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

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The chiral spin-flip luminophore $[Cr(ddpd)_2]^{3+}$ can be resolved into enantiopure material by chiral HPLC. The corresponding enantiomers show very high luminescence dissymmetry factors of up to $|g_{lum}| \approx 0.093$ in circularly polarized luminescence (CPL) measurements for the "ruby-like" phosphorescence transition $^2E/^2T_1 \rightarrow {}^4A_2$ in the near-IR region around $\lambda \approx 775$ nm.

The development of efficient luminophores capable of emitting “enantioenriched” light, i.e. the preferential emission of one form of either left- or right-circularly polarized luminescence (CPL), is a fascinating field in the photonic sciences due to many emerging applications (e.g. CPL bioanalytics, CP-OLEDs, etc.).[1,2] Naturally, the observation of CPL activity in isolated molecules is only possible for chiral, non-racemic compounds, ideally in enantiopure and configurationally stable systems. The extent of enantiomeric excess in the emitted, circularly polarized light is usually expressed as luminescence dissymmetry factor g_{lum} given as:

$$g_{lum}(\lambda) = 2\frac{I_L(\lambda) - I_R(\lambda)}{I_L(\lambda) + I_R(\lambda)}; \qquad [-2 \le g_{lum} \le +2]$$

with I_L and I_R being the intensities of left- and right-circularly polarized light at a specific emission wavelength λ, respectively. For practical CPL applications, large values of g_{lum} are desirable, as well as high general photoluminescence quantum efficiencies Φ_{lum}, especially at the emissive transition chosen for CPL observation and sizeable molar extinction coefficients ε at the excitation wavelength λ_{exc}. High values of g_{lum} are especially expected for luminescence bands which are electric dipole forbidden and magnetic dipole allowed.[3] Therefore, while organic and most inorganic transition metal luminophores have a rich history in the photophysics of enantiopure compounds, the nature of the most prevalent luminescent transitions does not bode well for the achievement of high dissymmetry factors and typically, relatively small values of ca. $10^{-4} < g_{lum} < 10^{-2}$ are the norm.[1,4] On the other hand, the best candidates for the realization of sizeable g_{lum} factors are enantiopure complexes with trivalent lanthanoid cations where g_{lum} is routinely a few orders of magnitudes larger (ca. $10^{-2} < g_{lum} < 1$) than in other systems[2] and can reach values of up to 1.38 in solution.[5] Despite the suitability of lanthanoids for the development of efficient CPL emitters, it is highly desirable to have alternatives based on other, more abundant elements. In addition, the most prevalent CPL-active transitions of lanthanoids (mostly for Eu^{3+} and Tb^{3+}) do not cover various spectral ranges, for example the important near-IR wavelength region from approx. 700-900 nm. One of the most promising avenues for the development of alternative CPL-emitters is based on the photophysics of chromium(III) complexes, best known for the optical properties (e.g. color, luminescence) of ruby. Especially the phosphorescent, spin-flip-transitions analogous to the R1- and R2-ruby laser lines ($^2E/^2T_1 \rightarrow {}^4A_2$) have many properties that are reminiscent of the best CPL-active lanthanoid transitions (excited and ground states in the weak coupling limit, strongly electric-dipole forbidden, magnetically allowed).[6] Despite encouraging proof-of-concept CPL studies in the solid state and at low-temperature, previous work on Cr^{3+}-CPL starting as early as 1967 was hampered by the fact that generally, molecular chromium(III) complexes only showed very low quantum efficiencies at room temperature in solution and the potential for realistic CPL-applications was therefore rather low.[7] This situation has changed recently with the development of the molecular ruby $[Cr(ddpd)_2]^{3+}$ (Figure 1)[8] which has extraordinarily high phosphorescence quantum yields Φ of up to 30% in deoxygenated solutions at room temperature, especially after reducing multiphonon quenching through deuteration of the ligands and the solvent (see Figure 1). In a seminal work in the area of CPL luminophores, Piguet et al.[9]

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Electronic Supplementary Information (ESI) available: Details of the chiral resolution, configurational stability, assignment of absolute configurations, CD spectroscopy, computational estimation of the racemization barriers. See DOI: 10.1039/x0xx00000x

