

# **Strong Circularly Polarized Luminescence of an Octahedral Chromium(III) Complex**

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## **Supplementary Information**

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## 1. Materials and Methods

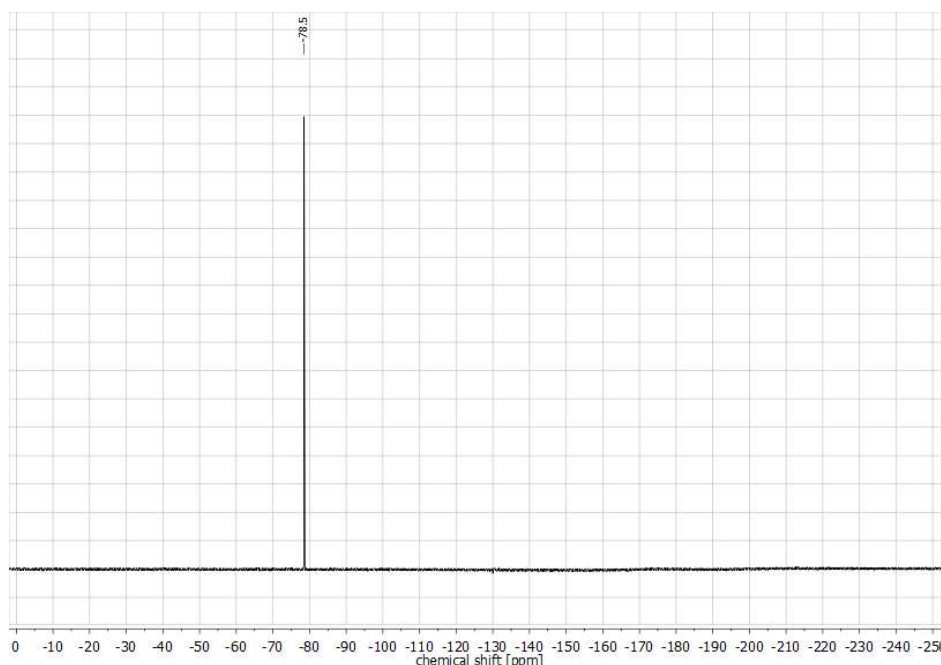
NMR spectra were recorded on a Bruker AVII+400 spectrometer ( $^1\text{H}$ : 400 MHz,  $^{19}\text{F}$ : 377 MHz) using  $\text{CD}_3\text{OD}$  ( $\geq 99.8\%$  D) as the solvent. The racemic Cr complex  $[\text{Cr}(\text{ddpd})_2](\text{BF}_4)_3$  was synthesized as described previously.<sup>1</sup> NMR-grade  $\text{D}_2\text{O}$  ( $>99.8\%$  D) was used for the photophysical measurements.

## 2. Chiral HPLC / Configurational Stability Test

All chiral HPLC runs of the  $[\text{Cr}(\text{ddpd})_2](\text{X})_3$  complexes (**rac-1** or enantioenriched samples) were performed on a Knauer Azura HPLC system (UV detection at  $\lambda = 300$  nm), equipped with a CHIRALPAK IC column (Daicel, particle size: 5  $\mu\text{m}$ , internal diameter: 4.6 mm, column length: 250 mm) using  $\text{CH}_2\text{Cl}_2/\text{MeOH}$  (90:10) with additional 0.5 vol.-%  $\text{NEt}_3$  and 0.3 vol.-%  $\text{CF}_3\text{COOH}$  as mobile phase with a flow of 1.0 mL/min. All samples were filtered through a membrane filter (nylon, 0.45  $\mu\text{m}$  pore size, 13 mm diameter) in a stainless steel filter holder prior to injection.

Racemic  $[\text{Cr}(\text{ddpd})_2](\text{BF}_4)_3$  (6.0 mg) was dissolved in  $\text{CH}_2\text{Cl}_2/\text{MeOH}$  (90:10, v/v, 5.5 mL) and filtered through a membrane filter (vide infra). The filter was washed with additional 0.5 mL of the solvent mixture, to yield a concentration of ca. 1 mg/mL. The solution was subjected to chiral HPLC in portions of 100  $\mu\text{L}$ . The collected fractions of the respective enantiomers were combined and the solvents were removed in vacuo at room temperature. After drying in vacuo, samples of the enantiomers were redissolved in the HPLC solvent mixture, filtered, and injected to verify the enantiopurity. After the HPLC purification, the enantiopure complexes contain additional triethylammonium trifluoroacetate ( $\text{HNEt}_3\text{CF}_3\text{COO}$ ). This raw material was washed repeatedly with  $\text{CH}_2\text{Cl}_2$  which slowly removes the slightly soluble impurity triethylammonium trifluoroacetate. This procedure yields material with only a minimum presence of the salt.

The counterions after chiral HPLC resolution was confirmed to be trifluoroacetate by mass spectrometry (ESI-MS, neg. mode:  $m/z(\%) = 113.11 \{31\%, [\text{CF}_3\text{COO}]^-\}, 226.96 \{100\%, [\text{2CF}_3\text{COO} + \text{H}]^-\}$ ) and by  $^{19}\text{F}$  NMR spectroscopy<sup>2</sup> (Figure S1):



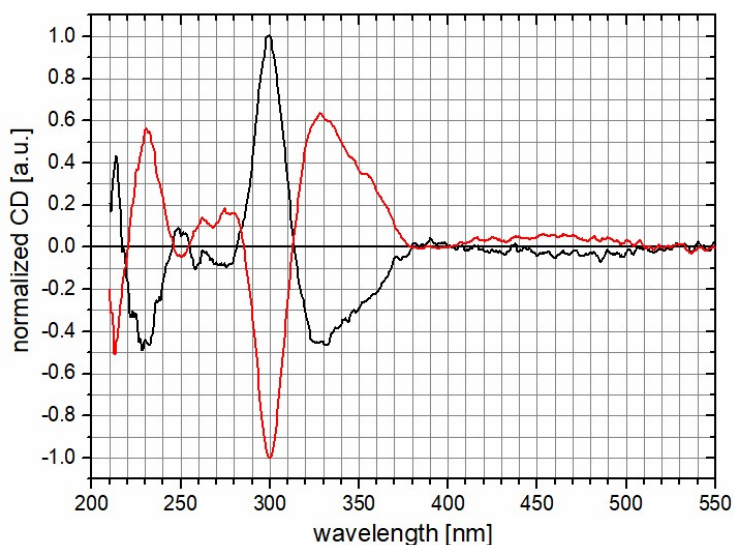
**Figure S1.**  $^{19}\text{F}$  NMR spectrum (377 MHz,  $\text{CD}_3\text{OD}$ ) of **(*M,M*)-1**.

#### Configurational stability test in solution

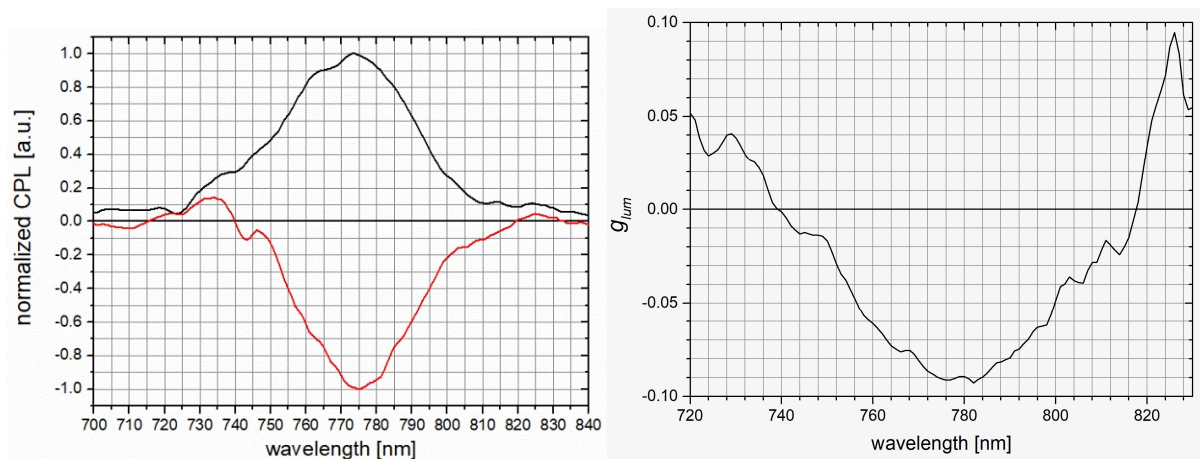
An enantiomerically pure sample of **(*M,M*)-1** (0.3 mg) was stirred at room temperature in  $\text{H}_2\text{O}$  (1.0 mL, HPLC grade). During the course of 48 h, samples of 100  $\mu\text{L}$  were taken at certain intervals (1h, 3h, 24 h, 48 h). These samples were immediately concentrated under a stream of air and the residues were taken up in  $\text{CH}_2\text{Cl}_2/\text{MeOH}$  (90:10, 100  $\mu\text{L}$ ). The solutions were filtered through a membrane filter (nylon, 0.45  $\mu\text{m}$  pore size), the filter was washed with additional solvent mixture (100  $\mu\text{L}$ ), and the combined filtrates were concentrated. For chiral HPLC analysis, the dry samples were redissolved in  $\text{CH}_2\text{Cl}_2/\text{MeOH}$  (90:10, 100  $\mu\text{L}$ ) directly before the run.

### 3. ECD and CPL measurements

The ECD spectra (Figure S2) were recorded with a Jasco J-715 spectropolarimeter (4 accumulations) on 10  $\mu\text{M}$  solutions in deoxygenated  $\text{D}_2\text{O}$ . CPL spectra were measured with a home-made spectrofluoropolarimeter<sup>3</sup> in the configuration described before.<sup>4</sup> The spectra were acquired on 10  $\mu\text{M}$  solutions in deoxygenated  $\text{D}_2\text{O}$  under 365 nm irradiation, with 4 sec integration time and 4 accumulations. The spectra were baseline corrected by subtracting the trace of the solvent.



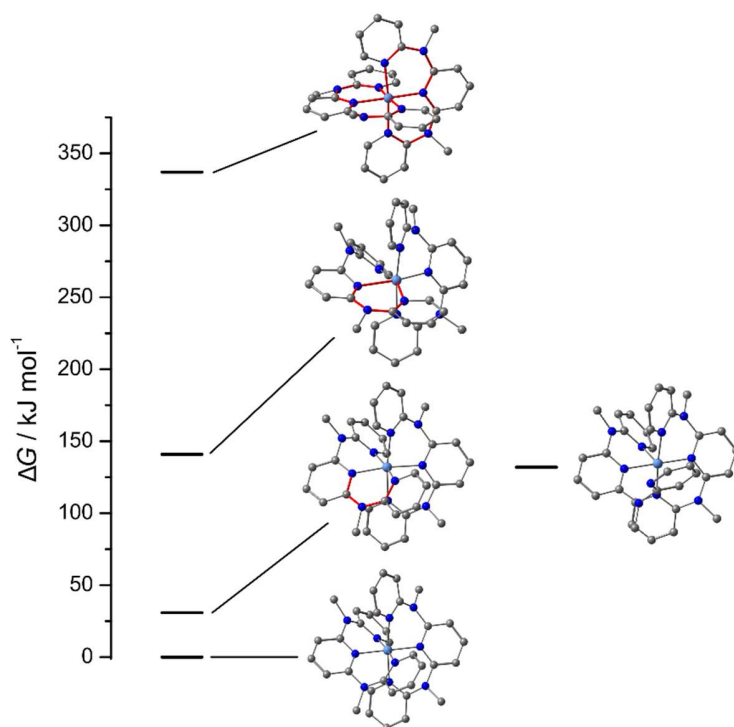
**Figure S2.** Normalized CD spectra (deoxygenated  $\text{D}_2\text{O}$ ,  $c = 10 \mu\text{M}$ ) of the first chiral HPLC fraction (black) and the second fraction (red) – Mirror-image relationship indicating the enantiomeric nature of both fractions.



**Figure S3.** Left: Normalized CPL spectra (deoxygenated  $\text{D}_2\text{O}$ ,  $c = 10 \mu\text{M}$ ) of the first chiral HPLC fraction (black) and the second fraction (red) – Right: Plot of  $g_{\text{lum}}$  vs. the wavelength for (*M,M*-1).

#### 4. Calculation of the Energy Barriers for Racemization Pathways

Racemization of (*M,M*)- or (*P,P*)-[Cr(ddpd)<sub>2</sub>]<sup>3+</sup> can occur without changing the coordination number via inverting the boat conformations of the four six-membered chelate rings. Using DFT optimizations with constrained dihedral angles in the chelate rings, geometries of [Cr(ddpd)<sub>2</sub>]<sup>3+</sup> with one half-chair, one flattened ring and with fully flattened ligands were optimized with free enthalpy differences of 31, 141 and 337 kJ/mol, respectively. These numbers show that the planarization of only one chelate ring is very unfavorable (Figure S4). Since completely flattened ligands might be avoided in the actual mechanism, a reaction path from (*M,M*)- to (*P,P*)-[Cr(ddpd)<sub>2</sub>]<sup>3+</sup> was calculated using the nudged elastic band (NEB) method. The NEB method indeed favors a stepwise minimum energy path (Figure 2 in the manuscript). The inversion of both chelate rings of the first ligand is followed by the planarization and subsequent inversion of the first chelate ring on the second ddpd ligand. Finally, the last six-membered chelate-ring inverts.



