An Unprecedented Family of Luminescent Iridium(III) Complexes Bearing A six-Membered Chelated Trideterminate C^N^C Ligand

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**Experimental Part**

**General Synthetic Procedures**

Commercial chemicals were used as supplied. All reactions were performed using standard Schlenk techniques under inert (N$_2$) atmosphere with reagent-grade solvents. Freshly distilled anhydrous THF was obtained from a Pure SolvTM solvent purification system (Innovative Technologies). Flash column chromatography was performed using silica gel (Silia-P from Silicycle, 60 Å, 40-63 μm). Analytical thin layer chromatography (TLC) was performed with silica plates with aluminum backings (250 μm with indicator F-254). Compounds were visualized under UV light. $^1$H, $^{13}$C and $^{19}$F solution-phase NMR spectra were recorded on a Bruker Avance spectrometer operating at 11.7 T (Larmor frequencies of 400, 101 and 376 MHz, respectively). The following abbreviations have been used for multiplicity assignments: “s” for singlet, “d” for doublet, “t” for triplet, “m” for multiplet and “br” for broad. $^1$H and $^{13}$C NMR spectra were referenced to the solvent peak. Melting points (Mps) were recorded using open-ended capillaries on an electrothermal melting point apparatus and are uncorrected. High-resolution mass spectra were recorded at the EPSRC UK National Mass Spectrometry Facility at Swansea University on a quadrupole time-of-flight (ESI-Q-TOF), model ABSciex 5600 Triple TOF in positive electrospray ionization mode and spectra were recorded using sodium formate solution as the calibrant.
Characterization of Precursors and Ligand

Figure S1. $^1$H NMR spectrum of Diphenyl(pyridin-2-yl)methanol (A1) in CDCl$_3$

Figure S2. $^{13}$C NMR spectrum of Diphenyl(pyridin-2-yl)methanol (A1) in CDCl$_3$
Figure S3. FT mass spectrum of Diphenyl(pyridin-2-yl)methanol (A1)

Figure S4. $^1$H NMR spectrum of Bis(4-(tert-butyl)phenyl)(pyridin-2-yl)methanol (A2) in CDCl$_3$
Figure S5. $^{13}$C NMR spectrum of Bis(4-(tert-butyl)phenyl)(pyridin-2-yl) methanol (A2) in CDCl$_3$

Figure S6. FT mass spectrum of Bis(4-(tert-butyl)phenyl)(pyridin-2-yl)methanol (A2)
Figure S7. $^1$H NMR spectrum of Pyridin-2-ylbis(4-(trifluoromethyl)phenyl)methanol (A3) in CDCl$_3$

Figure S8. $^{13}$C NMR spectrum of Pyridin-2-ylbis(4-(trifluoromethyl)phenyl)methanol (A3) in CDCl$_3$
Figure S9. $^{19}$F NMR spectrum of Pyridin-2-ylbis(4-(trifluoromethyl)phenyl)methanol (A3) in CDCl$_3$.

Figure S10. FT mass spectrum of Pyridin-2-ylbis(4-(trifluoromethyl)phenyl)methanol (A3).
Figure S11. $^1$H NMR spectrum of 2-benzhydrylpyridine (L1) in CDCl$_3$

Figure S12. $^{13}$C NMR spectrum of 2-benzhydrylpyridine (L1) in CDCl$_3$
Figure S13. FT mass spectrum of 2-benzhydrylpyridine (L1)

Figure S14. $^1$H NMR spectrum of 2-(bis(4-(tert-butyl)phenyl)methyl)pyridine (L2) in CDCl$_3$
Figure S15. $^{13}$C NMR spectrum of 2-(bis(4-(tert-butyl)phenyl)methyl)pyridine (L2) in CDCl$_3$

Figure S16. ASAP mass spectrum of 2-(bis(4-(tert-butyl)phenyl)methyl)pyridine (L2)
Figure S17. $^1$H NMR spectrum of 2-(bis(4-(trifluoromethyl)phenyl)methyl)pyridine (L3) in CDCl$_3$

Figure S18. $^{13}$C NMR spectrum of 2-(bis(4-(trifluoromethyl)phenyl)methyl)pyridine (L3) in CDCl$_3$
Figure S19. $^{19}$F NMR spectrum of 2-(bis(4-(trifluoromethyl)phenyl)methyl)pyridine (L3) in CDCl$_3$

Figure S20. FT mass spectrum of 2-(bis(4-(trifluoromethyl)phenyl)methyl)pyridine (L3)
Figure S21. $^1$H NMR spectrum of $[\text{Ir(bnpy)(d/Bubpy)Cl}]$ (1) in CD$_2$Cl$_2$

Figure S22. $^{13}$C NMR spectrum of $[\text{Ir(bnpy)(d/Bubpy)Cl}]$ (1) in CD$_2$Cl$_2$
Figure S23. ASAP mass spectrum of [Ir(bnpy)(dtBubpy)Cl] (1)

Figure S24. $^1$H NMR spectrum of [Ir(dtBubnpy)(dtBubpy)Cl] (2) in CD$_2$Cl$_2$
Figure S25. $^{13}$C NMR spectrum of [Ir(dtBubnpy)(dtBubpy)Cl] (2) in CD$_2$Cl$_2$

Figure S26. ASAP mass spectrum of [Ir(dtBubnpy)(dtBubpy)Cl] (2)
Figure S27. $^1$H NMR spectrum of [Ir(dtfmbnpy)(dtrBubpy)Cl] (3) in CD$_2$Cl$_2$

Figure S28. $^{13}$C NMR spectrum of [Ir(dtfmbnpy)(dtrBubpy)Cl] (3) in CD$_2$Cl$_2$
Figure S29. $^{19}$F NMR spectrum of [Ir(dtfnbnp)(drBubpy)Cl] (3) in CD$_2$Cl$_2$

Figure S30. ASAP mass spectrum of [Ir(dtfnbnp)(drBubpy)Cl] (3)
**X-ray crystal structures**