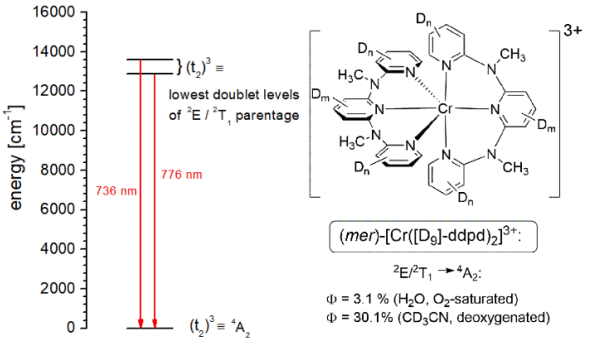


Figure 1. Energy level diagram for the metal-centered states in the chromium complex $[Cr(ddpd)_2]^{3+}$ showing the "ruby-like" spin-flip emission $^2E/^2T_1 \rightarrow {}^4A_2$ with very favorable general luminescence properties such as high quantum yields Φ, especially in the deuterated version shown.[8]

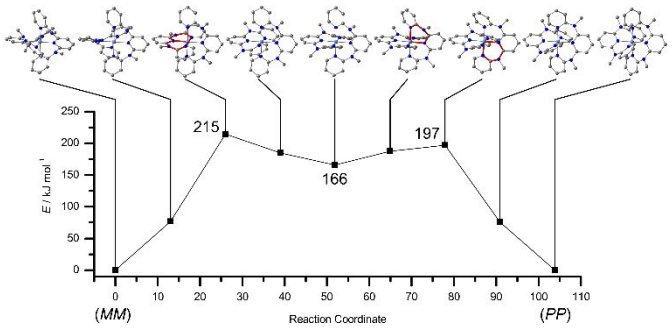
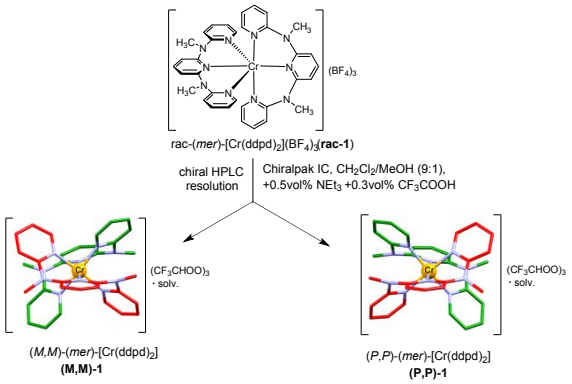


Figure 2. DFT calculations of the trajectory for the stepwise racemization of six-coordinate $[Cr(ddpd)_2]^{3+}$ (hydrogen atoms omitted; inverting chelate rings marked in red; see the ESI for details).

could show recently that a similar, enantiopure chromium(III) complex is indeed capable of combining sizeable general phosphorescence quantum yields (Φ = 5.2% in deoxygenated H_2O at room temperature) with unprecedentedly high values for the luminescence dissymmetry factors of up to $|g_{lum}| = 0.2$. In this communication, we show that the successful luminophore $[Cr(ddpd)_2]^{3+}$, which previously was employed in its racemic form, can also be resolved into enantiopure material and that the enantiomers exhibit very high g_{lum} values for a 3d-metal complex.

Despite its simplified depiction in Figure 1, the complex $[Cr(ddpd)_2]^{3+}$ is not achiral with D_{2d} symmetry as would be expected for a homoleptic, meridionally coordinated metal center with planar tridentate chelators such as tpy. Instead, the previously determined structure of racemic material in the solid state[8b] shows strongly twisted ddpd ligands with homochiral helicities (M,M or P,P), which effectively lowers the local symmetry to D_2, making the complex chiral (Scheme 1). Since the chirality of the complexes only relies on the conformations of the rather flexible ddpd ligands, it was not clear at the outset if these presumably rather "soft" stereogenic elements would be suitable to endow the complex with enough configurational stability in order to be able to obtain pure enantiomers and to prevent their rapid racemization once resolved.



Scheme 1. Chiral resolution of the racemic, meridional chromium(III) complex $[Cr(ddpd)_2]^{3+}$ into the (*M,M*)- and (*P,P*)-enantiomers (schematic representations, red and green colors used for carbon atoms in different ddpd units in order to clarify the helicity of each ligand).