**Figure S4.** Optimized geometries of [Cr(ddpd)<sub>2</sub>]<sup>3+</sup> with constrained chelate rings indicated in red (left) and of [Cr(ddpd)(κ<sup>2</sup>N-ddpd)]<sup>3+</sup> (right).

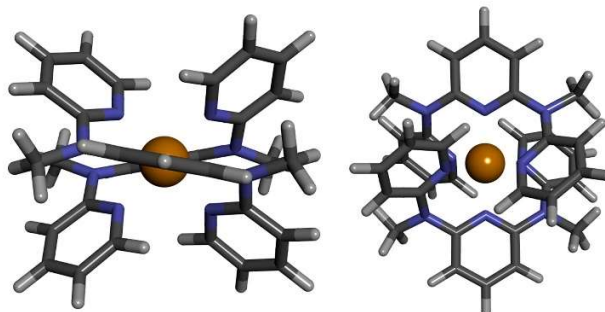
To investigate a conceivable dissociative pathway, the geometry of [Cr(ddpd)(κ<sup>2</sup>N-ddpd)]<sup>3+</sup> was optimized using DFT (Figure S4, right). This yielded a free enthalpy difference of 132 kJ/mol. It

was not possible to obtain the optimized geometry of 7-coordinate  $[\text{Cr}(\text{ddpd})_2(\text{H}_2\text{O})]^{3+}$ . Instead, the calculation yielded 6-coordinate  $[\text{Cr}(\text{ddpd})(\text{k}^2\text{N-ddpd})(\text{H}_2\text{O})]^{3+}$  with the dissociated pyridyl residue forming a hydrogen bond with the water ligand.

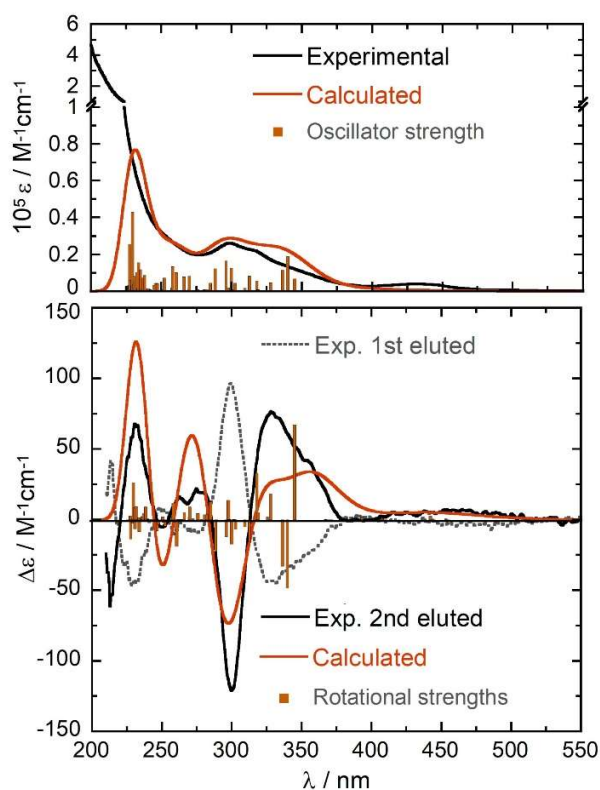
DFT calculations were carried out using the ORCA program package (version 4.1.1)<sup>5</sup> using the B3LYP functional.<sup>6-8</sup> Tight convergence criteria were chosen for geometry optimizations and frequency calculations (Keywords TightSCF and TightOpt, convergence criteria for the SCF part: energy change  $1.0 \times 10^{-8} E_h$ , 1-El. energy change  $1.0 \times 10^{-5} E_h$ , orbital gradient  $1.0 \times 10^{-5}$ , orbital rotation angle  $1.0 \times 10^{-5}$ , DIIS Error  $5.0 \times 10^{-7}$ ; for geometry optimizations: energy change:  $1.0 \times 10^{-6} E_h$ , max. gradient  $1.0 \times 10^{-4} E_h a_0^{-1}$ , RMS gradient  $3.0 \times 10^{-5} E_h a_0^{-1}$ , max. displacement  $1.0 \times 10^{-3} a_0$ , RMS displacement  $6.0 \times 10^{-4} a_0$ ). All calculations make use of the resolution of identity (Split-RI-J) approach for the Coulomb term in combination with the chain-of-spheres approximation for the exchange term (COSX).<sup>9,10</sup> The ZORA relativistic approximation was used to describe relativistic effects in all calculations.<sup>11</sup> To account for solvent effects, a conductor-like screening model (CPCM) modeling acetonitrile was used in all calculations.<sup>12</sup> Atom-pairwise dispersion correction was performed with the Becke-Johnson damping scheme (D3BJ).<sup>13,14</sup> For the geometries of the ground state and with (partly) planarized ligands geometry optimizations were performed using Ahlrichs' split valence triple- $\xi$  basis set def2-TZVPP which comprises polarization functions for all non-hydrogen atoms.<sup>15,16</sup> Dihedral angles were fixed to  $0^\circ$  for the calculations of the structures with (partly) planarized ligands. For ground state geometries the presence of energy minima was checked by numerical frequency calculations. Explicit counter ions and/or solvent molecules were not taken into account. NEB calculations were performed using Ahlrichs' split valence polarization basis set def2-SVP basis with ground state geometries optimized using the same basis set.<sup>13,14</sup> Seven intermediate images were calculated with initial path generation via the image dependent pair potential (IDPP) method<sup>17</sup> and optimized using the Limited-memory Broyden-Fletcher-Goldfarb-Shanno (L-BFGS) algorithm.<sup>18</sup> Tolerance for the maximum component of the atomic force perpendicular to the path was  $5.0 \times 10^{-4} E_h a_0^{-1}$  with a root-mean-square of  $2.0 \times 10^{-4} E_h a_0^{-1}$ . The spring constant was set to  $1.0 \times 10^{-1} E_h a_0^{-2}$ . CASSCF(7,12)-NEVPT2 calculations for metal-centered excited states were performed as previously described.<sup>19</sup>

## 5. Assignment of Absolute Configuration

To assign the absolute configuration of the enantiomers of  $[\text{Cr}(\text{ddpd})_2]^{3+}$  and the elution order of its enantioseparation, experimental electronic circular dichroism (ECD) spectra were compared with those calculated by means of density functional theory (DFT).<sup>20,21</sup> The X-ray geometry of **rac-1** served as starting point to produce a DFT-optimized geometry (M06/def2-SVP) with (*M,M*)-chirality and  $D_2$ -symmetry, shown in Figure S5. Excited state calculations were then run with the time-dependent DFT method (TD-DFT). After a minimal screening of functionals and basis sets,<sup>22</sup> final calculations were run at the CAM-B3LYP/def2-TZVP level of theory using a PCM solvent model for water. The comparison between experimental and calculated UV/ECD spectra is shown in Figure S6. The agreement is excellent between the ECD spectrum calculated for the (*M,M*)-enantiomer and the experimental trace recorded for the second eluted isomer. As it frequently happens with open-shell transition metal complexes with multi-chromophoric ligands, there is a very high densities of states in the short-wavelength region (see vertical bars in Figure S6).<sup>23,24</sup> Moreover, a clear distinction between metal-centered and ligand-centered transitions is challenging by TD-DFT methods. To extract the metal-centered transitions, CASSCF(7,12)-NEVPT2 calculations were performed additionally.<sup>19</sup>



**Figure S5.** DFT-optimized structure of the cationic metal complex in (*M,M*)-1 with  $D_2$  symmetry seen along two different  $C_2$  axes.



**Figure S6.** Comparison between the experimental and calculated UV/vis absorption (top) and ECD (bottom) spectra measured in D<sub>2</sub>O at 10<sup>-5</sup> M concentration, and TD-DFT-calculated spectra on **(M,M)-1** at the CAM-B3LYP/def2-TZVP/PCM//M06/def2-SVP level. Calculated spectra were plotted using an exponential bandwidth of 0.35 eV and red-shifted by 33 nm.

DFT/TD-DFT calculations for the assignment of absolute configurations were run with the Gaussian16 package,<sup>25</sup> using default grids and convergence criteria. The starting geometry was extracted from the published X-ray structure of a racemic form of [Cr(ddpd)<sub>2</sub>]<sup>3+</sup> and had (*M,M*)-configuration.<sup>1</sup> The tricationic metal complex was optimized at the M06/def2-SVP level in vacuo. TD-DFT calculations were run using B3LYP and CAM-B3LYP functionals, def2-SVP or def2-TZVP basis set on all atoms, either in vacuo or including IEF-PCM solvent model for water. All calculations were run for [Cr(ddpd)<sub>2</sub>]<sup>3+</sup> in its quartet state using unrestricted wavefunctions; ground and excited states were checked for wavefunction stability and spin contamination. Up to 100 excited states (roots) were considered. UV/vis absorption and ECD spectra were plotted using the software SpecDis.<sup>26,27</sup>

The absorption bands at wavelengths > 400 nm (the metal-centered quartet transitions) were reproduced by CASSCF(7,12)-NEVPT2 calculations on **(M,M)-1**.<sup>19</sup> The calculated overall positive CD intensity for **(M,M)-1** at wavelengths > 400 nm confirm the TD-DFT based

assignment of the second fraction as **(M,M)-1** (434 nm:  $R^*T = -4.5 \times 10^{40}$  cgs; 429 nm:  $R^*T = -3.4 \times 10^{40}$  cgs; 411 nm:  $R^*T = -12.5 \times 10^{40}$  cgs).

## 6. Cartesian Coordinates for Calculated Species

Cartesian Coordinates (in Å) for the optimized geometries of constrained chelate rings (Figure S3), NEB calculations (Figure 2 in the manuscript) and the five-coordinate complex  $[\text{Cr}(\text{ddpd})(\text{k}^2\text{N-ddpd})]^{3+}$  (Figure S4):

$[\text{Cr}(\text{ddpd})_2]^{3+}$  with one half-chair:

|    |              |              |              |
|----|--------------|--------------|--------------|
| 24 | 10.634778000 | 12.457922000 | 5.063104000  |
| 7  | 9.012260000  | 13.664918000 | 5.635481000  |
| 6  | 8.988788000  | 14.323422000 | 6.815651000  |
| 1  | 9.906857000  | 14.353730000 | 7.376477000  |
| 7  | 8.023550000  | 13.061364000 | 3.620616000  |
| 6  | 7.853464000  | 14.915969000 | 7.309190000  |
| 1  | 7.881250000  | 15.410296000 | 8.267528000  |
| 7  | 10.311847000 | 13.164149000 | 2.860345000  |
| 6  | 6.686841000  | 14.848172000 | 6.549204000  |
| 1  | 5.770218000  | 15.294113000 | 6.908482000  |
| 7  | 11.723999000 | 14.155526000 | 5.605300000  |
| 6  | 6.719747000  | 14.238368000 | 5.312428000  |
| 1  | 5.843488000  | 14.222993000 | 4.686366000  |
| 7  | 12.770385000 | 12.976580000 | 7.355545000  |
| 6  | 7.916525000  | 13.673981000 | 4.862550000  |
| 7  | 10.675374000 | 11.883625000 | 7.024539000  |
| 6  | 6.792570000  | 12.456893000 | 3.085861000  |
| 1  | 6.081305000  | 13.188704000 | 2.702507000  |
| 1  | 6.320176000  | 11.890852000 | 3.885604000  |
| 1  | 7.063798000  | 11.774641000 | 2.286610000  |
| 6  | 8.992063000  | 13.436078000 | 2.647376000  |
| 6  | 8.519165000  | 13.916158000 | 1.446198000  |
| 1  | 7.485388000  | 14.199501000 | 1.340121000  |
| 6  | 9.381664000  | 13.931210000 | 0.360928000  |
| 1  | 9.036715000  | 14.255496000 | -0.610361000 |

|   |              |              |              |
|---|--------------|--------------|--------------|
| 6 | 11.581457000 | 15.272372000 | 4.858994000  |
| 1 | 10.768409000 | 15.273750000 | 4.151787000  |
| 6 | 12.420948000 | 16.351434000 | 4.972497000  |
| 1 | 12.268261000 | 17.219349000 | 4.350055000  |
| 6 | 13.450647000 | 16.286541000 | 5.909878000  |
| 1 | 14.129938000 | 17.117066000 | 6.040228000  |
| 6 | 13.582005000 | 15.166956000 | 6.704374000  |
| 1 | 14.343604000 | 15.126253000 | 7.464158000  |
| 6 | 12.682566000 | 14.106280000 | 6.546050000  |
| 6 | 14.046400000 | 12.747368000 | 8.051935000  |
| 1 | 14.852787000 | 12.904238000 | 7.341405000  |
| 1 | 14.072411000 | 11.715946000 | 8.387468000  |
| 1 | 14.181768000 | 13.407238000 | 8.908358000  |
| 6 | 11.648433000 | 12.312220000 | 7.872617000  |
| 6 | 11.567818000 | 12.078455000 | 9.236330000  |
| 1 | 12.334931000 | 12.451694000 | 9.893339000  |
| 6 | 10.470498000 | 11.401125000 | 9.737729000  |
| 1 | 10.387762000 | 11.209123000 | 10.797944000 |
| 7 | 12.407366000 | 11.904387000 | 4.161282000  |
| 6 | 13.030561000 | 11.135963000 | 5.116522000  |
| 1 | 12.480530000 | 10.972363000 | 6.022358000  |
| 7 | 12.381619000 | 12.484167000 | 1.842861000  |
| 6 | 14.250428000 | 10.537432000 | 4.990494000  |
| 1 | 14.661751000 | 9.977766000  | 5.815737000  |
| 6 | 14.885378000 | 10.632590000 | 3.756944000  |
| 1 | 15.835661000 | 10.152799000 | 3.573021000  |
| 6 | 14.242446000 | 11.290358000 | 2.741931000  |
| 1 | 14.677081000 | 11.266910000 | 1.761090000  |
| 6 | 13.002396000 | 11.933904000 | 2.950504000  |
| 6 | 13.299545000 | 12.846543000 | 0.724082000  |
| 1 | 13.326499000 | 12.060477000 | -0.027337000 |
| 1 | 14.291229000 | 13.022435000 | 1.117535000  |
| 1 | 12.974913000 | 13.774340000 | 0.276488000  |
| 6 | 11.122849000 | 13.063139000 | 1.786942000  |