Single crystals of sufficient quality of 1-3 were grown from CH$_2$Cl$_2$/Et$_2$O at -18°C. X-ray diffraction data for compound 1 were collected at 150 K by using a Bruker D8 VENTURE with an Incoatec microfocus source equipped with a multilayer monochromator (Mo Kα radiation, λ = 0.71073 Å) and a PHOTON 100 detection system. Intensity data were collected using rotation frames accumulating area detector images. Data for compounds 2 and 3 were collected at 173 K by using a Rigaku FR-X Ultrahigh brilliance Microfocus RA generator/confocal optics and Rigaku XtaLAB P200 system, with Mo Kα radiation (λ = 0.71075 Å). Intensity data were collected using ω steps accumulating area detector images spanning at least a hemisphere of reciprocal space. All data were corrected for Lorentz polarization effects. A multiscan absorption correction was applied by using SADABS$^1$ (1) or CrystalClear$^2$ (2 and 3). Structures were solved by either dual-space (SHELX$^3$) or Patterson methods (PATTY$^4$) and refined by full-matrix least-squares against F$^2$ (SHELXL-2014)$^3$. In 1 the contribution of the disordered solvent to the calculated structure factors was calculated by the PLATON/SQUEEZE procedure.$^4$ Non-hydrogen atoms were refined anisotropically, and hydrogen atoms were refined using a riding model. CCDC 1519101–1519103 contain the supplementary crystallographic data for this paper. These data are provided free of charge by The Cambridge Crystallographic Data Centre. Table S1 contains a summary of crystallographic data.
### Table S1. Crystallographic data for complexes 1–3.

|       | 1                                      | 2                                      | 3                                      |
|-------|----------------------------------------|----------------------------------------|----------------------------------------|
| Formula | C$_{36}$H$_{57}$Cl Ir N$_3$            | C$_{46}$H$_{57}$Cl$_3$IrN$_3$          | C$_{30}$H$_{37}$Cl$_3$F$_6$IrN$_3$     |
| Formula weight | 739.36                                | 1021.46                                | 960.31                                 |
| Crystal colour, habit | Red, prism                            | Red, prism                             | Yellow, prism                          |
| Crystal dimensions (mm$^3$) | 0.14×0.08×0.06                        | 0.12×0.08×0.03                        | 0.07×0.02×0.02                        |
| Space group | $P2_12_12_1$                           | $P2_1/n$                               | $P\bar{1}$                            |
| a (Å) | 17.5788(6)                             | 16.6728(18)                            | 13.2316(11)                           |
| b (Å) | 18.3829(6)                             | 16.9537(14)                            | 15.2465(12)                           |
| c (Å) | 22.6662(8)                             | 17.3328(18)                            | 19.5943(19)                           |
| $\alpha$ (°) | 86.300(6)                              |                                        |                                        |
| $\beta$ (°) |                                        | 113.334(2)                             | 81.439(6)                             |
| $\gamma$ (°) |                                        |                                        | 77.394(6)                             |
| Volume (Å$^3$) | 7324.6(4)                             | 4498.7(8)                              | 3812.5(6)                             |
| Z | 8                                      | 4                                      | 4                                      |
| $\rho_{\text{calc}}$ (g cm$^{-3}$) | 1.341                                 | 1.508                                  | 1.673                                  |
| Temperature (K) | 150                                    | 173                                    | 173                                    |
| $\mu$ (mm$^{-1}$) | 3.743                                 | 3.308                                  | 3.784                                  |
| $\theta$ range | 2.915-27.484                          | 1.755-25.410                           | 1.592-25.242                           |
| Reflections collected | 45293                                 | 38432                                  | 62965                                  |
| Independant reflections ($R_{int}$) | 16770 (0.0455)                        | 8234 (0.0242)                          | 13863 (0.1140)                         |
| $R_1$ [$I>2\sigma(I)$] | 0.0541                                | 0.0256                                 | 0.0515                                 |
| w$R_2$ (all data) | 0.1329                                | 0.0728                                 | 0.0796                                 |
| Residual electron peak, hole | 1.551, -2.459                         | 1.32, -1.34                           | 1.21, -0.92                           |
**Electrochemistry**

Cyclic and differential pulse voltammetry measurements were performed on an Electrochemical Analyzer potentiostat model 600D from CH Instruments. Solutions for cyclic voltammetry were prepared in DCM and degassed with DCM-saturated nitrogen by bubbling for about 10 min prior to scanning. Tetra(n-butyl)ammoniumhexafluorophosphate (TBAPF\(_6\); ca. 0.1 M in DCM) was used as the supporting electrolyte. A Ag/Ag+ electrode (silver wire in a solution of 0.1 M KCl in H\(_2\)O) was used as the pseudoreference electrode; a glassy carbon electrode was used for the working electrode and a Pt electrode was used as the counter electrode. The redox potentials are reported relative to a saturated calomel electrode (SCE) electrode with a ferrocene/ferrocenium (Fc/Fc\(^+\)) redox couple as an internal reference (0.46 V vs. SCE).\(^6\)

**Photophysical data**

All samples were prepared in HPLC grade dichloromethane with varying concentrations in the order of micromolar. Absorption spectra were recorded at room temperature using a Shimadzu UV-1800 double beam spectrophotometer. Molar absorptivity determination was verified by linear least-squares fit of values obtained from at least four independent solutions at varying concentrations ranging from 8.22 \(\times\) 10\(^{-5}\) to 4.83 \(\times\) 10\(^{-6}\) M. The sample solutions for the emission spectra were prepared in HPLC grade dichloromethane and degassed via three freeze–pump–thaw cycles using an in-house designed quartz cuvette. Steady-state and time-resolved emission spectra were recorded at 298 K using Gilden photonics Fluorimeter. All samples for steady-state measurements were excited at 420 nm. The excited-state lifetimes of the complexes were obtained by time correlated single photon counting (TCSPC) at an excitation wavelength of 378 nm using an Edinburgh Instruments FLS980 fluorimeter using a pulsed diode laser, and PL emission was detected at the corresponding steady-state emission maximum for each complex. The PL decays were fitted with a single exponential decay function. Emission quantum yields were determined using the optically dilute method.\(^7\) A stock solution with absorbance of ca. 0.2 was prepared, and then four dilutions were prepared with dilution factors between 2 and 20 to obtain solutions with absorbances of ca. 0.103, 0.076, 0.052, and 0.026, respectively. The Beer–Lambert law was found to be linear at the concentrations of the solutions. The emission spectra were then measured after the solutions were degassed by nitrogen purging for fifteen minutes per sample prior to spectrum acquisition. For each sample, linearity between absorption and emission intensity was verified through linear regression analysis, and additional measurements were acquired until the
Pearson regression factor (R²) for the linear fit of the data set surpassed 0.9. Individual relative quantum yield values were calculated for each solution, and the values reported represent the slope value. The \( \Phi_s = \Phi_r (A_r/A_s)(I_s/I_r)(n_s/n_r)^2 \) equation was used to calculate the relative quantum yield of each of the sample, where \( \Phi_r \) is the absolute quantum yield of the reference, \( n \) is the refractive index of the solvent, \( A \) is the absorbance at the excitation wavelength, and \( I \) is the integrated area under the corrected emission curve. The subscripts \( s \) and \( r \) refer to the sample and reference, respectively. A solution of [Ru(bpy)₃]PF₆ in aerated MeCN at 298K (\( \Phi_{PL} = 1.8\% \)) was used as a reference.⁸

