Chemical Science

Controlling Dynamic Stereoisomerism in Transition-Metal Folded Baskets

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SUPPLEMENTARY INFORMATION
General

All chemicals were purchased from commercial sources, and used as received unless stated otherwise. All solvents were dried prior to use according to standard literature protocols. Chromatography purifications were performed using silica gel 60 (Sorbent Technologies 40-75µm, 200 x 400 mesh). Thin-layer chromatography (TLC) was performed on silica-gel plate w/UV254 (200µm). $^1$H and $^{13}$C NMR spectra were recorded, at 400 MHz and 100 MHz respectively, on a Bruker DPX-400 spectrometer unless otherwise noted. The NMR spectra were referenced using solvent residual signal as an internal standard. NMR samples were prepared with CDCl$_3$ and CD$_3$CN solvents that were purchased from Cambridge Isotope Laboratories. The chemical shift values are expressed as δ values (ppm) and the couple constants (J) are given in Hertz (Hz). The following abbreviations were used for signal multiplicities: s, singlet; d, doublet; t, triplet; m, multiplet; and br, broad. MALDI-TOF mass spectra were measured with 2,5-dihydroxybenzoic acid as matrix.

Synthesis

The preparation of baskets ($R$/S)-1 and model compounds ($R$/S)-2 was completed in accord with Scheme 1. Note that the synthesis of compounds ($R$/S)-7 was already reported (see G. Chelucci and coworkers Tetrahedron Asymmetry 2006, 17, 3163-3169) and we followed these protocols. Compound 8 was made in accord with our previously published procedure (Badjic and coworkers Org. Lett. 2007, 9, 2301). We hereby report a full characterization of new compounds ($R$/S)-1 and ($R$/S)-2 while only the $^1$H NMR characterization of the known compounds (see G. Chelucci and coworkers Tetrahedron Asymmetry 2006, 17, 3163-3169).

Chiral basket ($R_3$)-1: Compound ($R$)-7 (1.9 mg, 0.0158 mmol) was added to a solution of tris-anhydride 8 (2.0 mg, 0.00317 mmol) in 2 mL of toluene. The solution was heated to reflux and stirred for 1 h upon which 200 µL of neat pyridine was added. The resulting mixture was stirred for additional 12 h and then cooled down to room temperature. The mixture was concentrated under reduced pressure and the residue purified with thin-layer chromatography (SiO$_2$, acetone:benzene=3:1) to yield 1.64 mg of basket ($R_3$)-1 (55%) as a colorless oil. $^1$H NMR (500 MHz, CDCl$_3$, 300 K): δ = 8.60 (d, J=1.8 Hz, 3H), 8.46 (dd, J=4.8, 1.8 3H ), 7.78 (dt, J=7.9, 1.8, 1.8 3H ), 7.47 (d, J=5.6 6H), 7.20 (dd, J=7.9, 4.8 3H ), 5.44 (q, J=7.4 Hz, 3H), 4.49 (s, 6H), 2.58 (s, 6H), 1.79 (d, J=7.4 Hz, 9H); $^{13}$C NMR (100 MHz, CDCl$_3$, 300 K): δ = 167.80, 167.78, 156.93, 156.89, 149.33, 149.09, 137.99, 135.95, 135.17, 130.55, 130.43, 123.38, 116.18, 116.14, 65.98, 49.26, 47.31, 17.44 ppm; HRMS MALDI-TOF: $m/z$ calcd for C$_{60}$H$_{42}$N$_6$O$_6$: 943.327 [M + H]$^+$, found: 943.373.
**Figure S1:** $^1$H NMR spectrum (500 MHz) of basket $(R_3)$-1 (4.24 mM) in CDCl$_3$ at 300 K.