|   |              |              |              |
|---|--------------|--------------|--------------|
| 6 | 10.655760000 | 13.447958000 | 0.513660000  |
| 1 | 11.265631000 | 13.316654000 | -0.359127000 |
| 7 | 9.724951000  | 10.676627000 | 4.641404000  |
| 7 | 8.547356000  | 10.860690000 | 6.667809000  |
| 6 | 9.964005000  | 10.054126000 | 3.466213000  |
| 1 | 10.776119000 | 10.438644000 | 2.873739000  |
| 6 | 9.209638000  | 8.998397000  | 3.021854000  |
| 1 | 9.435634000  | 8.541129000  | 2.071347000  |
| 6 | 8.158960000  | 8.557380000  | 3.823543000  |
| 1 | 7.537966000  | 7.730830000  | 3.509103000  |
| 6 | 7.928233000  | 9.164088000  | 5.042300000  |
| 1 | 7.145750000  | 8.804330000  | 5.688828000  |
| 6 | 8.745514000  | 10.224855000 | 5.443607000  |
| 6 | 7.204427000  | 10.764324000 | 7.259408000  |
| 1 | 6.474333000  | 10.866185000 | 6.461947000  |
| 1 | 7.073526000  | 11.587815000 | 7.954754000  |
| 1 | 7.037441000  | 9.821929000  | 7.780421000  |
| 6 | 9.589483000  | 11.232808000 | 7.522374000  |
| 6 | 9.475457000  | 10.971381000 | 8.881844000  |
| 1 | 8.628884000  | 10.423993000 | 9.259006000  |

[Cr(ddpd)<sub>2</sub>]<sup>3+</sup> with one flattened ring:

|    |              |              |             |
|----|--------------|--------------|-------------|
| 24 | 10.634778000 | 12.457922000 | 5.063104000 |
| 7  | 9.012260000  | 13.664918000 | 5.635481000 |
| 6  | 8.988788000  | 14.323422000 | 6.815651000 |
| 1  | 9.906857000  | 14.353730000 | 7.376477000 |
| 7  | 8.023550000  | 13.061364000 | 3.620616000 |
| 6  | 7.853464000  | 14.915969000 | 7.309190000 |
| 1  | 7.881250000  | 15.410296000 | 8.267528000 |
| 7  | 10.311847000 | 13.164149000 | 2.860345000 |
| 6  | 6.686841000  | 14.848172000 | 6.549204000 |
| 1  | 5.770218000  | 15.294113000 | 6.908482000 |
| 7  | 11.723999000 | 14.155526000 | 5.605300000 |
| 6  | 6.719747000  | 14.238368000 | 5.312428000 |

|   |              |              |              |
|---|--------------|--------------|--------------|
| 1 | 5.843488000  | 14.222993000 | 4.686366000  |
| 7 | 12.770385000 | 12.976580000 | 7.355545000  |
| 6 | 7.916525000  | 13.673981000 | 4.862550000  |
| 7 | 10.675374000 | 11.883625000 | 7.024539000  |
| 6 | 6.792570000  | 12.456893000 | 3.085861000  |
| 1 | 6.081305000  | 13.188704000 | 2.702507000  |
| 1 | 6.320176000  | 11.890852000 | 3.885604000  |
| 1 | 7.063798000  | 11.774641000 | 2.286610000  |
| 6 | 8.992063000  | 13.436078000 | 2.647376000  |
| 6 | 8.519165000  | 13.916158000 | 1.446198000  |
| 1 | 7.485388000  | 14.199501000 | 1.340121000  |
| 6 | 9.381664000  | 13.931210000 | 0.360928000  |
| 1 | 9.036715000  | 14.255496000 | -0.610361000 |
| 6 | 11.581457000 | 15.272372000 | 4.858994000  |
| 1 | 10.768409000 | 15.273750000 | 4.151787000  |
| 6 | 12.420948000 | 16.351434000 | 4.972497000  |
| 1 | 12.268261000 | 17.219349000 | 4.350055000  |
| 6 | 13.450647000 | 16.286541000 | 5.909878000  |
| 1 | 14.129938000 | 17.117066000 | 6.040228000  |
| 6 | 13.582005000 | 15.166956000 | 6.704374000  |
| 1 | 14.343604000 | 15.126253000 | 7.464158000  |
| 6 | 12.682566000 | 14.106280000 | 6.546050000  |
| 6 | 14.046400000 | 12.747368000 | 8.051935000  |
| 1 | 14.852787000 | 12.904238000 | 7.341405000  |
| 1 | 14.072411000 | 11.715946000 | 8.387468000  |
| 1 | 14.181768000 | 13.407238000 | 8.908358000  |
| 6 | 11.648433000 | 12.312220000 | 7.872617000  |
| 6 | 11.567818000 | 12.078455000 | 9.236330000  |
| 1 | 12.334931000 | 12.451694000 | 9.893339000  |
| 6 | 10.470498000 | 11.401125000 | 9.737729000  |
| 1 | 10.387762000 | 11.209123000 | 10.797944000 |
| 7 | 12.407366000 | 11.904387000 | 4.161282000  |
| 6 | 13.030561000 | 11.135963000 | 5.116522000  |
| 1 | 12.480530000 | 10.972363000 | 6.022358000  |

|   |              |              |              |
|---|--------------|--------------|--------------|
| 7 | 12.381619000 | 12.484167000 | 1.842861000  |
| 6 | 14.250428000 | 10.537432000 | 4.990494000  |
| 1 | 14.661751000 | 9.977766000  | 5.815737000  |
| 6 | 14.885378000 | 10.632590000 | 3.756944000  |
| 1 | 15.835661000 | 10.152799000 | 3.573021000  |
| 6 | 14.242446000 | 11.290358000 | 2.741931000  |
| 1 | 14.677081000 | 11.266910000 | 1.761090000  |
| 6 | 13.002396000 | 11.933904000 | 2.950504000  |
| 6 | 13.299545000 | 12.846543000 | 0.724082000  |
| 1 | 13.326499000 | 12.060477000 | -0.027337000 |
| 1 | 14.291229000 | 13.022435000 | 1.117535000  |
| 1 | 12.974913000 | 13.774340000 | 0.276488000  |
| 6 | 11.122849000 | 13.063139000 | 1.786942000  |
| 6 | 10.655760000 | 13.447958000 | 0.513660000  |
| 1 | 11.265631000 | 13.316654000 | -0.359127000 |
| 7 | 9.724951000  | 10.676627000 | 4.641404000  |
| 7 | 8.547356000  | 10.860690000 | 6.667809000  |
| 6 | 9.964005000  | 10.054126000 | 3.466213000  |
| 1 | 10.776119000 | 10.438644000 | 2.873739000  |
| 6 | 9.209638000  | 8.998397000  | 3.021854000  |
| 1 | 9.435634000  | 8.541129000  | 2.071347000  |
| 6 | 8.158960000  | 8.557380000  | 3.823543000  |
| 1 | 7.537966000  | 7.730830000  | 3.509103000  |
| 6 | 7.928233000  | 9.164088000  | 5.042300000  |
| 1 | 7.145750000  | 8.804330000  | 5.688828000  |
| 6 | 8.745514000  | 10.224855000 | 5.443607000  |
| 6 | 7.204427000  | 10.764324000 | 7.259408000  |
| 1 | 6.474333000  | 10.866185000 | 6.461947000  |
| 1 | 7.073526000  | 11.587815000 | 7.954754000  |
| 1 | 7.037441000  | 9.821929000  | 7.780421000  |
| 6 | 9.589483000  | 11.232808000 | 7.522374000  |
| 6 | 9.475457000  | 10.971381000 | 8.881844000  |
| 1 | 8.628884000  | 10.423993000 | 9.259006000  |

[Cr(ddpd)<sub>2</sub>]<sup>3+</sup> with fully planarized ligands:

|    |              |              |              |
|----|--------------|--------------|--------------|
| 24 | 0.194337000  | 0.103937000  | 0.639206000  |
| 7  | -0.246153000 | -0.156350000 | 2.672886000  |
| 7  | 0.618343000  | 0.357652000  | -1.398737000 |
| 7  | -1.593250000 | -0.844703000 | 0.023159000  |
| 7  | 2.016210000  | 1.081091000  | 1.029588000  |
| 7  | -0.825627000 | 1.943944000  | 0.773424000  |
| 7  | 1.224679000  | -1.732966000 | 0.738023000  |
| 6  | -1.418095000 | -0.746003000 | 3.086621000  |
| 6  | -1.639387000 | -1.038176000 | 4.435719000  |
| 6  | -0.823148000 | -0.509479000 | 5.399402000  |
| 6  | 0.283946000  | 0.196679000  | 5.002836000  |
| 6  | 0.632985000  | 0.256544000  | 3.651253000  |
| 1  | -2.460280000 | -1.663427000 | 4.727119000  |
| 1  | 0.887652000  | 0.687481000  | 5.740332000  |
| 6  | -1.823493000 | -1.023373000 | -1.309588000 |
| 6  | -2.911174000 | -1.657256000 | -1.844718000 |
| 6  | -3.837952000 | -2.209046000 | -0.969525000 |
| 6  | -3.634075000 | -2.048509000 | 0.374641000  |
| 6  | -2.530619000 | -1.314578000 | 0.865212000  |
| 1  | -4.685310000 | -2.776341000 | -1.326408000 |
| 1  | -1.089384000 | -0.642435000 | -1.980832000 |
| 1  | -3.005250000 | -1.740268000 | -2.916610000 |
| 1  | -4.304479000 | -2.528924000 | 1.061799000  |
| 6  | 2.513331000  | 1.286023000  | 2.261256000  |
| 6  | 3.673381000  | 2.073600000  | 2.439943000  |
| 6  | 4.373011000  | 2.557502000  | 1.365628000  |
| 6  | 3.900248000  | 2.277711000  | 0.089770000  |
| 6  | 2.734373000  | 1.572940000  | -0.019611000 |
| 1  | 5.255210000  | 3.161256000  | 1.521234000  |
| 1  | 3.994858000  | 2.342284000  | 3.428528000  |
| 1  | 4.396387000  | 2.622383000  | -0.803956000 |
| 1  | 2.345873000  | 1.396239000  | -0.996089000 |
| 6  | 0.142642000  | 1.444224000  | -2.100378000 |

|   |              |              |              |
|---|--------------|--------------|--------------|
| 6 | 0.289967000  | 1.522571000  | -3.487468000 |
| 6 | 1.168744000  | 0.691192000  | -4.132288000 |
| 6 | 1.765335000  | -0.312754000 | -3.415013000 |
| 6 | 1.364149000  | -0.563522000 | -2.099068000 |
| 1 | -0.249774000 | 2.256602000  | -4.051746000 |
| 1 | 2.510365000  | -0.927090000 | -3.881523000 |
| 6 | -1.309495000 | 2.347989000  | 1.983583000  |
| 6 | -2.068055000 | 3.466358000  | 2.193043000  |
| 6 | -2.424879000 | 4.226165000  | 1.085317000  |
| 6 | -1.929575000 | 3.860448000  | -0.137339000 |
| 6 | -1.058557000 | 2.755484000  | -0.272533000 |
| 1 | -3.088248000 | 5.074535000  | 1.169951000  |
| 1 | -1.072200000 | 1.740289000  | 2.826155000  |
| 1 | -2.398160000 | 3.706954000  | 3.191723000  |
| 1 | -2.241996000 | 4.404691000  | -1.008109000 |
| 6 | 1.861797000  | -2.301377000 | -0.300935000 |
| 6 | 2.679712000  | -3.437683000 | -0.105416000 |
| 6 | 2.773719000  | -4.042941000 | 1.119068000  |
| 6 | 2.049249000  | -3.503221000 | 2.174848000  |
| 6 | 1.313815000  | -2.375028000 | 1.938278000  |
| 1 | 3.412684000  | -4.903672000 | 1.252240000  |
| 1 | 3.277932000  | -3.810911000 | -0.914473000 |
| 1 | 2.060579000  | -3.929821000 | 3.165914000  |
| 1 | 0.759711000  | -1.961549000 | 2.749538000  |
| 7 | -0.603340000 | 2.495703000  | -1.561162000 |
| 6 | -0.469229000 | 3.765601000  | -2.362512000 |
| 1 | -0.393997000 | 4.602914000  | -1.682995000 |
| 1 | 0.449819000  | 3.733689000  | -2.930679000 |
| 1 | -1.314899000 | 3.903995000  | -3.030909000 |
| 7 | 1.903071000  | -1.740922000 | -1.572922000 |
| 6 | 2.100194000  | -2.799458000 | -2.631260000 |
| 1 | 3.136906000  | -2.848222000 | -2.954414000 |
| 1 | 1.788721000  | -3.755406000 | -2.233364000 |
| 1 | 1.462050000  | -2.581458000 | -3.475882000 |

|   |              |              |              |
|---|--------------|--------------|--------------|
| 7 | -2.416820000 | -1.252510000 | 2.249372000  |
| 7 | 1.856759000  | 0.897996000  | 3.425948000  |
| 6 | -3.772441000 | -1.252288000 | 2.912106000  |
| 1 | -4.507846000 | -0.898993000 | 2.201860000  |
| 1 | -4.039971000 | -2.244449000 | 3.265339000  |
| 1 | -3.768696000 | -0.557684000 | 3.740022000  |
| 6 | 2.835074000  | 0.671047000  | 4.550497000  |
| 1 | 3.811123000  | 0.468602000  | 4.129956000  |
| 1 | 2.884380000  | 1.532285000  | 5.211657000  |
| 1 | 2.541895000  | -0.205284000 | 5.111028000  |
| 1 | -1.046693000 | -0.648688000 | 6.447246000  |
| 1 | 1.388717000  | 0.828658000  | -5.181000000 |