Table S2. Selected photophysical data for complexes 1-3

| \( \lambda_{abs} \) [nm] | \( \epsilon \) [M⁻¹cm⁻¹] | [a] |
|-------------------------|-------------------------|-----|
| 1                       | 294 (12008), 355 (3624), 404 (2704), 500 (696) |     |
| 2                       | 295 (14123), 359 (4697), 405 (3336), 510 (1114) |     |
| 3                       | 293 (15433), 343 (4989), 393 (4206), 468 (1131) |     |

[a] recorded in aerated CH₂Cl₂ at 298 K

Figure S31: Excited-state lifetime (\( \lambda_{exc} = 378 \) nm) decay profile of 1 in deaerated dichloromethane at room temperature.
Figure S32: Excited-state lifetime ($\lambda_{\text{exc}} = 378$ nm) decay profile of 2 in deaerated dichloromethane at room temperature.

Figure S33: Excited-state lifetime ($\lambda_{\text{exc}} = 378$ nm) decay profile of 3 in deaerated dichloromethane at room temperature.
DFT and TD-DFT calculations

To perform DFT and TD-DFT calculations, we have used the Gaussian09 program.\textsuperscript{9} Our calculations consisted in geometry optimization vibrational spectra determinations and TD-DFT calculations of the different structures. We have applied default procedures, integration grids, algorithms and parameters, except for improved energy (typically $10^{-10}$ \textit{a.u.}) and internal forces ($10^{-5}$ \textit{a.u.}) convergence thresholds and the use of the \textit{ultrafine} integration DFT grid. The ground-state geometrical parameters have been determined with the M06 functional.\textsuperscript{10} The vibrational spectrum has been subsequently determined analytically at the same level of theory and it has been checked that all structures correspond to true minima of the potential energy surface. At least, the first forty low-lying excited-states have been determined within the vertical TD-DFT approximation using the same functional that is suited for optical spectra.\textsuperscript{11-12} Phosphorescence wavelengths were obtained by first optimizing the lowest triplet excited-state with unrestricted DFT (M06 functional) and next computing the singlet ground-state energy on that structure. For all nuclei, we have used the LanL2DZ(5d,7f) basis set and pseudopotential augmented by additional \textit{d} (C, N, Cl) and \textit{f} (Ir) functions of contraction length one ($\alpha=0.938, 0.587, 0.736, 1.577$ and $0.648$ for C, N, F, Cl and Ir, respectively). During all steps, a modeling of bulk solvent effects (here CH\textsubscript{2}Cl\textsubscript{2}) through the Polarizable Continuum Model (PCM),\textsuperscript{13} using the linear-response approach for the TD-DFT part of the calculation.

The simulated TD-DFT spectra obtained by convoluting the vertical \textit{stick} contributions with a Gaussian of HWHH of 0.2 eV are displayed in Figure S35. Globally, the match with the experimental data (Figure 4) is very satisfying, giving confidence in the theoretical analysis. A list of the key singlet transitions is given in Table S3. For 1, PCM-TD-DFT calculations yield the lowest singlet excited-states at 489 nm ($f=0.004$) and 483 nm ($f=0.057$), which match well the weak experimental absorption band at ca. 500 nm (see Figure 4 in the main text). According to TD-DFT, the two lowest triplet excited-states are located in a very close region, 508 and 503 nm, respectively, though they present zero oscillator strengths due to the neglect of spin-orbit couplings in the non-relativistic approach used here. The $S_1$ (T\textsubscript{2}) and $S_2$ (T\textsubscript{1}) states mainly correspond to HOMO-1 to LUMO and HOMO to LUMO transitions, respectively. The occupied orbitals are shown in Figure S34 and a clear mixed charge-transfer (CT) character can be seen, the electron going from the metal, chlorine, and phenyl to the bipyridine (bpy) group. For the same compound, the next dipole-allowed transition found by TD-DFT are in the 420-370 nm region and correspond to the second maxima at ca. 400 nm
experimentally. The two transitions presenting the strongest $f$ in this spectra region are located by TD-DFT at 419 nm ($f=0.056$) and 382 nm ($f=0.093$). The first can be mainly ascribed to a HOMO-2 to LUMO transition and therefore corresponds to a metal+chlorine to dtBubpy charge transfer, whereas the second is a HOMO-1 to LUMO+1 transition, of MLCT/ILCT nature not involving the dtBubpy. In 2, the addition of the $t$Bu groups induces a small bathochromic displacement, the two lowest weakly allowed transitions appearing at 495 nm ($f=0.005$) and 493 nm ($f=0.053$), whereas the two next are at 423 nm ($f=0.055$) and 386 nm ($f=0.092$). The changes are indeed small as can be seen in both the calculated spectra and orbital energy levels (Figures S34 and S35). As expected, and consistently with the measurements, the CF$_3$ groups (3) induce qualitatively the opposite effect, with larger quantitative differences. Indeed, TD-DFT provides vertical transitions at 459 nm ($f=0.004$), 444 nm ($f=0.067$), 400 nm ($f=0.049$) and 369 nm ($f=0.099$). For 3, the two first transitions correspond to HOMO-1 to LUMO and HOMO to LUMO transitions, respectively, whereas the two latter excitations can be mainly ascribed to HOMO-2 to LUMO and HOMO-1 to LUMO+1 transitions, respectively. These orbitals are represented in Figure S34. The nature of the transitions and orbitals are thus not qualitatively modified by the trifluoromethyl substituents.
Table S3. Key singlet excited-states determined by TD-DFT. We provide the corresponding wavelength (in nm), oscillator strength (in parenthesis) and the dominating orbital character. Only states of interest for the analysis are given