**Figure S2:** $^{13}$C NMR spectrum (125 MHz) of chiral basket $(R_3)$-1 (4.24 mM) in CDCl$_3$ at 300 K.
**Figure S3**: High resolution MS (MALDI-TOF) spectrum of chiral basket ($R_3$)-1 showing a strong signal at 943.373 corresponding to its (M+H)$^+$ ion.
Chiral basket \((S_3)_1\): Compound \((S)-7\) (13.5 mg, 0.111 mmol) was added to a solution of \(tris\)-anhydride 8 (14 mg, 0.022 mmol) in 7 mL of toluene. The resulting solution was heated to reflux for 1 h upon which 700 µL of neat pyridine was added. The resulting mixture was stirred for 12 h and cooled down to room temperature. The mixture was concentrated under reduced pressure and the residue purified with thin-layer chromatography (SiO₂, acetone:benzene=3:1) to yield 17.6 mg of basket \((S_3)_1\) (84%) as a colorless oil.

\(^1\)H NMR (500 MHz, CDCl₃, 300 K): \(\delta = 8.60\) (d, \(J=1.8\) Hz, 3H), 8.46 (dd, \(J=4.8, 1.8\) 3H ), 7.78 (dt, \(J=7.9, 1.8, 1.8\) 3H ), 7.47 (d, \(J=5.6\) 6H), 7.20 (dd, \(J=7.9, 4.8\) 3H ), 5.44 (q, \(J=7.4\) Hz, 3H), 4.49 (s, 6H), 2.58 (s, 6H), 1.79 (d, \(J=7.4\) Hz, 9H) ppm; \(^{13}\)C NMR (100 MHz, CDCl₃, 300 K): \(\delta = 167.80, 167.76, 156.93, 156. 89, 149.30, 149.07, 137.97, 135.95, 135.16, 130.53, 130.41, 123.37, 116.17, 116.13, 65.96, 49.24, 47.29, 17.43 ppm; HRMS MALDI-TOF: \(m/z\) calcd for C₆₀H₄₂N₆O₆: 943.327 [M + H]+, found: 943.347.

**Figure S4:** \(^1\)H NMR spectrum (500 MHz) of chiral basket \((S_3)_1\) (27.57 mM) in CDCl₃ at 300 K.
Figure S5: $^{13}$C NMR spectrum (125 MHz) of chiral basket ($S_3$)-1 (27.57 mM) in CDCl$_3$ at 300 K.
**Figure S6**: High resolution MS spectrum (MALDI-TOF) of chiral basket $(S_3)$-1 showing a strong signal at 943.347 corresponding to its $(M+H)^+$ ion.

**Model compound (R)-2**: Compound (R)-7 (48 mg, 0.394 mmol) was added to a solution of phthalic anhydride (70 mg, 0.473 mmol) in 8 mL of toluene. The resulting solution was heated to reflux for 1 h upon which 800 µL of neat pyridine was added. The resulting mixture was stirred for additional 12 h and then cooled down to room temperature. The mixture was concentrated under reduced pressure and the residue purified via flash chromatography (SiO2, ethyl acetate:hexanes=1:1) to yield 96.6 mg of compound (R)-2 (81%) as a colorless oil.

$^1$H NMR (500 MHz, CDCl$_3$, 300 K): $\delta = 8.70$ (d, $J=2.3$ Hz, 1H), 8.50 (dd, $J=4.8, 1.8, 1H$), 7.87 (dt, $J=7.9, 1.8, 1.8, 1H$), 7.80 (dd, $J=5.5, 3.0, 2H$), 7.68 (dd, $J=5.5, 3.0, 2H$), 7.25 (dd, $J=7.9, 4.8, 1H$), 5.58 (q, $J=7.4$ Hz, 1H), 1.92 (d, $J=7.4$ Hz, 3H) ppm; $^{13}$C NMR (100 MHz, CDCl$_3$, 300 K): $\delta = 168.0, 149.4, 149.2, 135.8, 135.2, 134.2, 131.9, 123.44, 123.42, 47.5, 17.4$ ppm; HRMS ESI: $m/z$ calcd forC$_{15}$H$_{12}$N$_2$O$_2$: 253.0999 $[M + H]^+$, found: 253.0968.
Figure S7: Variable temperature $^1$H NMR spectrum (500 MHz) of model compound $(R)$-2 (0.158 M) in CDCl$_3$ at (a) 298.0, (b) 283.0, (c) 268, (d) 253.0, (e) 238.0, (f) 223.0, (g) 208.0 and (h) 193.0 K.
Figure S8: $^{13}$C NMR spectrum (125 MHz) of model compound (R)-2 (0.158 M) in CDCl$_3$ at 300 K.
Figure S9: High resolution MS (ESI) spectrum of model compound (R)-2 showing a strong signal at 253.0968 corresponding to its (M+H)$^+$ ion.