In order to evaluate this question, we performed DFT calculations along possible racemization trajectories (Figure 2, see ESI for details). The highest energy species was calculated at 215 kJ/mol higher in energy than the ground state (D_2-symmetric enantiomers). These results suggest that racemization of **(M,M)-1** or **(P,P)-1** without a change in coordination number is rather unlikely and a dissociative or associative pathway might be followed instead (if racemization occurs at all). Pathways with 5- or 7-coordinate intermediates $[Cr(ddpd)(k^2N\text{-}ddpd)]^{3+}$ or $[Cr(ddpd)_2(H_2O)]^{3+}$ are either high in energy (calculated free dissociation enthalpy of 132 kJ/mol) or inaccessible (H_2O coordination to Cr proved unfeasible). This suggests considerable configurational stability of $[Cr(ddpd)_2]^{3+}$. The practical resolution of the two enantiomers proved to be surprisingly difficult and to date we were only successful by employing chiral HPLC using highly optimized conditions (see ESI for details). The racemic material **rac-1** clearly shows two peaks with a peak area ratio very close to 50:50 (Figure 3A) which, despite considerable efforts, could not be baseline-separated completely. For separations on a larger scale necessary for the spectroscopic work, it proved impossible to cleanly obtain the first fraction without contamination by the second fraction and consequently gave only an enantiomeric excess of 80%. In contrast, sampling only the middle and tail portions of the second fraction provided enantiopure material (100% ee). Nevertheless, CD spectra of both fractions in deoxygenated D_2O showed a mirror-image pattern indicative of their enantiomeric relationship (see Figure S2 in the ESI).

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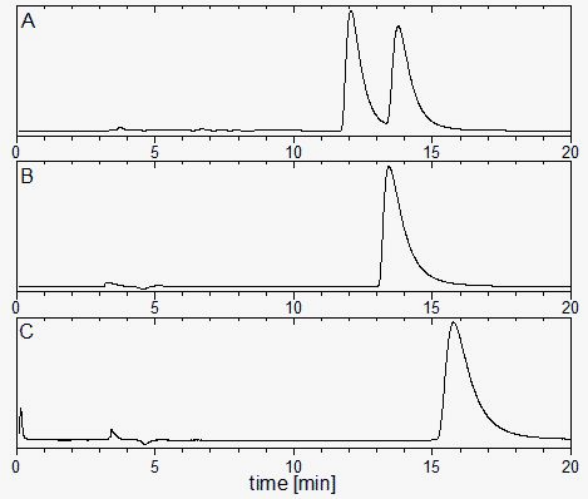

Figure 3. Chiral HPLC traces (Chiralpak IC, CH_2Cl_2/MeOH/NEt_3/CF_3COOH 90:10:0.3:0.5, UV detection at 300 nm) for the preparative resolution of **rac-1** (A) and the corresponding analytical runs after the separation (B: **(P,P)-1** and C: **(M,M)-1**; see text for assignment of the configurations).

The counterions for the tricationic chromium complex enantiomers after chiral HPLC resolution were assumed to be trifluoroacetates due to the large excess of the trifluoroacetic acid additive used in the HPLC eluents. ^{19}F NMR spectra of the compounds confirmed this by showing resonances around ca. −78 ppm, which can unambiguously be assigned to free trifluoroacetate (see ESI).[10] The configurational stability under the experimental conditions was assessed by stirring enantiopure material in H_2O at room temperature. The enantiopurity of the dissolved complex was monitored over 48 h by taking samples at certain intervals and determining the enantiomeric excess by chiral HPLC. Over the course of this timeframe, no deterioration of the enantiomeric excess through racemization was detectable. Similarly, enantiomerically resolved material was configurationally stable in the solid state over extended periods (several weeks) of storage at room temperature. The absolute configuration of the resolved enantiomers **(M,M)-1** and **(P,P)-1** was elucidated via computational methods (TD-DFT, CASSCF(7,12)-NEVPT2[11]) by calculating the CD spectrum of **(M,M)-1** (see ESI for details). The good agreement of the TD-DFT derived spectral shape in the region of the ligand-centered UV-transitions (ca. λ < 350 nm) with the experimental CD spectrum of the second HPLC fraction permits the assignment of the first HPLC fraction as **(P,P)-1** and the second as **(M,M)-1** (see Figure 3). The metal centered transitions > 400 nm display an overall positive rotatory strength according to CASSCF-NEVPT calculations on **(M,M)-1** confirming the assignment based on TD-DFT (see ESI). Finally, the CPL properties of the phosphorescent near-IR emission bands (λ_{em} ≈ 738/775 nm) were measured for the enantiopure complex **(M,M)-1** in deoxygenated D_2O (see Figure 4 and Figure S3 in the ESI). The CPL measurement confirmed a large maximum value for g_{lum} = −0.093 at 775 nm (and a positive g_{lum} for the weaker high-energy transition), which is less than the value recently obtained by Piguet[9] ($|g_{lum}|$ < 0.2) but which still represents a very large dissymmetry factor for a 3d-metal complex and

