000  | -0.586162000 | 0.533691000  |

44

exo-4t2N-O

|    |              |              |              |
|----|--------------|--------------|--------------|
| 46 | 0.245517000  | -0.288222000 | -0.476701000 |
| 6  | -2.601759000 | 0.398573000  | -0.473120000 |
| 6  | -3.485460000 | 0.141646000  | 0.769479000  |
| 6  | -2.186622000 | -1.689427000 | 0.659120000  |
| 6  | -1.698213000 | -0.865268000 | -0.537483000 |
| 6  | -2.518030000 | -0.607380000 | 1.687220000  |
| 1  | -3.006218000 | -0.992794000 | 2.575326000  |
| 1  | -1.656101000 | -0.023083000 | 1.990073000  |
| 6  | -4.478891000 | -0.964000000 | 0.402041000  |
| 1  | -4.996185000 | -0.756054000 | -0.527436000 |
| 6  | -3.587824000 | -2.228223000 | 0.331821000  |
| 1  | -3.617911000 | -2.711556000 | -0.636742000 |
| 1  | -3.946941000 | 1.037618000  | 1.162354000  |
| 1  | -1.492594000 | -2.454047000 | 0.969131000  |
| 1  | -1.835409000 | -1.399089000 | -1.466623000 |
| 1  | -3.224168000 | 0.519361000  | -1.355243000 |
| 6  | -1.811621000 | 1.652795000  | -0.349437000 |
| 8  | -0.594965000 | 1.674878000  | -0.299138000 |
| 8  | -2.512417000 | 2.753223000  | -0.302303000 |
| 6  | -1.809141000 | 3.987229000  | -0.188089000 |
| 1  | -2.568811000 | 4.751542000  | -0.158465000 |
| 1  | -1.220499000 | 4.000910000  | 0.718331000  |
| 1  | -1.161208000 | 4.129124000  | -1.041684000 |
| 6  | 0.720443000  | -2.171521000 | -0.687010000 |
| 7  | 1.018694000  | -3.270836000 | -0.804388000 |

|   |              |              |              |
|---|--------------|--------------|--------------|
| 1 | -5.233166000 | -1.057221000 | 1.174622000  |
| 1 | -3.895830000 | -2.962484000 | 1.067785000  |
| 6 | 4.571708000  | 1.210485000  | 0.855011000  |
| 6 | 3.070652000  | 0.948199000  | 1.152102000  |
| 6 | 3.666802000  | -0.861423000 | -0.027179000 |
| 6 | 4.982613000  | -0.039545000 | 0.039281000  |
| 1 | 4.726211000  | 2.136165000  | 0.314793000  |
| 1 | 5.129014000  | 1.276208000  | 1.782169000  |
| 1 | 5.362858000  | 0.206115000  | -0.944131000 |
| 1 | 5.748494000  | -0.608983000 | 0.551971000  |
| 6 | 3.094977000  | -0.567249000 | 1.361406000  |
| 1 | 2.118400000  | -1.003700000 | 1.517152000  |
| 1 | 3.760566000  | -0.870306000 | 2.161569000  |
| 6 | 2.390181000  | 1.042254000  | -0.193330000 |
| 1 | 1.934673000  | 1.933868000  | -0.580727000 |
| 6 | 2.753701000  | -0.037058000 | -0.898641000 |
| 1 | 2.636926000  | -0.183385000 | -1.955694000 |
| 1 | 2.653899000  | 1.556741000  | 1.941579000  |
| 1 | 3.777324000  | -1.896218000 | -0.308783000 |

44

exo-4t2N-N

|    |              |              |              |
|----|--------------|--------------|--------------|
| 46 | 0.067810000  | -0.069147000 | -0.473792000 |
| 6  | -1.979132000 | 0.251595000  | -0.385810000 |
| 6  | -2.606169000 | 0.419951000  | 1.000584000  |
| 6  | -3.465493000 | -1.543879000 | 0.318144000  |
| 6  | -2.580442000 | -1.104566000 | -0.860389000 |
| 6  | -2.671572000 | -1.019165000 | 1.514288000  |
| 1  | -3.218215000 | -1.115489000 | 2.445427000  |
| 1  | -1.699352000 | -1.482799000 | 1.631142000  |
| 6  | -4.099241000 | 0.733350000  | 0.817811000  |
| 1  | -4.261907000 | 1.542363000  | 0.115937000  |
| 6  | -4.683228000 | -0.613810000 | 0.322212000  |
| 1  | -5.145050000 | -0.540760000 | -0.655898000 |
| 1  | -2.083041000 | 1.121982000  | 1.631843000  |
| 1  | -3.707300000 | -2.598568000 | 0.312907000  |
| 1  | -3.133638000 | -1.042256000 | -1.790279000 |
| 1  | -2.242306000 | 1.053257000  | -1.060750000 |
| 6  | 0.182085000  | 1.816661000  | 0.101081000  |

|   |              |              |              |
|---|--------------|--------------|--------------|
| 8 | 0.288798000  | 2.198918000  | 1.226432000  |
| 8 | 0.164194000  | 2.674160000  | -0.932428000 |
| 6 | 0.270777000  | 4.054643000  | -0.609908000 |
| 1 | 0.229877000  | 4.581611000  | -1.551487000 |
| 1 | -0.545805000 | 4.363435000  | 0.029334000  |
| 1 | 1.204989000  | 4.261641000  | -0.104246000 |
| 6 | -1.433586000 | -1.986411000 | -1.075333000 |
| 7 | -0.455170000 | -2.565510000 | -1.197082000 |
| 1 | -4.548804000 | 1.027593000  | 1.760008000  |
| 1 | -5.436308000 | -0.991259000 | 1.003399000  |
| 6 | 4.639207000  | -0.129403000 | 0.468632000  |
| 6 | 3.220607000  | 0.462791000  | 0.687389000  |
| 6 | 2.822490000  | -1.733608000 | 0.490250000  |
| 6 | 4.364483000  | -1.646996000 | 0.335242000  |
| 1 | 5.128013000  | 0.288064000  | -0.402609000 |
| 1 | 5.265236000  | 0.083172000  | 1.327002000  |
| 1 | 4.703931000  | -2.055769000 | -0.608040000 |
| 1 | 4.849887000  | -2.205529000 | 1.126854000  |
| 6 | 2.593144000  | -0.642401000 | 1.538705000  |
| 1 | 1.551316000  | -0.460394000 | 1.765733000  |
| 1 | 3.138512000  | -0.822963000 | 2.457948000  |
| 6 | 2.518091000  | 0.251191000  | -0.632133000 |
| 1 | 2.494137000  | 0.972875000  | -1.426734000 |
| 6 | 2.279152000  | -1.066362000 | -0.750271000 |
| 1 | 2.033210000  | -1.590875000 | -1.654097000 |
| 1 | 3.196939000  | 1.465407000  | 1.084955000  |
| 1 | 2.441653000  | -2.721532000 | 0.700671000  |

44

exo-4t2N-N'

|    |              |              |              |
|----|--------------|--------------|--------------|
| 46 | 0.064512000  | -0.157482000 | -0.536156000 |
| 6  | -1.989896000 | 0.122779000  | -0.539811000 |
| 6  | -2.658305000 | 0.653724000  | 0.730785000  |
| 6  | -3.453099000 | -1.446503000 | 0.614079000  |
| 6  | -2.550022000 | -1.328385000 | -0.624979000 |
| 6  | -2.702228000 | -0.583711000 | 1.628330000  |
| 1  | -3.270182000 | -0.431599000 | 2.539164000  |
| 1  | -1.722247000 | -0.966464000 | 1.886995000  |
| 6  | -4.153028000 | 0.858725000  | 0.438805000  |

|            |              |              |              |
|------------|--------------|--------------|--------------|
| 1          | -4.314775000 | 1.430516000  | -0.466784000 |
| 6          | -4.692639000 | -0.590118000 | 0.335628000  |
| 1          | -5.132731000 | -0.809795000 | -0.630358000 |
| 1          | -2.171110000 | 1.520721000  | 1.149798000  |
| 1          | -3.668893000 | -2.467043000 | 0.901689000  |
| 1          | -3.082126000 | -1.542780000 | -1.544446000 |
| 1          | -2.252092000 | 0.696731000  | -1.416825000 |
| 6          | 0.135219000  | 1.814913000  | -0.621665000 |
| 8          | 0.134332000  | 2.468989000  | -1.618620000 |
| 8          | 0.232101000  | 2.385920000  | 0.591866000  |
| 6          | 0.319878000  | 3.804481000  | 0.614979000  |
| 1          | 0.387760000  | 4.079804000  | 1.656968000  |
| 1          | 1.195742000  | 4.145185000  | 0.078294000  |
| 1          | -0.557155000 | 4.250500000  | 0.164520000  |
| 6          | -1.379640000 | -2.203651000 | -0.566954000 |
| 7          | -0.386750000 | -2.767693000 | -0.507505000 |
| 1          | -4.634213000 | 1.394322000  | 1.250152000  |
| 1          | -5.452269000 | -0.781904000 | 1.083832000  |
| 6          | 4.650752000  | -0.011387000 | 0.379820000  |
| 6          | 3.227499000  | 0.596399000  | 0.505743000  |
| 6          | 2.849402000  | -1.605010000 | 0.680522000  |
| 6          | 4.389574000  | -1.532047000 | 0.503950000  |
| 1          | 5.129754000  | 0.259366000  | -0.552475000 |
| 1          | 5.279789000  | 0.346970000  | 1.186026000  |
| 1          | 4.728225000  | -2.089690000 | -0.359892000 |
| 1          | 4.884331000  | -1.946110000 | 1.374583000  |
| 6          | 2.614822000  | -0.356146000 | 1.534020000  |
| 1          | 1.570463000  | -0.152003000 | 1.730973000  |
| 1          | 3.164701000  | -0.376641000 | 2.468121000  |
| 6          | 2.519137000  | 0.162824000  | -0.754934000 |
| 1          | 2.479752000  | 0.744238000  | -1.656459000 |
| 6          | 2.292759000  | -1.157579000 | -0.649255000 |
| 1          | 2.045930000  | -1.827258000 | -1.451368000 |
| 1          | 3.201334000  | 1.652149000  | 0.728013000  |
| 1          | 2.477117000  | -2.546307000 | 1.054828000  |
| 44         |              |              |              |
| exo-4c2N-O |              |              |              |
| 46         | 0.292053000  | 0.686613000  | -0.215455000 |

|   |              |              |              |
|---|--------------|--------------|--------------|
| 6 | -2.430571000 | -0.457855000 | -0.610208000 |
| 6 | -3.119325000 | -1.415328000 | 0.384607000  |
| 6 | -0.990767000 | -2.126007000 | 0.350941000  |
| 6 | -0.950302000 | -0.945862000 | -0.634232000 |
| 6 | -1.998709000 | -1.650357000 | 1.397397000  |
| 1 | -2.250531000 | -2.410954000 | 2.128114000  |
| 1 | -1.685231000 | -0.754475000 | 1.921430000  |
| 6 | -3.223974000 | -2.786243000 | -0.288555000 |
| 1 | -3.652287000 | -2.720739000 | -1.281884000 |
| 6 | -1.759968000 | -3.289795000 | -0.292738000 |
| 1 | -1.398070000 | -3.514894000 | -1.288943000 |
| 1 | -4.058284000 | -1.039257000 | 0.767467000  |
| 1 | -0.026511000 | -2.419651000 | 0.737642000  |
| 1 | -0.701637000 | -1.290049000 | -1.632259000 |
| 1 | -2.914070000 | -0.511429000 | -1.581382000 |
| 6 | -2.526779000 | 0.957856000  | -0.168525000 |
| 8 | -1.548433000 | 1.620409000  | 0.124927000  |
| 8 | -3.725332000 | 1.464256000  | -0.108720000 |
| 6 | -3.846160000 | 2.827437000  | 0.303911000  |
| 1 | -4.900709000 | 3.046986000  | 0.264470000  |
| 1 | -3.466362000 | 2.947132000  | 1.308376000  |
| 1 | -3.293355000 | 3.469789000  | -0.366220000 |
| 6 | 1.230477000  | 2.487213000  | 0.142203000  |
| 7 | 1.704260000  | 3.511961000  | 0.336023000  |
| 1 | -3.862168000 | -3.440975000 | 0.293058000  |
| 1 | -1.659315000 | -4.193355000 | 0.299359000  |
| 6 | 4.642736000  | -0.464418000 | -0.383780000 |
| 6 | 3.552836000  | 0.566646000  | 0.012192000  |
| 6 | 2.671702000  | -1.385966000 | 0.676678000  |
| 6 | 4.037710000  | -1.812266000 | 0.079525000  |
| 1 | 4.863957000  | -0.444840000 | -1.443764000 |
| 1 | 5.562999000  | -0.243340000 | 0.142707000  |
| 1 | 3.929386000  | -2.526541000 | -0.727614000 |
| 1 | 4.647566000  | -2.276975000 | 0.845065000  |
| 6 | 3.054373000  | -0.053156000 | 1.317576000  |
| 1 | 2.224504000  | 0.484626000  | 1.752788000  |
| 1 | 3.842391000  | -0.157878000 | 2.053780000  |
| 6 | 2.415329000  | 0.254489000  | -0.928101000 |



|   |             |              |              |
|---|-------------|--------------|--------------|
| 1 | 2.345997000 | 0.669941000  | -1.916041000 |
| 6 | 1.879885000 | -0.933539000 | -0.528998000 |
| 1 | 1.372181000 | -1.621667000 | -1.172564000 |
| 1 | 3.869785000 | 1.595245000  | 0.040422000  |
| 1 | 2.204660000 | -2.129024000 | 1.305747000  |

44

exo-4c2N-OMe

|    |              |              |              |
|----|--------------|--------------|--------------|
| 46 | 0.256338000  | 0.655145000  | -0.194570000 |
| 6  | -2.536514000 | -0.283875000 | -0.666102000 |
| 6  | -3.346285000 | -1.162527000 | 0.312166000  |
| 6  | -1.262211000 | -1.971990000 | 0.485910000  |
| 6  | -1.102039000 | -0.865231000 | -0.571776000 |
| 6  | -2.320550000 | -1.388484000 | 1.421784000  |
| 1  | -2.660926000 | -2.092736000 | 2.172533000  |
| 1  | -2.005595000 | -0.477568000 | 1.918474000  |
| 6  | -3.466960000 | -2.562753000 | -0.294377000 |
| 1  | -3.804277000 | -2.531891000 | -1.323592000 |
| 6  | -2.038166000 | -3.138647000 | -0.143622000 |
| 1  | -1.610379000 | -3.451872000 | -1.088733000 |
| 1  | -4.290527000 | -0.718264000 | 0.594051000  |
| 1  | -0.342133000 | -2.280146000 | 0.960263000  |
| 1  | -0.828344000 | -1.287035000 | -1.532040000 |
| 1  | -2.943827000 | -0.363253000 | -1.668391000 |
| 6  | -2.719029000 | 1.158109000  | -0.297859000 |
| 8  | -3.734616000 | 1.763583000  | -0.346753000 |
| 8  | -1.574214000 | 1.749613000  | 0.140546000  |
| 6  | -1.697721000 | 3.126103000  | 0.558332000  |
| 1  | -0.721267000 | 3.424240000  | 0.894017000  |
| 1  | -2.014343000 | 3.723867000  | -0.282707000 |
| 1  | -2.432150000 | 3.184227000  | 1.347051000  |
| 6  | 1.373262000  | 2.378476000  | 0.114851000  |
| 7  | 1.914031000  | 3.372281000  | 0.296805000  |
| 1  | -4.187376000 | -3.151307000 | 0.261146000  |
| 1  | -2.033669000 | -4.001023000 | 0.514554000  |
| 6  | 4.479400000  | -0.889588000 | -0.536274000 |
| 6  | 3.506874000  | 0.261879000  | -0.163815000 |
| 6  | 2.538449000  | -1.540544000 | 0.756049000  |
| 6  | 3.814464000  | -2.133347000 | 0.102414000  |

|   |             |              |              |
|---|-------------|--------------|--------------|
| 1 | 4.614075000 | -0.987222000 | -1.606340000 |
| 1 | 5.453350000 | -0.697002000 | -0.103899000 |
| 1 | 3.586586000 | -2.908437000 | -0.619030000 |
| 1 | 4.447631000 | -2.573446000 | 0.863306000  |
| 6 | 3.073494000 | -0.191498000 | 1.230603000  |
| 1 | 2.327841000 | 0.450927000  | 1.674764000  |
| 1 | 3.910889000 | -0.293563000 | 1.910180000  |
| 6 | 2.277936000 | -0.043058000 | -0.984474000 |
| 1 | 2.162512000 | 0.275267000  | -2.004302000 |
| 6 | 1.691791000 | -1.140689000 | -0.428392000 |
| 1 | 1.083692000 | -1.842893000 | -0.958082000 |
| 1 | 3.904921000 | 1.257685000  | -0.260309000 |
| 1 | 2.067047000 | -2.180774000 | 1.486825000  |