**Model compound (S)-2:** Compound (S)-7 (48 mg, 0.394 mmol) was added to a solution of phthalic anhydride (70 mg, 0.473 mmol) in 8 mL of toluene. The resulting solution was heated to reflux and stirred for 1h upon which 800 µL of neat pyridine was added. The resulting mixture was stirred for 12 h and then cooled down to room temperature. The mixture was concentrated under reduced pressure and the residue purified via flash chromatography (SiO$_2$, ethyl acetate:hexane=1:1) to yield 75 mg of model compound (S)-2 (63%) as a colorless oil.

$^1$H NMR (500 MHz, CDCl$_3$, 300 K): $\delta = 8.71$ (d, $J=2.3$ Hz, 1H), 8.51 (dd, $J=4.8$, 1.8, 1H ), 7.88 (dt, $J=7.9$, 1.8, 1.8, 1H ), 7.81 (dd, $J=5.5$, 3.0, 2H), 7.69 (dd, $J=5.5$, 3.0, 2H ), 7.26 (dd, $J=7.9$, 4.8, 1H), 5.59 (q, $J=7.4$ Hz, 1H), 1.93 (d, $J=7.4$ Hz, 3H) ppm; $^{13}$C NMR (100 MHz, CDCl$_3$, 300 K): $\delta = 168.0$, 149.4, 149.2, 135.8, 135.2, 134.2, 131.9, 123.4, 123.4, 47.5, 17.4 ppm; HRMS ESI: m/z calcd forC$_{15}$H$_{12}$N$_2$O$_2$: 253.0999 [M + H]$^+$, found: 253.0970.
Figure S10: $^1$H NMR spectrum (500 MHz) of model compound (S)-2 (0.238 M) in CDCl$_3$ at 300 K.
**Figure S11:** $^{13}$C NMR spectrum (125 MHz) of model compound (S)-2 (0.238 M) in CDCl$_3$ at 300 K.

**Figure S12:** High resolution MS (ESI) spectrum of model compound (S)-2 showing a strong signal at 253.0970 corresponding to its (M+H)$^+$ ion.
**Compound (R₄)-5**: Ti(OEt)₄ (1.74 mL, 7.42 mmol) was added to a solution of 3-acetylpyridine 3 (494 mg, 4.08 mmol) and compound (R₄)-4 (501 mg, 4.12 mmol) in dry dichloromethane (16 mL). The resulting solution was stirred at reflux for 60 h. After cooling to room temperature, the solvent was removed under vacuum and the residue extracted with ethyl acetate (80 mL). Upon a slow addition of brine (16 mL), the mixture was filtered through a pad of Celite. The organic phase was dried over MgSO₄ and the solvent evaporated in vacuum to give a solid residue. The residue was purified with flash chromatography (SiO₂, ethyl acetate: hexanes=4:1) to give 694 mg of (R₄)-5 (75%) as a yellow oil. ¹H NMR (250 MHz, CDCl₃, 300 K): δ = 9.09 (s, 1H), 8.71 (d, J=4.8, 1H), 8.15 (dt, J=8.1, 1.8, 1.8, 1H), 7.37 (dd, J=8.1, 4.8, 1H), 2.80 (s, 3H), 1.33 (s, 9H) ppm.