NEB #1:

|    |              |              |              |
|----|--------------|--------------|--------------|
| 24 | -0.000085000 | 0.000888000  | 0.000253000  |
| 7  | -0.091023000 | -2.052760000 | -0.086249000 |
| 6  | 0.884859000  | -2.745412000 | -0.715287000 |
| 1  | 1.569522000  | -2.167731000 | -1.316003000 |
| 7  | -2.053586000 | -1.988559000 | 1.210512000  |
| 6  | 1.027682000  | -4.103621000 | -0.588001000 |
| 1  | 1.834570000  | -4.611595000 | -1.094810000 |
| 7  | -2.034199000 | -0.000496000 | -0.095014000 |
| 6  | 0.113162000  | -4.788757000 | 0.210524000  |
| 1  | 0.191126000  | -5.859726000 | 0.339944000  |
| 7  | 0.191078000  | 0.000730000  | -2.048492000 |
| 6  | -0.917198000 | -4.099316000 | 0.815357000  |
| 1  | -1.659811000 | -4.628061000 | 1.389924000  |
| 7  | 2.084339000  | 1.382703000  | -1.840314000 |
| 6  | -1.013260000 | -2.713917000 | 0.635101000  |
| 7  | 2.034201000  | 0.000888000  | 0.095121000  |
| 6  | -2.748954000 | -2.603010000 | 2.350455000  |
| 1  | -3.457787000 | -3.374198000 | 2.046916000  |
| 1  | -2.003352000 | -3.036342000 | 3.012078000  |
| 1  | -3.276702000 | -1.822135000 | 2.890063000  |

|   |              |              |              |
|---|--------------|--------------|--------------|
| 6 | -2.741265000 | -0.981898000 | 0.517110000  |
| 6 | -4.129131000 | -0.996776000 | 0.477268000  |
| 1 | -4.680242000 | -1.792662000 | 0.950207000  |
| 6 | -4.787647000 | -0.004343000 | -0.226778000 |
| 1 | -5.867933000 | -0.005771000 | -0.278452000 |
| 6 | -0.720389000 | -0.644303000 | -2.810685000 |
| 1 | -1.402524000 | -1.297362000 | -2.289596000 |
| 6 | -0.804839000 | -0.470693000 | -4.168658000 |
| 1 | -1.562409000 | -0.992885000 | -4.733790000 |
| 6 | 0.103455000  | 0.393239000  | -4.778645000 |
| 1 | 0.070643000  | 0.559943000  | -5.846784000 |
| 6 | 1.070820000  | 1.016322000  | -4.017874000 |
| 1 | 1.810652000  | 1.642911000  | -4.488205000 |
| 6 | 1.108687000  | 0.788073000  | -2.636729000 |
| 6 | 2.752816000  | 2.576395000  | -2.377955000 |
| 1 | 1.997895000  | 3.219069000  | -2.823507000 |
| 1 | 3.216004000  | 3.109347000  | -1.552780000 |
| 1 | 3.511485000  | 2.335932000  | -3.123538000 |
| 6 | 2.756371000  | 0.683018000  | -0.827381000 |
| 6 | 4.143650000  | 0.708206000  | -0.775871000 |
| 1 | 4.707954000  | 1.236641000  | -1.526175000 |
| 6 | 4.788086000  | -0.002297000 | 0.221174000  |
| 1 | 5.868473000  | -0.003467000 | 0.270665000  |
| 7 | -0.101451000 | 2.054480000  | 0.078163000  |
| 6 | 0.811060000  | 2.747861000  | 0.795175000  |
| 1 | 1.437790000  | 2.170547000  | 1.456366000  |
| 7 | -1.934740000 | 1.988628000  | -1.395804000 |
| 6 | 0.963433000  | 4.106340000  | 0.682394000  |
| 1 | 1.719495000  | 4.614691000  | 1.262000000  |
| 6 | 0.125404000  | 4.791020000  | -0.196391000 |
| 1 | 0.213854000  | 5.862124000  | -0.317499000 |
| 6 | -0.844054000 | 4.100825000  | -0.894041000 |
| 1 | -1.531124000 | 4.629019000  | -1.534482000 |
| 6 | -0.954095000 | 2.715103000  | -0.724783000 |

|   |              |              |              |
|---|--------------|--------------|--------------|
| 6 | -2.520893000 | 2.602876000  | -2.595770000 |
| 1 | -3.258181000 | 3.371081000  | -2.359871000 |
| 1 | -1.717448000 | 3.040026000  | -3.182950000 |
| 1 | -2.991999000 | 1.821051000  | -3.184119000 |
| 6 | -2.682154000 | 0.979352000  | -0.771655000 |
| 6 | -4.067538000 | 0.990093000  | -0.864528000 |
| 1 | -4.572760000 | 1.785304000  | -1.386928000 |
| 7 | -0.000085000 | 0.000888000  | 2.057842000  |
| 7 | 1.904605000  | -1.380694000 | 2.027339000  |
| 6 | -0.978914000 | 0.645323000  | 2.731730000  |
| 1 | -1.609491000 | 1.298395000  | 2.149429000  |
| 6 | -1.189844000 | 0.471230000  | 4.075831000  |
| 1 | -1.997146000 | 0.993153000  | 4.567620000  |
| 6 | -0.342265000 | -0.392603000 | 4.767781000  |
| 1 | -0.475188000 | -0.560001000 | 5.828001000  |
| 6 | 0.692439000  | -1.014952000 | 4.100703000  |
| 1 | 1.385517000  | -1.641683000 | 4.637599000  |
| 6 | 0.858960000  | -0.786050000 | 2.729244000  |
| 6 | 2.519009000  | -2.575039000 | 2.624769000  |
| 1 | 1.725247000  | -3.216521000 | 2.998739000  |
| 1 | 3.055729000  | -3.108540000 | 1.845933000  |
| 1 | 3.205183000  | -2.335618000 | 3.437753000  |
| 6 | 2.667406000  | -0.682739000 | 1.079844000  |
| 6 | 4.053615000  | -0.711065000 | 1.155133000  |
| 1 | 4.545432000  | -1.240114000 | 1.954334000  |

NEB #2:

|    |              |              |              |
|----|--------------|--------------|--------------|
| 24 | 0.000155000  | 0.001794000  | -0.004132000 |
| 7  | 0.026286000  | -2.085673000 | -0.238049000 |
| 6  | 1.096243000  | -2.670703000 | -0.835707000 |
| 1  | 1.891774000  | -2.016887000 | -1.169825000 |
| 7  | -2.115204000 | -2.251242000 | 0.773056000  |
| 6  | 1.205271000  | -4.035369000 | -1.020321000 |
| 1  | 2.092850000  | -4.449524000 | -1.492427000 |

|   |              |              |              |
|---|--------------|--------------|--------------|
| 7 | -2.082294000 | -0.007366000 | -0.096421000 |
| 6 | 0.141562000  | -4.842206000 | -0.598478000 |
| 1 | 0.166986000  | -5.919165000 | -0.753320000 |
| 7 | 0.037142000  | 0.018060000  | -2.119496000 |
| 6 | -0.966911000 | -4.252093000 | -0.007878000 |
| 1 | -1.815182000 | -4.862513000 | 0.280610000  |
| 7 | 2.265054000  | 0.861554000  | -2.156993000 |
| 6 | -1.005112000 | -2.853799000 | 0.166531000  |
| 7 | 2.104100000  | -0.003401000 | 0.099589000  |
| 6 | -2.905193000 | -3.121321000 | 1.661438000  |
| 1 | -3.570224000 | -3.797351000 | 1.108566000  |
| 1 | -2.216327000 | -3.713417000 | 2.267541000  |
| 1 | -3.502672000 | -2.495115000 | 2.327106000  |
| 6 | -2.780670000 | -1.127886000 | 0.259489000  |
| 6 | -4.175669000 | -1.168541000 | 0.156569000  |
| 1 | -4.714703000 | -2.084302000 | 0.367475000  |
| 6 | -4.861150000 | -0.026016000 | -0.235092000 |
| 1 | -5.947584000 | -0.034460000 | -0.294175000 |
| 6 | -1.056146000 | -0.424363000 | -2.794423000 |
| 1 | -1.926735000 | -0.677273000 | -2.206656000 |
| 6 | -1.099006000 | -0.561279000 | -4.167556000 |
| 1 | -2.018248000 | -0.887617000 | -4.646817000 |
| 6 | 0.072741000  | -0.309590000 | -4.889760000 |
| 1 | 0.110044000  | -0.465851000 | -5.965922000 |
| 6 | 1.202866000  | 0.118426000  | -4.210455000 |
| 1 | 2.129057000  | 0.278071000  | -4.750848000 |
| 6 | 1.153446000  | 0.316242000  | -2.813730000 |
| 6 | 3.133168000  | 1.693967000  | -3.013319000 |
| 1 | 2.498838000  | 2.291135000  | -3.670195000 |
| 1 | 3.712873000  | 2.370068000  | -2.382608000 |
| 1 | 3.818815000  | 1.095461000  | -3.626990000 |
| 6 | 2.856476000  | 0.369297000  | -0.983726000 |
| 6 | 4.255858000  | 0.297236000  | -0.952935000 |
| 1 | 4.835771000  | 0.493206000  | -1.846110000 |

|   |              |              |              |
|---|--------------|--------------|--------------|
| 6 | 4.896633000  | -0.032444000 | 0.231603000  |
| 1 | 5.983591000  | -0.045470000 | 0.283601000  |
| 7 | 0.005808000  | 2.089502000  | 0.218200000  |
| 6 | 1.028331000  | 2.682458000  | 0.886760000  |
| 1 | 1.807947000  | 2.034338000  | 1.265706000  |
| 7 | -2.059132000 | 2.242746000  | -0.949483000 |
| 6 | 1.107965000  | 4.046893000  | 1.088940000  |
| 1 | 1.959218000  | 4.467503000  | 1.618541000  |
| 6 | 0.061347000  | 4.843378000  | 0.609122000  |
| 1 | 0.060753000  | 5.918930000  | 0.775519000  |
| 6 | -0.997656000 | 4.244747000  | -0.058775000 |
| 1 | -1.831160000 | 4.848227000  | -0.400013000 |
| 6 | -1.005246000 | 2.848271000  | -0.250652000 |
| 6 | -2.778034000 | 3.119364000  | -1.890270000 |
| 1 | -3.491275000 | 3.783465000  | -1.385070000 |
| 1 | -2.045792000 | 3.723586000  | -2.429847000 |
| 1 | -3.313910000 | 2.498606000  | -2.611080000 |
| 6 | -2.756211000 | 1.107007000  | -0.512844000 |
| 6 | -4.155424000 | 1.127424000  | -0.550633000 |
| 1 | -4.684026000 | 2.035779000  | -0.812966000 |
| 7 | -0.174112000 | 0.003333000  | 2.106641000  |
| 7 | 2.032938000  | -0.856935000 | 2.364465000  |
| 6 | -1.324372000 | 0.455268000  | 2.671777000  |
| 1 | -2.136057000 | 0.702659000  | 2.003286000  |
| 6 | -1.496817000 | 0.604713000  | 4.033323000  |
| 1 | -2.456018000 | 0.937535000  | 4.421440000  |
| 6 | -0.400529000 | 0.355726000  | 4.865961000  |
| 1 | -0.466349000 | 0.520095000  | 5.939582000  |
| 6 | 0.787602000  | -0.080902000 | 4.299436000  |
| 1 | 1.659058000  | -0.238427000 | 4.924873000  |
| 6 | 0.869378000  | -0.293084000 | 2.906588000  |
| 6 | 2.799042000  | -1.697009000 | 3.305267000  |
| 1 | 2.093856000  | -2.274369000 | 3.904958000  |
| 1 | 3.421291000  | -2.390232000 | 2.736777000  |

|   |             |              |             |
|---|-------------|--------------|-------------|
| 1 | 3.436316000 | -1.104871000 | 3.974410000 |
| 6 | 2.742298000 | -0.386540000 | 1.250140000 |
| 6 | 4.140183000 | -0.345605000 | 1.349629000 |
| 1 | 4.630218000 | -0.555862000 | 2.291486000 |