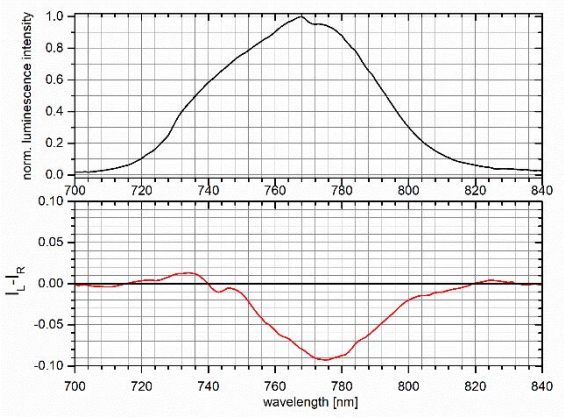

Figure 4. Steady-state emission (top, black) and CPL spectra (bottom, red) of the near-IR luminescence band $^2E/^2T_1 \rightarrow {}^4A_2$ of **(M,M)-1** in solution at room temperature (deoxygenated D_2O, c = 10 µM, λ_{exc} = 365 nm).

which is on a par with many lanthanoid-based CPL emitters.[2] Together with the superior general luminescence properties of $[Cr(ddpd)_2]^{3+}$ (e.g. phosphorescence quantum yields up to 30% in solution) and high stability (configurational, thermal, photochemical), its resolved enantiomers are excellent candidates for the development of very efficient NIR-CPL luminophores based on the earth-abundant and cheap element chromium. Moreover, thanks to their ruby-like emission, optically active chromium(III) compounds could be advantageously used in the field of chiral optoelectronics and photonics.

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Conflicts of interest

There are no conflicts to declare.

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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}H: 400 MHz, ^{19}F: 377 MHz) using CD_3OD (≥ 99.8% D) as the solvent. The racemic Cr complex $[Cr(ddpd)_2](BF_4)_3$ was synthesized as described previously.[1] NMR-grade D_2O (>99.8%D) was used for the photophysical measurements.

2. Chiral HPLC / Configurational Stability Test

All chiral HPLC runs of the $[Cr(ddpd)_2](X)_3$ complexes (**rac-1** or enantioenriched samples) were performed on a Knauer Azura HPLC system (UV detection at λ = 300 nm), equipped with a CHIRALPAK IC column (Daicel, particle size: 5 µm, internal diameter: 4.6 mm, column length: 250 mm) using CH_2Cl_2/MeOH (90:10) with additional 0.5 vol.-% NEt_3 and 0.3 vol.-% CF_3COOH as mobile phase with a flow of 1.0 mL/min. All samples were filtered through a membrane filter (nylon, 0.45 µm pore size, 13 mm diameter) in a stainless steel filter holder prior to injection.