44

exo-4c2N-N

|    |              |              |              |
|----|--------------|--------------|--------------|
| 46 | -0.146828000 | -0.517633000 | -0.216906000 |
| 6  | 2.709190000  | -1.038781000 | -0.574761000 |
| 6  | 3.760917000  | -0.668617000 | 0.479516000  |
| 6  | 2.520093000  | 1.193312000  | 0.270812000  |
| 6  | 1.827503000  | 0.236998000  | -0.703552000 |
| 6  | 2.965506000  | 0.259097000  | 1.397621000  |
| 1  | 3.594233000  | 0.746480000  | 2.134152000  |
| 1  | 2.145337000  | -0.230328000 | 1.909261000  |
| 6  | 4.721311000  | 0.314941000  | -0.197476000 |
| 1  | 5.072080000  | -0.051226000 | -1.155590000 |
| 6  | 3.877707000  | 1.609331000  | -0.317798000 |
| 1  | 3.787377000  | 1.954346000  | -1.340780000 |
| 1  | 4.242928000  | -1.520154000 | 0.941457000  |
| 1  | 1.913722000  | 2.032339000  | 0.577956000  |
| 1  | 1.834446000  | 0.603786000  | -1.721967000 |
| 1  | 3.152468000  | -1.394032000 | -1.497221000 |
| 6  | -1.828692000 | -1.543148000 | 0.356488000  |
| 8  | -2.237907000 | -1.588232000 | 1.476521000  |
| 8  | -2.347262000 | -2.307963000 | -0.617182000 |
| 6  | -3.342357000 | -3.244408000 | -0.226594000 |
| 1  | -3.626215000 | -3.769874000 | -1.126286000 |
| 1  | -2.945922000 | -3.937527000 | 0.503425000  |
| 1  | -4.199511000 | -2.739653000 | 0.200377000  |

|   |              |              |              |
|---|--------------|--------------|--------------|
| 6 | 1.735875000  | -2.026062000 | -0.110754000 |
| 7 | 0.849121000  | -2.659896000 | 0.249343000  |
| 1 | 5.594523000  | 0.470483000  | 0.424466000  |
| 1 | 4.320954000  | 2.415349000  | 0.258075000  |
| 6 | -3.272089000 | 2.688081000  | -0.231686000 |
| 6 | -2.777636000 | 1.334886000  | 0.339724000  |
| 6 | -0.904166000 | 2.563698000  | 0.256956000  |
| 6 | -1.979683000 | 3.538443000  | -0.284068000 |
| 1 | -3.743701000 | 2.578504000  | -1.200521000 |
| 1 | -4.004262000 | 3.123979000  | 0.437329000  |
| 1 | -1.748051000 | 3.892562000  | -1.281156000 |
| 1 | -2.052959000 | 4.406709000  | 0.360150000  |
| 6 | -1.711028000 | 1.819980000  | 1.320939000  |
| 1 | -1.178145000 | 1.010236000  | 1.799690000  |
| 1 | -2.114875000 | 2.483250000  | 2.076771000  |
| 6 | -1.931508000 | 0.761189000  | -0.771108000 |
| 1 | -2.355221000 | 0.234817000  | -1.605077000 |
| 6 | -0.777850000 | 1.512352000  | -0.823676000 |
| 1 | -0.218077000 | 1.687389000  | -1.721464000 |
| 1 | -3.549021000 | 0.692676000  | 0.731816000  |
| 1 | 0.010929000  | 3.042100000  | 0.569190000  |

44

exo-4c2N-N'

|    |              |              |              |
|----|--------------|--------------|--------------|
| 46 | -0.119450000 | -0.517793000 | -0.402886000 |
| 6  | 2.770152000  | -0.913296000 | -0.590930000 |
| 6  | 3.744281000  | -0.619791000 | 0.557632000  |
| 6  | 2.455620000  | 1.218335000  | 0.452226000  |
| 6  | 1.855795000  | 0.343980000  | -0.651676000 |
| 6  | 2.863993000  | 0.190398000  | 1.509259000  |
| 1  | 3.430143000  | 0.619940000  | 2.328009000  |
| 1  | 2.031375000  | -0.370263000 | 1.917253000  |
| 6  | 4.709559000  | 0.451958000  | 0.040569000  |
| 1  | 5.129104000  | 0.191826000  | -0.924467000 |
| 6  | 3.831226000  | 1.727745000  | -0.006960000 |
| 1  | 3.790605000  | 2.169152000  | -0.995455000 |
| 1  | 4.226227000  | -1.499011000 | 0.964518000  |
| 1  | 1.804834000  | 2.006610000  | 0.799918000  |
| 1  | 1.912130000  | 0.809498000  | -1.627419000 |

|   |              |              |              |
|---|--------------|--------------|--------------|
| 1 | 3.278034000  | -1.164371000 | -1.514218000 |
| 6 | -1.803768000 | -1.686050000 | -0.245884000 |
| 8 | -2.344554000 | -2.253091000 | -1.145719000 |
| 8 | -2.161348000 | -1.890400000 | 1.033064000  |
| 6 | -3.164778000 | -2.870110000 | 1.261840000  |
| 1 | -3.313336000 | -2.900958000 | 2.331074000  |
| 1 | -4.086371000 | -2.601263000 | 0.761287000  |
| 1 | -2.841395000 | -3.836900000 | 0.899621000  |
| 6 | 1.804160000  | -1.966915000 | -0.284109000 |
| 7 | 0.919596000  | -2.655330000 | -0.036270000 |
| 1 | 5.538269000  | 0.569853000  | 0.728215000  |
| 1 | 4.211602000  | 2.485234000  | 0.670768000  |
| 6 | -3.342277000 | 2.583671000  | -0.199047000 |
| 6 | -2.833102000 | 1.180495000  | 0.218438000  |
| 6 | -1.006468000 | 2.462136000  | 0.428410000  |
| 6 | -2.081715000 | 3.469718000  | -0.049930000 |
| 1 | -3.746619000 | 2.591089000  | -1.203528000 |
| 1 | -4.131329000 | 2.904442000  | 0.470449000  |
| 1 | -1.800705000 | 3.961495000  | -0.973039000 |
| 1 | -2.228235000 | 4.240586000  | 0.697439000  |
| 6 | -1.851405000 | 1.559333000  | 1.326878000  |
| 1 | -1.315576000 | 0.709718000  | 1.727873000  |
| 1 | -2.326392000 | 2.103075000  | 2.135158000  |
| 6 | -1.897211000 | 0.787620000  | -0.898386000 |
| 1 | -2.246411000 | 0.356318000  | -1.816967000 |
| 6 | -0.772807000 | 1.570686000  | -0.771620000 |
| 1 | -0.158844000 | 1.877454000  | -1.595448000 |
| 1 | -3.607264000 | 0.470605000  | 0.462070000  |
| 1 | -0.132611000 | 2.920107000  | 0.864510000  |

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exo-4tT-O

|    |              |              |              |
|----|--------------|--------------|--------------|
| 46 | 0.089587000  | -0.917431000 | -0.259583000 |
| 6  | -2.066827000 | 1.009219000  | -0.634531000 |
| 6  | -3.024908000 | 1.368256000  | 0.524796000  |
| 6  | -2.756922000 | -0.854191000 | 0.733287000  |
| 6  | -1.878546000 | -0.525817000 | -0.477087000 |
| 6  | -2.581028000 | 0.385929000  | 1.610040000  |
| 1  | -3.238371000 | 0.398854000  | 2.472103000  |

|           |              |              |              |
|-----------|--------------|--------------|--------------|
| 1         | -1.561111000 | 0.532158000  | 1.947594000  |
| 6         | -4.407041000 | 0.819463000  | 0.160696000  |
| 1         | -4.716925000 | 1.118766000  | -0.833827000 |
| 6         | -4.226425000 | -0.711370000 | 0.305593000  |
| 1         | -4.434457000 | -1.248795000 | -0.611273000 |
| 1         | -3.019020000 | 2.420022000  | 0.777003000  |
| 1         | -2.529374000 | -1.804978000 | 1.187625000  |
| 1         | -2.196036000 | -1.061093000 | -1.359980000 |
| 1         | -2.511610000 | 1.283652000  | -1.586724000 |
| 6         | -0.776709000 | 1.745937000  | -0.548346000 |
| 8         | 0.294954000  | 1.199853000  | -0.366494000 |
| 8         | -0.864520000 | 3.041754000  | -0.687693000 |
| 6         | 0.340457000  | 3.798856000  | -0.617768000 |
| 1         | 0.046958000  | 4.825139000  | -0.768988000 |
| 1         | 0.803981000  | 3.674692000  | 0.350894000  |
| 1         | 1.027689000  | 3.480839000  | -1.388993000 |
| 6         | -0.319684000 | -2.826171000 | -0.198652000 |
| 7         | -0.513453000 | -3.953978000 | -0.152530000 |
| 1         | -5.150176000 | 1.194641000  | 0.854496000  |
| 1         | -4.884568000 | -1.110811000 | 1.068894000  |
| 6         | 3.650342000  | 0.651468000  | 0.740520000  |
| 6         | 3.766265000  | 0.569808000  | -0.645269000 |
| 6         | 3.030812000  | -0.383195000 | 1.407874000  |
| 1         | 4.254228000  | 1.366415000  | -1.180303000 |
| 1         | 2.940761000  | -0.347544000 | 2.479173000  |
| 6         | 3.275785000  | -0.510094000 | -1.336603000 |
| 6         | 2.533604000  | -1.484325000 | 0.720258000  |
| 1         | 3.384292000  | -0.559838000 | -2.404875000 |
| 1         | 2.103702000  | -2.307253000 | 1.260507000  |
| 6         | 2.652611000  | -1.551755000 | -0.657601000 |
| 1         | 2.322631000  | -2.427195000 | -1.184772000 |
| 6         | 4.188344000  | 1.840603000  | 1.475272000  |
| 1         | 3.642121000  | 2.741188000  | 1.211868000  |
| 1         | 4.113605000  | 1.708478000  | 2.546961000  |
| 1         | 5.230585000  | 2.013760000  | 1.229761000  |
| 42        |              |              |              |
| exo-4tT-N |              |              |              |
| 46        | 0.010043000  | -0.420453000 | -0.362279000 |

|   |              |              |              |
|---|--------------|--------------|--------------|
| 6 | -1.879086000 | 0.393765000  | -0.425607000 |
| 6 | -2.438949000 | 0.993234000  | 0.865999000  |
| 6 | -3.747168000 | -0.811843000 | 0.567548000  |
| 6 | -2.797249000 | -0.846552000 | -0.642288000 |
| 6 | -2.840358000 | -0.249023000 | 1.662325000  |
| 1 | -3.387154000 | -0.017074000 | 2.569137000  |
| 1 | -2.004057000 | -0.890481000 | 1.912258000  |
| 6 | -3.815546000 | 1.602325000  | 0.554817000  |
| 1 | -3.784757000 | 2.254194000  | -0.309787000 |
| 6 | -4.709874000 | 0.356631000  | 0.332839000  |
| 1 | -5.157006000 | 0.326882000  | -0.654228000 |
| 1 | -1.762233000 | 1.672158000  | 1.362873000  |
| 1 | -4.231796000 | -1.757852000 | 0.769383000  |
| 1 | -3.332296000 | -0.836815000 | -1.584930000 |
| 1 | -1.924831000 | 1.077657000  | -1.259960000 |
| 6 | 0.662808000  | 1.421935000  | -0.126310000 |
| 8 | 1.162603000  | 1.845285000  | 0.871987000  |
| 8 | 0.541435000  | 2.182389000  | -1.225412000 |
| 6 | 1.048665000  | 3.506300000  | -1.135422000 |
| 1 | 0.859759000  | 3.961263000  | -2.096392000 |
| 1 | 0.545194000  | 4.058469000  | -0.352553000 |
| 1 | 2.110625000  | 3.498163000  | -0.927163000 |
| 6 | -1.905684000 | -2.006152000 | -0.644899000 |
| 7 | -1.098167000 | -2.814855000 | -0.624503000 |
| 1 | -4.172744000 | 2.192109000  | 1.391969000  |
| 1 | -5.519480000 | 0.320345000  | 1.051688000  |
| 6 | 3.698592000  | -0.248592000 | 0.918452000  |
| 6 | 3.839453000  | -0.032961000 | -0.449475000 |
| 6 | 2.795702000  | -1.200404000 | 1.343277000  |
| 1 | 4.545514000  | 0.701629000  | -0.795294000 |
| 1 | 2.677055000  | -1.387934000 | 2.395457000  |
| 6 | 3.084084000  | -0.728591000 | -1.361176000 |
| 6 | 2.029808000  | -1.915484000 | 0.433742000  |
| 1 | 3.207178000  | -0.547474000 | -2.413379000 |
| 1 | 1.370807000  | -2.691956000 | 0.776973000  |
| 6 | 2.163114000  | -1.677774000 | -0.927115000 |
| 1 | 1.631193000  | -2.284827000 | -1.636913000 |
| 6 | 4.468862000  | 0.574831000  | 1.900512000  |

|            |              |              |              |
|------------|--------------|--------------|--------------|
| 1          | 3.936707000  | 1.500463000  | 2.097635000  |
| 1          | 4.590783000  | 0.055612000  | 2.843036000  |
| 1          | 5.451374000  | 0.829033000  | 1.520601000  |
| 42         |              |              |              |
| exo-4tT-N' |              |              |              |
| 46         | -0.028543000 | -0.508525000 | -0.338213000 |
| 6          | -1.920655000 | 0.269678000  | -0.579410000 |
| 6          | -2.456776000 | 1.214558000  | 0.497278000  |
| 6          | -3.769925000 | -0.593726000 | 0.748777000  |
| 6          | -2.840261000 | -0.977963000 | -0.415278000 |
| 6          | -2.843974000 | 0.253466000  | 1.621962000  |
| 1          | -3.374878000 | 0.737166000  | 2.434001000  |
| 1          | -2.003513000 | -0.294707000 | 2.030096000  |
| 6          | -3.838494000 | 1.716978000  | 0.048663000  |
| 1          | -3.822423000 | 2.095938000  | -0.965829000 |
| 6          | -4.736196000 | 0.463900000  | 0.205558000  |
| 1          | -5.199255000 | 0.155912000  | -0.724875000 |
| 1          | -1.770467000 | 2.002929000  | 0.766760000  |
| 1          | -4.251304000 | -1.440057000 | 1.220537000  |
| 1          | -3.390190000 | -1.237537000 | -1.312468000 |
| 1          | -1.986068000 | 0.686802000  | -1.573580000 |
| 6          | 0.597633000  | 1.300515000  | -0.800365000 |
| 8          | 0.712610000  | 1.741223000  | -1.901945000 |
| 8          | 0.936948000  | 2.020775000  | 0.283255000  |
| 6          | 1.443050000  | 3.324657000  | 0.035482000  |
| 1          | 1.648774000  | 3.752564000  | 1.005632000  |
| 1          | 2.348107000  | 3.280085000  | -0.556539000 |
| 1          | 0.714497000  | 3.925862000  | -0.492820000 |
| 6          | -1.948237000 | -2.093020000 | -0.097688000 |
| 7          | -1.140433000 | -2.865062000 | 0.142990000  |
| 1          | -4.181311000 | 2.522083000  | 0.689512000  |
| 1          | -5.534050000 | 0.637842000  | 0.917395000  |
| 6          | 3.741377000  | -0.084828000 | 0.792831000  |
| 6          | 3.833045000  | -0.188138000 | -0.593217000 |
| 6          | 2.828235000  | -0.879736000 | 1.451813000  |
| 1          | 4.539646000  | 0.427366000  | -1.122017000 |
| 1          | 2.744753000  | -0.819912000 | 2.522296000  |
| 6          | 3.034034000  | -1.055268000 | -1.295800000 |

|   |             |              |              |
|---|-------------|--------------|--------------|
| 6 | 2.018382000 | -1.767188000 | 0.754711000  |
| 1 | 3.118176000 | -1.118138000 | -2.364981000 |
| 1 | 1.358389000 | -2.426319000 | 1.288272000  |
| 6 | 2.116409000 | -1.859497000 | -0.625709000 |
| 1 | 1.555270000 | -2.604591000 | -1.159946000 |
| 6 | 4.597823000 | 0.891376000  | 1.537315000  |
| 1 | 4.211905000 | 1.900224000  | 1.426218000  |
| 1 | 4.626051000 | 0.664477000  | 2.595473000  |
| 1 | 5.614619000 | 0.889032000  | 1.161713000  |

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exo-4tTr-O

|    |              |              |              |
|----|--------------|--------------|--------------|
| 46 | 0.316804000  | -0.004508000 | -0.177929000 |
| 6  | -2.559055000 | 0.063017000  | -0.621438000 |
| 6  | -3.542082000 | -0.464127000 | 0.449917000  |
| 6  | -1.871937000 | -1.968727000 | 0.483455000  |
| 6  | -1.402402000 | -0.976124000 | -0.583778000 |
| 6  | -2.584889000 | -1.058967000 | 1.484090000  |
| 1  | -3.106205000 | -1.603084000 | 2.263562000  |
| 1  | -1.927468000 | -0.331753000 | 1.947329000  |
| 6  | -4.202166000 | -1.723662000 | -0.117592000 |
| 1  | -4.608361000 | -1.561214000 | -1.109218000 |
| 6  | -3.054672000 | -2.762724000 | -0.093646000 |
| 1  | -2.830807000 | -3.165805000 | -1.073507000 |
| 1  | -4.242171000 | 0.284130000  | 0.796111000  |
| 1  | -1.081510000 | -2.590442000 | 0.871683000  |
| 1  | -1.264425000 | -1.454600000 | -1.542289000 |
| 1  | -3.050622000 | 0.109535000  | -1.588997000 |
| 6  | -2.094212000 | 1.446205000  | -0.326620000 |
| 8  | -0.935395000 | 1.724895000  | -0.076950000 |
| 8  | -3.022088000 | 2.363539000  | -0.357765000 |
| 6  | -2.637957000 | 3.709222000  | -0.087328000 |
| 1  | -3.542397000 | 4.290073000  | -0.168850000 |
| 1  | -2.224280000 | 3.787752000  | 0.908175000  |
| 1  | -1.905886000 | 4.041953000  | -0.809593000 |
| 6  | 1.268237000  | -1.700485000 | -0.350803000 |
| 7  | 1.842740000  | -2.685612000 | -0.455979000 |
| 1  | -5.023679000 | -2.030926000 | 0.518872000  |
| 1  | -3.300560000 | -3.599767000 | 0.549965000  |



|   |             |              |              |
|---|-------------|--------------|--------------|
| 6 | 2.938478000 | 0.705284000  | 1.777919000  |
| 6 | 2.190010000 | 1.531395000  | 0.949200000  |
| 6 | 3.945694000 | -0.067443000 | 1.253625000  |
| 1 | 1.435394000 | 2.175599000  | 1.361880000  |
| 1 | 4.505493000 | -0.719768000 | 1.900105000  |
| 6 | 2.484952000 | 1.577246000  | -0.404615000 |
| 6 | 4.238527000 | -0.046269000 | -0.105781000 |
| 1 | 1.954054000 | 2.255047000  | -1.048755000 |
| 6 | 3.507430000 | 0.793831000  | -0.920184000 |
| 1 | 3.720138000 | 0.829440000  | -1.973730000 |
| 1 | 2.726117000 | 0.669763000  | 2.830948000  |
| 6 | 5.271012000 | -0.966141000 | -0.673402000 |
| 1 | 4.827404000 | -1.942097000 | -0.846101000 |
| 1 | 5.652855000 | -0.599463000 | -1.618231000 |
| 1 | 6.104792000 | -1.094400000 | 0.006837000  |