| Compound | $\lambda_{\text{max}}$ ($\ell$) | Dominant MO character |
|----------|-----------------|----------------------|
| 1        | 489 (0.004)     | HOMO-1 / LUMO        |
|          | 483 (0.057)     | HOMO / LUMO          |
|          | 419 (0.056)     | HOMO-2 / LUMO        |
|          | 382 (0.093)     | HOMO-1 / LUMO+1      |
|          | 373 (0.016)     | HOMO / LUMO +2       |
| 2        | 495 (0.005)     | HOMO-1 / LUMO        |
|          | 493 (0.053)     | HOMO / LUMO          |
|          | 423 (0.055)     | HOMO-2 / LUMO        |
|          | 386 (0.092)     | HOMO-1 / LUMO+1      |
|          | 379 (0.015)     | HOMO / LUMO +2       |
| 3        | 459 (0.004)     | HOMO-1 / LUMO        |
|          | 444 (0.067)     | HOMO / LUMO          |
|          | 400 (0.049)     | HOMO-2 / LUMO        |
|          | 369 (0.099)     | HOMO-1 / LUMO+1      |
|          | 349 (0.019)     | HOMO / LUMO +2       |

In Figure S34, we provide the orbital energies for the five highest occupied and five lowest unoccupied molecular orbitals of the three complexes. As can be seen, the addition of $t$Bu groups has a very small influence on the key MOs playing a role in the visible absorption. In contrast, the addition of the trifluoromethyl moieties induces a stabilization of all MOs. As a consequence of their topologies, this stabilization is quantitatively larger for the HOMO than for the LUMO, which is consistent with the observed blue-shift of the spectrum when going from 1 to 3.
Figure S34: Energy orbital diagram for the 1, 2 and 3 with representation of the key MOs for 1 and 3. The blue and red bars represent occupied and unoccupied levels, respectively.

Figure S35: Theoretical absorption spectra computed in the vertical approximation, and convoluted with a Gaussian of HWHH of 0.2 eV.

We have also optimized the structure of the lowest triplet excited-state of the three complexes. The corresponding spin density for the three compounds can be found in Figure S36. As can be seen, the triplet presents contributions on the metal centre, bipyridine and chlorine atom, but the last ligand has no direct contribution. As stated in the main text, the computed vertical
phosphorescence wavelengths are 613 nm, 622 nm and 573 nm, for 1, 2, and 3, respectively. These values nicely match the room-temperature measurements. The 0-0 phosphorescence that accounts for vibrational relaxation effects and that are typically more comparable to low-temperature experiments attain 596 nm, 577 nm and 546 nm, that is are only slightly shifted.

Figure S36: Density difference plots obtained for the lowest triplet state of the three compounds. We show both the top (top) and side (bottom) views. A contour threshold of 0.002 au has been used for all compounds.

Below are the Cartesian coordinates for all structures, in Å, has obtained by DFT, considering restricted (ground-state, S0) and unrestricted (excited-state, T1) calculations.

**1 (S0)**

|   | X             | Y             | Z          |
|---|---------------|---------------|------------|
| 77 | -0.3562030    | -0.9737670    | 0.0000000  |
| 17 | -2.6936210    | -0.3396900    | 0.0000000  |
| 6  | -0.6401330    | -2.4286690    | 1.3736700  |
| 6  | -1.4801350    | -2.3092800    | 2.4988050  |
| 1  | -2.0810950    | -1.4040060    | 2.6228700  |
| 6  | -1.5851210    | -3.3313630    | 3.4522890  |
| 1  | -2.2494180    | -3.2051590    | 4.3094090  |
| 6  | -0.8489840    | -4.5131670    | 3.3070160  |
| 1  | -0.9277600    | -5.3106150    | 4.0467760  |
| 6  | -0.0174030    | -4.6602530    | 2.1899470  |
| 1  | 0.5557320     | -5.5814080    | 2.0512030  |
| 6  | 0.0744430     | -3.6393090    | 1.2389120  |
| 6  | 0.9316560     | -3.8102730    | 0.0000000  |
| 1  | 1.4087300     | -4.8017270    | 0.0000000  |
| 6  | 2.0208810     | -2.7700950    | 0.0000000  |
| 6  | 3.3722110     | -3.1237410    | 0.0000000  |
| 1  | 3.6355950     | -4.1809250    | 0.0000000  |
| 6  | 4.3551160     | -2.1374690    | 0.0000000  |
| 1  | 5.4113410 | -2.4029350 | 0.0000000 |
| 6  | 3.9511810 | -0.7929500 | 0.0000000 |
| 1  | 4.6685770 | 0.0183120 | 0.0000000 |
| 6  | 2.5933670 | -0.5137140 | 0.0000000 |
| 1  | 2.2443590 | 0.5172210 | 0.0000000 |
| 6  | 0.0744430 | 0.7311400 | 3.7313090 |
| 1  | 0.0485970 | 0.6653300 | 0.7311400 |
| 6  | 0.0343450 | 3.0691390 | 2.9033010 |
| 6  | -0.0465700 | 3.1207280 | -1.5034480 |
| 1  | -0.0831190 | 4.0874160 | -1.0023710 |
| 6  | -0.0782430 | 1.9543050 | -0.7414440 |
| 6  | -0.0782430 | 1.9543050 | 0.7414440 |
| 6  | -0.0465700 | 3.1207280 | 1.5034480 |
| 1  | -0.0831190 | 4.0874160 | 1.0023710 |
| 6  | 0.0343450 | 3.0691390 | 2.9033010 |
| 6  | 0.0968660 | 1.7935280 | -3.4758210 |
| 1  | 0.1750000 | 1.6520620 | -4.5515290 |
| 6  | 0.0343450 | 3.0691390 | 2.9033010 |
| 6  | -0.0465700 | 3.1207280 | -1.5034480 |
| 1  | -0.0831190 | 4.0874160 | -1.0023710 |
| 6  | -0.0782430 | 1.9543050 | -0.7414440 |
| 6  | -0.0782430 | 1.9543050 | 0.7414440 |
| 6  | -0.0465700 | 3.1207280 | 1.5034480 |
| 1  | -0.0831190 | 4.0874160 | 1.0023710 |
| 6  | 0.0343450 | 3.0691390 | 2.9033010 |
| 6  | 0.0968660 | 1.7935280 | 3.4758210 |
| 1  | 0.1750000 | 1.6520620 | 4.5515290 |
| 6  | 0.0485970 | 0.6653300 | 3.7455770 |
| 1  | 0.0810960 | -0.3388950 | 3.0862780 |
| 6  | 0.0569960 | 4.3556000 | 3.7169970 |
| 6  | 1.2735450 | 5.1966890 | 4.3949020 |
| 6  | 2.2111700 | 4.5655060 | 3.4835770 |
| 1  | 1.2425650 | 5.4707770 | 3.2345170 |
| 1  | 1.2971080 | 6.1284310 | 3.8813830 |
| 1  | -2.1197620 | 4.5612870 | 3.7343750 |
| 1  | -1.2293140 | 6.0758380 | 4.0219000 |
| 1  | -1.3384970 | 5.4113230 | 2.3817770 |
| 1  | 0.1599260 | 5.0040150 | 5.7603780 |
| 6  | -0.7116900 | 3.5062340 | 5.5852560 |
| 1  | 1.0704190 | 3.5443150 | 5.4835630 |
| 6  | 0.0569960 | 4.3556000 | -3.7169970 |
| 6  | -1.2342350 | 5.1430430 | -3.4420260 |
|   | 6     | 1.2735450 | 5.1966890 | -3.2980270 |
|---|-------|-----------|-----------|------------|
| 6 | 0.1493580 | 4.0839320 | -5.2192750 |
| 1 | -2.1197620 | 4.5612870 | -3.7343750 |
| 1 | -1.3384970 | 5.4113230 | -2.3817770 |
| 1 | -1.2293140 | 6.0758380 | -4.0241900 |
| 1 | 2.2111700  | 4.6535060 | -3.4835770 |
| 1 | 1.2971080  | 6.1284310 | -3.8813830 |
| 1 | 1.2425650  | 5.4707770 | -2.3345170 |
| 1 | 0.1599260  | 5.0401570 | -5.7603780 |
| 1 | 1.0704190  | 3.5431500 | -5.4835630 |
| 1 | -0.7116900 | 3.5062340 | -5.5852560 |