Racemic $[Cr(ddpd)_2](BF_4)_3$ (6.0 mg) was dissolved in CH_2Cl_2/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 µL. 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 ($HNEt_3CF_3COO$). This raw material was washed repeatedly with CH_2Cl_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%, $[CF_3COO]^-$}, 226.96 {100%, $[2CF_3COO + H]^-$}) and by ^{19}F NMR spectroscopy[2] (Figure S1):

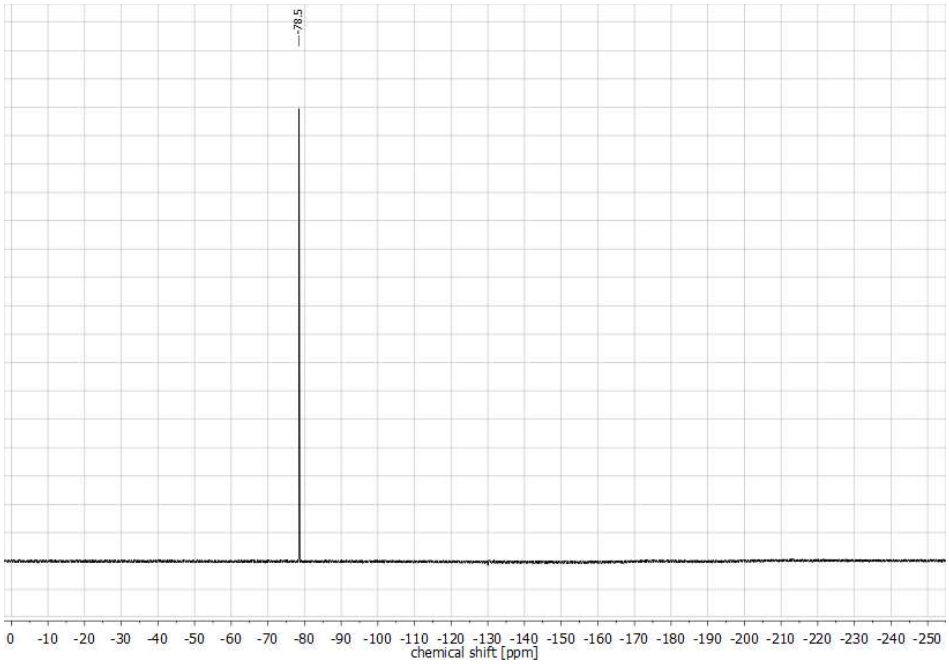

Figure S1. ^{19}F NMR spectrum (377 MHz, CD_3OD) of **(*M,M*)-1**.

Configurational stability test in solution

An enantiomerically pure sample of **(*M,M*)-1** (0.3 mg) was stirred at room temperature in H_2O (1.0 mL, HPLC grade). During the course of 48 h, samples of 100 µl 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 CH_2Cl_2/MeOH (90:10, 100 µL). The solutions were filtered through a membrane filter (nylon, 0.45 µm pore size), the filter was washed with additional solvent mixture (100 µL), and the combined filtrates were concentrated. For chiral HPLC analysis, the dry samples were redissolved in CH_2Cl_2/MeOH (90:10, 100 µL) 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 µM solutions in deoxygenated D_2O. CPL spectra were measured with a home-made spectrofluoropolarimeter[3] in the configuration described before.[4] The spectra were acquired on 10 µM solutions in deoxygenated D_2O under 365 nm irradiation, with 4 sec integration time and 4 accumulations. The spectra were baseline corrected by subtracting the trace of the solvent.

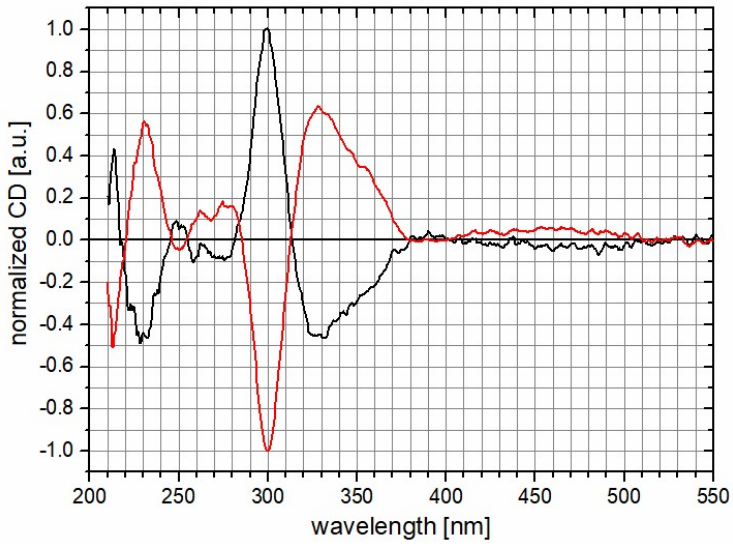

Figure S2. Normalized CD spectra (deoxygenated D_2O, c = 10 µM) of the first chiral HPLC fraction (black) and the second fraction (red) – Mirror-image relationship indicating the enantiomeric nature of both fractions.