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exo-4tTr-N

|    |              |              |              |
|----|--------------|--------------|--------------|
| 46 | 0.035826000  | 0.357085000  | -0.162710000 |
| 6  | -1.899642000 | -0.148409000 | -0.543704000 |
| 6  | -2.869835000 | -0.033997000 | 0.631261000  |
| 6  | -2.860944000 | -2.247169000 | 0.225124000  |
| 6  | -1.888811000 | -1.678630000 | -0.824787000 |
| 6  | -2.606145000 | -1.320913000 | 1.414577000  |
| 1  | -3.313164000 | -1.483283000 | 2.220172000  |
| 1  | -1.601054000 | -1.390697000 | 1.813755000  |
| 6  | -4.285281000 | -0.302016000 | 0.094570000  |
| 1  | -4.505634000 | 0.297830000  | -0.779299000 |
| 6  | -4.268646000 | -1.821900000 | -0.204480000 |
| 1  | -4.464781000 | -2.050980000 | -1.245813000 |
| 1  | -2.782642000 | 0.895657000  | 1.168994000  |
| 1  | -2.745008000 | -3.309401000 | 0.394791000  |
| 1  | -2.174798000 | -1.938245000 | -1.837456000 |
| 1  | -2.215505000 | 0.427717000  | -1.399047000 |
| 6  | -0.560902000 | 2.256878000  | -0.170011000 |
| 8  | -1.654770000 | 2.724206000  | -0.228249000 |
| 8  | 0.525751000  | 3.058041000  | -0.104308000 |
| 6  | 0.280058000  | 4.457640000  | -0.115539000 |
| 1  | 1.249306000  | 4.930716000  | -0.059570000 |

|   |              |              |              |
|---|--------------|--------------|--------------|
| 1 | -0.228797000 | 4.748496000  | -1.024951000 |
| 1 | -0.328662000 | 4.745732000  | 0.731294000  |
| 6 | -0.511393000 | -2.113228000 | -0.617104000 |
| 7 | 0.592521000  | -2.323030000 | -0.414919000 |
| 1 | -5.028768000 | -0.062834000 | 0.846880000  |
| 1 | -5.011047000 | -2.348162000 | 0.383357000  |
| 6 | 2.777125000  | -0.264711000 | 1.801806000  |
| 6 | 2.395840000  | 0.821285000  | 1.021870000  |
| 6 | 3.445256000  | -1.321373000 | 1.234616000  |
| 1 | 1.935145000  | 1.681076000  | 1.468991000  |
| 1 | 3.732529000  | -2.158906000 | 1.846036000  |
| 6 | 2.701294000  | 0.823312000  | -0.329690000 |
| 6 | 3.748243000  | -1.336991000 | -0.123595000 |
| 1 | 2.463848000  | 1.683369000  | -0.926804000 |
| 6 | 3.373623000  | -0.254752000 | -0.890754000 |
| 1 | 3.607037000  | -0.241946000 | -1.940829000 |
| 1 | 2.558130000  | -0.269540000 | 2.854301000  |
| 6 | 4.419351000  | -2.525534000 | -0.735231000 |
| 1 | 3.692554000  | -3.312971000 | -0.910790000 |
| 1 | 4.875996000  | -2.277208000 | -1.685178000 |
| 1 | 5.186675000  | -2.926080000 | -0.082858000 |

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exo-4tTr-N'

|    |              |              |              |
|----|--------------|--------------|--------------|
| 46 | 0.086408000  | 0.385544000  | -0.127451000 |
| 6  | -1.770348000 | -0.361688000 | -0.519584000 |
| 6  | -2.760429000 | -0.392838000 | 0.646994000  |
| 6  | -2.449635000 | -2.579196000 | 0.222996000  |
| 6  | -1.553794000 | -1.875552000 | -0.812381000 |
| 6  | -2.330834000 | -1.638904000 | 1.422372000  |
| 1  | -3.014795000 | -1.902410000 | 2.221149000  |
| 1  | -1.328225000 | -1.574838000 | 1.828308000  |
| 6  | -4.123326000 | -0.843620000 | 0.097248000  |
| 1  | -4.416793000 | -0.272703000 | -0.775019000 |
| 6  | -3.898572000 | -2.344226000 | -0.214887000 |
| 1  | -4.054434000 | -2.587082000 | -1.259803000 |
| 1  | -2.803375000 | 0.529235000  | 1.204064000  |
| 1  | -2.193224000 | -3.617534000 | 0.385668000  |
| 1  | -1.798051000 | -2.159825000 | -1.829440000 |

|   |              |              |              |
|---|--------------|--------------|--------------|
| 1 | -2.161710000 | 0.163012000  | -1.376855000 |
| 6 | -0.601036000 | 2.238015000  | -0.085957000 |
| 8 | 0.151980000  | 3.134872000  | 0.164388000  |
| 8 | -1.885908000 | 2.470540000  | -0.359749000 |
| 6 | -2.301694000 | 3.829636000  | -0.333607000 |
| 1 | -3.353804000 | 3.820816000  | -0.576090000 |
| 1 | -2.144708000 | 4.259261000  | 0.646876000  |
| 1 | -1.752375000 | 4.411518000  | -1.061652000 |
| 6 | -0.133654000 | -2.136656000 | -0.601214000 |
| 7 | 0.986648000  | -2.217839000 | -0.397797000 |
| 1 | -4.898860000 | -0.715178000 | 0.844535000  |
| 1 | -4.567671000 | -2.971201000 | 0.361968000  |
| 6 | 2.927184000  | 0.074863000  | 1.791740000  |
| 6 | 2.378451000  | 1.131390000  | 1.073823000  |
| 6 | 3.718955000  | -0.852266000 | 1.160352000  |
| 1 | 1.812825000  | 1.899614000  | 1.565190000  |
| 1 | 4.134903000  | -1.668967000 | 1.724233000  |
| 6 | 2.645510000  | 1.237759000  | -0.281833000 |
| 6 | 3.984718000  | -0.764261000 | -0.202828000 |
| 1 | 2.280670000  | 2.088372000  | -0.826330000 |
| 6 | 3.445075000  | 0.289857000  | -0.908529000 |
| 1 | 3.649534000  | 0.384633000  | -1.960547000 |
| 1 | 2.740102000  | -0.007937000 | 2.847216000  |
| 6 | 4.798647000  | -1.818600000 | -0.883884000 |
| 1 | 4.191037000  | -2.700353000 | -1.064121000 |
| 1 | 5.174623000  | -1.473104000 | -1.838830000 |
| 1 | 5.643134000  | -2.121045000 | -0.275238000 |

42

exo-4cT-O

|    |              |              |              |
|----|--------------|--------------|--------------|
| 46 | 0.345574000  | 0.330619000  | -0.184351000 |
| 6  | -2.573462000 | -0.066762000 | -0.547302000 |
| 6  | -3.429610000 | -0.765857000 | 0.530877000  |
| 6  | -1.572594000 | -2.020754000 | 0.425489000  |
| 6  | -1.263938000 | -0.907763000 | -0.582841000 |
| 6  | -2.359199000 | -1.268980000 | 1.500491000  |
| 1  | -2.768305000 | -1.915318000 | 2.269128000  |
| 1  | -1.790049000 | -0.477977000 | 1.975685000  |
| 6  | -3.936960000 | -2.078014000 | -0.071933000 |

|           |              |              |              |
|-----------|--------------|--------------|--------------|
| 1         | -4.409769000 | -1.929631000 | -1.035603000 |
| 6         | -2.657218000 | -2.945247000 | -0.151729000 |
| 1         | -2.425715000 | -3.256994000 | -1.163258000 |
| 1         | -4.208721000 | -0.138107000 | 0.941335000  |
| 1         | -0.705406000 | -2.566656000 | 0.770534000  |
| 1         | -1.111760000 | -1.314673000 | -1.577839000 |
| 1         | -3.106390000 | -0.061010000 | -1.494122000 |
| 6         | -2.290182000 | 1.356375000  | -0.224421000 |
| 8         | -1.162955000 | 1.774366000  | -0.031056000 |
| 8         | -3.321618000 | 2.150693000  | -0.167337000 |
| 6         | -3.078403000 | 3.527582000  | 0.129044000  |
| 1         | -4.048066000 | 3.998320000  | 0.122957000  |
| 1         | -2.610767000 | 3.622989000  | 1.098416000  |
| 1         | -2.435016000 | 3.962001000  | -0.622468000 |
| 6         | 1.810952000  | 1.765888000  | 0.169921000  |
| 7         | 2.590131000  | 2.580814000  | 0.377115000  |
| 1         | -4.674356000 | -2.528558000 | 0.581967000  |
| 1         | -2.758284000 | -3.843679000 | 0.447642000  |
| 6         | 1.746047000  | -1.476711000 | -0.763233000 |
| 6         | 2.750289000  | -0.970920000 | -1.600913000 |
| 6         | 1.951953000  | -1.460527000 | 0.615486000  |
| 1         | 2.614396000  | -1.000154000 | -2.666566000 |
| 1         | 1.244675000  | -1.928329000 | 1.273348000  |
| 6         | 3.899019000  | -0.461954000 | -1.066968000 |
| 6         | 3.130108000  | -0.941446000 | 1.139418000  |
| 1         | 4.654780000  | -0.056869000 | -1.715720000 |
| 1         | 3.269007000  | -0.921481000 | 2.205034000  |
| 6         | 4.104761000  | -0.430991000 | 0.315344000  |
| 1         | 0.943411000  | -2.047590000 | -1.185731000 |
| 6         | 5.319832000  | 0.228148000  | 0.875405000  |
| 1         | 5.537695000  | -0.121173000 | 1.876788000  |
| 1         | 6.189078000  | 0.058970000  | 0.250919000  |
| 1         | 5.140451000  | 1.298855000  | 0.922214000  |
| 42        |              |              |              |
| exo-4cT-N |              |              |              |
| 46        | 0.030712000  | 0.349372000  | -0.125596000 |
| 6         | 2.020472000  | -0.358866000 | -0.631433000 |
| 6         | 2.746204000  | -1.319140000 | 0.317094000  |

|   |              |              |              |
|---|--------------|--------------|--------------|
| 6 | 3.956041000  | 0.560704000  | 0.537224000  |
| 6 | 2.880050000  | 0.929368000  | -0.491929000 |
| 6 | 3.192787000  | -0.396187000 | 1.452674000  |
| 1 | 3.841947000  | -0.884765000 | 2.170394000  |
| 1 | 2.373102000  | 0.070343000  | 1.985969000  |
| 6 | 4.101330000  | -1.702908000 | -0.298435000 |
| 1 | 4.000500000  | -2.035559000 | -1.324402000 |
| 6 | 4.921549000  | -0.394154000 | -0.173356000 |
| 1 | 5.246311000  | -0.006505000 | -1.132143000 |
| 1 | 2.167115000  | -2.179870000 | 0.624800000  |
| 1 | 4.431395000  | 1.412061000  | 1.006267000  |
| 1 | 3.298917000  | 1.319454000  | -1.411486000 |
| 1 | 2.020898000  | -0.710033000 | -1.657549000 |
| 6 | -1.733961000 | 1.245868000  | 0.396912000  |
| 8 | -2.328654000 | 1.114528000  | 1.427877000  |
| 8 | -2.164953000 | 2.113909000  | -0.541034000 |
| 6 | -3.304825000 | 2.891340000  | -0.215076000 |
| 1 | -3.475540000 | 3.543316000  | -1.059407000 |
| 1 | -4.169698000 | 2.260280000  | -0.050318000 |
| 1 | -3.128061000 | 3.475495000  | 0.678694000  |
| 6 | 1.883987000  | 1.874204000  | 0.014872000  |
| 7 | 0.981726000  | 2.462807000  | 0.414839000  |
| 1 | 4.568852000  | -2.508069000 | 0.259334000  |
| 1 | 5.809584000  | -0.542363000 | 0.429029000  |
| 6 | -0.801666000 | -1.926615000 | -0.103185000 |
| 6 | -1.000952000 | -1.403360000 | -1.380322000 |
| 6 | -1.885969000 | -2.099878000 | 0.756604000  |
| 1 | -0.204532000 | -1.402999000 | -2.099517000 |
| 1 | -1.715977000 | -2.493546000 | 1.742294000  |
| 6 | -2.302759000 | -1.084651000 | -1.784079000 |
| 6 | -3.159497000 | -1.773522000 | 0.363093000  |
| 1 | -2.471889000 | -0.699091000 | -2.772408000 |
| 6 | -3.352261000 | -1.278631000 | -0.931347000 |
| 1 | -4.348757000 | -1.029643000 | -1.251499000 |
| 1 | 0.157459000  | -2.316120000 | 0.173904000  |
| 6 | -4.312851000 | -1.882901000 | 1.305819000  |
| 1 | -4.114248000 | -2.597573000 | 2.094383000  |
| 1 | -4.489836000 | -0.917208000 | 1.769831000  |

|            |              |              |              |
|------------|--------------|--------------|--------------|
| 1          | -5.219570000 | -2.179871000 | 0.791864000  |
| 42         |              |              |              |
| exo-4cT-N' |              |              |              |
| 46         | 0.049363000  | 0.270967000  | -0.352953000 |
| 6          | 2.038480000  | -0.585569000 | -0.514405000 |
| 6          | 2.665581000  | -1.171004000 | 0.752154000  |
| 6          | 3.899090000  | 0.678263000  | 0.423887000  |
| 6          | 2.931673000  | 0.660316000  | -0.767319000 |
| 6          | 3.038532000  | 0.086847000  | 1.540843000  |
| 1          | 3.614895000  | -0.121878000 | 2.435097000  |
| 1          | 2.188515000  | 0.702849000  | 1.809763000  |
| 6          | 4.056944000  | -1.733792000 | 0.418863000  |
| 1          | 4.031618000  | -2.387025000 | -0.444928000 |
| 6          | 4.899366000  | -0.456159000 | 0.175678000  |
| 1          | 5.325393000  | -0.414261000 | -0.820099000 |
| 1          | 2.039843000  | -1.882718000 | 1.275630000  |
| 1          | 4.352937000  | 1.641831000  | 0.613947000  |
| 1          | 3.450180000  | 0.686126000  | -1.718215000 |
| 1          | 2.078628000  | -1.262393000 | -1.360446000 |
| 6          | -1.712412000 | 1.309329000  | -0.273732000 |
| 8          | -2.531127000 | 1.430267000  | -1.136891000 |
| 8          | -1.846159000 | 1.964554000  | 0.900601000  |
| 6          | -2.946013000 | 2.851823000  | 1.014640000  |
| 1          | -2.864613000 | 3.308084000  | 1.990542000  |
| 1          | -2.908432000 | 3.609951000  | 0.243186000  |
| 1          | -3.885489000 | 2.319548000  | 0.929883000  |
| 6          | 1.929021000  | 1.724761000  | -0.750187000 |
| 7          | 1.010718000  | 2.414650000  | -0.712570000 |
| 1          | 4.455004000  | -2.308957000 | 1.248684000  |
| 1          | 5.720856000  | -0.387609000 | 0.878495000  |
| 6          | -0.969314000 | -1.638988000 | 0.729956000  |
| 6          | -0.808605000 | -1.956316000 | -0.616726000 |
| 6          | -2.249216000 | -1.386213000 | 1.236296000  |
| 1          | 0.132467000  | -2.315380000 | -0.981458000 |
| 1          | -2.360873000 | -1.148466000 | 2.278581000  |
| 6          | -1.935642000 | -1.996240000 | -1.445293000 |
| 6          | -3.352432000 | -1.441746000 | 0.425063000  |
| 1          | -1.820888000 | -2.239554000 | -2.485340000 |

|             |              |              |              |
|-------------|--------------|--------------|--------------|
| 6           | -3.173414000 | -1.745481000 | -0.930141000 |
| 1           | -4.032771000 | -1.770575000 | -1.576396000 |
| 1           | -0.144168000 | -1.730008000 | 1.411078000  |
| 6           | -4.722165000 | -1.141409000 | 0.943398000  |
| 1           | -4.726160000 | -1.045418000 | 2.021407000  |
| 1           | -5.085808000 | -0.210547000 | 0.519300000  |
| 1           | -5.425404000 | -1.919709000 | 0.667581000  |
| 61          |              |              |              |
| exo-TSLFR-O |              |              |              |
| 46          | 0.836083000  | -0.336048000 | 0.630095000  |
| 15          | -1.521865000 | -0.062169000 | -0.010794000 |
| 6           | -1.901857000 | -1.196474000 | -1.388176000 |
| 6           | -1.598003000 | -2.542973000 | -1.218235000 |
| 6           | -2.423341000 | -0.779504000 | -2.601909000 |
| 6           | -1.825137000 | -3.450349000 | -2.230015000 |
| 1           | -1.189746000 | -2.885955000 | -0.282887000 |
| 6           | -2.642515000 | -1.688888000 | -3.620170000 |
| 1           | -2.658152000 | 0.256407000  | -2.758791000 |
| 6           | -2.347427000 | -3.023436000 | -3.436947000 |
| 1           | -1.590531000 | -4.488514000 | -2.079686000 |
| 1           | -3.046119000 | -1.349579000 | -4.556938000 |
| 1           | -2.519418000 | -3.728650000 | -4.229664000 |
| 6           | -2.784476000 | -0.435578000 | 1.243478000  |
| 6           | -3.959221000 | -1.112195000 | 0.947253000  |
| 6           | -2.560599000 | -0.005050000 | 2.545151000  |
| 6           | -4.896276000 | -1.350066000 | 1.932879000  |
| 1           | -4.145236000 | -1.460427000 | -0.051808000 |
| 6           | -3.503439000 | -0.238754000 | 3.525486000  |
| 1           | -1.649199000 | 0.504993000  | 2.799329000  |
| 6           | -4.670760000 | -0.911530000 | 3.222534000  |
| 1           | -5.801026000 | -1.878262000 | 1.691681000  |
| 1           | -3.317045000 | 0.099131000  | 4.528493000  |
| 1           | -5.400060000 | -1.098516000 | 3.990002000  |
| 6           | -1.946629000 | 1.590678000  | -0.633799000 |
| 6           | -0.941404000 | 2.348955000  | -1.217862000 |
| 6           | -3.229318000 | 2.113512000  | -0.553938000 |
| 6           | -1.223122000 | 3.598891000  | -1.732578000 |
| 1           | 0.065642000  | 1.973850000  | -1.261255000 |