**Compound (R₄, S)-6**: 2.22 mL of 1.0 M solution of L-Selectride (2.22 mmol) in THF was added dropwise at -78°C to a solution of compound (R₄)-5 (500 mg, 2.22 mmol) in dry THF (20 mL). After 6 h, the reaction mixture was quenched with saturated solution of NH₄Cl (30 mL) and extracted with 30 mL of ethyl acetate. The organic phase was dried over MgSO₄ and the solvent evaporated under reduced pressure. The solid residue was purified with flash chromatography (SiO₂, dichloromethane:methanol=9:1) to give 323 mg of (R₄, S)-6 (64%) as a yellow oil. ¹H NMR (250 MHz, CDCl₃, 300 K): δ = 8.54 (s, 1H), 8.47 (d, J=4.8, 1H), 7.60 (td, J=7.9, 1.8, 1.8, 1H), 7.22 (dd, J=7.9, 4.8, 1H), 4.56 (q, J=6.7, 1H), 1.51 (d, J=6.7, 3H), 1.15 (s, 9H) ppm.

**Compound (R₄, R)-6**: 5.0 mL of 1.0 M solution of DIBAL (5 mmol) in THF was added dropwise, at -78°C, to a solution of compound (R₄)-5 (500 mg, 2.22 mmol) in dry THF (20 mL). After 6 h the reaction mixture was quenched with methanol (10 mL) at -78°C and then warmed up to room temperature. The solvent was evaporated under reduced pressure, upon which 2 M NaOH (20 mL) was added and the crude mixture extracted with 30 mL of ethyl acetate. The organic phase was dried over MgSO₄ and the solvent evaporated under reduced pressure. The solid residue was purified with flash chromatography (SiO₂, dichloromethane:methanol=9:1) to give 404 mg of (R₄, R)-6 (80%) as a yellow oil. ¹H NMR (250 MHz, CDCl₃, 300 K): δ = 8.63 (s, 1H), 8.56 (d, J=4.8, 1H), 7.71 (dt, J=7.9, 1.8, 1.8, 1H), 7.31 (dd, J=7.9, 4.8, 1H), 4.60 (q, J=6.7, 1H), 1.56 (d, J=6.7, 3H), 1.24 (s, 9H) ppm.

**Compound (S)-7**: Compound (R₄, S)-6 (318 mg, 1.4 mmol) was dissolved in 28 mL of methanol upon which 28 mL of 6 M HCl (in methanol) was added. The reaction mixture was stirred at room temperature for one hour. Methanol was evaporated under reduced pressure and 10 ml of H₂O was added. Upon the extraction of aqueous solution with diethyl ether (3 X 20 mL), 2 M NaOH was added dropwise until pH~12. The organic layer was extracted with dichloromethane (3 X 20 mL) and dried with MgSO₄. The solvent was evaporated under reduced pressure to give 95 mg of (S)-7 as a colorless oil (yield 55%). ¹H NMR (250 MHz, CDCl₃, 300 K): δ = 8.59 (d, J=1.8, 1H), 8.49 (dd, J=4.8, 1.8, 1H), 7.71 (td, J=7.9, 1.8, 1.8, 1H), 7.25 (dd, J=7.9, 4.8, 1H), 4.18 (q, J=6.7, 1H), 1.41 (d, J=6.7, 3H) ppm.

**Compound (R)-7**: Compound (R₄, R)-6 (230 mg, 1.02 mmol) was dissolved in 20 mL of methanol upon which 20 ml of 6 M HCl (in methanol) was added. The reaction mixture was stirred at room temperature for one hour. Methanol was evaporated under reduced pressure and 10 ml of H₂O was added. Upon the extraction of aqueous solution with diethyl ether (3 X 20 mL), 2 M NaOH was added dropwise until pH~12. The organic layer was extracted with dichloromethane (3 X 20 mL) and dried with MgSO₄.
solvent was evaporated under reduced pressure to give 68 mg of \((R)-7\) (55%) as a colorless oil. NMR (250 MHz, CDCl\(_3\), 300 K): \(\delta = 8.55\) (d, \(J=1.8\), 1H), 8.44 (dd, \(J=4.8\), 1.8, 1H), 7.67 (td, \(J=7.9\), 1.8, 1.8, 1H), 7.22 (dd, \(J=7.9\), 4.8, 1H), 4.14 (q, \(J=6.7\), 1H), 1.37 (d, \(J=6.7\), 3H) ppm.