NEB #3:

|    |              |              |              |
|----|--------------|--------------|--------------|
| 24 | 0.032777000  | -0.005506000 | -0.005640000 |
| 7  | 0.135490000  | -2.085428000 | -0.357432000 |
| 6  | 1.305511000  | -2.666196000 | -0.732429000 |
| 1  | 2.187828000  | -2.049313000 | -0.732143000 |
| 7  | -2.149429000 | -2.385790000 | 0.249844000  |
| 6  | 1.435747000  | -3.997865000 | -1.076402000 |
| 1  | 2.414561000  | -4.388019000 | -1.341970000 |
| 7  | -2.068771000 | -0.004481000 | -0.102766000 |
| 6  | 0.285378000  | -4.790660000 | -1.093103000 |
| 1  | 0.322268000  | -5.830309000 | -1.410400000 |
| 7  | -0.001115000 | 0.193761000  | -2.091156000 |
| 6  | -0.915148000 | -4.220218000 | -0.702784000 |
| 1  | -1.827863000 | -4.804478000 | -0.721321000 |
| 7  | 2.378510000  | 0.142651000  | -2.330466000 |
| 6  | -0.959106000 | -2.872647000 | -0.293795000 |
| 7  | 2.138992000  | -0.005112000 | 0.101184000  |
| 6  | -2.986583000 | -3.391910000 | 0.935268000  |
| 1  | -3.613383000 | -3.968290000 | 0.244338000  |
| 1  | -2.329315000 | -4.074550000 | 1.477809000  |
| 1  | -3.627511000 | -2.879080000 | 1.655820000  |
| 6  | -2.773118000 | -1.177861000 | -0.062892000 |
| 6  | -4.164682000 | -1.206363000 | -0.216270000 |
| 1  | -4.682137000 | -2.155200000 | -0.284233000 |
| 6  | -4.873967000 | -0.016106000 | -0.248726000 |
| 1  | -5.960421000 | -0.020644000 | -0.306431000 |
| 6  | -1.184925000 | 0.249987000  | -2.757175000 |
| 1  | -2.041021000 | 0.591122000  | -2.206878000 |
| 6  | -1.353440000 | -0.100707000 | -4.081016000 |

|   |              |              |              |
|---|--------------|--------------|--------------|
| 1 | -2.331209000 | 0.007273000  | -4.542977000 |
| 6 | -0.255023000 | -0.638518000 | -4.757306000 |
| 1 | -0.350063000 | -1.029195000 | -5.767712000 |
| 6 | 0.971904000  | -0.649031000 | -4.115307000 |
| 1 | 1.844185000  | -1.047514000 | -4.620132000 |
| 6 | 1.096441000  | -0.128664000 | -2.808067000 |
| 6 | 3.344519000  | 0.478749000  | -3.408043000 |
| 1 | 2.789806000  | 0.865440000  | -4.260960000 |
| 1 | 4.016515000  | 1.262513000  | -3.056440000 |
| 1 | 3.928082000  | -0.394832000 | -3.723960000 |
| 6 | 2.908883000  | 0.038710000  | -1.045866000 |
| 6 | 4.309688000  | -0.050651000 | -0.990339000 |
| 1 | 4.896700000  | -0.118846000 | -1.891986000 |
| 6 | 4.954721000  | -0.048693000 | 0.228534000  |
| 1 | 6.041245000  | -0.065245000 | 0.279117000  |
| 7 | 0.096252000  | 2.074982000  | 0.347389000  |
| 6 | 1.228695000  | 2.657434000  | 0.822071000  |
| 1 | 2.115973000  | 2.048617000  | 0.863072000  |
| 7 | -2.133003000 | 2.378402000  | -0.443990000 |
| 6 | 1.314835000  | 3.979285000  | 1.215354000  |
| 1 | 2.266239000  | 4.372773000  | 1.562525000  |
| 6 | 0.155076000  | 4.757409000  | 1.173716000  |
| 1 | 0.153984000  | 5.786140000  | 1.526397000  |
| 6 | -1.003175000 | 4.188235000  | 0.670512000  |
| 1 | -1.920177000 | 4.764300000  | 0.630353000  |
| 6 | -0.997830000 | 2.854845000  | 0.216535000  |
| 6 | -2.903506000 | 3.399946000  | -1.183470000 |
| 1 | -3.594910000 | 3.959726000  | -0.542053000 |
| 1 | -2.198322000 | 4.095465000  | -1.643436000 |
| 1 | -3.471507000 | 2.906550000  | -1.975528000 |
| 6 | -2.775128000 | 1.163465000  | -0.213015000 |
| 6 | -4.175735000 | 1.179755000  | -0.206877000 |
| 1 | -4.704854000 | 2.124347000  | -0.192382000 |
| 7 | -0.197758000 | -0.201455000 | 2.070794000  |

|   |              |              |             |
|---|--------------|--------------|-------------|
| 7 | 2.146913000  | -0.122357000 | 2.543710000 |
| 6 | -1.439643000 | -0.256843000 | 2.622362000 |
| 1 | -2.235494000 | -0.622442000 | 2.001303000 |
| 6 | -1.738323000 | 0.126107000  | 3.914002000 |
| 1 | -2.754012000 | 0.015546000  | 4.283791000 |
| 6 | -0.717160000 | 0.701255000  | 4.675566000 |
| 1 | -0.913989000 | 1.120456000  | 5.659573000 |
| 6 | 0.565704000  | 0.710232000  | 4.154318000 |
| 1 | 1.381096000  | 1.134107000  | 4.728547000 |
| 6 | 0.822150000  | 0.151098000  | 2.882779000 |
| 6 | 3.002328000  | -0.420596000 | 3.721330000 |
| 1 | 2.365143000  | -0.755640000 | 4.537337000 |
| 1 | 3.685678000  | -1.233411000 | 3.474091000 |
| 1 | 3.572076000  | 0.459286000  | 4.044413000 |
| 6 | 2.798724000  | -0.064632000 | 1.314039000 |
| 6 | 4.202375000  | -0.024263000 | 1.383969000 |
| 1 | 4.709761000  | 0.029592000  | 2.333512000 |

NEB #4:

|    |              |              |              |
|----|--------------|--------------|--------------|
| 24 | 0.039588000  | 0.004986000  | -0.005317000 |
| 7  | 0.145396000  | -2.086943000 | -0.310670000 |
| 6  | 1.347273000  | -2.692151000 | -0.503749000 |
| 1  | 2.226333000  | -2.121150000 | -0.263895000 |
| 7  | -2.196971000 | -2.405408000 | 0.025278000  |
| 6  | 1.501279000  | -3.996728000 | -0.932113000 |
| 1  | 2.501098000  | -4.403409000 | -1.059677000 |
| 7  | -2.099240000 | 0.004037000  | -0.110648000 |
| 6  | 0.351506000  | -4.743258000 | -1.199531000 |
| 1  | 0.414381000  | -5.756163000 | -1.589667000 |
| 7  | 0.115096000  | 0.309567000  | -2.072088000 |
| 6  | -0.882105000 | -4.170100000 | -0.934208000 |
| 1  | -1.795617000 | -4.729793000 | -1.103956000 |
| 7  | 2.329711000  | -0.515862000 | -2.272898000 |
| 6  | -0.959336000 | -2.853190000 | -0.442011000 |

|   |              |              |              |
|---|--------------|--------------|--------------|
| 7 | 2.102298000  | 0.005306000  | 0.092148000  |
| 6 | -3.044638000 | -3.458567000 | 0.627803000  |
| 1 | -3.651489000 | -3.996080000 | -0.109119000 |
| 1 | -2.395853000 | -4.169113000 | 1.143804000  |
| 1 | -3.705220000 | -2.996259000 | 1.364806000  |
| 6 | -2.805439000 | -1.169105000 | -0.188252000 |
| 6 | -4.195918000 | -1.192068000 | -0.356079000 |
| 1 | -4.704029000 | -2.135058000 | -0.513238000 |
| 6 | -4.914944000 | -0.010935000 | -0.288513000 |
| 1 | -6.000350000 | -0.016581000 | -0.360625000 |
| 6 | -1.015069000 | 0.751533000  | -2.684921000 |
| 1 | -1.746063000 | 1.224529000  | -2.056212000 |
| 6 | -1.264411000 | 0.622189000  | -4.034173000 |
| 1 | -2.209620000 | 0.965280000  | -4.444986000 |
| 6 | -0.269125000 | 0.039952000  | -4.825947000 |
| 1 | -0.414481000 | -0.110008000 | -5.893563000 |
| 6 | 0.933241000  | -0.315792000 | -4.240358000 |
| 1 | 1.729615000  | -0.698610000 | -4.863435000 |
| 6 | 1.115030000  | -0.165505000 | -2.844991000 |
| 6 | 3.273933000  | -1.225352000 | -3.160893000 |
| 1 | 2.722706000  | -1.955737000 | -3.750368000 |
| 1 | 3.797280000  | -0.532925000 | -3.830739000 |
| 1 | 4.001137000  | -1.761943000 | -2.555775000 |
| 6 | 2.861304000  | -0.099093000 | -1.047823000 |
| 6 | 4.253879000  | 0.050756000  | -1.000927000 |
| 1 | 4.821662000  | 0.132818000  | -1.918801000 |
| 6 | 4.900308000  | -0.003222000 | 0.223453000  |
| 1 | 5.987079000  | -0.007941000 | 0.274910000  |
| 7 | 0.098298000  | 2.093747000  | 0.317434000  |
| 6 | 1.273741000  | 2.700965000  | 0.627988000  |
| 1 | 2.174606000  | 2.142687000  | 0.441428000  |
| 7 | -2.205340000 | 2.413459000  | -0.228325000 |
| 6 | 1.376828000  | 3.993149000  | 1.107848000  |
| 1 | 2.357726000  | 4.406542000  | 1.326644000  |

|   |              |              |              |
|---|--------------|--------------|--------------|
| 6 | 0.199687000  | 4.718210000  | 1.308298000  |
| 1 | 0.217645000  | 5.717978000  | 1.735256000  |
| 6 | -1.001194000 | 4.144141000  | 0.921558000  |
| 1 | -1.931858000 | 4.690565000  | 1.029851000  |
| 6 | -1.021409000 | 2.847475000  | 0.375108000  |
| 6 | -2.986383000 | 3.485939000  | -0.886636000 |
| 1 | -3.676867000 | 3.994837000  | -0.204288000 |
| 1 | -2.286554000 | 4.216000000  | -1.298486000 |
| 1 | -3.554309000 | 3.050766000  | -1.712383000 |
| 6 | -2.822327000 | 1.169870000  | -0.114823000 |
| 6 | -4.223983000 | 1.177205000  | -0.126563000 |
| 1 | -4.758537000 | 2.113961000  | -0.033297000 |
| 7 | -0.090508000 | -0.292323000 | 2.060919000  |
| 7 | 2.106619000  | 0.515033000  | 2.469742000  |
| 6 | -1.277153000 | -0.719152000 | 2.569571000  |
| 1 | -1.964958000 | -1.166139000 | 1.876415000  |
| 6 | -1.639041000 | -0.604658000 | 3.894574000  |
| 1 | -2.621722000 | -0.936543000 | 4.216458000  |
| 6 | -0.707286000 | -0.051946000 | 4.778925000  |
| 1 | -0.941468000 | 0.082797000  | 5.832666000  |
| 6 | 0.544254000  | 0.294769000  | 4.302018000  |
| 1 | 1.289840000  | 0.657728000  | 4.995745000  |
| 6 | 0.843631000  | 0.162335000  | 2.925115000  |
| 6 | 2.967720000  | 1.221158000  | 3.442243000  |
| 1 | 2.366219000  | 1.946089000  | 3.988388000  |
| 1 | 3.436808000  | 0.526104000  | 4.148555000  |
| 1 | 3.741150000  | 1.763938000  | 2.903368000  |
| 6 | 2.751306000  | 0.103991000  | 1.297790000  |
| 6 | 4.141579000  | -0.054082000 | 1.381409000  |
| 1 | 4.622021000  | -0.143498000 | 2.347450000  |