|               |              |              |              |
|---------------|--------------|--------------|--------------|
| 6             | -3.505155000 | 3.366868000  | -1.061027000 |
| 1             | -4.013879000 | 1.547736000  | -0.086755000 |
| 6             | -2.503319000 | 4.109425000  | -1.655050000 |
| 1             | -0.437049000 | 4.176604000  | -2.183784000 |
| 1             | -4.501212000 | 3.764390000  | -0.987971000 |
| 1             | -2.718694000 | 5.087015000  | -2.047173000 |
| 6             | 3.840686000  | 0.172164000  | 0.397881000  |
| 6             | 4.527020000  | -0.729487000 | -0.658229000 |
| 6             | 2.949543000  | -2.071358000 | 0.192915000  |
| 6             | 2.776500000  | -0.778600000 | 0.999421000  |
| 6             | 3.354456000  | -1.552869000 | -1.188917000 |
| 1             | 3.667703000  | -2.342589000 | -1.863081000 |
| 1             | 2.602161000  | -0.948618000 | -1.679500000 |
| 6             | 5.339918000  | -1.791696000 | 0.090398000  |
| 1             | 5.962262000  | -1.357291000 | 0.863269000  |
| 6             | 4.255055000  | -2.739301000 | 0.657988000  |
| 1             | 4.300566000  | -2.835732000 | 1.735230000  |
| 1             | 5.098628000  | -0.177908000 | -1.393717000 |
| 1             | 2.098324000  | -2.745199000 | 0.227782000  |
| 1             | 2.944856000  | -0.926803000 | 2.053322000  |
| 1             | 4.549460000  | 0.491664000  | 1.149494000  |
| 6             | 3.304327000  | 1.411693000  | -0.259845000 |
| 8             | 2.383983000  | 1.446941000  | -1.029059000 |
| 8             | 4.001092000  | 2.487004000  | 0.066418000  |
| 6             | 3.581578000  | 3.719057000  | -0.498446000 |
| 1             | 4.263715000  | 4.463776000  | -0.118972000 |
| 1             | 3.628678000  | 3.678179000  | -1.578508000 |
| 1             | 2.569647000  | 3.946398000  | -0.192060000 |
| 6             | 0.885254000  | 0.675802000  | 2.302634000  |
| 7             | 0.867145000  | 1.278536000  | 3.276439000  |
| 1             | 5.995125000  | -2.315739000 | -0.595462000 |
| 1             | 4.344138000  | -3.734518000 | 0.235753000  |
| 61            |              |              |              |
| exo-TSLFR-OMe |              |              |              |
| 46            | -0.887954000 | -0.197152000 | -0.605361000 |
| 15            | 1.481622000  | -0.100474000 | 0.032495000  |
| 6             | 1.741815000  | -0.885680000 | 1.657364000  |
| 6             | 1.352467000  | -2.212559000 | 1.810077000  |



|   |              |              |              |
|---|--------------|--------------|--------------|
| 6 | 2.216840000  | -0.201787000 | 2.764578000  |
| 6 | 1.453380000  | -2.841942000 | 3.031259000  |
| 1 | 0.976444000  | -2.762529000 | 0.964467000  |
| 6 | 2.309435000  | -0.831441000 | 3.992444000  |
| 1 | 2.516456000  | 0.825203000  | 2.675227000  |
| 6 | 1.932056000  | -2.150291000 | 4.128885000  |
| 1 | 1.154818000  | -3.869939000 | 3.128607000  |
| 1 | 2.680125000  | -0.285956000 | 4.841301000  |
| 1 | 2.006820000  | -2.638339000 | 5.083539000  |
| 6 | 2.585166000  | -0.995565000 | -1.104839000 |
| 6 | 3.632541000  | -1.799890000 | -0.681292000 |
| 6 | 2.365739000  | -0.831135000 | -2.467224000 |
| 6 | 4.448032000  | -2.427406000 | -1.602431000 |
| 1 | 3.813616000  | -1.945236000 | 0.367592000  |
| 6 | 3.187941000  | -1.452858000 | -3.383943000 |
| 1 | 1.554238000  | -0.215715000 | -2.813035000 |
| 6 | 4.228374000  | -2.253353000 | -2.954021000 |
| 1 | 5.254934000  | -3.050880000 | -1.261976000 |
| 1 | 3.009450000  | -1.314799000 | -4.434669000 |
| 1 | 4.863734000  | -2.742290000 | -3.670189000 |
| 6 | 2.222474000  | 1.551965000  | 0.165598000  |
| 6 | 1.394367000  | 2.662007000  | 0.139707000  |
| 6 | 3.595335000  | 1.735527000  | 0.274800000  |
| 6 | 1.925044000  | 3.934097000  | 0.240911000  |
| 1 | 0.336120000  | 2.533661000  | 0.011543000  |
| 6 | 4.123720000  | 3.003825000  | 0.376109000  |
| 1 | 4.254975000  | 0.886940000  | 0.270865000  |
| 6 | 3.287534000  | 4.105647000  | 0.362124000  |
| 1 | 1.272988000  | 4.787581000  | 0.207053000  |
| 1 | 5.187536000  | 3.134877000  | 0.456818000  |
| 1 | 3.701715000  | 5.095151000  | 0.432455000  |
| 6 | -3.948792000 | 0.321185000  | -0.477568000 |
| 6 | -4.580384000 | -0.581949000 | 0.611174000  |
| 6 | -2.955609000 | -1.871434000 | -0.226659000 |
| 6 | -2.823788000 | -0.580486000 | -1.038671000 |
| 6 | -3.377107000 | -1.352869000 | 1.150384000  |
| 1 | -3.658422000 | -2.146525000 | 1.833901000  |
| 1 | -2.645512000 | -0.717750000 | 1.633242000  |

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|---|--------------|--------------|--------------|
| 6 | -5.354920000 | -1.694791000 | -0.104944000 |
| 1 | -6.016056000 | -1.304093000 | -0.868333000 |
| 6 | -4.236001000 | -2.594100000 | -0.684817000 |
| 1 | -4.284433000 | -2.687095000 | -1.762122000 |
| 1 | -5.168803000 | -0.037865000 | 1.338374000  |
| 1 | -2.080936000 | -2.518870000 | -0.256665000 |
| 1 | -2.940610000 | -0.733983000 | -2.099145000 |
| 1 | -4.673257000 | 0.538500000  | -1.250861000 |
| 6 | -3.590840000 | 1.678584000  | 0.065543000  |
| 8 | -4.137108000 | 2.686312000  | -0.256358000 |
| 8 | -2.641287000 | 1.652048000  | 1.005373000  |
| 6 | -2.308499000 | 2.902913000  | 1.585092000  |
| 1 | -1.516918000 | 2.703084000  | 2.291308000  |
| 1 | -1.974377000 | 3.595848000  | 0.824894000  |
| 1 | -3.165835000 | 3.327224000  | 2.090373000  |
| 6 | -0.847874000 | 0.966674000  | -2.176978000 |
| 7 | -0.748195000 | 1.633226000  | -3.102768000 |
| 1 | -5.965385000 | -2.242848000 | 0.603044000  |
| 1 | -4.278006000 | -3.594062000 | -0.267129000 |

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exo-TSrot-O

|    |              |              |              |
|----|--------------|--------------|--------------|
| 46 | 1.013459000  | -0.481452000 | 0.390583000  |
| 15 | -1.394737000 | -0.086877000 | -0.063395000 |
| 6  | -1.746115000 | 1.600564000  | -0.656852000 |
| 6  | -0.983653000 | 2.085969000  | -1.713032000 |
| 6  | -2.697169000 | 2.430230000  | -0.083396000 |
| 6  | -1.179896000 | 3.362032000  | -2.195382000 |
| 1  | -0.222913000 | 1.469228000  | -2.158144000 |
| 6  | -2.886985000 | 3.713312000  | -0.561444000 |
| 1  | -3.291546000 | 2.080090000  | 0.739303000  |
| 6  | -2.133361000 | 4.180004000  | -1.618899000 |
| 1  | -0.578410000 | 3.720844000  | -3.010274000 |
| 1  | -3.627198000 | 4.345754000  | -0.105668000 |
| 1  | -2.282733000 | 5.177941000  | -1.989373000 |
| 6  | -2.141230000 | -1.170101000 | -1.322355000 |
| 6  | -2.985119000 | -0.696805000 | -2.316185000 |
| 6  | -1.855795000 | -2.529363000 | -1.268080000 |
| 6  | -3.536040000 | -1.565326000 | -3.238283000 |

|   |              |              |              |
|---|--------------|--------------|--------------|
| 1 | -3.214300000 | 0.350357000  | -2.378762000 |
| 6 | -2.414395000 | -3.393589000 | -2.186549000 |
| 1 | -1.196960000 | -2.916494000 | -0.512273000 |
| 6 | -3.253267000 | -2.914372000 | -3.174059000 |
| 1 | -4.185972000 | -1.184658000 | -4.005320000 |
| 1 | -2.185531000 | -4.442211000 | -2.131795000 |
| 1 | -3.681532000 | -3.589662000 | -3.892611000 |
| 6 | -2.442901000 | -0.299121000 | 1.405318000  |
| 6 | -1.875429000 | -0.105557000 | 2.655649000  |
| 6 | -3.784518000 | -0.643374000 | 1.320939000  |
| 6 | -2.637608000 | -0.231852000 | 3.799527000  |
| 1 | -0.828421000 | 0.125062000  | 2.737117000  |
| 6 | -4.544679000 | -0.775140000 | 2.464567000  |
| 1 | -4.235510000 | -0.819709000 | 0.361792000  |
| 6 | -3.973306000 | -0.565846000 | 3.704957000  |
| 1 | -2.183437000 | -0.085813000 | 4.762494000  |
| 1 | -5.581456000 | -1.048097000 | 2.387312000  |
| 1 | -4.565320000 | -0.675611000 | 4.595464000  |
| 6 | 3.657267000  | 0.664863000  | 0.445744000  |
| 6 | 4.612320000  | 0.389516000  | -0.722729000 |
| 6 | 3.722237000  | -1.628345000 | -0.304282000 |
| 6 | 3.008823000  | -0.732954000 | 0.707139000  |
| 6 | 3.871983000  | -0.694680000 | -1.505024000 |
| 1 | 4.471991000  | -1.116290000 | -2.303790000 |
| 1 | 2.928614000  | -0.358449000 | -1.918436000 |
| 6 | 5.799779000  | -0.399189000 | -0.162474000 |
| 1 | 6.231467000  | 0.072928000  | 0.712780000  |
| 6 | 5.185372000  | -1.787241000 | 0.140871000  |
| 1 | 5.262303000  | -2.064045000 | 1.185376000  |
| 1 | 4.881617000  | 1.280069000  | -1.272753000 |
| 1 | 3.219609000  | -2.566914000 | -0.477403000 |
| 1 | 3.151491000  | -1.059048000 | 1.725995000  |
| 1 | 4.186784000  | 0.987470000  | 1.336019000  |
| 6 | 2.678535000  | 1.777420000  | 0.147344000  |
| 8 | 2.458995000  | 2.257576000  | -0.923256000 |
| 8 | 2.059294000  | 2.188219000  | 1.257334000  |
| 6 | 1.235475000  | 3.343641000  | 1.148106000  |
| 1 | 0.846303000  | 3.519542000  | 2.138727000  |

|             |              |              |              |
|-------------|--------------|--------------|--------------|
| 1           | 1.825982000  | 4.188929000  | 0.820625000  |
| 1           | 0.429588000  | 3.182632000  | 0.447783000  |
| 6           | 0.856145000  | -2.344945000 | 0.942037000  |
| 7           | 0.712022000  | -3.438679000 | 1.248467000  |
| 1           | 6.584270000  | -0.472121000 | -0.906646000 |
| 1           | 5.673851000  | -2.565873000 | -0.434375000 |
| 61          |              |              |              |
| exo-4tP-piO |              |              |              |
| 46          | 0.847710000  | -0.212191000 | 0.716076000  |
| 15          | -1.501007000 | -0.076939000 | 0.015577000  |
| 6           | -2.021724000 | -1.641559000 | -0.763999000 |
| 6           | -1.900780000 | -2.809358000 | -0.018001000 |
| 6           | -2.464870000 | -1.731078000 | -2.073280000 |
| 6           | -2.231323000 | -4.031067000 | -0.562028000 |
| 1           | -1.553589000 | -2.761410000 | 0.999922000  |
| 6           | -2.787085000 | -2.958952000 | -2.622140000 |
| 1           | -2.558090000 | -0.844381000 | -2.671394000 |
| 6           | -2.674568000 | -4.108732000 | -1.869738000 |
| 1           | -2.138810000 | -4.922861000 | 0.030947000  |
| 1           | -3.127703000 | -3.011812000 | -3.640323000 |
| 1           | -2.926976000 | -5.061769000 | -2.297861000 |
| 6           | -2.759601000 | 0.240172000  | 1.289703000  |
| 6           | -3.993993000 | -0.392978000 | 1.304545000  |
| 6           | -2.465872000 | 1.174829000  | 2.274922000  |
| 6           | -4.920691000 | -0.094598000 | 2.283776000  |
| 1           | -4.235573000 | -1.124624000 | 0.556047000  |
| 6           | -3.397766000 | 1.474823000  | 3.247281000  |
| 1           | -1.510304000 | 1.667218000  | 2.288100000  |
| 6           | -4.624797000 | 0.840893000  | 3.254890000  |
| 1           | -5.872713000 | -0.593982000 | 2.286201000  |
| 1           | -3.157859000 | 2.200151000  | 4.003126000  |
| 1           | -5.346308000 | 1.071839000  | 4.017694000  |
| 6           | -1.773237000 | 1.200523000  | -1.246181000 |
| 6           | -0.682400000 | 1.658883000  | -1.970567000 |
| 6           | -3.030878000 | 1.726307000  | -1.510444000 |
| 6           | -0.851797000 | 2.610850000  | -2.957394000 |
| 1           | 0.307275000  | 1.294600000  | -1.759466000 |
| 6           | -3.196036000 | 2.680423000  | -2.492044000 |

|   |              |              |              |
|---|--------------|--------------|--------------|
| 1 | -3.882273000 | 1.398954000  | -0.942455000 |
| 6 | -2.106421000 | 3.120929000  | -3.219844000 |
| 1 | 0.002982000  | 2.958690000  | -3.507900000 |
| 1 | -4.173327000 | 3.084462000  | -2.684859000 |
| 1 | -2.235880000 | 3.868297000  | -3.981785000 |
| 6 | 3.909804000  | 0.076153000  | 0.281257000  |
| 6 | 4.354953000  | -1.055506000 | -0.664467000 |
| 6 | 2.737214000  | -2.021489000 | 0.540355000  |
| 6 | 2.786888000  | -0.604688000 | 1.106486000  |
| 6 | 3.047115000  | -1.792011000 | -0.942287000 |
| 1 | 3.188504000  | -2.716322000 | -1.491497000 |
| 1 | 2.326440000  | -1.175578000 | -1.464142000 |
| 6 | 5.114231000  | -2.091455000 | 0.174246000  |
| 1 | 5.876566000  | -1.635806000 | 0.794470000  |
| 6 | 3.998871000  | -2.771782000 | 1.006232000  |
| 1 | 4.153122000  | -2.682142000 | 2.073926000  |
| 1 | 4.896136000  | -0.705521000 | -1.532780000 |
| 1 | 1.820570000  | -2.568947000 | 0.767639000  |
| 1 | 2.974646000  | -0.557232000 | 2.167830000  |
| 1 | 4.717104000  | 0.379302000  | 0.935129000  |
| 6 | 3.457552000  | 1.309278000  | -0.454806000 |
| 8 | 2.793223000  | 1.312190000  | -1.451830000 |
| 8 | 3.888379000  | 2.407083000  | 0.135372000  |
| 6 | 3.406700000  | 3.644727000  | -0.367238000 |
| 1 | 3.913968000  | 4.408402000  | 0.201217000  |
| 1 | 3.632332000  | 3.740310000  | -1.420734000 |
| 1 | 2.339751000  | 3.713129000  | -0.208381000 |
| 6 | 1.023517000  | 1.491121000  | 1.660489000  |
| 7 | 1.055890000  | 2.500917000  | 2.199861000  |
| 1 | 5.607795000  | -2.808759000 | -0.470640000 |
| 1 | 3.920576000  | -3.827852000 | 0.773114000  |