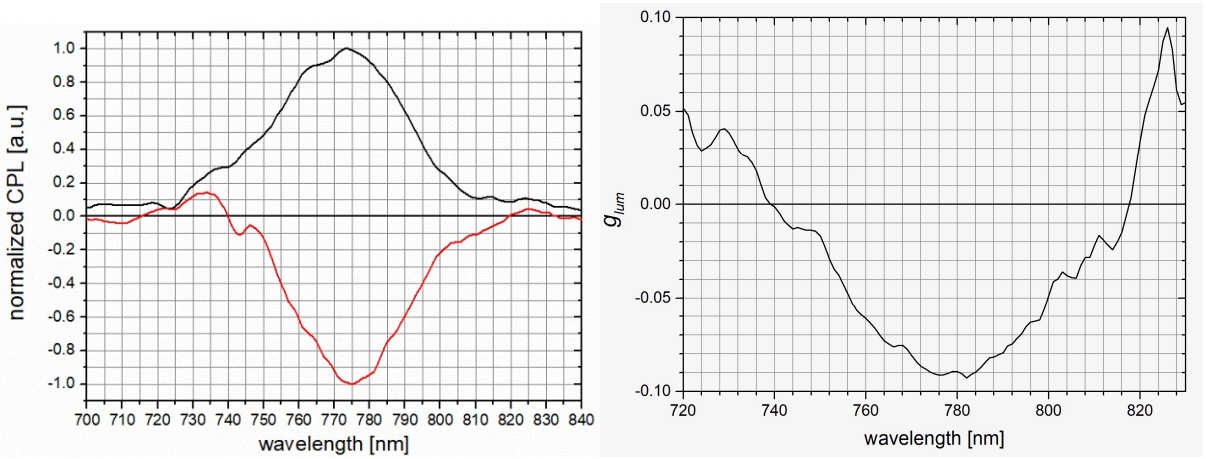

Figure S3. Left: Normalized CPL spectra (deoxygenated D_2O, c = 10 µM) of the first chiral HPLC fraction (black) and the second fraction (red) – Right: Plot of g_{lum} vs. the wavelength for (***M,M*-1**).

4. Calculation of the Energy Barriers for Racemization Pathways

Racemization of (*M,M*)- or (*P,P*)-$[Cr(ddpd)_2]^{3+}$ 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 $[Cr(ddpd)_2]^{3+}$ 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*)-$[Cr(ddpd)_2]^{3+}$ 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.

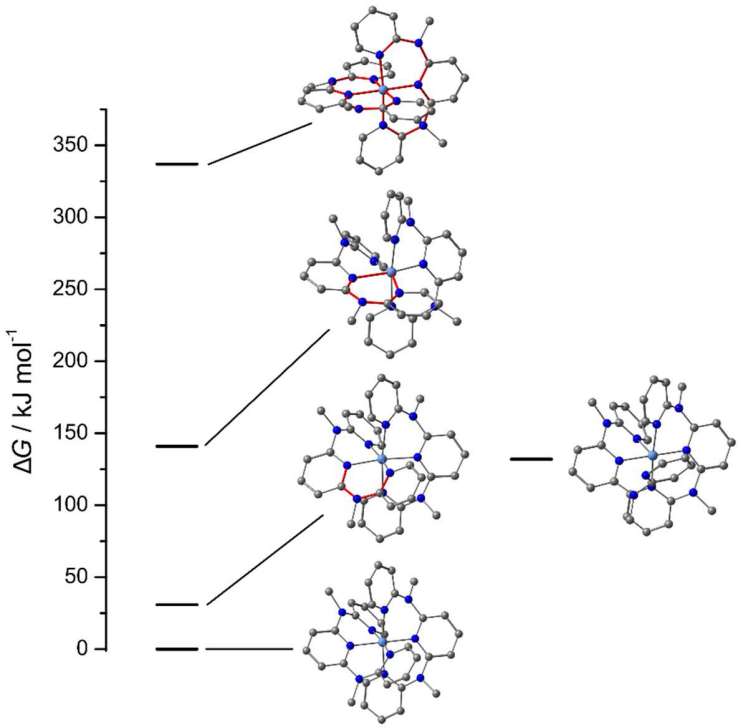

Figure S4. Optimized geometries of $[Cr(ddpd)_2]^{3+}$ with constrained chelate rings indicated in red (left) and of $[Cr(ddpd)(\kappa^2N\text{-ddpd})]^{3+}$ (right).