| 2 (S₀) |
|--------|
| 77     | 0.1651330 | -0.5248250 | 0.0000000 |
| 17     | -2.2474190 | -0.2712040 | 0.0000000 |
| 6      | 0.1082600 | -2.0013020 | 1.3760750 |
| 6      | -0.7273580 | -1.9886250 | 2.5040460 |
| 1      | -1.4453230 | -1.1677450 | 2.5994960 |
| 6      | -0.6972100 | -2.9868000 | 3.4973800 |
| 6      | 0.2087510  | -4.0446560 | 3.363420 |
| 1      | 0.2709360  | -4.8424150 | 4.0766790 |
| 6      | 1.0448510  | -4.0943730 | 2.2116550 |
| 1      | 1.7396410  | -4.9305170 | 2.0894570 |
| 6      | 0.9923390  | -3.0941780 | 1.2412600 |
| 6      | 1.8611140  | -3.1421550 | 0.0000000 |
| 1      | 2.4799480  | -4.0522100 | 0.0000000 |
| 6      | 2.7832650  | -1.9495300 | 0.0000000 |
| 6      | 4.1725090  | -2.0960870 | 0.0000000 |
| 1      | 4.5916780  | -3.1017650 | 0.0000000 |
| 6      | 4.9966840  | -0.9737850 | 0.0000000 |
| 1      | 6.0807640  | -1.0782540 | 0.0000000 |
| 6      | 4.3973050  | 0.2891340  | 0.0000000 |
| 1      | 4.9845040  | 1.2047250  | 0.0000000 |
| 6      | 3.0120590  | 0.3683370  | 0.0000000 |
| 1      | 2.5119450  | 1.3352530  | 0.0000000 |
| 7      | 2.2109680  | -0.7198950 | 0.0000000 |
| 6      | 0.9923390  | -3.0941780 | -1.2412600 |
| 6      | 1.0448510  | -4.0943730 | -2.2116550 |
| 1      | 1.7396410  | -4.9305170 | -2.0894570 |
| 1      | 0.2087510  | -4.0446560 | -3.336420 |
| 1      | 0.2709360  | -4.8424150 | -4.0766790 |
| 6      | -0.6972100 | -2.9868000 | -3.4973800 |
| 6      | -0.7273580 | -1.9886250 | -2.5040460 |
| 1      | -1.4453230 | -1.1677450 | -2.5994960 |
| 6      | 0.1082600  | -2.0013020 | -1.3760750 |
| 7      | 0.1993970  | 1.2100630  | -1.3280320 |
| 6      | 0.3007550  | 1.1612600  | -2.6607970 |
| 1      | 0.5019460  | 0.1764440  | -3.0819860 |
| 6      | 0.1489750  | 2.2797240  | -3.4777680 |
|   | 1   | 2   | 3   | 4   |
|---|-----|-----|-----|-----|
| 1 | 0.2397500 | 2.1507560 | -4.5544580 |
| 6 | -0.1235450 | 3.5272170 | -2.9044410 |
| 6 | -0.1989940 | 3.5660480 | -1.5038130 |
| 1 | -0.3929600 | 4.5135380 | -1.0023490 |
| 6 | -0.0303150 | 2.4113780 | -0.7416100 |
| 6 | -0.1989940 | 3.5660480 | -1.5038130 |
| 1 | -0.3929600 | 4.5135380 | 1.0023490 |
| 6 | -0.1235450 | 3.5272170 | 2.9044410 |
| 6 | 0.1489750 | 2.2797240 | 3.4777680 |
| 1 | 0.2397500 | 2.1507560 | 4.5544580 |
| 6 | -0.3007550 | 1.1612600 | 2.6607970 |
| 6 | -0.3267670 | 4.7981930 | 3.7175370 |
| 1 | 1.7512920 | 5.4490310 | 3.5141000 |
| 1 | 0.6778860 | 6.0956460 | 2.2506070 |
| 1 | 0.6003170 | 6.7519470 | 3.8974030 |
| 1 | -2.5078380 | 4.6403130 | 3.7015290 |
| 1 | -1.8847940 | 6.2800830 | 4.0078610 |
| 1 | -1.8581230 | 5.6142150 | 2.3629820 |
| 1 | -0.3712330 | 5.4858140 | 5.7622680 |
| 1 | -0.9674140 | 3.8266940 | 5.5746530 |
| 1 | 0.7836440 | 4.1666460 | 5.4991040 |
| 1 | -0.3267670 | 4.7981930 | -3.7175370 |
| 1 | -1.7264820 | 5.3618140 | 3.4240720 |
| 1 | -0.2116290 | 4.5429140 | 5.2211550 |
| 1 | 1.7512920 | 5.4490310 | 3.5141000 |
| 1 | 0.6778860 | 6.0956460 | 2.2506070 |
| 1 | 0.6003170 | 6.7519470 | 3.8974030 |
| 1 | -2.5078380 | 4.6403130 | 3.7015290 |
| 1 | 1.7512920 | 5.4490310 | -3.5141000 |
| 1 | 0.6003170 | 6.7519470 | -3.8974030 |
| 1 | 0.6778860 | 6.0956460 | -2.2506070 |
| 1 | 0.3712330 | 5.4858140 | -5.7622680 |
| 1 | 0.7836440 | 4.1666460 | -5.4991040 |
| 1 | -0.9674140 | 3.8266940 | -5.5746530 |
| 1 | 1.6508070 | -2.8856580 | -4.6880560 |
| 1 | -3.1016580 | -2.9499240 | -4.1849180 |
| 1 | -1.4283340 | -1.5526520 | -5.4205830 |
| 1 | -1.4472620 | -4.0178000 | -5.6976590 |
| 1 | -3.2957620 | -3.9078500 | -3.6803430 |
| 1 | -3.3222620 | -2.1443510 | -3.4704190 |
| 1 | -3.8037410 | -2.8580190 | -5.0283460 |
| 1 | -0.3896650 | -1.4692680 | -5.7755120 |
| 1 | -2.0949180 | -1.4813160 | -6.2939300 |
|   | -1.6363540 | -0.6886980 | -4.7729140 |
|---|------------|------------|------------|
| 1 | -2.1511610 | -3.8962620 | -6.5342040 |
| 1 | -0.4292610 | -4.0156860 | -6.1153300 |
| 1 | -1.6341350 | -5.0045770 | -5.2490850 |
| 6 | -1.6508070 | -2.8856580 |  4.6880560 |
| 6 | -1.4283340 | -1.5526520 |  5.4205830 |
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| 1 | -1.6363540 | -0.6886980 |  4.7729140 |
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| 1 | -3.2957620 | -3.9078500 |  3.6803430 |
| 3   (Sₐ)    | 0.1424290 | -0.5137470 |  0.0000000 |
| 77 | -2.2612220 | -0.2571000 |  0.0000000 |
| 17 | 0.0749880 | -1.9916350 |  1.3689810 |
| 6  | -0.7683020 | -1.9870250 |  2.4913470 |
| 1  | -1.4953510 | -1.1787670 |  2.6170850 |
| 6  | -0.7104150 | -3.0075430 |  3.4507530 |
| 6  | 0.1760600 | -4.0772900 |  3.3146500 |
| 1  | 0.2160520 | -4.8681420 |  4.0623880 |
| 6  | 1.0074380 | -4.1176000 |  2.1899150 |
| 1  | 1.7008900 | -4.9448190 |  2.0537360 |
| 6  | 0.9529030 | -3.0919180 |  1.2373350 |
| 6  | 1.8279210 | -3.1362430 |  0.0000000 |
| 1  | 2.4424340 | -4.0478980 |  0.0000000 |
| 6  | 2.7552950 | -1.9463270 |  0.0000000 |
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| 6  | 4.9724050 | -0.9846170 |  0.0000000 |