NEB #5:

|    |              |              |              |
|----|--------------|--------------|--------------|
| 24 | -0.000119000 | -0.017389000 | -0.007602000 |
| 7  | 0.061697000  | -2.109661000 | -0.237910000 |

|   |              |              |              |
|---|--------------|--------------|--------------|
| 6 | 1.196488000  | -2.725336000 | -0.657547000 |
| 1 | 2.061873000  | -2.107171000 | -0.808256000 |
| 7 | -2.164787000 | -2.315602000 | 0.554159000  |
| 6 | 1.304480000  | -4.086939000 | -0.866785000 |
| 1 | 2.253815000  | -4.505288000 | -1.190570000 |
| 7 | -2.097207000 | -0.006112000 | -0.105421000 |
| 6 | 0.172356000  | -4.881134000 | -0.663060000 |
| 1 | 0.192790000  | -5.951294000 | -0.856575000 |
| 7 | 0.018339000  | 0.207549000  | -2.104004000 |
| 6 | -0.990207000 | -4.274337000 | -0.216269000 |
| 1 | -1.890982000 | -4.857796000 | -0.061123000 |
| 7 | 2.342853000  | -0.293136000 | -2.286015000 |
| 6 | -1.014141000 | -2.885395000 | 0.011778000  |
| 7 | 2.131704000  | -0.027686000 | 0.095437000  |
| 6 | -2.971947000 | -3.189263000 | 1.425447000  |
| 1 | -3.613977000 | -3.880497000 | 0.866328000  |
| 1 | -2.293081000 | -3.762267000 | 2.062235000  |
| 1 | -3.599225000 | -2.562712000 | 2.063753000  |
| 6 | -2.797348000 | -1.171373000 | 0.064567000  |
| 6 | -4.179089000 | -1.239431000 | -0.124033000 |
| 1 | -4.683182000 | -2.197014000 | -0.070472000 |
| 6 | -4.895865000 | -0.071653000 | -0.342814000 |
| 1 | -5.978933000 | -0.096915000 | -0.442886000 |
| 6 | -1.125751000 | 0.479556000  | -2.782368000 |
| 1 | -2.053357000 | 0.252225000  | -2.285720000 |
| 6 | -1.162508000 | 0.963476000  | -4.077301000 |
| 1 | -2.122177000 | 1.151485000  | -4.552320000 |
| 6 | 0.051046000  | 1.210477000  | -4.724639000 |
| 1 | 0.081984000  | 1.652028000  | -5.718190000 |
| 6 | 1.224440000  | 0.844544000  | -4.082285000 |
| 1 | 2.185332000  | 0.977240000  | -4.567998000 |
| 6 | 1.177282000  | 0.290087000  | -2.791634000 |
| 6 | 3.175086000  | -0.983707000 | -3.294731000 |
| 1 | 3.867204000  | -0.310805000 | -3.814617000 |

|   |              |              |              |
|---|--------------|--------------|--------------|
| 1 | 2.510873000  | -1.438260000 | -4.033104000 |
| 1 | 3.737331000  | -1.779792000 | -2.799192000 |
| 6 | 2.907515000  | -0.083986000 | -1.034579000 |
| 6 | 4.306395000  | -0.032536000 | -0.984681000 |
| 1 | 4.875551000  | 0.002741000  | -1.904558000 |
| 6 | 4.950673000  | -0.040311000 | 0.239927000  |
| 1 | 6.036623000  | -0.043916000 | 0.297207000  |
| 7 | 0.029803000  | 2.072859000  | 0.208708000  |
| 6 | 1.152572000  | 2.680331000  | 0.671304000  |
| 1 | 2.018966000  | 2.060017000  | 0.808462000  |
| 7 | -2.164636000 | 2.323856000  | -0.690217000 |
| 6 | 1.252581000  | 4.033964000  | 0.929190000  |
| 1 | 2.195123000  | 4.445154000  | 1.280890000  |
| 6 | 0.119210000  | 4.828342000  | 0.736696000  |
| 1 | 0.129278000  | 5.891641000  | 0.966404000  |
| 6 | -1.028622000 | 4.232014000  | 0.240275000  |
| 1 | -1.925243000 | 4.820269000  | 0.082392000  |
| 6 | -1.040751000 | 2.853636000  | -0.052147000 |
| 6 | -2.902491000 | 3.259135000  | -1.561517000 |
| 1 | -3.611651000 | 3.884795000  | -1.007638000 |
| 1 | -2.179645000 | 3.898196000  | -2.071336000 |
| 1 | -3.447687000 | 2.687931000  | -2.315581000 |
| 6 | -2.807754000 | 1.133407000  | -0.369423000 |
| 6 | -4.208750000 | 1.128121000  | -0.425243000 |
| 1 | -4.746234000 | 2.060018000  | -0.545010000 |
| 7 | -0.193585000 | -0.216069000 | 2.085343000  |
| 7 | 2.102985000  | 0.280811000  | 2.480786000  |
| 6 | -1.403117000 | -0.450626000 | 2.655998000  |
| 1 | -2.271765000 | -0.244183000 | 2.056169000  |
| 6 | -1.575716000 | -0.874178000 | 3.961330000  |
| 1 | -2.579803000 | -1.036310000 | 4.345965000  |
| 6 | -0.437254000 | -1.095691000 | 4.739900000  |
| 1 | -0.512119000 | -1.491689000 | 5.750195000  |
| 6 | 0.799364000  | -0.767346000 | 4.203933000  |

|   |             |              |             |
|---|-------------|--------------|-------------|
| 1 | 1.705778000 | -0.882347000 | 4.789351000 |
| 6 | 0.888666000 | -0.273855000 | 2.890540000 |
| 6 | 2.829071000 | 1.027739000  | 3.529799000 |
| 1 | 3.462944000 | 0.387482000  | 4.154167000 |
| 1 | 2.093763000 | 1.518678000  | 4.171418000 |
| 1 | 3.440566000 | 1.797583000  | 3.051070000 |
| 6 | 2.787941000 | 0.031838000  | 1.298294000 |
| 6 | 4.183524000 | -0.038055000 | 1.391985000 |
| 1 | 4.654842000 | -0.070162000 | 2.365970000 |

NEB #6:

|    |              |              |              |
|----|--------------|--------------|--------------|
| 24 | -0.034485000 | -0.014860000 | 0.027437000  |
| 7  | -0.030470000 | -2.076273000 | -0.306279000 |
| 6  | 1.054003000  | -2.660895000 | -0.874154000 |
| 1  | 1.711690000  | -2.011383000 | -1.432825000 |
| 7  | -2.162279000 | -2.285072000 | 0.624939000  |
| 6  | 1.328926000  | -4.008253000 | -0.762258000 |
| 1  | 2.215386000  | -4.420241000 | -1.235629000 |
| 7  | -2.107239000 | 0.016850000  | -0.090977000 |
| 6  | 0.447255000  | -4.799144000 | -0.010814000 |
| 1  | 0.647304000  | -5.857384000 | 0.142220000  |
| 7  | -0.003321000 | 0.242100000  | -2.085777000 |
| 6  | -0.710058000 | -4.233839000 | 0.501273000  |
| 1  | -1.434400000 | -4.850319000 | 1.020847000  |
| 7  | 2.362806000  | -0.001233000 | -2.289062000 |
| 6  | -0.958476000 | -2.862879000 | 0.280645000  |
| 7  | 2.111461000  | -0.053096000 | 0.117375000  |
| 6  | -3.087829000 | -3.065443000 | 1.461422000  |
| 1  | -3.543600000 | -3.903162000 | 0.919277000  |
| 1  | -2.542919000 | -3.449462000 | 2.327817000  |
| 1  | -3.873874000 | -2.400356000 | 1.820938000  |
| 6  | -2.736082000 | -1.204093000 | -0.079774000 |
| 6  | -3.998021000 | -1.391374000 | -0.624243000 |
| 1  | -4.429121000 | -2.385799000 | -0.667511000 |

|   |              |              |              |
|---|--------------|--------------|--------------|
| 6 | -4.691003000 | -0.280318000 | -1.101705000 |
| 1 | -5.664339000 | -0.394855000 | -1.570942000 |
| 6 | -1.162061000 | 0.369789000  | -2.782808000 |
| 1 | -2.055667000 | -0.011674000 | -2.320430000 |
| 6 | -1.247967000 | 0.904030000  | -4.053888000 |
| 1 | -2.214407000 | 0.962676000  | -4.546164000 |
| 6 | -0.075811000 | 1.373483000  | -4.651101000 |
| 1 | -0.093451000 | 1.867005000  | -5.619483000 |
| 6 | 1.126918000  | 1.150707000  | -3.998422000 |
| 1 | 2.063610000  | 1.448509000  | -4.455794000 |
| 6 | 1.143772000  | 0.508212000  | -2.746194000 |
| 6 | 3.241093000  | -0.504410000 | -3.373285000 |
| 1 | 3.832803000  | -1.337398000 | -2.987878000 |
| 1 | 2.610056000  | -0.877587000 | -4.182059000 |
| 1 | 3.913172000  | 0.266331000  | -3.766403000 |
| 6 | 2.897331000  | 0.010093000  | -1.005323000 |
| 6 | 4.299331000  | 0.016555000  | -0.932395000 |
| 1 | 4.886369000  | 0.172173000  | -1.826880000 |
| 6 | 4.925893000  | -0.193807000 | 0.281401000  |
| 1 | 6.009901000  | -0.250909000 | 0.343670000  |
| 7 | -0.034797000 | 2.047473000  | 0.264276000  |
| 6 | 1.128116000  | 2.628182000  | 0.660139000  |
| 1 | 1.822803000  | 1.993392000  | 1.185739000  |
| 7 | -2.319085000 | 2.409630000  | -0.362130000 |
| 6 | 1.447715000  | 3.949798000  | 0.426395000  |
| 1 | 2.394766000  | 4.346910000  | 0.778176000  |
| 6 | 0.543715000  | 4.714255000  | -0.318556000 |
| 1 | 0.786269000  | 5.728400000  | -0.627840000 |
| 6 | -0.685980000 | 4.163712000  | -0.641750000 |
| 1 | -1.409974000 | 4.752333000  | -1.191714000 |
| 6 | -0.997755000 | 2.840512000  | -0.256595000 |
| 6 | -3.332435000 | 3.491308000  | -0.316374000 |
| 1 | -2.915909000 | 4.331470000  | 0.237755000  |
| 1 | -3.631371000 | 3.824176000  | -1.316128000 |

|   |              |              |              |
|---|--------------|--------------|--------------|
| 1 | -4.202993000 | 3.134673000  | 0.234664000  |
| 6 | -2.823010000 | 1.118062000  | -0.457815000 |
| 6 | -4.131179000 | 0.974951000  | -0.969225000 |
| 1 | -4.670780000 | 1.839739000  | -1.326336000 |
| 7 | -0.234891000 | -0.258962000 | 2.103213000  |
| 7 | 2.091018000  | 0.032568000  | 2.536534000  |
| 6 | -1.470789000 | -0.398613000 | 2.650700000  |
| 1 | -2.306233000 | -0.121483000 | 2.030580000  |
| 6 | -1.697748000 | -0.827949000 | 3.944301000  |
| 1 | -2.717274000 | -0.912037000 | 4.309716000  |
| 6 | -0.594130000 | -1.165408000 | 4.730702000  |
| 1 | -0.717591000 | -1.575777000 | 5.730037000  |
| 6 | 0.673816000  | -0.940520000 | 4.217477000  |
| 1 | 1.553905000  | -1.157392000 | 4.811586000  |
| 6 | 0.828760000  | -0.425881000 | 2.916734000  |
| 6 | 2.891032000  | 0.602657000  | 3.644766000  |
| 1 | 3.571104000  | 1.352268000  | 3.233998000  |
| 1 | 2.210312000  | 1.097686000  | 4.340491000  |
| 1 | 3.472357000  | -0.152640000 | 4.185496000  |
| 6 | 2.757328000  | -0.150880000 | 1.325415000  |
| 6 | 4.144763000  | -0.313897000 | 1.417105000  |
| 1 | 4.603945000  | -0.495710000 | 2.379661000  |

NEB #7:

|    |              |              |              |
|----|--------------|--------------|--------------|
| 24 | -0.019576000 | -0.044455000 | -0.060631000 |
| 7  | 0.000444000  | -2.123900000 | -0.320824000 |
| 6  | 1.202565000  | -2.744778000 | -0.465349000 |
| 1  | 1.959945000  | -2.198978000 | -0.998767000 |
| 7  | -2.340120000 | -2.471877000 | -0.075810000 |
| 6  | 1.482059000  | -4.010071000 | 0.005511000  |
| 1  | 2.457566000  | -4.451544000 | -0.177497000 |
| 7  | -2.113883000 | -0.056896000 | -0.131269000 |
| 6  | 0.494985000  | -4.648006000 | 0.766220000  |
| 1  | 0.692183000  | -5.592409000 | 1.268470000  |

|   |              |              |              |
|---|--------------|--------------|--------------|
| 7 | 0.037554000  | 0.327001000  | -2.130050000 |
| 6 | -0.762719000 | -4.072764000 | 0.842368000  |
| 1 | -1.545862000 | -4.566472000 | 1.404895000  |
| 7 | 2.305014000  | -0.398269000 | -2.315206000 |
| 6 | -1.026150000 | -2.859041000 | 0.165343000  |
| 7 | 2.082449000  | -0.089418000 | 0.065443000  |
| 6 | -3.328663000 | -3.575026000 | -0.077585000 |
| 1 | -2.811594000 | -4.525147000 | -0.015076000 |
| 1 | -4.024969000 | -3.476801000 | 0.760754000  |
| 1 | -3.878128000 | -3.594203000 | -1.016829000 |
| 6 | -2.836226000 | -1.203085000 | -0.375541000 |
| 6 | -4.172547000 | -1.126485000 | -0.810586000 |
| 1 | -4.738891000 | -2.015784000 | -1.030907000 |
| 6 | -4.789132000 | 0.100360000  | -0.954287000 |
| 1 | -5.805938000 | 0.158447000  | -1.334288000 |
| 6 | -1.072423000 | 0.793170000  | -2.757701000 |
| 1 | -1.986787000 | 0.826449000  | -2.189177000 |
| 6 | -1.100990000 | 1.203689000  | -4.076272000 |
| 1 | -2.037057000 | 1.542068000  | -4.511454000 |
| 6 | 0.096909000  | 1.192412000  | -4.794825000 |
| 1 | 0.143879000  | 1.560945000  | -5.816676000 |
| 6 | 1.236189000  | 0.706208000  | -4.174591000 |
| 1 | 2.181275000  | 0.702328000  | -4.703780000 |
| 6 | 1.175579000  | 0.233236000  | -2.849074000 |
| 6 | 3.176485000  | -1.058265000 | -3.308568000 |
| 1 | 3.759885000  | -1.832321000 | -2.805368000 |
| 1 | 2.542223000  | -1.533520000 | -4.059253000 |
| 1 | 3.861167000  | -0.359906000 | -3.805344000 |
| 6 | 2.866367000  | -0.161216000 | -1.057569000 |
| 6 | 4.260237000  | -0.071480000 | -0.989971000 |
| 1 | 4.846671000  | -0.041472000 | -1.899286000 |
| 6 | 4.883775000  | -0.026239000 | 0.248236000  |
| 1 | 5.969107000  | -0.006712000 | 0.321068000  |
| 7 | 0.147406000  | 2.054845000  | 0.097376000  |