To investigate a conceivable dissociative pathway, the geometry of $[Cr(ddpd)(\kappa^2N\text{-ddpd})]^{3+}$ 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 $[Cr(ddpd)_2(H_2O)]^{3+}$. Instead, the calculation yielded 6-coordinate $[Cr(ddpd)(k^2N\text{-}ddpd)(H_2O)]^{3+}$ 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)[5] using the B3LYP functional.[6-8] Tight convergence criteria were chosen for geometry optimizations and frequency calculations (Keywords TightSCF and TightOpt, convergence criteria for the SCF part: energy change 1.0×10^{-8} E_h, 1-El. energy change 1.0×10^{-5} E_h, orbital gradient 1.0×10^{-5}, orbital rotation angle 1.0×10^{-5}, DIIS Error 5.0×10^{-7}; for geometry optimizations: energy change: 1.0×10^{-6} E_h, max. gradient 1.0×10^{-4} E_h a_0^{-1}, RMS gradient 3.0×10^{-5} E_h a_0^{-1}, max. displacement 1.0×10^{-3} a_0, RMS displacement 6.0×10^{-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).[9,10] The ZORA relativistic approximation was used to describe relativistic effects in all calculations.[11] To account for solvent effects, a conductor-like screening model (CPCM) modeling acetonitrile was used in all calculations.[12] Atom-pairwise dispersion correction was performed with the Becke-Johnson damping scheme (D3BJ).[13,14] For the geometries of the ground state and with (partly) planarized ligands geometry optimizations were performed using Ahlrichs' split valence triple-ξ basis set def2-TZVPP which comprises polarization functions for all non-hydrogen atoms.[15,16] Dihedral angles were fixed to 0° 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.[13,14] Seven intermediate images were calculated with initial path generation via the image dependent pair potential (IDPP) method[17] and optimized using the Limited-memory Broyden-Fletcher-Goldfarb-Shanno (L-BFGS) algorithm.[18] Tolerance for the maximum component of the atomic force perpendicular to the path was 5.0×10^{-4} Eh a_0^{-1} with a root-mean-square of 2.0×10^{-4} Eh a_0^{-1}. The spring constant was set to 1.0×10^{-1} Eh a_0^{-2}.
CASSCF(7,12)-NEVPT2 calculations for metal-centered excited states were performed as previously described.[19]

5. Assignment of Absolute Configuration

To assign the absolute configuration of the enantiomers of $[Cr(ddpd)_2]^{3+}$ 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).[20,21] 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,[22] 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).[23,24] 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.[19]

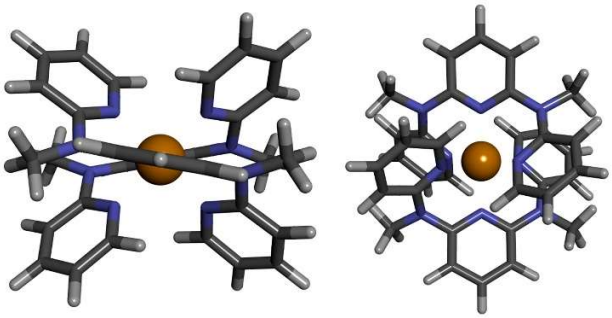

Figure S5. DFT-optimized structure of the cationic metal complex in **(*M,M*)-1** with D_2 symmetry seen along two different C_2 axes.