**Figure S13:** 2-D \(^1\)H-\(^1\)H NOESY Spectrum (400 MHz, 298 K) of 0.16 M solution of \((R)-2\) in CD\(_3\)CN; mixing time 400 ms.
Figure S14: A series of $^1$H NMR spectra (400 MHz, CD$_3$CN, 298 K) recorded on addition of 1.60 M standard solution of AgBF$_4$ to 80.0 mM solution of (R)-2.
Figure S15: UV-Vis and CD titration of 0.0635 mM (R)-2 solution recorded upon incremental addition of 0.0, 0.2, 0.4, 0.6, 0.8, 1.0 molar equivalents of 0.292 mM solution of AgBF₄ in CH₃CN.
Figure S16: 2-D $^1$H-$^1$H NOESY Spectrum (400 MHz, 298 K) of 2.12 mM solution of (R)-1 in CD$_3$CN.
Figure S17: 2-D $^1$H-$^1$H NOESY Spectrum (400 MHz, 298 K) of 2.12 mM solution of ($R$)-1 in CD$_3$CN after the addition of 1 molar equivalent of 10.6 mM AgBF$_4$. 
**Figure S18:** Variable temperature $^1$H NMR (400 MHz) spectra of 13.6 mM solution of (R)-1 in CD$_2$Cl$_2$.

**Figure S19:** Variable temperature $^1$H NMR (400 MHz) spectra of 3.39 mM solution of (R)-1 upon the addition of 3.0 molar equivalents of 0.169 M AgBF$_4$ in CD$_3$CN.
**Computational Studies**

The Monte Carlo/Molecular Mechanics (MC/MM) calculations were performed using MacroModel v9.7 from the Schrödinger ‘09 software suite (using the Maestro v9.0 interface). The Monte Carlo multiple minimum search protocol was used for the conformational search, generating 5,000 starting structures for \((R)-2\) and 10,000 for \((R_3)-1\). The MM3 force field, as implemented in MacroModel, was used to optimize the conformations. The GB/SA model as implemented in MacroModel was utilized for the calculation of the aqueous solvent. Structures within 20 kcal/mol of the lowest energy conformation were retained in the final results. Six unique conformations were found for the search of \((R)-2\). The top two conformations are presented in the paper; DFT optimization of the bottom four conformations caused the geometries to adopt either the 1st or 2nd best conformation. 207 conformations were found for \((R_3)-1\) when no solvent was included and 247 conformations when water was used as a solvent. The lowest energy values of the four distinct conformations of \((R_3)-1\) (three in, two in, one in and none in) were included in the paper. The energies of all conformations are included in the supporting information as a table.

Density functional theory (DFT) calculations were performed using the Turbomole 5.10 software package. Geometry optimizations were performed using the B3LYP and BHLYP functionals in conjunction with the resolution-of-the-identity (RI) approximation, decreasing the time required for the calculations with a minimal loss of accuracy. For \((R)-2\), all atoms were treated using the TZVP basis set, whereas for Ag(I)-(\(R_3\))-1, only the silver atom was treated with TZVP and all other atoms were treated with the SV(P) basis set. Optimizations were performed using the jobex module implemented in Turbomole. The analytical second derivative was calculated for each structure to verify that no imaginary frequencies were present, thus confirming the structure as a minimum. These calculations were done using the aoforce module available in Turbomole. Thermodynamic corrections were calculated using the freeh module available in Turbomole.