|   |              |              |              |
|---|--------------|--------------|--------------|
| 6 | 1.357708000  | 2.662122000  | -0.027287000 |
| 1 | 2.233261000  | 2.038367000  | 0.020356000  |
| 7 | -2.209716000 | 2.315444000  | 0.367429000  |
| 6 | 1.528816000  | 4.018349000  | -0.219233000 |
| 1 | 2.534046000  | 4.425088000  | -0.285812000 |
| 6 | 0.388819000  | 4.811795000  | -0.371030000 |
| 1 | 0.465525000  | 5.869578000  | -0.612818000 |
| 6 | -0.852890000 | 4.215449000  | -0.229931000 |
| 1 | -1.755015000 | 4.799894000  | -0.369071000 |
| 6 | -0.951885000 | 2.838625000  | 0.062737000  |
| 6 | -3.166973000 | 3.293772000  | 0.926995000  |
| 1 | -2.622662000 | 3.957827000  | 1.601521000  |
| 1 | -3.661383000 | 3.898050000  | 0.156114000  |
| 1 | -3.924658000 | 2.755977000  | 1.499767000  |
| 6 | -2.787671000 | 1.140295000  | -0.131088000 |
| 6 | -4.106245000 | 1.246193000  | -0.582469000 |
| 1 | -4.584062000 | 2.213404000  | -0.662606000 |
| 7 | -0.239768000 | -0.366738000 | 2.018168000  |
| 7 | 1.990907000  | 0.356615000  | 2.430787000  |
| 6 | -1.424589000 | -0.775440000 | 2.546036000  |
| 1 | -2.273362000 | -0.800400000 | 1.883998000  |
| 6 | -1.603635000 | -1.122157000 | 3.871995000  |
| 1 | -2.589004000 | -1.419995000 | 4.219944000  |
| 6 | -0.491202000 | -1.101470000 | 4.717053000  |
| 1 | -0.565003000 | -1.423068000 | 5.753551000  |
| 6 | 0.717932000  | -0.661537000 | 4.203333000  |
| 1 | 1.601331000  | -0.637589000 | 4.830772000  |
| 6 | 0.809228000  | -0.251937000 | 2.858940000  |
| 6 | 2.706142000  | 1.131206000  | 3.465806000  |
| 1 | 3.322695000  | 1.887195000  | 2.974562000  |
| 1 | 1.964882000  | 1.637743000  | 4.088261000  |
| 1 | 3.343610000  | 0.505511000  | 4.101629000  |
| 6 | 2.706596000  | 0.054318000  | 1.275088000  |
| 6 | 4.102884000  | 0.005847000  | 1.390565000  |

|   |             |             |             |
|---|-------------|-------------|-------------|
| 1 | 4.565081000 | 0.017045000 | 2.369666000 |
|---|-------------|-------------|-------------|

NEB #8:

|    |              |              |              |
|----|--------------|--------------|--------------|
| 24 | 0.003573000  | -0.016832000 | -0.027468000 |
| 7  | 0.063272000  | -2.125565000 | -0.069508000 |
| 6  | 1.183687000  | -2.751683000 | 0.374933000  |
| 1  | 2.039587000  | -2.130759000 | 0.585298000  |
| 7  | -2.164118000 | -2.295173000 | -0.925016000 |
| 6  | 1.276337000  | -4.114269000 | 0.572484000  |
| 1  | 2.218265000  | -4.550655000 | 0.893796000  |
| 7  | -2.102266000 | -0.021340000 | -0.100981000 |
| 6  | 0.121289000  | -4.878614000 | 0.390983000  |
| 1  | 0.119829000  | -5.944841000 | 0.604510000  |
| 7  | 0.094779000  | 0.230039000  | -2.109024000 |
| 6  | -1.034433000 | -4.250372000 | -0.044957000 |
| 1  | -1.944671000 | -4.825021000 | -0.157444000 |
| 7  | 2.222523000  | -0.827568000 | -2.171038000 |
| 6  | -1.032499000 | -2.867679000 | -0.325509000 |
| 7  | 2.087403000  | 0.014460000  | 0.079029000  |
| 6  | -2.961383000 | -3.242478000 | -1.732926000 |
| 1  | -2.281817000 | -3.947127000 | -2.213276000 |
| 1  | -3.685136000 | -3.796586000 | -1.121787000 |
| 1  | -3.491900000 | -2.692126000 | -2.510526000 |
| 6  | -2.800232000 | -1.103721000 | -0.565878000 |
| 6  | -4.197591000 | -1.052017000 | -0.702872000 |
| 1  | -4.756391000 | -1.927585000 | -1.001543000 |
| 6  | -4.868472000 | 0.128067000  | -0.440422000 |
| 1  | -5.943083000 | 0.188785000  | -0.590710000 |
| 6  | -0.925683000 | 0.863306000  | -2.742068000 |
| 1  | -1.746806000 | 1.206438000  | -2.126372000 |
| 6  | -0.951073000 | 1.076260000  | -4.106338000 |
| 1  | -1.802454000 | 1.575460000  | -4.561173000 |

|   |              |              |              |
|---|--------------|--------------|--------------|
| 6 | 0.149434000  | 0.646742000  | -4.856568000 |
| 1 | 0.192695000  | 0.823907000  | -5.928740000 |
| 6 | 1.207188000  | 0.018950000  | -4.215778000 |
| 1 | 2.081482000  | -0.277868000 | -4.782406000 |
| 6 | 1.161589000  | -0.183256000 | -2.822218000 |
| 6 | 3.033356000  | -1.724772000 | -3.014136000 |
| 1 | 3.577530000  | -2.417889000 | -2.369588000 |
| 1 | 2.360449000  | -2.300596000 | -3.653023000 |
| 1 | 3.748753000  | -1.178750000 | -3.642037000 |
| 6 | 2.838521000  | -0.353206000 | -1.002862000 |
| 6 | 4.235828000  | -0.307976000 | -0.955666000 |
| 1 | 4.821960000  | -0.531409000 | -1.838373000 |
| 6 | 4.865129000  | 0.042790000  | 0.231475000  |
| 1 | 5.950978000  | 0.052760000  | 0.292533000  |
| 7 | 0.065736000  | 2.101774000  | -0.005374000 |
| 6 | 1.175346000  | 2.734045000  | -0.467265000 |
| 1 | 1.999684000  | 2.112484000  | -0.785925000 |
| 7 | -2.138376000 | 2.198056000  | 0.867444000  |
| 6 | 1.290614000  | 4.107717000  | -0.543196000 |
| 1 | 2.215671000  | 4.553842000  | -0.899016000 |
| 6 | 0.181579000  | 4.879826000  | -0.181866000 |
| 1 | 0.204793000  | 5.963227000  | -0.273698000 |
| 6 | -0.967164000 | 4.244532000  | 0.263853000  |
| 1 | -1.849039000 | 4.828464000  | 0.498982000  |
| 6 | -0.999984000 | 2.838327000  | 0.363778000  |
| 6 | -2.988784000 | 3.027489000  | 1.741989000  |
| 1 | -2.343904000 | 3.595649000  | 2.415446000  |
| 1 | -3.619637000 | 3.725976000  | 1.177886000  |
| 1 | -3.626536000 | 2.371407000  | 2.337187000  |
| 6 | -2.787546000 | 1.114645000  | 0.244087000  |
| 6 | -4.162627000 | 1.226478000  | 0.029200000  |
| 1 | -4.673983000 | 2.160218000  | 0.223415000  |
| 7 | -0.114431000 | -0.268662000 | 2.057283000  |
| 7 | 1.961044000  | 0.853797000  | 2.331537000  |

|   |              |              |             |
|---|--------------|--------------|-------------|
| 6 | -1.183826000 | -0.913555000 | 2.590170000 |
| 1 | -1.933104000 | -1.275834000 | 1.899790000 |
| 6 | -1.351401000 | -1.107774000 | 3.946950000 |
| 1 | -2.236834000 | -1.617910000 | 4.316982000 |
| 6 | -0.347900000 | -0.643450000 | 4.804273000 |
| 1 | -0.420302000 | -0.801095000 | 5.878220000 |
| 6 | 0.760371000  | -0.003592000 | 4.268279000 |
| 1 | 1.563598000  | 0.319662000  | 4.919463000 |
| 6 | 0.858518000  | 0.180776000  | 2.874442000 |
| 6 | 2.652358000  | 1.778645000  | 3.245828000 |
| 1 | 3.239222000  | 2.483080000  | 2.653383000 |
| 1 | 1.901645000  | 2.337941000  | 3.808312000 |
| 1 | 3.315332000  | 1.257737000  | 3.948191000 |
| 6 | 2.707617000  | 0.399960000  | 1.233972000 |
| 6 | 4.102904000  | 0.383546000  | 1.339582000 |
| 1 | 4.583921000  | 0.622341000  | 2.279603000 |

NEB #9:

|    |              |              |              |
|----|--------------|--------------|--------------|
| 24 | -0.000063000 | 0.000898000  | -0.000217000 |
| 7  | -0.094015000 | -2.054296000 | -0.023984000 |
| 6  | 0.820932000  | -2.779434000 | 0.657817000  |
| 1  | 1.445687000  | -2.233707000 | 1.347168000  |
| 7  | -1.928109000 | -1.921579000 | -1.492264000 |
| 6  | 0.977984000  | -4.130034000 | 0.477428000  |
| 1  | 1.735575000  | -4.664290000 | 1.031131000  |
| 7  | -2.034245000 | -0.000423000 | -0.094029000 |
| 6  | 0.142935000  | -4.772783000 | -0.435243000 |
| 1  | 0.234961000  | -5.836238000 | -0.609585000 |
| 7  | 0.190601000  | 0.102451000  | -2.046433000 |
| 6  | -0.828492000 | -4.051921000 | -1.098178000 |
| 1  | -1.513479000 | -4.549922000 | -1.764480000 |
| 7  | 2.087367000  | -1.283409000 | -1.907801000 |
| 6  | -0.943953000 | -2.676885000 | -0.859438000 |
| 7  | 2.034258000  | 0.000820000  | 0.093942000  |

|   |              |              |              |
|---|--------------|--------------|--------------|
| 6 | -2.513472000 | -2.477389000 | -2.720669000 |
| 1 | -1.708796000 | -2.879284000 | -3.330935000 |
| 1 | -3.245649000 | -3.260958000 | -2.522555000 |
| 1 | -2.990699000 | -1.669601000 | -3.267655000 |
| 6 | -2.679341000 | -0.948759000 | -0.816729000 |
| 6 | -4.064891000 | -0.962338000 | -0.906443000 |
| 1 | -4.568017000 | -1.732619000 | -1.467118000 |
| 6 | -4.788042000 | -0.004322000 | -0.218322000 |
| 1 | -5.868458000 | -0.005770000 | -0.267105000 |
| 6 | -0.723014000 | 0.781649000  | -2.775489000 |
| 1 | -1.406302000 | 1.406660000  | -2.222602000 |
| 6 | -0.808095000 | 0.674601000  | -4.140300000 |
| 1 | -1.567523000 | 1.222048000  | -4.678415000 |
| 6 | 0.101893000  | -0.156011000 | -4.792526000 |
| 1 | 0.068163000  | -0.270568000 | -5.867466000 |
| 6 | 1.071727000  | -0.812947000 | -4.063973000 |
| 1 | 1.812977000  | -1.414035000 | -4.564615000 |
| 6 | 1.109930000  | -0.652401000 | -2.673365000 |
| 6 | 2.757167000  | -2.448248000 | -2.503948000 |
| 1 | 3.220605000  | -3.020792000 | -1.706016000 |
| 1 | 2.002917000  | -3.068630000 | -2.981066000 |
| 1 | 3.515187000  | -2.170602000 | -3.237038000 |
| 6 | 2.757518000  | -0.634854000 | -0.860409000 |
| 6 | 4.144801000  | -0.662676000 | -0.808231000 |
| 1 | 4.709745000  | -1.152785000 | -1.583556000 |
| 6 | 4.787972000  | -0.002587000 | 0.223608000  |
| 1 | 5.868296000  | -0.003842000 | 0.274444000  |
| 7 | -0.098385000 | 2.056067000  | 0.014275000  |
| 6 | 0.875084000  | 2.781851000  | -0.579995000 |
| 1 | 1.561680000  | 2.236408000  | -1.207952000 |
| 7 | -2.060215000 | 1.921840000  | 1.306970000  |
| 6 | 1.013300000  | 4.132749000  | -0.386666000 |
| 1 | 1.818674000  | 4.667314000  | -0.867918000 |
| 6 | 0.095908000  | 4.775182000  | 0.443405000  |