| 6  | 6.0557160 | -1.0951800 |  0.0000000 |
| 6  | 4.3804160 |  0.2811690 |  0.0000000 |
| 6  | 4.9731570 |  1.1930510 |  0.0000000 |
| 6  | 2.9956060 |  0.3693930 |  0.0000000 |
| 1  | 2.5013850 |  1.3391600 |  0.0000000 |
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| 6  | 0.1760600 | -4.0772900 | -4.0623880 |
| 6  | -0.7104150 | -3.0075430 | -3.4507530 |
| 6  | -0.7683020 | -1.9870250 | -2.4913470 |
|   |        |        |        |
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| 1 | -1.495351 | -1.178767 | -2.617085 |
| 6 | 0.074988 | -1.991635 | -1.368981 |
| 7 | 0.185246 | 1.212263 | -1.328061 |
| 6 | 0.287609 | 1.163461 | -2.661130 |
| 1 | 0.484579 | 0.180038 | -3.091684 |
| 6 | 0.146523 | 2.283620 | -3.477107 |
| 1 | 0.239072 | 2.155168 | -4.553202 |
| 6 | -0.118638 | 3.532313 | -2.903590 |
| 6 | -0.196296 | 3.570862 | -1.503045 |
| 1 | -0.384420 | 4.519216 | -1.001294 |
| 6 | -0.036559 | 2.415322 | 0.741292 |
| 6 | -0.196296 | 3.570862 | 1.503045 |
| 1 | -0.384420 | 4.519216 | 1.001294 |
| 6 | -0.118638 | 3.532313 | 2.903590 |
| 6 | 0.146523 | 2.283620 | 3.477107 |
| 1 | 0.239072 | 2.155168 | 4.553202 |
| 6 | 0.287609 | 1.163461 | 2.661130 |
| 1 | 0.484579 | 0.180038 | 3.091684 |
| 7 | 0.185246 | 1.212263 | 1.328061 |
| 6 | 0.287609 | 1.163461 | -2.661130 |
| 1 | 0.484579 | 0.180038 | -3.091684 |
| 6 | 0.146523 | 2.283620 | -3.477107 |
| 1 | 0.239072 | 2.155168 | -4.553202 |
| 6 | -0.118638 | 3.532313 | -2.903590 |
| 6 | -0.196296 | 3.570862 | -1.503045 |
| 1 | -0.384420 | 4.519216 | -1.001294 |
| 6 | -0.036559 | 2.415322 | 0.741292 |
| 6 | -0.196296 | 3.570862 | 1.503045 |
| 6 | -0.118638 | 3.532313 | 2.903590 |
| 1 | 0.185246 | 1.212263 | 1.328061 |
| 6 | -0.312520 | 4.804598 | 3.716378 |
| 6 | 0.758591 | 5.829703 | 3.310289 |
| 6 | -1.709892 | 5.375236 | 3.424936 |
| 6 | -0.195542 | 4.549263 | 5.219792 |
| 1 | 1.768861 | 5.443647 | 3.507530 |
| 1 | 0.695989 | 6.095809 | 2.246144 |
| 1 | 0.625754 | 6.752705 | 3.892788 |
| 1 | -2.494540 | 4.658191 | 3.704381 |
| 1 | -1.861808 | 6.294518 | 4.008679 |
| 1 | -1.842158 | 5.628089 | 2.364040 |
| 1 | -0.348209 | 5.493485 | 5.760456 |
| 1 | -0.954938 | 3.838116 | 5.575557 |
| 1 (T₁) | 77 | -0.4250580 | -0.9757230 | 0.0000000 |
|-------|----|-------------|-------------|-------------|
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|       | 6  | -1.4667750 | -3.4180190 | 3.4473550 |
|       | 1  | -2.1332170 | -3.3380050 | 4.3070600 |
|       | 6  | -0.6828440 | -4.5668930 | 3.2731400 |
|       | 1  | -0.7230070 | -5.3773770 | 4.0009780 |
|       | 6  | 0.1539840  | -4.6622060 | 2.1568300 |
|       | 1  | 0.7730510  | -5.5500970 | 2.0080560 |
|       | 6  | 0.2016370  | -3.6194630 | 1.2270690 |
|       | 6  | 1.0879250  | -3.7143390 | 0.0000000 |
|       | 1  | 1.6364680  | -4.6664050 | 0.0000000 |
|       | 6  | 2.0928610  | -2.5945960 | 0.0000000 |
|       | 6  | 3.4644170  | -2.8463080 | 0.0000000 |
|       | 1  | 3.8104360  | -3.8787800 | 0.0000000 |
|       | 6  | 4.3655570  | -1.7837800 | 0.0000000 |
|       | 1  | 5.4387610  | -1.9688860 | 0.0000000 |
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|   | -0.5760680 | -2.4536040 | -1.3811480 |
|   | -0.1441020 |  0.6825030 | -1.3365670 |
|   | -0.0078010 |  0.6315640 | -2.6719040 |
|   |  0.0287240 | -0.3702620 | -3.1062710 |
|   |  0.0752370 |  1.7486840 | -3.4853960 |
|   |  1.8079000 |  1.6073730 | -4.5580420 |
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|   | -0.1113680 |  3.1026750 | -1.5165780 |
|   | -0.1582310 |  4.0722610 | -1.0189510 |
|   | -0.1494290 |  1.9283790 | -0.7117030 |
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|   | -0.1113680 |  3.1026750 |  1.5165780 |
|   | -0.1582310 |  4.0722610 |  1.0189510 |
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|   |  1.8079000 |  1.6073730 |  4.5580420 |
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|   |  0.0448660 |  4.3290350 |  3.7190840 |
|   |  1.2683250 |  5.1605400 |  3.3017910 |
|   | -1.2340470 |  5.1444700 |  3.4724600 |
|   |  0.1490480 |  4.0465450 |  5.2197740 |
|   |  2.1993080 |  4.5991950 |  3.4685430 |
|   |  1.2286900 |  5.4439900 |  2.2408950 |
|   |  1.3159370 |  6.0858260 |  3.8957580 |
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|   | -1.3437400 |  5.4271530 |  2.4164550 |
|   |  0.1737720 |  4.9983180 |  5.7695890 |
|   | -0.7128500 |  3.4717800 |  5.5889570 |
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|   |  0.0448660 |  4.3290350 | -3.7190840 |
|   | -1.2340470 |  5.1444700 | -3.4724600 |
|   |  1.2683250 |  5.1605400 | -3.3017910 |
|   |  0.1490480 |  4.0465450 | -5.2197740 |
|   | -2.1263070 |  4.5718170 | -3.7639820 |
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|   |         |         |         |         |
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| 1 | 0.1737720 | 4.9983180 | -5.7695890 |
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2 (T$_1$)