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exo-4tP-piOMe

|    |              |             |              |
|----|--------------|-------------|--------------|
| 46 | -0.843891000 | 0.175084000 | 0.647583000  |
| 15 | 1.523410000  | 0.058285000 | 0.018764000  |
| 6  | 2.085210000  | 1.656052000 | -0.659744000 |
| 6  | 1.874073000  | 2.794632000 | 0.110505000  |
| 6  | 2.660770000  | 1.796811000 | -1.911776000 |

|   |              |              |              |
|---|--------------|--------------|--------------|
| 6 | 2.243067000  | 4.038347000  | -0.353385000 |
| 1 | 1.425568000  | 2.706555000  | 1.085245000  |
| 6 | 3.021549000  | 3.046568000  | -2.381416000 |
| 1 | 2.828721000  | 0.933331000  | -2.527411000 |
| 6 | 2.816902000  | 4.167376000  | -1.604952000 |
| 1 | 2.079208000  | 4.907080000  | 0.258056000  |
| 1 | 3.465197000  | 3.139378000  | -3.356139000 |
| 1 | 3.099551000  | 5.137557000  | -1.971145000 |
| 6 | 2.722529000  | -0.321393000 | 1.332171000  |
| 6 | 3.949373000  | 0.318828000  | 1.434991000  |
| 6 | 2.393203000  | -1.307582000 | 2.253868000  |
| 6 | 4.833792000  | -0.022937000 | 2.438641000  |
| 1 | 4.218083000  | 1.089179000  | 0.736363000  |
| 6 | 3.283576000  | -1.650294000 | 3.250875000  |
| 1 | 1.442354000  | -1.805951000 | 2.200632000  |
| 6 | 4.503013000  | -1.009119000 | 3.346398000  |
| 1 | 5.779878000  | 0.482545000  | 2.509858000  |
| 1 | 3.016038000  | -2.414604000 | 3.957362000  |
| 1 | 5.191409000  | -1.273644000 | 4.128644000  |
| 6 | 1.866089000  | -1.151242000 | -1.293765000 |
| 6 | 0.841228000  | -1.481313000 | -2.168302000 |
| 6 | 3.108037000  | -1.747032000 | -1.458047000 |
| 6 | 1.058770000  | -2.370464000 | -3.201204000 |
| 1 | -0.135898000 | -1.053484000 | -2.030856000 |
| 6 | 3.322711000  | -2.642953000 | -2.485473000 |
| 1 | 3.907942000  | -1.520272000 | -0.777787000 |
| 6 | 2.300340000  | -2.952345000 | -3.361109000 |
| 1 | 0.256361000  | -2.617329000 | -3.872397000 |
| 1 | 4.287574000  | -3.102879000 | -2.598730000 |
| 1 | 2.468159000  | -3.653105000 | -4.158758000 |
| 6 | -4.047150000 | -0.013461000 | 0.573396000  |
| 6 | -4.531366000 | 0.959777000  | -0.528853000 |
| 6 | -2.632502000 | 1.904551000  | 0.164283000  |
| 6 | -2.749843000 | 0.669615000  | 1.049403000  |
| 6 | -3.223324000 | 1.424192000  | -1.162458000 |
| 1 | -3.361951000 | 2.228454000  | -1.876714000 |
| 1 | -2.667275000 | 0.622970000  | -1.627604000 |
| 6 | -5.004525000 | 2.249294000  | 0.159712000  |

|   |              |              |              |
|---|--------------|--------------|--------------|
| 1 | -5.678963000 | 2.047236000  | 0.982430000  |
| 6 | -3.688020000 | 2.926659000  | 0.621799000  |
| 1 | -3.654081000 | 3.098933000  | 1.689740000  |
| 1 | -5.265151000 | 0.529213000  | -1.197098000 |
| 1 | -1.622900000 | 2.339554000  | 0.116697000  |
| 1 | -2.787390000 | 0.889699000  | 2.107199000  |
| 1 | -4.762948000 | -0.040309000 | 1.384119000  |
| 6 | -3.985255000 | -1.448586000 | 0.115771000  |
| 8 | -4.681049000 | -2.303372000 | 0.567785000  |
| 8 | -3.123661000 | -1.667291000 | -0.872499000 |
| 6 | -2.958915000 | -3.024611000 | -1.257378000 |
| 1 | -2.237254000 | -3.019469000 | -2.060354000 |
| 1 | -2.586301000 | -3.600439000 | -0.421587000 |
| 1 | -3.897809000 | -3.441303000 | -1.595684000 |
| 6 | -1.031849000 | -1.552133000 | 1.543442000  |
| 7 | -1.074033000 | -2.581986000 | 2.042494000  |
| 1 | -5.533398000 | 2.878536000  | -0.546111000 |
| 1 | -3.539867000 | 3.880205000  | 0.127620000  |

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exo-4t2P-O

|    |              |              |              |
|----|--------------|--------------|--------------|
| 46 | -0.282678000 | 0.718400000  | -0.518815000 |
| 15 | 2.119217000  | 0.201418000  | -0.197699000 |
| 6  | 2.773358000  | -0.746169000 | -1.617053000 |
| 6  | 2.920273000  | -0.076007000 | -2.836867000 |
| 6  | 2.998185000  | -2.121031000 | -1.571678000 |
| 6  | 3.320890000  | -0.765270000 | -3.970733000 |
| 1  | 2.707129000  | 0.985450000  | -2.903451000 |
| 6  | 3.399550000  | -2.806348000 | -2.711836000 |
| 1  | 2.852692000  | -2.671944000 | -0.651101000 |
| 6  | 3.568608000  | -2.131180000 | -3.910736000 |
| 1  | 3.433835000  | -0.230203000 | -4.907212000 |
| 1  | 3.574253000  | -3.875319000 | -2.656906000 |
| 1  | 3.884130000  | -2.667557000 | -4.799244000 |
| 6  | 3.196317000  | 1.685447000  | -0.082637000 |
| 6  | 4.507650000  | 1.693661000  | -0.553385000 |
| 6  | 2.713411000  | 2.796502000  | 0.606447000  |
| 6  | 5.321910000  | 2.798085000  | -0.345311000 |
| 1  | 4.900926000  | 0.839912000  | -1.092608000 |

|   |              |              |              |
|---|--------------|--------------|--------------|
| 6 | 3.535753000  | 3.892054000  | 0.825712000  |
| 1 | 1.689835000  | 2.812415000  | 0.964933000  |
| 6 | 4.838540000  | 3.898547000  | 0.347544000  |
| 1 | 6.337693000  | 2.795915000  | -0.725716000 |
| 1 | 3.152860000  | 4.750701000  | 1.366551000  |
| 1 | 5.475143000  | 4.761341000  | 0.511626000  |
| 6 | 2.665914000  | -0.634068000 | 1.346351000  |
| 6 | 1.888746000  | -0.431833000 | 2.485554000  |
| 6 | 3.873246000  | -1.321775000 | 1.471443000  |
| 6 | 2.294809000  | -0.922501000 | 3.719477000  |
| 1 | 0.957645000  | 0.118995000  | 2.410247000  |
| 6 | 4.272629000  | -1.824819000 | 2.700841000  |
| 1 | 4.513765000  | -1.462484000 | 0.609092000  |
| 6 | 3.483961000  | -1.628627000 | 3.827760000  |
| 1 | 1.677124000  | -0.752462000 | 4.594573000  |
| 1 | 5.211060000  | -2.362890000 | 2.781196000  |
| 1 | 3.802536000  | -2.016748000 | 4.789266000  |
| 6 | -2.189394000 | 3.150329000  | -0.659954000 |
| 6 | -3.633378000 | 3.408484000  | -0.166003000 |
| 6 | -3.512720000 | 1.171066000  | -0.259870000 |
| 6 | -2.164425000 | 1.614453000  | -0.897054000 |
| 6 | -3.810118000 | 2.236909000  | 0.799235000  |
| 1 | -4.824643000 | 2.157867000  | 1.202169000  |
| 1 | -3.105388000 | 2.254803000  | 1.630030000  |
| 6 | -4.612046000 | 3.050806000  | -1.295118000 |
| 1 | -4.294475000 | 3.471252000  | -2.252580000 |
| 6 | -4.610554000 | 1.500530000  | -1.286552000 |
| 1 | -4.405889000 | 1.064821000  | -2.266447000 |
| 1 | -3.775599000 | 4.411713000  | 0.240820000  |
| 1 | -3.570409000 | 0.146486000  | 0.094040000  |
| 1 | -2.233285000 | 1.455039000  | -1.973066000 |
| 1 | -1.981574000 | 3.702087000  | -1.576972000 |
| 6 | -1.242360000 | 3.695092000  | 0.376638000  |
| 8 | -1.086450000 | 5.004176000  | 0.230724000  |
| 8 | -0.723505000 | 3.087659000  | 1.275824000  |
| 6 | 0.398766000  | 2.202185000  | -1.695618000 |
| 7 | 0.810143000  | 2.971879000  | -2.450419000 |
| 1 | -5.606853000 | 3.451475000  | -1.082733000 |



|    |              |              |              |
|----|--------------|--------------|--------------|
| 1  | -5.576789000 | 1.109322000  | -0.952192000 |
| 15 | -1.246468000 | -1.375980000 | 0.188397000  |
| 6  | -1.958364000 | -1.401863000 | 1.875603000  |
| 6  | -1.973710000 | -0.205021000 | 2.590865000  |
| 6  | -2.435982000 | -2.562752000 | 2.491054000  |
| 6  | -2.478173000 | -0.163373000 | 3.885264000  |
| 6  | -2.942226000 | -2.518519000 | 3.780467000  |
| 6  | -2.967254000 | -1.316763000 | 4.478781000  |
| 1  | -1.586859000 | 0.700222000  | 2.134222000  |
| 1  | -2.393314000 | -3.512852000 | 1.971285000  |
| 1  | -2.484833000 | 0.776226000  | 4.426441000  |
| 1  | -3.311456000 | -3.426205000 | 4.245314000  |
| 1  | -3.361120000 | -1.284587000 | 5.488957000  |
| 6  | -0.209325000 | -2.907874000 | 0.173064000  |
| 6  | -0.106768000 | -3.692877000 | -0.976462000 |
| 6  | 0.499981000  | -3.301861000 | 1.309345000  |
| 6  | 0.671890000  | -4.841835000 | -0.985748000 |
| 6  | 1.281783000  | -4.448169000 | 1.298277000  |
| 6  | 1.368287000  | -5.224944000 | 0.151029000  |
| 1  | -0.645335000 | -3.420422000 | -1.874647000 |
| 1  | 0.440271000  | -2.720164000 | 2.219094000  |
| 1  | 0.728963000  | -5.439301000 | -1.888974000 |
| 1  | 1.821173000  | -4.733248000 | 2.194700000  |
| 1  | 1.972223000  | -6.125941000 | 0.145276000  |
| 6  | -2.567074000 | -1.864353000 | -0.999033000 |
| 6  | -2.385921000 | -1.507897000 | -2.335707000 |
| 6  | -3.701110000 | -2.593663000 | -0.646855000 |
| 6  | -3.307496000 | -1.889062000 | -3.301328000 |
| 6  | -4.629363000 | -2.961913000 | -1.610727000 |
| 6  | -4.432849000 | -2.616077000 | -2.940503000 |
| 1  | -1.522852000 | -0.916870000 | -2.622855000 |
| 1  | -3.880790000 | -2.865714000 | 0.385059000  |
| 1  | -3.148483000 | -1.604662000 | -4.335650000 |
| 1  | -5.511784000 | -3.520632000 | -1.318383000 |
| 1  | -5.159281000 | -2.905742000 | -3.691934000 |
| 6  | -0.246685000 | 5.671384000  | 1.143702000  |
| 1  | -0.543047000 | 5.465523000  | 2.173916000  |
| 1  | 0.790601000  | 5.361643000  | 1.004705000  |

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| 1            | -0.342180000 | 6.734361000  | 0.928619000  |
| 95           |              |              |              |
| exo-4t2P-OMe |              |              |              |
| 46           | 0.236693000  | 0.780943000  | 0.568315000  |
| 15           | -2.148178000 | 0.176974000  | 0.178505000  |
| 6            | -2.834133000 | -0.849680000 | 1.526819000  |
| 6            | -3.184918000 | -0.214022000 | 2.722051000  |
| 6            | -2.895266000 | -2.240933000 | 1.458162000  |
| 6            | -3.618475000 | -0.957302000 | 3.809025000  |
| 1            | -3.102024000 | 0.863351000  | 2.810208000  |
| 6            | -3.334716000 | -2.979794000 | 2.549204000  |
| 1            | -2.595717000 | -2.760775000 | 0.557038000  |
| 6            | -3.702165000 | -2.341159000 | 3.724022000  |
| 1            | -3.887144000 | -0.449121000 | 4.728514000  |
| 1            | -3.382556000 | -4.060770000 | 2.476039000  |
| 1            | -4.045544000 | -2.919713000 | 4.574925000  |
| 6            | -3.306254000 | 1.605960000  | 0.093331000  |
| 6            | -4.685654000 | 1.403284000  | 0.180531000  |
| 6            | -2.830873000 | 2.893668000  | -0.134257000 |
| 6            | -5.564922000 | 2.464475000  | 0.039193000  |
| 1            | -5.081136000 | 0.411935000  | 0.369972000  |
| 6            | -3.712869000 | 3.957198000  | -0.282022000 |
| 1            | -1.769473000 | 3.089955000  | -0.166915000 |
| 6            | -5.079322000 | 3.745539000  | -0.196147000 |
| 1            | -6.632968000 | 2.291642000  | 0.116145000  |
| 1            | -3.315568000 | 4.952506000  | -0.445863000 |
| 1            | -5.768029000 | 4.576848000  | -0.302537000 |
| 6            | -2.564078000 | -0.639890000 | -1.415951000 |
| 6            | -1.759571000 | -0.322439000 | -2.510116000 |
| 6            | -3.678822000 | -1.452756000 | -1.619971000 |
| 6            | -2.052950000 | -0.809963000 | -3.776193000 |
| 1            | -0.889933000 | 0.310379000  | -2.368512000 |
| 6            | -3.966955000 | -1.950177000 | -2.883014000 |
| 1            | -4.330305000 | -1.705078000 | -0.792303000 |
| 6            | -3.155821000 | -1.631002000 | -3.964270000 |
| 1            | -1.414598000 | -0.551654000 | -4.614087000 |
| 1            | -4.835006000 | -2.585189000 | -3.023852000 |
| 1            | -3.386471000 | -2.017473000 | -4.951140000 |

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| 6  | 1.912676000  | 3.346072000  | 0.598538000  |
| 6  | 3.358196000  | 3.702554000  | 0.174673000  |
| 6  | 3.455024000  | 1.478714000  | 0.462410000  |
| 6  | 2.026567000  | 1.834300000  | 0.963279000  |
| 6  | 3.744887000  | 2.481162000  | -0.658662000 |
| 1  | 4.799494000  | 2.483589000  | -0.951757000 |
| 1  | 3.136354000  | 2.357085000  | -1.550039000 |
| 6  | 4.270098000  | 3.545053000  | 1.403647000  |
| 1  | 3.835037000  | 4.007712000  | 2.292740000  |
| 6  | 4.422466000  | 2.006727000  | 1.537833000  |
| 1  | 4.177217000  | 1.636727000  | 2.535362000  |
| 1  | 3.439401000  | 4.677901000  | -0.311004000 |
| 1  | 3.635320000  | 0.436871000  | 0.212914000  |
| 1  | 2.037952000  | 1.773646000  | 2.049802000  |
| 1  | 1.603345000  | 3.930322000  | 1.464677000  |
| 6  | 0.944397000  | 3.772389000  | -0.478654000 |
| 8  | 0.298149000  | 4.776067000  | -0.443213000 |
| 8  | 0.896303000  | 2.961492000  | -1.550492000 |
| 6  | 0.112570000  | 3.401929000  | -2.638954000 |
| 1  | 0.263365000  | 2.678207000  | -3.439603000 |
| 1  | -0.944632000 | 3.443335000  | -2.373220000 |
| 1  | 0.426099000  | 4.394632000  | -2.966583000 |
| 6  | -0.514023000 | 2.107744000  | 1.873212000  |
| 7  | -0.948842000 | 2.725100000  | 2.745120000  |
| 1  | 5.234831000  | 4.028569000  | 1.229096000  |
| 1  | 5.447667000  | 1.693050000  | 1.317095000  |
| 15 | 1.348147000  | -1.262171000 | -0.132009000 |
| 6  | 2.163771000  | -1.311641000 | -1.772067000 |
| 6  | 2.221469000  | -0.131972000 | -2.511006000 |
| 6  | 2.688124000  | -2.482448000 | -2.328225000 |
| 6  | 2.813373000  | -0.114102000 | -3.768579000 |
| 6  | 3.279145000  | -2.463047000 | -3.581615000 |
| 6  | 3.346086000  | -1.276746000 | -4.303177000 |
| 1  | 1.800710000  | 0.777486000  | -2.098500000 |
| 1  | 2.618453000  | -3.420478000 | -1.789838000 |
| 1  | 2.856814000  | 0.813819000  | -4.328280000 |
| 1  | 3.683531000  | -3.378239000 | -4.000131000 |
| 1  | 3.807660000  | -1.263768000 | -5.284654000 |

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| 6 | 0.384101000  | -2.840216000 | -0.146942000 |
| 6 | 0.324806000  | -3.665170000 | 0.976690000  |
| 6 | -0.308735000 | -3.231099000 | -1.295011000 |
| 6 | -0.396785000 | -4.851226000 | 0.949661000  |
| 6 | -1.030811000 | -4.415244000 | -1.320620000 |
| 6 | -1.075324000 | -5.231960000 | -0.198318000 |
| 1 | 0.852347000  | -3.394504000 | 1.881947000  |
| 1 | -0.280823000 | -2.616768000 | -2.185391000 |
| 1 | -0.421940000 | -5.479707000 | 1.833075000  |
| 1 | -1.557301000 | -4.698625000 | -2.225171000 |
| 1 | -1.633358000 | -6.161790000 | -0.221147000 |
| 6 | 2.626036000  | -1.658015000 | 1.133214000  |
| 6 | 2.360161000  | -1.286130000 | 2.451771000  |
| 6 | 3.814014000  | -2.329854000 | 0.851339000  |
| 6 | 3.254212000  | -1.594836000 | 3.467581000  |
| 6 | 4.713433000  | -2.626373000 | 1.866129000  |
| 6 | 4.434348000  | -2.264462000 | 3.176562000  |
| 1 | 1.453556000  | -0.738352000 | 2.686210000  |
| 1 | 4.057887000  | -2.611990000 | -0.164623000 |
| 1 | 3.030032000  | -1.298564000 | 4.486317000  |
| 1 | 5.638373000  | -3.140484000 | 1.628539000  |
| 1 | 5.138841000  | -2.496753000 | 3.967755000  |

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exo-TS4\_5tP-O

|    |              |              |              |
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| 46 | 0.654505000  | -0.597194000 | 0.389940000  |
| 15 | -1.580224000 | -0.067588000 | -0.013068000 |
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| 6  | -2.575322000 | -2.622430000 | -0.349939000 |
| 6  | -3.137020000 | -1.136724000 | -2.131648000 |
| 6  | -3.233369000 | -3.648513000 | -0.990980000 |
| 1  | -2.094295000 | -2.810457000 | 0.594248000  |
| 6  | -3.787502000 | -2.170513000 | -2.781482000 |
| 1  | -3.105678000 | -0.165586000 | -2.587988000 |
| 6  | -3.841508000 | -3.424940000 | -2.213149000 |
| 1  | -3.266295000 | -4.624785000 | -0.542075000 |
| 1  | -4.252947000 | -1.988845000 | -3.733395000 |
| 1  | -4.349187000 | -4.226556000 | -2.718246000 |
| 6  | -2.572473000 | 0.255584000  | 1.481774000  |