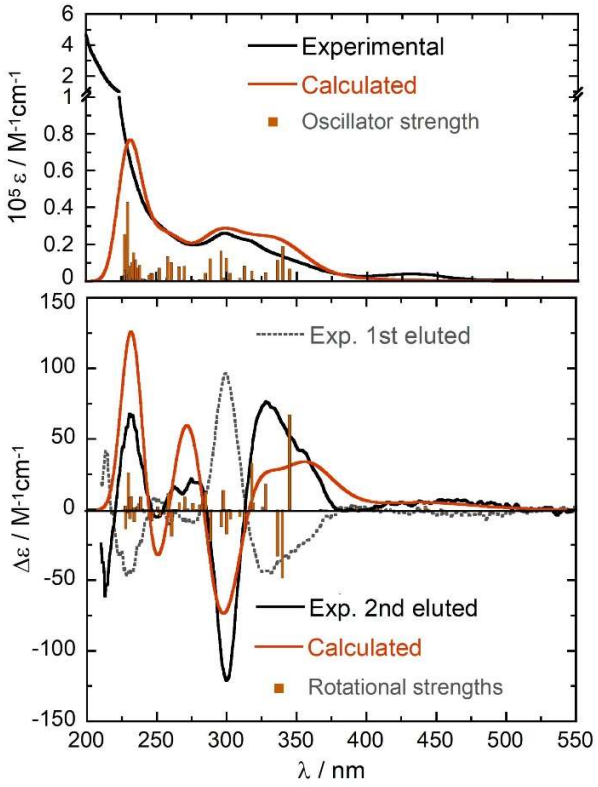

Figure S6. Comparison between the experimental and calculated UV/vis absorption (top) and ECD (bottom) spectra measured in D_2O at 10^{-5} M concentration, and TD-DFT-calculated spectra on ***(M,M)*-1** at the CAM-B3LYP/def2-TZVP/PCM//M06/def2-SVP level. Calculated spectra were plotted using an exponential 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,[25] using default grids and convergence criteria. The starting geometry was extracted from the published X-ray structure of a racemic form of $[Cr(ddpd)_2]^{3+}$ and had (*M,M*)-configuration.[1] 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 $[Cr(ddpd)_2]^{3+}$ 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.[26,27]

The absorption bands at wavelengths > 400 nm (the metal-centered quartet transitions) were reproduced by CASSCF(7,12)-NEVPT2 calculations on **(M,M)-1**.[19] 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 = –4.5x10^{40} cgs; 429 nm: R^*T = –3.4x10^{40} cgs; 411 nm: R^*T = -12.5x10^{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 [Cr(ddpd)(k^{2}N-ddpd)]$^{3+}$ (Figure S4):

[Cr(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

$[Cr(ddpd)_2]^{3+}$ 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

$[Cr(ddpd)_2]^{3+}$ 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^2*N*-ddpd)]$^{3+}$:

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

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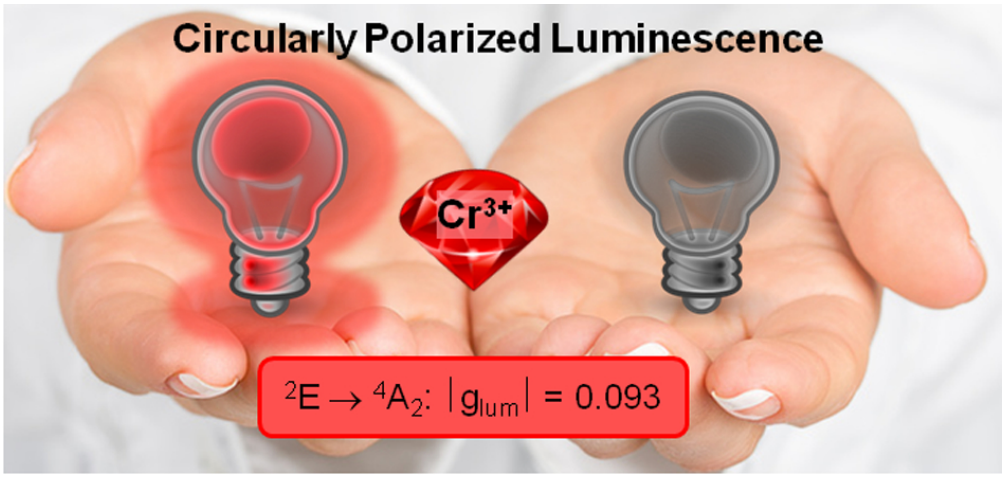

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