|   |         |         |         |         |
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| 1 | -1.4281090 | -1.2462210 | 2.6423080 |
| 6 | -0.5866880 | -3.0411450 | 3.4945370 |
| 6 | 0.3681360 | -4.0529500 | 3.3011480 |
| 1 | 0.4783160 | -4.8564060 | 4.0289950 |
| 6 | 1.1994910 | -4.0415700 | 2.1749210 |
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| 6 | 0.1454460 | -1.9940480 | -1.3822090 |
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| 6 | 0.2264800 | 1.1413990 | -2.6724670 |
| 1 | 0.4314180 | 0.1594600 | -3.1067990 |
| 6 | 0.1138210 | 2.2547120 | -3.4878620 |
| 1 | 0.2350120 | 2.1301600 | -4.5612840 |
| 6 | -0.1762390 | 3.5212670 | -2.8952500 |
| 6 | -0.2827070 | 3.5609970 | -1.5176670 |
| 1 | -0.4873460 | 4.5099840 | -1.0201700 |
| 6 | -0.1210530 | 2.3977060 | -0.7120120 |
| 6 | -0.1210530 | 2.3977060 | 0.7120120 |
| 6 | -0.2827070 | 3.5609970 | 1.5176670 |
|   |     |     |     |     |     |     |
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| 6 | -0.1762390 | 3.5212670 | 2.8952500 |
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| 1 | 0.2350120  | 2.1301600 | 4.5612840 |
| 6 | 0.2264800  | 1.1413990 | 2.6724670 |
| 6 | 0.2264800  | 1.1413990 | 2.6724670 |
| 7 | 0.0900380  | 1.1701460 | 1.3368860 |
| 6 | -0.3497800 | 4.7932950 | 3.7217250 |
| 6 | -0.3497800 | 4.7932950 | 3.7217250 |
| 1 | 1.7326830  | 5.4163830 | 3.4919990 |
| 1 | 0.6468540  | 6.0910210 | 2.2553410 |
| 1 | 0.6117090  | 6.7357860 | 3.9111280 |
| 1 | -2.5317030 | 4.6744350 | 3.7448610 |
| 1 | -1.8791500 | 6.3020970 | 4.0594550 |
| 1 | -1.8879530 | 5.6510200 | 2.4064370 |
| 1 | -0.3559810 | 5.4705150 | 5.7738690 |
| 1 | -0.9715450 | 3.8170220 | 5.5834620 |
| 1 | 0.7801420  | 4.1395490 | 5.4838450 |
| 6 | -0.3497800 | 4.7932950 | -3.7217250 |
| 6 | -1.7432460 | 5.3871480 | -3.4630730 |
| 6 | 0.7232770  | 5.8163740 | -3.3165410 |
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| 6  | -1.2687080 | -4.1558970 |  5.6738180 |
| 1  | -0.2998240 | -1.5752400 |  5.8054200 |
| 1  | -1.5802460 | -0.8105540 |  4.8345360 |
| 1  | -1.9981190 | -1.6548440 |  6.3389910 |
| 1  | -3.1486600 | -4.0566530 |  3.6786810 |
| 1  | -3.6725250 | -3.0694530 |  5.0666870 |
| 1  | -3.2442220 | -2.2885230 |  4.8345360 |
| 1  | -1.9657440 | -4.0814210 |  6.5210360 |
| 1  | -1.4257640 | -5.1371510 |  5.2022880 |
| 1  | -0.2470260 | -4.1261930 |  6.0809300 |