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| 6 | -3.906598000 | -0.104134000 | 1.601973000  |
| 6 | -1.954063000 | 0.917356000  | 2.534995000  |
| 6 | -4.612046000 | 0.197030000  | 2.750548000  |
| 1 | -4.399237000 | -0.627753000 | 0.803620000  |
| 6 | -2.664180000 | 1.224393000  | 3.677397000  |
| 1 | -0.914972000 | 1.186229000  | 2.467452000  |
| 6 | -3.993107000 | 0.864265000  | 3.788405000  |
| 1 | -5.644578000 | -0.091233000 | 2.832687000  |
| 1 | -2.172638000 | 1.737208000  | 4.483997000  |
| 1 | -4.542416000 | 1.097382000  | 4.682737000  |
| 6 | -1.780499000 | 1.444313000  | -1.008671000 |
| 6 | -0.690705000 | 1.919921000  | -1.721869000 |
| 6 | -2.981714000 | 2.139097000  | -1.070720000 |
| 6 | -0.806745000 | 3.055888000  | -2.500848000 |
| 1 | 0.259170000  | 1.420817000  | -1.651773000 |
| 6 | -3.094911000 | 3.273822000  | -1.845135000 |
| 1 | -3.830253000 | 1.799990000  | -0.505127000 |
| 6 | -2.007063000 | 3.731760000  | -2.565625000 |
| 1 | 0.048331000  | 3.414243000  | -3.044390000 |
| 1 | -4.028993000 | 3.804750000  | -1.881722000 |
| 1 | -2.095025000 | 4.619549000  | -3.165748000 |
| 6 | 3.998827000  | -0.044548000 | 0.328764000  |
| 6 | 4.551036000  | -1.040158000 | -0.712364000 |
| 6 | 2.772908000  | -2.133401000 | 0.103055000  |
| 6 | 2.827112000  | -0.835647000 | 0.967043000  |
| 6 | 3.273175000  | -1.670687000 | -1.263026000 |
| 1 | 3.473006000  | -2.500834000 | -1.931776000 |
| 1 | 2.625982000  | -0.959259000 | -1.754119000 |
| 6 | 5.184338000  | -2.214275000 | 0.041848000  |
| 1 | 5.848955000  | -1.881799000 | 0.830218000  |
| 6 | 3.957673000  | -2.991072000 | 0.580220000  |
| 1 | 3.971265000  | -3.115721000 | 1.655711000  |
| 1 | 5.208302000  | -0.577758000 | -1.436894000 |
| 1 | 1.838871000  | -2.686744000 | 0.115377000  |
| 1 | 3.071660000  | -1.114648000 | 1.976262000  |
| 1 | 4.735546000  | 0.187238000  | 1.084524000  |
| 6 | 3.621576000  | 1.256448000  | -0.332660000 |
| 8 | 2.776093000  | 1.390711000  | -1.166880000 |

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| 8 | 4.389511000 | 2.248960000  | 0.084324000  |
| 6 | 4.103491000 | 3.535174000  | -0.441315000 |
| 1 | 4.814461000 | 4.204861000  | 0.017010000  |
| 1 | 4.216825000 | 3.541129000  | -1.517309000 |
| 1 | 3.093739000 | 3.825038000  | -0.185300000 |
| 6 | 1.706784000 | 0.469654000  | 1.628608000  |
| 7 | 1.873049000 | 1.330702000  | 2.376123000  |
| 1 | 5.767741000 | -2.827852000 | -0.634083000 |
| 1 | 3.897213000 | -3.980019000 | 0.139853000  |

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exo-TS4\_5tP-OMe

|    |              |              |              |
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| 46 | -0.724179000 | 0.509152000  | 0.372179000  |
| 15 | 1.545561000  | 0.104783000  | 0.008516000  |
| 6  | 2.518078000  | 1.535347000  | -0.578287000 |
| 6  | 2.299591000  | 2.760250000  | 0.039953000  |
| 6  | 3.448371000  | 1.463238000  | -1.603007000 |
| 6  | 3.004777000  | 3.880358000  | -0.344918000 |
| 1  | 1.571061000  | 2.835025000  | 0.828376000  |
| 6  | 4.147457000  | 2.588855000  | -1.997036000 |
| 1  | 3.629548000  | 0.529255000  | -2.101297000 |
| 6  | 3.930406000  | 3.797208000  | -1.368120000 |
| 1  | 2.827021000  | 4.819175000  | 0.147571000  |
| 1  | 4.862960000  | 2.517535000  | -2.796227000 |
| 1  | 4.475032000  | 4.671538000  | -1.675366000 |
| 6  | 2.466532000  | -0.478613000 | 1.467044000  |
| 6  | 3.806682000  | -0.181586000 | 1.672925000  |
| 6  | 1.797034000  | -1.261653000 | 2.397749000  |
| 6  | 4.467580000  | -0.666218000 | 2.783561000  |
| 1  | 4.337699000  | 0.434693000  | 0.971372000  |
| 6  | 2.463472000  | -1.750968000 | 3.503449000  |
| 1  | 0.751808000  | -1.478114000 | 2.272573000  |
| 6  | 3.797696000  | -1.454666000 | 3.698609000  |
| 1  | 5.504322000  | -0.424947000 | 2.934370000  |
| 1  | 1.931037000  | -2.353320000 | 4.216645000  |
| 1  | 4.312359000  | -1.829332000 | 4.565026000  |
| 6  | 1.839748000  | -1.172125000 | -1.261322000 |
| 6  | 1.068183000  | -1.133105000 | -2.415777000 |
| 6  | 2.781593000  | -2.178935000 | -1.123693000 |

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| 6             | 1.248465000  | -2.063274000 | -3.416991000 |
| 1             | 0.316039000  | -0.372010000 | -2.527809000 |
| 6             | 2.953835000  | -3.120023000 | -2.121642000 |
| 1             | 3.379702000  | -2.238396000 | -0.233968000 |
| 6             | 2.192761000  | -3.062243000 | -3.270435000 |
| 1             | 0.646337000  | -2.015383000 | -4.306287000 |
| 1             | 3.684060000  | -3.898959000 | -1.996862000 |
| 1             | 2.327889000  | -3.794822000 | -4.045397000 |
| 6             | -4.111128000 | -0.091704000 | 0.484909000  |
| 6             | -4.707100000 | 0.774696000  | -0.646622000 |
| 6             | -2.871028000 | 1.923656000  | -0.074450000 |
| 6             | -2.885964000 | 0.741815000  | 0.942477000  |
| 6             | -3.455832000 | 1.307378000  | -1.341992000 |
| 1             | -3.682602000 | 2.052807000  | -2.096437000 |
| 1             | -2.841658000 | 0.532622000  | -1.776871000 |
| 6             | -5.280909000 | 2.048793000  | -0.017704000 |
| 1             | -5.912676000 | 1.832339000  | 0.834919000  |
| 6             | -4.015381000 | 2.855826000  | 0.361911000  |
| 1             | -3.967652000 | 3.102527000  | 1.415029000  |
| 1             | -5.412731000 | 0.235423000  | -1.264136000 |
| 1             | -1.934185000 | 2.463490000  | -0.188386000 |
| 1             | -3.055580000 | 1.139380000  | 1.927063000  |
| 1             | -4.808309000 | -0.183497000 | 1.305824000  |
| 6             | -3.910509000 | -1.513614000 | 0.021761000  |
| 8             | -4.664028000 | -2.393141000 | 0.299677000  |
| 8             | -2.868407000 | -1.679012000 | -0.782820000 |
| 6             | -2.594845000 | -3.011006000 | -1.189026000 |
| 1             | -1.695392000 | -2.959902000 | -1.783191000 |
| 1             | -2.438342000 | -3.637971000 | -0.322194000 |
| 1             | -3.415854000 | -3.407240000 | -1.771562000 |
| 6             | -1.734330000 | -0.530385000 | 1.675482000  |
| 7             | -1.878206000 | -1.343693000 | 2.477359000  |
| 1             | -5.884256000 | 2.588116000  | -0.738062000 |
| 1             | -3.963307000 | 3.786504000  | -0.191898000 |
| 61            |              |              |              |
| exo-TS4_5tP-N |              |              |              |
| 46            | -0.940589000 | 0.014227000  | 0.115939000  |
| 15            | 1.377579000  | 0.109653000  | -0.085081000 |

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| 6 | 1.324810000  | -1.693873000 | -2.179157000 |
| 6 | 3.477015000  | -1.440994000 | -1.168602000 |
| 6 | 1.855331000  | -2.600379000 | -3.077244000 |
| 1 | 0.273804000  | -1.471386000 | -2.203807000 |
| 6 | 4.004356000  | -2.348846000 | -2.062493000 |
| 1 | 4.115071000  | -1.007117000 | -0.421061000 |
| 6 | 3.194212000  | -2.927172000 | -3.021948000 |
| 1 | 1.215350000  | -3.058999000 | -3.808825000 |
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| 1 | 3.605448000  | -3.638134000 | -3.715804000 |
| 6 | 1.941775000  | 1.740871000  | -0.677487000 |
| 6 | 2.760497000  | 1.917984000  | -1.780486000 |
| 6 | 1.473318000  | 2.862765000  | -0.001299000 |
| 6 | 3.113730000  | 3.189507000  | -2.194508000 |
| 1 | 3.123565000  | 1.066832000  | -2.324973000 |
| 6 | 1.835233000  | 4.128191000  | -0.409202000 |
| 1 | 0.818355000  | 2.748041000  | 0.845444000  |
| 6 | 2.656867000  | 4.295102000  | -1.509055000 |
| 1 | 3.747572000  | 3.311034000  | -3.054370000 |
| 1 | 1.467820000  | 4.984527000  | 0.126636000  |
| 1 | 2.932982000  | 5.282799000  | -1.831386000 |
| 6 | 2.293714000  | -0.122271000 | 1.475437000  |
| 6 | 1.781041000  | -1.020412000 | 2.401344000  |
| 6 | 3.471883000  | 0.546464000  | 1.772649000  |
| 6 | 2.444082000  | -1.261131000 | 3.587029000  |
| 1 | 0.850159000  | -1.518993000 | 2.197547000  |
| 6 | 4.130775000  | 0.311101000  | 2.963158000  |
| 1 | 3.873792000  | 1.263076000  | 1.080187000  |
| 6 | 3.620897000  | -0.596139000 | 3.870142000  |
| 1 | 2.034168000  | -1.957915000 | 4.295533000  |
| 1 | 5.040323000  | 0.840620000  | 3.182610000  |
| 1 | 4.132591000  | -0.776146000 | 4.798308000  |
| 6 | -3.192698000 | -0.467620000 | 0.145203000  |
| 6 | -3.718957000 | -0.044224000 | -1.233380000 |
| 6 | -4.425787000 | 1.613425000  | 0.104023000  |
| 6 | -3.592641000 | 0.742090000  | 1.073154000  |
| 6 | -3.624224000 | 1.480349000  | -1.188989000 |



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| 1 | -4.108761000 | 1.958736000  | -2.032277000 |
| 1 | -2.611052000 | 1.858116000  | -1.111625000 |
| 6 | -5.239340000 | -0.237819000 | -1.226545000 |
| 1 | -5.524640000 | -1.236860000 | -0.920367000 |
| 6 | -5.715126000 | 0.857080000  | -0.238967000 |
| 1 | -6.194546000 | 0.449487000  | 0.643856000  |
| 1 | -3.212707000 | -0.545545000 | -2.043786000 |
| 1 | -4.584948000 | 2.614957000  | 0.479865000  |
| 1 | -4.191253000 | 0.398502000  | 1.908809000  |
| 1 | -3.779076000 | -1.297111000 | 0.509639000  |
| 6 | -1.849282000 | -1.761993000 | 0.046126000  |
| 8 | -1.882880000 | -2.417247000 | -0.955950000 |
| 8 | -1.745028000 | -2.329307000 | 1.271691000  |
| 6 | -1.581855000 | -3.738233000 | 1.286254000  |
| 1 | -1.535041000 | -4.018938000 | 2.328109000  |
| 1 | -2.418262000 | -4.227537000 | 0.803472000  |
| 1 | -0.670165000 | -4.028186000 | 0.780060000  |
| 6 | -2.511878000 | 1.540925000  | 1.649244000  |
| 7 | -1.729229000 | 2.231993000  | 2.106752000  |
| 1 | -5.650019000 | -0.073386000 | -2.216492000 |
| 1 | -6.426689000 | 1.527556000  | -0.705131000 |

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|    |              |              |              |
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| 6  | -3.136012000 | 1.059967000  | -0.649706000 |
| 6  | -2.559562000 | 1.785880000  | -1.692206000 |
| 6  | -4.296456000 | 1.552771000  | -0.055279000 |
| 6  | -3.136473000 | 2.962883000  | -2.145231000 |
| 1  | -1.646122000 | 1.422995000  | -2.152366000 |
| 6  | -4.869141000 | 2.736767000  | -0.500376000 |
| 1  | -4.759439000 | 1.015101000  | 0.762809000  |
| 6  | -4.294283000 | 3.442101000  | -1.547977000 |
| 1  | -2.674481000 | 3.512980000  | -2.957594000 |
| 1  | -5.771163000 | 3.107668000  | -0.025378000 |
| 1  | -4.743261000 | 4.366721000  | -1.894243000 |
| 6  | -3.202892000 | -1.730951000 | -1.246754000 |
| 6  | -3.980859000 | -1.338294000 | -2.335889000 |

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| 6 | -3.665781000 | -4.037906000 | -1.798388000 |
| 1 | -2.431149000 | -3.430512000 | -0.163503000 |
| 6 | -4.438148000 | -3.637617000 | -2.881479000 |
| 1 | -5.193607000 | -1.960308000 | -3.989834000 |
| 1 | -3.534426000 | -5.092474000 | -1.581502000 |
| 1 | -4.917416000 | -4.377136000 | -3.514131000 |
| 6 | -2.991425000 | -0.895979000 | 1.497810000  |
| 6 | -2.165668000 | -0.690353000 | 2.602269000  |
| 6 | -4.283219000 | -1.383623000 | 1.705731000  |
| 6 | -2.628007000 | -0.936383000 | 3.888300000  |
| 1 | -1.143735000 | -0.358051000 | 2.453677000  |
| 6 | -4.743715000 | -1.633523000 | 2.989993000  |
| 1 | -4.930322000 | -1.580737000 | 0.858533000  |
| 6 | -3.918381000 | -1.405620000 | 4.083984000  |
| 1 | -1.970633000 | -0.775132000 | 4.735479000  |
| 1 | -5.748706000 | -2.014430000 | 3.136564000  |
| 1 | -4.278184000 | -1.606887000 | 5.087327000  |
| 6 | 2.697290000  | -3.260733000 | -0.587864000 |
| 6 | 4.040588000  | -2.681829000 | -1.091020000 |
| 6 | 2.537897000  | -1.228338000 | -1.903803000 |
| 6 | 1.649948000  | -2.279119000 | -1.188201000 |
| 6 | 3.784858000  | -1.174308000 | -1.022607000 |
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| 1 | 3.594373000  | -0.819508000 | -0.010845000 |
| 6 | 4.124547000  | -2.923745000 | -2.603060000 |
| 1 | 3.901757000  | -3.960529000 | -2.866867000 |
| 6 | 3.092409000  | -1.917024000 | -3.167928000 |
| 1 | 2.305329000  | -2.393351000 | -3.757680000 |
| 1 | 4.903280000  | -3.054487000 | -0.534972000 |
| 1 | 2.058494000  | -0.281233000 | -2.130736000 |
| 1 | 1.060813000  | -2.797301000 | -1.938285000 |
| 1 | 2.528459000  | -4.261716000 | -0.983406000 |
| 6 | 2.719582000  | -3.404751000 | 0.912861000  |
| 8 | 2.736515000  | -4.676693000 | 1.276736000  |
| 8 | 2.797905000  | -2.506384000 | 1.702118000  |

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| 6  | 0.167052000  | -2.559491000 | 0.021270000  |
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| 1  | 3.573154000  | -1.175503000 | -3.812436000 |
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| 6  | 2.047930000  | 1.721539000  | 1.735202000  |
| 6  | 2.422882000  | 0.516814000  | 2.324608000  |
| 6  | 2.369644000  | 2.920506000  | 2.378975000  |
| 6  | 3.122314000  | 0.507774000  | 3.526558000  |
| 6  | 3.063359000  | 2.908739000  | 3.578465000  |
| 6  | 3.442681000  | 1.700570000  | 4.154622000  |
| 1  | 2.186435000  | -0.431237000 | 1.857002000  |
| 1  | 2.072612000  | 3.868200000  | 1.944657000  |
| 1  | 3.408220000  | -0.444584000 | 3.958505000  |
| 1  | 3.306349000  | 3.845604000  | 4.068407000  |
| 1  | 3.984105000  | 1.694816000  | 5.094839000  |
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| 6  | 0.272930000  | 4.374475000  | -0.304854000 |
| 6  | -1.028698000 | 3.047588000  | 1.210332000  |
| 6  | -0.565356000 | 5.458202000  | -0.069482000 |
| 6  | -1.858161000 | 4.130199000  | 1.452575000  |
| 6  | -1.629503000 | 5.340806000  | 0.810754000  |
| 1  | 1.107004000  | 4.490761000  | -0.985454000 |
| 1  | -1.223987000 | 2.107726000  | 1.714664000  |
| 1  | -0.376950000 | 6.399742000  | -0.574379000 |
| 1  | -2.691493000 | 4.024549000  | 2.138037000  |
| 1  | -2.281248000 | 6.187780000  | 0.995944000  |
| 6  | 2.366647000  | 2.255604000  | -1.102328000 |
| 6  | 1.950571000  | 2.362195000  | -2.432669000 |
| 6  | 3.697119000  | 2.531380000  | -0.796997000 |
| 6  | 2.833278000  | 2.755918000  | -3.425647000 |
| 6  | 4.585792000  | 2.916352000  | -1.794677000 |
| 6  | 4.157748000  | 3.033447000  | -3.108052000 |
| 1  | 0.922135000  | 2.134762000  | -2.695870000 |
| 1  | 4.048242000  | 2.444827000  | 0.223842000  |
| 1  | 2.489479000  | 2.838845000  | -4.451001000 |
| 1  | 5.618713000  | 3.126146000  | -1.538555000 |
| 1  | 4.852542000  | 3.335454000  | -3.884163000 |

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| 1 | 3.535125000 | -4.482355000 | 3.176896000 |
| 1 | 1.761580000 | -4.564943000 | 3.086407000 |
| 1 | 2.734430000 | -6.027705000 | 2.763985000 |