|   |              |              |             |
|---|--------------|--------------|-------------|
| 1 | 0.170352000  | 5.838793000  | 0.624908000 |
| 6 | -0.932474000 | 4.053667000  | 1.013302000 |
| 1 | -1.677116000 | 4.551217000  | 1.612609000 |
| 6 | -1.023244000 | 2.678249000  | 0.766384000 |
| 6 | -2.756418000 | 2.477486000  | 2.476310000 |
| 1 | -2.011826000 | 2.883242000  | 3.156270000 |
| 1 | -3.470400000 | 3.258121000  | 2.211314000 |
| 1 | -3.278261000 | 1.668681000  | 2.979164000 |
| 6 | -2.744312000 | 0.946349000  | 0.567197000 |
| 6 | -4.132362000 | 0.955737000  | 0.531715000 |
| 1 | -4.685600000 | 1.725377000  | 1.043662000 |
| 7 | 0.000431000  | -0.100820000 | 2.054912000 |
| 7 | 1.901729000  | 1.285307000  | 2.091530000 |
| 6 | -0.976292000 | -0.780550000 | 2.696596000 |
| 1 | -1.605736000 | -1.405497000 | 2.082946000 |
| 6 | -1.186603000 | -0.673977000 | 4.047809000 |
| 1 | -1.992107000 | -1.221648000 | 4.513846000 |
| 6 | -0.340684000 | 0.156668000  | 4.781231000 |
| 1 | -0.472707000 | 0.270529000  | 5.848654000 |
| 6 | 0.691615000  | 0.814275000  | 4.145058000 |
| 1 | 1.383274000  | 1.415154000  | 4.712272000 |
| 6 | 0.857815000  | 0.654380000  | 2.763788000 |
| 6 | 2.514828000  | 2.449441000  | 2.747062000 |
| 1 | 3.051291000  | 3.021384000  | 1.995673000 |
| 1 | 1.720429000  | 3.071107000  | 3.151920000 |
| 1 | 3.201681000  | 2.170699000  | 3.546955000 |
| 6 | 2.666300000  | 0.634897000  | 1.111932000 |
| 6 | 4.052325000  | 0.659347000  | 1.190498000 |
| 1 | 4.543487000  | 1.148785000  | 2.015027000 |

[Cr(ddpd)(κ<sup>2</sup>N-ddpd)]<sup>3+</sup>:

|    |              |              |             |
|----|--------------|--------------|-------------|
| 24 | 10.575316000 | 13.219758000 | 5.444876000 |
| 7  | 9.220212000  | 14.762761000 | 5.390157000 |
| 6  | 9.283273000  | 15.709474000 | 6.356467000 |

|   |              |              |              |
|---|--------------|--------------|--------------|
| 1 | 10.150087000 | 15.685090000 | 6.995260000  |
| 7 | 8.176461000  | 13.847927000 | 3.481868000  |
| 6 | 8.302071000  | 16.648586000 | 6.539339000  |
| 1 | 8.392949000  | 17.371182000 | 7.335150000  |
| 7 | 10.462683000 | 13.169813000 | 3.403808000  |
| 6 | 7.205398000  | 16.632045000 | 5.680085000  |
| 1 | 6.407240000  | 17.351928000 | 5.791786000  |
| 7 | 12.048815000 | 14.581253000 | 5.458148000  |
| 6 | 7.156265000  | 15.709211000 | 4.656661000  |
| 1 | 6.338948000  | 15.720568000 | 3.956603000  |
| 7 | 13.006406000 | 13.587617000 | 7.362994000  |
| 6 | 8.196116000  | 14.785657000 | 4.515384000  |
| 7 | 10.662239000 | 13.214466000 | 7.499392000  |
| 6 | 6.874511000  | 13.588752000 | 2.838441000  |
| 1 | 6.585524000  | 14.380065000 | 2.148012000  |
| 1 | 6.124521000  | 13.493856000 | 3.617991000  |
| 1 | 6.938883000  | 12.647745000 | 2.302495000  |
| 6 | 9.322191000  | 13.509302000 | 2.745747000  |
| 6 | 9.260582000  | 13.513674000 | 1.359953000  |
| 1 | 8.355615000  | 13.807409000 | 0.857230000  |
| 6 | 10.392226000 | 13.188544000 | 0.636273000  |
| 1 | 10.364015000 | 13.193733000 | -0.443937000 |
| 6 | 12.088153000 | 15.497462000 | 4.458418000  |
| 1 | 11.186191000 | 15.619465000 | 3.883774000  |
| 6 | 13.215683000 | 16.215393000 | 4.165872000  |
| 1 | 13.206837000 | 16.921170000 | 3.350464000  |
| 6 | 14.356459000 | 15.993509000 | 4.938185000  |
| 1 | 15.273101000 | 16.525051000 | 4.726354000  |
| 6 | 14.306116000 | 15.117285000 | 5.999437000  |
| 1 | 15.164310000 | 14.987612000 | 6.635296000  |
| 6 | 13.115502000 | 14.429016000 | 6.272061000  |
| 6 | 14.249115000 | 13.157131000 | 8.023011000  |
| 1 | 14.955376000 | 12.850784000 | 7.256497000  |
| 1 | 14.022792000 | 12.299703000 | 8.648061000  |

|   |              |              |              |
|---|--------------|--------------|--------------|
| 1 | 14.691056000 | 13.945184000 | 8.632460000  |
| 6 | 11.826603000 | 13.500241000 | 8.124646000  |
| 6 | 11.877589000 | 13.693169000 | 9.496360000  |
| 1 | 12.810314000 | 13.932566000 | 9.978012000  |
| 6 | 10.700580000 | 13.624996000 | 10.224853000 |
| 1 | 10.718484000 | 13.804201000 | 11.290519000 |
| 7 | 11.886052000 | 11.646787000 | 5.346574000  |
| 6 | 11.943383000 | 10.738103000 | 6.348745000  |
| 1 | 11.162092000 | 10.787138000 | 7.085504000  |
| 7 | 12.764419000 | 12.553811000 | 3.354761000  |
| 6 | 12.956274000 | 9.823745000  | 6.469374000  |
| 1 | 12.960744000 | 9.133470000  | 7.298420000  |
| 6 | 13.964130000 | 9.827998000  | 5.507002000  |
| 1 | 14.782842000 | 9.124979000  | 5.563613000  |
| 6 | 13.902166000 | 10.725262000 | 4.462388000  |
| 1 | 14.653200000 | 10.711065000 | 3.691328000  |
| 6 | 12.836740000 | 11.630271000 | 4.392884000  |
| 6 | 14.019521000 | 12.855486000 | 2.645789000  |
| 1 | 14.295945000 | 12.081518000 | 1.930607000  |
| 1 | 14.807487000 | 12.963889000 | 3.385144000  |
| 1 | 13.899161000 | 13.800306000 | 2.126328000  |
| 6 | 11.573672000 | 12.856574000 | 2.685439000  |
| 6 | 11.561146000 | 12.864331000 | 1.297222000  |
| 1 | 12.442459000 | 12.586171000 | 0.745964000  |
| 7 | 8.796380000  | 10.294477000 | 7.505101000  |
| 7 | 8.411884000  | 12.625492000 | 7.525155000  |
| 6 | 8.972676000  | 9.151339000  | 6.838390000  |
| 1 | 9.100185000  | 8.261078000  | 7.440872000  |
| 6 | 9.013496000  | 9.071229000  | 5.444998000  |
| 1 | 9.178490000  | 8.119840000  | 4.961749000  |
| 6 | 8.822385000  | 10.227041000 | 4.713206000  |
| 1 | 8.824058000  | 10.211241000 | 3.632354000  |
| 6 | 8.602258000  | 11.422602000 | 5.405207000  |
| 1 | 8.279979000  | 12.309550000 | 4.880093000  |

|   |             |              |              |
|---|-------------|--------------|--------------|
| 6 | 8.611536000 | 11.402789000 | 6.794056000  |
| 6 | 7.093843000 | 12.719608000 | 8.166048000  |
| 1 | 6.344597000 | 12.463533000 | 7.421857000  |
| 1 | 6.928875000 | 13.742152000 | 8.496018000  |
| 1 | 6.997735000 | 12.038272000 | 9.013741000  |
| 6 | 9.522676000 | 13.059206000 | 8.233240000  |
| 6 | 9.508013000 | 13.310528000 | 9.597654000  |
| 1 | 8.596922000 | 13.197415000 | 10.161198000 |

## 7. References

- 1 S. Otto, M. Grabolle, C. Förster, C. Kreitner, U. Resch-Genger and K. Heinze, *Angew. Chem. Int. Ed.*, 2015, **54**, 11572.
- 2 J. W. Emsley and L. Phillips, *Prog. Nucl. Magn. Reson. Spectrosc.*, 1971, **7**, 1.
- 3 F. Zinna, T. Bruhn, C. A. Guido, J. Ahrens, M. Bröring, L. Di Bari and G. Pescitelli, *Chem. Eur. J.*, 2016, **22**, 16089.
- 4 F. Zinna, L. Arrico and L. Di Bari, *Chem. Commun.*, 2019, **55**, 6607.
- 5 F. Neese, *WIREs Comput. Mol. Sci.*, 2012, **2**, 73.
- 6 A. D. Becke, *J. Chem. Phys.*, 1993, **98**, 5648.
- 7 C. Lee, W. Yang and R. G. Parr, *Phys. Rev. B*, 1988, **37**, 785.
- 8 B. Miehlisch, A. Savin, H. Stoll and H. Preuss, *Chem. Phys. Lett.*, 1989, **157**, 200.
- 9 F. Neese, F. Wennmohs, A. Hansen and U. Becker, *Chem. Phys.*, 2009, **356**, 98.
- 10 R. Izsák and F. Neese, *J. Chem. Phys.*, 2011, **135**, 144105.
- 11 D. A. Pantazis, X.-Y. Chen, C. R. Landis and F. Neese, *J. Chem. Theory Comput.*, 2008, **4**, 908.
- 12 S. Sinnecker, A. Rajendran, A. Klamt, M. Diedenhofen and F. Neese, *J. Phys. Chem. A*, 2006, **110**, 2235.
- 13 S. Grimme, J. Antony, S. Ehrlich and H. Krieg, *J. Chem. Phys.*, 2010, **132**, 154104.
- 14 S. Grimme, S. Ehrlich and L. Goerigk, *J. Comput. Chem.*, 2011, **32**, 1456.
- 15 F. Weigend and R. Ahlrichs, *Phys. Chem. Chem. Phys.*, 2005, **7**, 3297.
- 16 F. Weigend, *Phys. Chem. Chem. Phys.*, 2006, **8**, 1057.
- 17 S. Smidstrup, A. Pedersen, K. Stokbro and H. Jónsson, *J. Chem. Phys.*, 2014, **140**, 214106.
- 18 J. Nocedal, *Math. Comp.*, 1980, **35**, 773.
- 19 S. Otto, J. P. Harris, K. Heinze and C. Reber, *Angew. Chem. Int. Ed.*, 2018, **57**, 11069.
- 20 J. Autschbach in *Comprehensive Inorganic Chemistry II*, 2nd ed. (Eds. J. Reedijk, K. Poeppelmeier), Elsevier, Amsterdam, 2013; pp. 407.
- 21 M. Srebro-Hooper and J. Autschbach, *Annu. Rev. Phys. Chem.*, 2017, **68**, 399.
- 22 G. Pescitelli and T. Bruhn, *Chirality*, 2016, **28**, 466.
- 23 M. Enamullah, A. Uddin, G. Pescitelli, R. Berardozi, G. Makhoulfi, V. Vasylyeva, A. C. Chamayou and C. Janiak, *Dalton Trans.*, 2014, **43**, 3313.
- 24 G. Pescitelli, S. Lüdeke, A.-C. Chamayou, M. Marolt, V. Justus, M. Górecki, L. Arrico, L. Di Bari, M. A. Islam, I. Gruber, M. Enamullah and C. Janiak, *Inorg. Chem.*, 2018, **57**, 13397.
- 25 Gaussian 16 (Revision A.03): M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, G. A. Petersson, H. Nakatsuji, X. Li, M. Caricato, A. V. Marenich, J. Bloino, B. G. Janesko, R. Gomperts, B. Mennucci, H. P. Hratchian, J. V. Ortiz, A. F. Izmaylov, J. L. Sonnenberg, D. Williams-Young, F. Ding, F. Lipparini, F. Egidi, J. Goings, B. Peng, A. Petrone, T. Henderson, D. Ranasinghe, V. G. Zakrzewski, J. Gao, N. Rega, G. Zheng, W. Liang, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, K. Throssell, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. J. Bearpark, J. J. Heyd, E. N. Brothers, K. N. Kudin, V. N. Staroverov, T. A. Keith, R. Kobayashi, J. Normand, K.

- Raghavachari, A. P. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, J. M. Millam, M. Klene, C. Adamo, R. Cammi, J. W. Ochterski, R. L. Martin, K. Morokuma, O. Farkas, J. B. Foresman and D. J. Fox, Gaussian, Inc., Wallingford CT, 2016.
- 26 T. Bruhn, A. Schaumlöffel, Y. Hemberger and G. Bringmann, *Chirality*, 2013, **25**, 243.
- 27 T. Bruhn, A. Schaumlöffel, Y. Hemberger and G. Pescitelli, SpecDis (version 1.71), Berlin, Germany, 2017; Web: <https://specdis-software.jimdo.com> (last access: August 11, 2019).