### 3 (T₁)

| 77 |  0.0424830 | -0.4878170 |  0.0000000 |
| 17 | -2.2910920 | -0.4508140 |  0.0000000 |
|  6 |  0.1312370 | -1.9817760 |  1.3790600 |
|  6 | -0.7018400 | -2.0505000 |  2.5069460 |
|  1 | -1.4842690 | -1.3002630 |  2.6547460 |
|  6 | -0.5710580 | -3.0873670 |  3.4381160 |
|  6 |  0.3915210 | -4.0855430 |  3.2749040 |
|  1 |  0.4901580 | -4.8872170 |  4.0053070 |
|  6 |  1.2263170 | -4.0335500 |  2.1556520 |
|  1 |  1.9843420 | -4.8046680 |  2.0065600 |
|  6 |  1.0954240 | -2.9986190 |  1.2277770 |
|  6 |  1.9834420 | -2.9464700 |  0.0000000 |
|  1 |  2.6815040 | -3.7941050 |  0.0000000 |
|  6 |  2.7908300 | -1.6759660 |  0.0000000 |
|  6 |  4.1844610 | -1.7027970 |  0.0000000 |
|  6 |  4.6932690 | -2.6654660 |  0.0000000 |
|  6 |  4.9006620 | -0.5076860 |  0.0000000 |
|  1 |  5.9895840 | -0.5156040 |  0.0000000 |
|  6 |  4.1959420 |  0.6988790 |  0.0000000 |
|  6 |  4.7029400 |  1.6605530 |  0.0000000 |
|  6 |  2.8100420 |  0.6607410 |  0.0000000 |
|  1 |  2.2240820 |  1.5778150 |  0.0000000 |
|  7 |  2.1194820 | -0.5006620 |  0.0000000 |
|  6 |  1.0954240 | -2.9986190 | -1.2277770 |
|  6 |  1.2263170 | -4.0335500 | -2.1556520 |
|  1 |  1.9843420 | -4.8046680 | -2.0065600 |
|  6 |  0.3915210 | -4.0855430 | -3.2749040 |
|  1 |  0.4901580 | -4.8872170 | -4.0053070 |
|  6 | -0.5710580 | -3.0873670 | -3.4381160 |
|  6 | -0.7018400 | -2.0505000 | -2.5069460 |
|  1 | -1.4842690 | -1.3002630 | -2.6547460 |
|  6 |  0.3915210 | -4.0855430 | -3.2749040 |
|  7 |  0.5046970 |  1.1779420 | -1.3348030 |
|  6 |  0.1906150 |  1.1464330 | -2.6720220 |
|  1 |  0.3861830 |  0.1643370 | -3.1083010 |
|  6 |  0.0882480 |  2.2608650 | -3.4847760 |
|  1 |  0.2067110 |  2.1354990 | -4.5579030 |
|   |       |        |        |        |
|---|-------|--------|--------|--------|
| 1 | -0.4984970 | 4.5235450 | -1.0201310 |
| 6 | -0.1924130 | 3.5314680 | 2.8938390 |
| 6 | -0.3015200 | 3.5731580 | 1.5174950 |
| 1 | -0.4984970 | 4.5235450 | 1.0201310 |
| 6 | -0.1924130 | 3.5314680 | 2.8938390 |
| 6 | -0.3015200 | 3.5731580 | 1.5174950 |
| 1 | -0.4984970 | 4.5235450 | 1.0201310 |
| 6 | -0.1924130 | 3.5314680 | 2.8938390 |
| 6 | -0.3015200 | 3.5731580 | 1.5174950 |
| 1 | -0.4984970 | 4.5235450 | 1.0201310 |
| 6 | -0.1924130 | 3.5314680 | 2.8938390 |
| 6 | -0.3015200 | 3.5731580 | 1.5174950 |
| 1 | -0.4984970 | 4.5235450 | 1.0201310 |
| 6 | -0.1924130 | 3.5314680 | 2.8938390 |
| 6 | -0.3015200 | 3.5731580 | 1.5174950 |
| 1 | -0.4984970 | 4.5235450 | 1.0201310 |
| 6 | -0.1924130 | 3.5314680 | 2.8938390 |
| 6 | -0.3015200 | 3.5731580 | 1.5174950 |
| 1 | -0.4984970 | 4.5235450 | 1.0201310 |
| 6 | -0.1924130 | 3.5314680 | 2.8938390 |
| 6 | -0.3015200 | 3.5731580 | 1.5174950 |
| 1 | -0.4984970 | 4.5235450 | 1.0201310 |
| 6 | -0.1924130 | 3.5314680 | 2.8938390 |
| 6 | -0.3015200 | 3.5731580 | 1.5174950 |
| 1 | -0.4984970 | 4.5235450 | 1.0201310 |
| 6 | -0.1924130 | 3.5314680 | 2.8938390 |
| 6 | -0.3015200 | 3.5731580 | 1.5174950 |
| 1 | -0.4984970 | 4.5235450 | 1.0201310 |
| 6 | -0.1924130 | 3.5314680 | 2.8938390 |
| 6 | -0.3015200 | 3.5731580 | 1.5174950 |
| 1 | -0.4984970 | 4.5235450 | 1.0201310 |
| 6 | -0.1924130 | 3.5314680 | 2.8938390 |
| 6 | -0.3015200 | 3.5731580 | 1.5174950 |
| 1 | -0.4984970 | 4.5235450 | 1.0201310 |
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