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|    |              |              |              |
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| 6  | -2.515032000 | 1.959645000  | -1.567973000 |
| 6  | -4.201627000 | 1.756465000  | 0.123799000  |
| 6  | -3.041838000 | 3.182232000  | -1.955542000 |
| 1  | -1.642401000 | 1.565387000  | -2.078418000 |
| 6  | -4.723721000 | 2.986242000  | -0.255532000 |
| 1  | -4.665006000 | 1.212355000  | 0.937331000  |
| 6  | -4.149441000 | 3.699711000  | -1.297501000 |
| 1  | -2.580078000 | 3.737197000  | -2.764715000 |
| 1  | -5.586695000 | 3.385788000  | 0.266450000  |
| 1  | -4.559390000 | 4.659445000  | -1.592847000 |
| 6  | -3.270700000 | -1.523269000 | -1.288336000 |
| 6  | -4.027033000 | -1.037037000 | -2.354822000 |
| 6  | -3.173903000 | -2.907279000 | -1.109669000 |
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| 6  | -4.572112000 | -3.280316000 | -3.036487000 |
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| 1  | -5.076660000 | -3.961724000 | -3.713173000 |
| 6  | -3.058820000 | -0.840266000 | 1.501866000  |
| 6  | -2.251292000 | -0.693359000 | 2.628716000  |
| 6  | -4.365690000 | -1.301943000 | 1.667093000  |
| 6  | -2.744664000 | -0.973085000 | 3.895806000  |
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| 6  | -4.857278000 | -1.587226000 | 2.932542000  |
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| 6  | -4.049155000 | -1.418898000 | 4.049582000  |

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| 1  | -4.433327000 | -1.647779000 | 5.037813000  |
| 6  | 2.454313000  | -3.533362000 | -0.502169000 |
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| 6  | 2.534197000  | -1.459181000 | -1.754689000 |
| 6  | 1.525719000  | -2.427657000 | -1.081156000 |
| 6  | 3.761352000  | -1.554059000 | -0.849448000 |
| 1  | 4.634330000  | -1.039892000 | -1.261879000 |
| 1  | 3.587520000  | -1.200725000 | 0.165402000  |
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| 6  | 2.442571000  | -3.866443000 | 0.970451000  |
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| 6  | 2.233148000  | -3.124445000 | 3.159639000  |
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| 6  | 2.341003000  | 1.653767000  | 1.571410000  |
| 6  | 2.710932000  | 0.466974000  | 2.200078000  |
| 6  | 2.808349000  | 2.865589000  | 2.087936000  |
| 6  | 3.551793000  | 0.489492000  | 3.307803000  |
| 6  | 3.642098000  | 2.886079000  | 3.194729000  |
| 6  | 4.018798000  | 1.695713000  | 3.805639000  |
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| 1  | 2.515911000  | 3.801315000  | 1.625851000  |

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| 1 | 3.839831000  | -0.442526000 | 3.780997000  |
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| 6 | 0.242177000  | 3.102961000  | 0.357049000  |
| 6 | 0.478697000  | 4.313115000  | -0.292340000 |
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| 6 | -1.540650000 | 4.159489000  | 1.602840000  |
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| 1 | 1.268176000  | 4.391181000  | -1.029676000 |
| 1 | -0.990857000 | 2.105173000  | 1.811831000  |
| 1 | -0.090228000 | 6.368588000  | -0.511999000 |
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| 6 | 2.557478000  | 2.472081000  | -3.678459000 |
| 6 | 4.498231000  | 2.590901000  | -2.272931000 |
| 6 | 3.922325000  | 2.689635000  | -3.529917000 |
| 1 | 0.720786000  | 1.970781000  | -2.707022000 |
| 1 | 4.185380000  | 2.211122000  | -0.189804000 |
| 1 | 2.098065000  | 2.539349000  | -4.658595000 |
| 1 | 5.563448000  | 2.753028000  | -2.148455000 |
| 1 | 4.533180000  | 2.929603000  | -4.393312000 |

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| 6  | -2.596141000 | -2.726085000 | -0.837819000 |
| 6  | -3.976822000 | -1.116135000 | -1.930082000 |
| 6  | -3.196525000 | -3.736015000 | -1.559870000 |
| 1  | -1.806468000 | -2.956442000 | -0.144876000 |
| 6  | -4.570199000 | -2.126043000 | -2.664166000 |
| 1  | -4.287089000 | -0.100068000 | -2.088310000 |
| 6  | -4.185688000 | -3.437883000 | -2.477784000 |
| 1  | -2.883686000 | -4.754511000 | -1.415350000 |

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| 6 | -4.468196000 | -0.613614000 | 1.600653000  |
| 6 | -2.647206000 | 0.501444000  | 2.664058000  |
| 6 | -5.197260000 | -0.536395000 | 2.772364000  |
| 1 | -4.903121000 | -1.090399000 | 0.742070000  |
| 6 | -3.378318000 | 0.590888000  | 3.830206000  |
| 1 | -1.641329000 | 0.880534000  | 2.628480000  |
| 6 | -4.656864000 | 0.069930000  | 3.887858000  |
| 1 | -6.188123000 | -0.952312000 | 2.811042000  |
| 1 | -2.945376000 | 1.055561000  | 4.697833000  |
| 1 | -5.224131000 | 0.128705000  | 4.799347000  |
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| 6 | -1.772897000 | 1.851553000  | -1.862286000 |
| 6 | -3.693005000 | 2.200584000  | -0.490339000 |
| 6 | -2.054463000 | 3.008774000  | -2.557352000 |
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| 6 | -3.968671000 | 3.368416000  | -1.177306000 |
| 1 | -4.337649000 | 1.900351000  | 0.314490000  |
| 6 | -3.154157000 | 3.772880000  | -2.214608000 |
| 1 | -1.409213000 | 3.320197000  | -3.359097000 |
| 1 | -4.822121000 | 3.960441000  | -0.898967000 |
| 1 | -3.369235000 | 4.680983000  | -2.748604000 |
| 6 | 5.379026000  | 0.561390000  | 0.338430000  |
| 6 | 6.289762000  | -0.035854000 | -0.738563000 |
| 6 | 5.286857000  | -1.857714000 | 0.105643000  |
| 6 | 4.651794000  | -0.708202000 | 0.920055000  |
| 6 | 5.453557000  | -1.202484000 | -1.263687000 |
| 1 | 5.995259000  | -1.828930000 | -1.962223000 |
| 1 | 4.521623000  | -0.893117000 | -1.718960000 |
| 6 | 7.435816000  | -0.767573000 | -0.035224000 |
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| 1 | 6.820049000  | -2.058348000 | 1.650503000  |
| 1 | 6.599774000  | 0.694507000  | -1.470260000 |
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| 1 | 4.849602000  | -0.813254000 | 1.979548000  |

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| 1 | 5.946361000 | 1.030115000  | 1.133011000  |
| 6 | 4.429228000 | 1.609547000  | -0.187108000 |
| 8 | 4.268795000 | 1.872478000  | -1.336870000 |
| 8 | 3.792061000 | 2.204982000  | 0.807967000  |
| 6 | 2.767954000 | 3.128613000  | 0.452080000  |
| 1 | 2.409448000 | 3.540325000  | 1.382115000  |
| 1 | 3.167650000 | 3.907616000  | -0.181893000 |
| 1 | 1.968165000 | 2.612789000  | -0.061319000 |
| 6 | 3.206722000 | -0.684002000 | 0.764851000  |
| 7 | 2.079920000 | -0.668474000 | 0.629617000  |
| 1 | 8.192788000 | -1.059206000 | -0.752889000 |
| 1 | 7.158646000 | -2.927975000 | 0.178502000  |

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| 46 | -0.027209000 | -0.497099000 | -0.387191000 |
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| 6  | 3.498764000  | 1.992366000  | 1.293080000  |
| 6  | 2.026206000  | 1.681827000  | 3.604843000  |
| 1  | 1.006115000  | 0.130805000  | 2.559218000  |
| 6  | 3.732124000  | 2.815449000  | 2.379718000  |
| 1  | 4.078104000  | 2.126978000  | 0.398930000  |
| 6  | 3.001452000  | 2.659623000  | 3.538984000  |
| 1  | 1.446844000  | 1.557452000  | 4.502180000  |
| 1  | 4.487726000  | 3.577926000  | 2.316491000  |
| 1  | 3.184300000  | 3.299014000  | 4.383838000  |
| 6  | 3.146921000  | -1.605152000 | 0.370487000  |
| 6  | 4.187071000  | -1.601449000 | 1.287284000  |
| 6  | 2.843313000  | -2.791895000 | -0.283899000 |
| 6  | 4.911045000  | -2.752116000 | 1.537204000  |
| 1  | 4.434147000  | -0.700052000 | 1.816704000  |
| 6  | 3.573094000  | -3.937513000 | -0.045051000 |
| 1  | 2.019134000  | -2.813157000 | -0.974611000 |
| 6  | 4.609458000  | -3.920979000 | 0.868934000  |
| 1  | 5.710773000  | -2.732288000 | 2.255791000  |
| 1  | 3.325168000  | -4.846319000 | -0.563396000 |
| 1  | 5.172464000  | -4.815937000 | 1.064191000  |



|   |              |              |              |
|---|--------------|--------------|--------------|
| 6 | 3.055438000  | 0.608203000  | -1.439667000 |
| 6 | 2.379614000  | 1.515521000  | -2.244779000 |
| 6 | 4.376513000  | 0.311653000  | -1.739854000 |
| 6 | 3.012981000  | 2.127193000  | -3.306799000 |
| 1 | 1.345202000  | 1.727314000  | -2.040345000 |
| 6 | 5.008530000  | 0.914145000  | -2.810917000 |
| 1 | 4.917703000  | -0.398136000 | -1.142348000 |
| 6 | 4.330563000  | 1.826502000  | -3.593655000 |
| 1 | 2.473584000  | 2.828211000  | -3.918033000 |
| 1 | 6.031347000  | 0.667505000  | -3.032956000 |
| 1 | 4.822447000  | 2.293715000  | -4.427818000 |
| 6 | -5.364363000 | 0.478159000  | -0.596178000 |
| 6 | -6.194317000 | 0.127221000  | 0.652235000  |
| 6 | -5.253018000 | -1.841772000 | 0.130962000  |
| 6 | -4.642936000 | -0.884615000 | -0.915281000 |
| 6 | -5.342950000 | -0.931780000 | 1.353320000  |
| 1 | -5.859634000 | -1.399624000 | 2.183025000  |
| 1 | -4.385081000 | -0.564772000 | 1.694415000  |
| 6 | -7.386950000 | -0.709453000 | 0.180960000  |
| 1 | -7.927756000 | -0.239567000 | -0.631466000 |
| 6 | -6.727478000 | -2.050190000 | -0.229505000 |
| 1 | -6.863746000 | -2.283054000 | -1.279188000 |
| 1 | -6.462567000 | 0.992688000  | 1.240689000  |
| 1 | -4.686683000 | -2.755382000 | 0.242642000  |
| 1 | -4.861746000 | -1.201857000 | -1.927342000 |
| 1 | -6.002392000 | 0.732719000  | -1.430320000 |
| 6 | -4.414850000 | 1.643781000  | -0.471616000 |
| 8 | -4.177026000 | 2.384159000  | -1.374370000 |
| 8 | -3.868479000 | 1.741961000  | 0.727843000  |
| 6 | -2.865291000 | 2.739841000  | 0.892285000  |
| 1 | -2.579464000 | 2.698928000  | 1.931319000  |
| 1 | -2.016159000 | 2.515473000  | 0.261816000  |
| 1 | -3.259786000 | 3.714442000  | 0.641372000  |
| 6 | -3.195213000 | -0.822655000 | -0.797205000 |
| 7 | -2.066902000 | -0.770748000 | -0.686016000 |
| 1 | -8.088082000 | -0.855463000 | 0.993705000  |
| 1 | -7.135852000 | -2.878436000 | 0.335797000  |

exo-5-O

|   |              |              |              |
|---|--------------|--------------|--------------|
| 6 | 2.883228000  | 0.200987000  | -0.646225000 |
| 6 | 1.842844000  | 0.952729000  | 0.188641000  |
| 6 | 1.187689000  | -1.186546000 | 0.359720000  |
| 6 | 2.448442000  | -1.279096000 | -0.503611000 |
| 6 | 1.546038000  | -0.042755000 | 1.308067000  |
| 1 | 0.728445000  | 0.253810000  | 1.952071000  |
| 1 | 2.415519000  | -0.257830000 | 1.917895000  |
| 6 | 0.510514000  | 0.941343000  | -0.592168000 |
| 1 | 0.653311000  | 1.231313000  | -1.625533000 |
| 6 | 0.076629000  | -0.568160000 | -0.495243000 |
| 1 | 0.056279000  | -0.988747000 | -1.493039000 |
| 1 | 2.142497000  | 1.947536000  | 0.485922000  |
| 1 | 0.887876000  | -2.113866000 | 0.823842000  |
| 6 | -0.445232000 | 1.879465000  | -0.019925000 |
| 7 | -1.173837000 | 2.622973000  | 0.437440000  |
| 6 | -1.303568000 | -0.761297000 | 0.078444000  |
| 8 | -2.231081000 | -0.399704000 | -0.795753000 |
| 8 | -1.543700000 | -1.184112000 | 1.165079000  |
| 1 | 2.262276000  | -1.756594000 | -1.458457000 |
| 1 | 2.904235000  | 0.538127000  | -1.676159000 |
| 6 | -3.577646000 | -0.428883000 | -0.341553000 |
| 1 | -3.851986000 | -1.429441000 | -0.036683000 |
| 1 | -3.702961000 | 0.248491000  | 0.491851000  |
| 1 | -4.177493000 | -0.109704000 | -1.179278000 |
| 1 | 3.209546000  | -1.860117000 | 0.002802000  |
| 1 | 3.873942000  | 0.360023000  | -0.238793000 |

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exo-5-OMe

|   |             |              |              |
|---|-------------|--------------|--------------|
| 6 | 2.928329000 | 0.059466000  | -0.243522000 |
| 6 | 1.800339000 | 0.873797000  | 0.398076000  |
| 6 | 0.968231000 | -1.208836000 | 0.349265000  |
| 6 | 2.374569000 | -1.387502000 | -0.229256000 |
| 6 | 1.209815000 | -0.119941000 | 1.395115000  |
| 1 | 0.306701000 | 0.231152000  | 1.874409000  |
| 1 | 1.921171000 | -0.421989000 | 2.154920000  |
| 6 | 0.654912000 | 0.990449000  | -0.628918000 |
| 1 | 1.016713000 | 1.319272000  | -1.595082000 |

|   |              |              |              |
|---|--------------|--------------|--------------|
| 6 | 0.125633000  | -0.488593000 | -0.719376000 |
| 1 | 0.339966000  | -0.871521000 | -1.707030000 |
| 1 | 2.108553000  | 1.832700000  | 0.789660000  |
| 1 | 0.514443000  | -2.122727000 | 0.704599000  |
| 6 | -0.345028000 | 1.959755000  | -0.202532000 |
| 7 | -1.112784000 | 2.724808000  | 0.140995000  |
| 6 | -1.371229000 | -0.602352000 | -0.585896000 |
| 8 | -1.781423000 | -0.645760000 | 0.671790000  |
| 8 | -2.106870000 | -0.640374000 | -1.522451000 |
| 1 | 2.363625000  | -1.844593000 | -1.211302000 |
| 1 | 3.168888000  | 0.408550000  | -1.241001000 |
| 6 | -3.187911000 | -0.654132000 | 0.877656000  |
| 1 | -3.627684000 | 0.245972000  | 0.471126000  |
| 1 | -3.633985000 | -1.517408000 | 0.403298000  |
| 1 | -3.328366000 | -0.693272000 | 1.946493000  |
| 1 | 2.968376000  | -2.023530000 | 0.416131000  |
| 1 | 3.831471000  | 0.140154000  | 0.348432000  |

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endo-3tP-O

|    |              |              |              |
|----|--------------|--------------|--------------|
| 6  | 1.024045000  | -2.247278000 | -0.480568000 |
| 7  | 1.021814000  | -3.389734000 | -0.397340000 |
| 6  | 1.025192000  | 1.833384000  | -0.760914000 |
| 8  | 1.083260000  | 2.443591000  | 0.438754000  |
| 8  | 0.971033000  | 2.471650000  | -1.770881000 |
| 46 | 1.065642000  | -0.190592000 | -0.628816000 |
| 15 | -1.142646000 | -0.156787000 | 0.018610000  |
| 6  | -2.277499000 | -1.138011000 | -1.009568000 |
| 6  | -1.814010000 | -1.969904000 | -2.014651000 |
| 6  | -3.648975000 | -1.034706000 | -0.798964000 |
| 6  | -2.702859000 | -2.690481000 | -2.789763000 |
| 1  | -0.761563000 | -2.073353000 | -2.185135000 |
| 6  | -4.532223000 | -1.759495000 | -1.567669000 |
| 1  | -4.030788000 | -0.381033000 | -0.036540000 |
| 6  | -4.059070000 | -2.589347000 | -2.567400000 |
| 1  | -2.327098000 | -3.334223000 | -3.563639000 |
| 1  | -5.588842000 | -1.672234000 | -1.391158000 |
| 1  | -4.748392000 | -3.151848000 | -3.170850000 |
| 6  | -1.203282000 | -0.835659000 | 1.699636000  |

|   |              |              |              |
|---|--------------|--------------|--------------|
| 6 | -1.932063000 | -1.966049000 | 2.023363000  |
| 6 | -0.430217000 | -0.221654000 | 2.678308000  |
| 6 | -1.903104000 | -2.466425000 | 3.311337000  |
| 1 | -2.509220000 | -2.471677000 | 1.273392000  |
| 6 | -0.410974000 | -0.717896000 | 3.963088000  |
| 1 | 0.159908000  | 0.643548000  | 2.431562000  |
| 6 | -1.149114000 | -1.842744000 | 4.282159000  |
| 1 | -2.465222000 | -3.350974000 | 3.548925000  |
| 1 | 0.188713000  | -0.234519000 | 4.712711000  |
| 1 | -1.125775000 | -2.236115000 | 5.282201000  |
| 6 | -2.022487000 | 1.438249000  | 0.107381000  |
| 6 | -2.155330000 | 2.174439000  | -1.063082000 |
| 6 | -2.599805000 | 1.917743000  | 1.271370000  |
| 6 | -2.853255000 | 3.361931000  | -1.066896000 |
| 1 | -1.702471000 | 1.827966000  | -1.973635000 |
| 6 | -3.296465000 | 3.112040000  | 1.266178000  |
| 1 | -2.515569000 | 1.363814000  | 2.186394000  |
| 6 | -3.425954000 | 3.834711000  | 0.099275000  |
| 1 | -2.944595000 | 3.920921000  | -1.980170000 |
| 1 | -3.739439000 | 3.471526000  | 2.177238000  |
| 1 | -3.969047000 | 4.762423000  | 0.095823000  |
| 6 | 3.853147000  | -1.077099000 | 1.099074000  |
| 6 | 4.355410000  | -1.406118000 | -0.322861000 |
| 6 | 4.449159000  | 0.830418000  | -0.263260000 |
| 6 | 3.909028000  | 0.468819000  | 1.138315000  |
| 1 | 5.902722000  | -0.317163000 | -1.458552000 |
| 1 | 6.214507000  | -0.379791000 | 0.283644000  |
| 6 | 3.369794000  | -0.888460000 | -1.353770000 |
| 1 | 2.911354000  | -1.498304000 | -2.105593000 |
| 6 | 3.423708000  | 0.456062000  | -1.319317000 |
| 1 | 3.019684000  | 1.133297000  | -2.044414000 |
| 1 | 4.644438000  | -2.436436000 | -0.462602000 |
| 1 | 4.831301000  | 1.837321000  | -0.348497000 |
| 1 | 2.951664000  | 0.928682000  | 1.334907000  |
| 1 | 2.870059000  | -1.480989000 | 1.286131000  |
| 6 | 5.443487000  | -0.326172000 | -0.477782000 |
| 6 | 1.059653000  | 3.864990000  | 0.436970000  |
| 1 | 0.134953000  | 4.228456000  | 0.008951000  |

|                |              |              |              |
|----------------|--------------|--------------|--------------|
| 1              | 1.136612000  | 4.165162000  | 1.471384000  |
| 1              | 1.889826000  | 4.262418000  | -0.131787000 |
| 1              | 4.601339000  | 0.816476000  | 1.896500000  |
| 1              | 4.528458000  | -1.509836000 | 1.827681000  |
| 61             |              |              |              |
| endo-TS3_4tP-O |              |              |              |
| 6              | 0.924366000  | -2.481211000 | -0.580636000 |
| 7              | 0.806240000  | -3.619625000 | -0.542532000 |
| 6              | 1.628457000  | 1.661083000  | -0.819555000 |
| 8              | 1.724193000  | 2.249749000  | 0.367384000  |
| 8              | 1.208790000  | 2.209712000  | -1.790200000 |
| 46             | 1.163614000  | -0.491013000 | -0.649731000 |
| 15             | -1.161771000 | -0.107986000 | 0.001052000  |
| 6              | -2.420310000 | -0.834556000 | -1.104238000 |
| 6              | -2.098308000 | -1.926457000 | -1.897431000 |
| 6              | -3.716033000 | -0.332381000 | -1.151931000 |
| 6              | -3.050780000 | -2.501794000 | -2.715969000 |
| 1              | -1.111459000 | -2.344289000 | -1.867924000 |
| 6              | -4.664067000 | -0.907804000 | -1.971536000 |
| 1              | -3.989717000 | 0.515179000  | -0.552377000 |
| 6              | -4.332584000 | -1.994637000 | -2.757170000 |
| 1              | -2.783169000 | -3.349173000 | -3.320314000 |
| 1              | -5.660515000 | -0.505168000 | -1.996851000 |
| 1              | -5.070807000 | -2.441908000 | -3.398147000 |
| 6              | -1.450686000 | -0.867037000 | 1.630077000  |
| 6              | -2.623171000 | -1.528759000 | 1.957456000  |
| 6              | -0.444752000 | -0.774940000 | 2.581577000  |
| 6              | -2.788988000 | -2.077193000 | 3.213907000  |
| 1              | -3.406238000 | -1.631388000 | 1.230434000  |
| 6              | -0.614457000 | -1.313113000 | 3.839835000  |
| 1              | 0.480947000  | -0.286911000 | 2.334417000  |
| 6              | -1.788573000 | -1.966920000 | 4.157948000  |
| 1              | -3.699617000 | -2.596711000 | 3.450932000  |
| 1              | 0.174990000  | -1.235519000 | 4.565043000  |
| 1              | -1.917814000 | -2.398847000 | 5.133758000  |
| 6              | -1.766045000 | 1.605540000  | 0.193525000  |
| 6              | -1.850340000 | 2.405730000  | -0.939905000 |
| 6              | -2.134577000 | 2.141346000  | 1.417023000  |

|   |              |              |              |
|---|--------------|--------------|--------------|
| 6 | -2.311873000 | 3.701076000  | -0.852428000 |
| 1 | -1.550447000 | 2.018097000  | -1.895966000 |
| 6 | -2.586164000 | 3.445698000  | 1.505644000  |
| 1 | -2.080571000 | 1.542542000  | 2.306351000  |
| 6 | -2.681667000 | 4.225806000  | 0.372482000  |
| 1 | -2.375351000 | 4.303469000  | -1.740304000 |
| 1 | -2.871056000 | 3.844746000  | 2.462349000  |
| 1 | -3.040465000 | 5.236893000  | 0.440629000  |
| 6 | 3.756998000  | -1.330247000 | 1.136801000  |
| 6 | 4.158609000  | -1.452714000 | -0.334821000 |
| 6 | 4.241704000  | 0.766720000  | 0.015195000  |
| 6 | 3.760706000  | 0.199810000  | 1.361396000  |
| 1 | 5.614040000  | -0.195299000 | -1.424766000 |
| 1 | 6.051380000  | -0.468702000 | 0.264796000  |
| 6 | 3.099934000  | -0.850249000 | -1.252656000 |
| 1 | 3.020035000  | -1.256020000 | -2.246374000 |
| 6 | 3.201017000  | 0.577902000  | -1.086719000 |
| 1 | 3.325727000  | 1.161912000  | -1.980887000 |
| 1 | 4.460252000  | -2.446864000 | -0.628464000 |
| 1 | 4.629486000  | 1.773548000  | 0.075211000  |
| 1 | 2.795966000  | 0.591613000  | 1.643422000  |
| 1 | 2.803021000  | -1.793987000 | 1.338437000  |
| 6 | 5.223055000  | -0.338766000 | -0.424172000 |
| 6 | 1.361304000  | 3.626992000  | 0.434548000  |
| 1 | 0.306605000  | 3.752695000  | 0.243118000  |
| 1 | 1.603179000  | 3.942448000  | 1.437652000  |
| 1 | 1.928022000  | 4.197328000  | -0.289522000 |
| 1 | 4.462086000  | 0.482914000  | 2.137617000  |
| 1 | 4.497630000  | -1.818078000 | 1.760346000  |

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endo-4tP-O

|    |              |              |              |
|----|--------------|--------------|--------------|
| 46 | 0.922554000  | -0.591497000 | -0.511324000 |
| 15 | -1.406811000 | 0.003169000  | 0.007448000  |
| 6  | -2.600123000 | -0.192991000 | -1.357514000 |
| 6  | -2.508656000 | -1.335755000 | -2.143204000 |
| 6  | -3.600769000 | 0.729925000  | -1.626806000 |
| 6  | -3.405499000 | -1.548153000 | -3.170006000 |
| 1  | -1.742001000 | -2.064040000 | -1.951655000 |

|   |              |              |              |
|---|--------------|--------------|--------------|
| 6 | -4.491642000 | 0.516795000  | -2.660444000 |
| 1 | -3.688972000 | 1.620900000  | -1.034007000 |
| 6 | -4.396294000 | -0.622728000 | -3.433217000 |
| 1 | -3.323498000 | -2.438343000 | -3.766615000 |
| 1 | -5.260201000 | 1.242083000  | -2.858507000 |
| 1 | -5.089865000 | -0.788219000 | -4.237879000 |
| 6 | -2.129158000 | -0.953293000 | 1.374759000  |
| 6 | -3.500394000 | -1.085277000 | 1.544804000  |
| 6 | -1.278128000 | -1.564607000 | 2.281760000  |
| 6 | -4.007066000 | -1.801413000 | 2.608730000  |
| 1 | -4.175953000 | -0.637120000 | 0.839659000  |
| 6 | -1.785306000 | -2.277791000 | 3.349919000  |
| 1 | -0.215041000 | -1.501504000 | 2.140273000  |
| 6 | -3.149760000 | -2.395912000 | 3.515173000  |
| 1 | -5.070846000 | -1.901774000 | 2.726298000  |
| 1 | -1.113368000 | -2.753182000 | 4.040860000  |
| 1 | -3.545864000 | -2.959844000 | 4.340272000  |
| 6 | -1.595041000 | 1.745232000  | 0.515169000  |
| 6 | -1.200224000 | 2.735363000  | -0.377152000 |
| 6 | -2.057942000 | 2.124124000  | 1.764442000  |
| 6 | -1.291763000 | 4.067202000  | -0.038072000 |
| 1 | -0.822664000 | 2.461502000  | -1.346167000 |
| 6 | -2.135118000 | 3.461057000  | 2.110982000  |
| 1 | -2.363342000 | 1.378542000  | 2.473875000  |
| 6 | -1.758482000 | 4.434814000  | 1.211086000  |
| 1 | -0.997736000 | 4.820535000  | -0.746895000 |
| 1 | -2.497428000 | 3.736645000  | 3.084867000  |
| 1 | -1.827289000 | 5.473946000  | 1.477881000  |
| 6 | 3.551907000  | -1.579545000 | 1.388240000  |
| 6 | 3.659476000  | -2.005751000 | -0.079413000 |
| 6 | 4.891384000  | -0.122016000 | 0.001191000  |
| 6 | 4.373020000  | -0.267235000 | 1.437144000  |
| 1 | 5.372709000  | -1.716262000 | -1.434132000 |
| 1 | 5.842112000  | -2.078872000 | 0.228861000  |
| 6 | 2.865512000  | -1.055482000 | -0.980317000 |
| 1 | 2.856029000  | -1.448590000 | -1.988542000 |
| 6 | 3.719502000  | 0.242487000  | -0.935573000 |
| 1 | 4.118480000  | 0.494321000  | -1.915530000 |

|   |             |              |              |
|---|-------------|--------------|--------------|
| 1 | 3.413033000 | -3.043608000 | -0.248042000 |
| 1 | 5.741055000 | 0.539745000  | -0.098257000 |
| 1 | 3.785874000 | 0.584765000  | 1.763620000  |
| 1 | 2.523764000 | -1.443667000 | 1.695976000  |
| 6 | 5.101995000 | -1.585057000 | -0.392498000 |
| 6 | 2.929599000 | 1.422805000  | -0.502128000 |
| 8 | 1.736752000 | 1.371202000  | -0.260288000 |
| 8 | 3.592153000 | 2.543961000  | -0.405446000 |
| 6 | 2.875042000 | 3.704816000  | 0.006017000  |
| 1 | 3.605509000 | 4.496802000  | 0.046830000  |
| 1 | 2.099184000 | 3.938473000  | -0.709142000 |
| 1 | 2.427839000 | 3.546192000  | 0.976960000  |
| 6 | 0.483069000 | -2.469760000 | -0.784292000 |
| 7 | 0.204364000 | -3.567297000 | -0.956947000 |
| 1 | 3.989337000 | -2.331219000 | 2.035883000  |
| 1 | 5.207200000 | -0.348263000 | 2.124232000  |

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endo-TS4\_5tP-O

|    |              |              |              |
|----|--------------|--------------|--------------|
| 46 | -0.826783000 | -0.056440000 | 0.300042000  |
| 15 | 1.475260000  | 0.060617000  | -0.019619000 |
| 6  | 2.445685000  | -0.092622000 | 1.517367000  |
| 6  | 2.153693000  | -1.159377000 | 2.361116000  |
| 6  | 3.429028000  | 0.810029000  | 1.890314000  |
| 6  | 2.847357000  | -1.322100000 | 3.541468000  |
| 1  | 1.377663000  | -1.857296000 | 2.100458000  |
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| 1  | 3.664643000  | 1.645256000  | 1.258204000  |
| 6  | 3.828435000  | -0.418466000 | 3.905474000  |
| 1  | 2.612580000  | -2.153013000 | 4.181820000  |
| 1  | 4.872284000  | 1.359250000  | 3.357617000  |
| 1  | 4.362819000  | -0.544524000 | 4.829944000  |
| 6  | 2.168851000  | -1.230677000 | -1.106494000 |
| 6  | 3.367403000  | -1.878153000 | -0.852260000 |
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| 1  | 3.927795000  | -1.644358000 | 0.033580000  |
| 6  | 1.939993000  | -2.516497000 | -3.126417000 |
| 1  | 0.513402000  | -1.092503000 | -2.446021000 |



|   |              |              |              |
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| 6 | 3.137810000  | -3.153961000 | -2.865166000 |
| 1 | 4.774880000  | -3.334508000 | -1.510477000 |
| 1 | 1.375835000  | -2.766863000 | -4.006584000 |
| 1 | 3.510317000  | -3.901414000 | -3.542118000 |
| 6 | 2.085303000  | 1.609064000  | -0.776755000 |
| 6 | 1.355479000  | 2.770256000  | -0.565776000 |
| 6 | 3.236654000  | 1.677769000  | -1.548624000 |
| 6 | 1.776117000  | 3.974491000  | -1.094279000 |
| 1 | 0.445230000  | 2.728274000  | 0.005794000  |
| 6 | 3.652777000  | 2.879445000  | -2.085564000 |
| 1 | 3.809644000  | 0.789150000  | -1.738354000 |
| 6 | 2.925928000  | 4.031312000  | -1.856059000 |
| 1 | 1.199748000  | 4.864987000  | -0.919388000 |
| 1 | 4.544791000  | 2.915018000  | -2.684706000 |
| 1 | 3.250303000  | 4.966471000  | -2.275749000 |
| 6 | -3.207424000 | -1.798818000 | -1.482102000 |
| 6 | -3.532818000 | -2.196457000 | -0.041291000 |
| 6 | -4.813847000 | -0.384161000 | -0.369389000 |
| 6 | -4.081958000 | -0.540790000 | -1.706702000 |
| 1 | -5.434044000 | -1.950767000 | 1.038661000  |
| 1 | -5.622873000 | -2.390875000 | -0.659717000 |
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| 6 | -5.014015000 | -1.836444000 | 0.045729000  |
| 6 | -3.328657000 | 1.473673000  | 0.398161000  |
| 8 | -2.257050000 | 1.788252000  | -0.045231000 |
| 8 | -4.273114000 | 2.367170000  | 0.631408000  |
| 6 | -3.970885000 | 3.721774000  | 0.325490000  |
| 1 | -4.857793000 | 4.282386000  | 0.575338000  |
| 1 | -3.130149000 | 4.062373000  | 0.914068000  |
| 1 | -3.737531000 | 3.829823000  | -0.724812000 |
| 6 | -1.249891000 | -1.767261000 | 1.098144000  |

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| 7          | -0.861605000 | -2.765633000 | 1.537093000  |
| 1          | -4.800962000 | -0.697556000 | -2.502128000 |
| 1          | -3.483319000 | -2.593757000 | -2.164847000 |
| 61         |              |              |              |
| endo-5tP-O |              |              |              |
| 46         | 0.006298000  | -0.419260000 | 0.434651000  |
| 15         | 2.167298000  | -0.086533000 | 0.040255000  |
| 6          | 3.312268000  | -0.608195000 | 1.372775000  |
| 6          | 3.000665000  | -1.768351000 | 2.069697000  |
| 6          | 4.460972000  | 0.085677000  | 1.721318000  |
| 6          | 3.825714000  | -2.234206000 | 3.071894000  |
| 1          | 2.095687000  | -2.297001000 | 1.828144000  |
| 6          | 5.281968000  | -0.372989000 | 2.734331000  |
| 1          | 4.717957000  | 0.993175000  | 1.207316000  |
| 6          | 4.969519000  | -1.535623000 | 3.408500000  |
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| 1          | 5.607969000  | -1.891387000 | 4.197083000  |
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| 6          | 4.128084000  | -1.475812000 | -1.490008000 |
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| 6          | 2.065787000  | 2.627089000  | 0.557882000  |
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| 6          | 2.394388000  | 3.958547000  | 0.415686000  |
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| 6          | 3.888674000  | 3.397262000  | -1.358827000 |
| 1          | 4.032495000  | 1.333462000  | -1.845399000 |
| 6          | 3.307021000  | 4.348393000  | -0.546721000 |
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|   |              |              |              |
|---|--------------|--------------|--------------|
| 1 | 4.594298000  | 3.691832000  | -2.114911000 |
| 1 | 3.556532000  | 5.387398000  | -0.666075000 |
| 6 | -4.983724000 | -1.689055000 | -1.268857000 |
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| 1 | -7.018113000 | -1.801760000 | 1.423615000  |
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| 6 | -5.530086000 | 0.290151000  | 0.854163000  |
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| 1 | -4.868038000 | -3.026746000 | 0.485962000  |
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| 1 | -3.957894000 | -1.415456000 | -1.479238000 |
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| 8 | -5.446368000 | 2.654725000  | 0.732233000  |
| 8 | -3.920275000 | 1.503023000  | -0.391077000 |
| 6 | -3.300168000 | 2.707468000  | -0.824837000 |
| 1 | -2.413401000 | 2.403129000  | -1.357291000 |
| 1 | -3.968691000 | 3.260908000  | -1.470654000 |
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| 1 | -5.222214000 | -2.542836000 | -1.890814000 |
| 1 | -6.757978000 | -0.814142000 | -2.195960000 |

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|   |              |              |              |
|---|--------------|--------------|--------------|
| 6 | -2.145021000 | 0.444503000  | 1.073988000  |
| 6 | -2.038296000 | 0.731109000  | -0.423954000 |
| 6 | -1.209890000 | -1.351379000 | -0.248834000 |
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| 1 | -2.216629000 | -0.694085000 | -2.094754000 |
| 1 | -3.318033000 | -1.007780000 | -0.753838000 |
| 6 | -0.550937000 | 0.912235000  | -0.812338000 |
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| 6 | -0.003890000 | -0.559906000 | -0.756883000 |
| 1 | 0.196818000  | -0.854007000 | -1.782048000 |
| 1 | -2.653932000 | 1.551028000  | -0.767213000 |
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| 6 | 3.547855000  | -0.103549000 | -0.012114000 |
| 1 | 4.179395000  | 0.536489000  | -0.607789000 |
| 1 | 3.498904000  | 0.258511000  | 1.005506000  |
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