Excited state calculations were performed using the escf package in Turbomole. The first 50 excitations were evaluated for the \((R)-2\) and Ag(I)-(\(R_3\))-1 systems using time-dependent density functional theory (TD-DFT) with the functionals used in optimization (TD-B3LYP and TD-BHLYP). The excitation values, oscillator strengths and rotatory strengths are included in this document for all calculations. A uniform 0.3 eV Gaussian line broadening was applied to the oscillator and rotatory values, in order to simulate UV and CD spectra, respectively. Previous work on organic systems using TD-DFT calculations suggests a uniform phase shift to the energy of excitations. For \((R)-2\) and Ag(I)-(\(R_3\))-1, a shift of -0.85 eV was applied to the TD-BHLYP results and -0.15 eV for the TD-B3LYP calculations. The phase shift values were chosen to align the UV spectra with the experimental peak at 220 nm. While the BHLYP results required a more significant shift than the B3LYP system, the theoretical CD spectrum of Ag(I)-(\(R_3\))-1 calculated using B3LYP only went out to 265 nm, whereas the BHLYP calculation provided information through 215 nm. Thus, we have decided to only include the BHLYP results in the paper and have put the B3LYP results in the supporting information. Due to hardware limitations, calculation of additional excited states for B3LYP is unfeasible, as the escf module in Turbomole is limited to one processor and the excited state...
calculations performed for this paper were on the order of 275 hours, 25 hours short of the time limit for the hardware.

**Figure S20.** Comparison of relative bottom-of-the-well energy ($E_{bw}$) and free energy ($G$ at 298 K) values (in kcal/mol) from a variety of DFT methods for the optimization of ($R$)-2.

<table>
<thead>
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<th>Conformer</th>
<th>RI-BP86/TZVP</th>
<th>RI-B3LYP/TZVP</th>
<th>RI-BHLYP/TZVP</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>$E_{bw}$</td>
<td>$G_{298}$</td>
<td>$E_{bw}$</td>
</tr>
<tr>
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<tr>
<td>B</td>
<td>0.7</td>
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</tr>
</tbody>
</table>

**Figure S21.** Comparison of relative bottom-of-the-well energy ($E_{bw}$) and free energy ($G$ at 298 K) values (in kcal/mol) from a variety of DFT methods for the optimization of Ag(I)-($R_3$)-1.

<table>
<thead>
<tr>
<th>Helical Sense</th>
<th>RI-BP86/TZVP</th>
<th>RI-B3LYP/SV(P),TZVP</th>
<th>RI-BHLYP/SV(P),TZVP</th>
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<tr>
<td></td>
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<td>$M$</td>
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<td>5.2</td>
<td>6.5</td>
</tr>
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</table>
**Figure S22.** Calculated UV-Vis spectra of \((R)-2\) (Conformer A) using the TD-B3LYP and TD-BHLYP functionals with a TZVP basis set. The B3LYP spectra was shifted by -0.15 eV and the BHLYP spectra was shifted by -0.85 eV. A 0.3 eV Gaussian line-broadening was applied to each excitation and the spectra were normalized to the experimental peak at 220 nm.
Figure S23. Calculated UV-Vis spectra of (R)-2(Conformer A) using the second-order approximate coupled-cluster model (RI-CC2/TZVP//RI-BHLYP/TZVP). The spectrum was shifted by -0.6 eV. A 0.3 eV Gaussian line-broadening was applied to each excitation and the spectrum was normalized to the experimental peak at 220 nm.
**Figure S24.** Calculated CD spectra of (R)-2 (Conformer A) using the TD-B3LYP and TD-BHLYP functionals with a TZVP basis set. The B3LYP spectra was shifted by -0.15 eV and the BHLYP spectra was shifted by -0.85 eV. A 0.3 eV Gaussian line-broadening was applied to each excitation and the spectra were normalized to the experimental peak at 235 nm.
**Figure S25.** Calculated UV-Vis spectra of Ag(I)-(R$_3$)-I($P$) using the TD-B3LYP and TD-BHLYP functionals with a TZVP basis set. The B3LYP spectra was shifted by -0.15 eV and the BHLYP spectra was shifted by -0.85 eV. A 0.3 eV Gaussian line-broadening was applied to each excitation and the spectra were normalized to the experimental peak at 220 nm.
**Figure S26.** Calculated CD spectra of Ag(I)-(R₃)-I(P) using the TD-B3LYP and TD-BHLYP functionals with a TZVP basis set. The B3LYP spectra was shifted by -0.15 eV and the BHLYP spectra was shifted by -0.85 eV and a 0.3 eV Gaussian line-broadening was applied to each excitation. The B3LYP spectrum was normalized to the experimental peak at 260 nm and the BHLYP spectrum was normalized to 220 nm.
Figure S27. Calculated CD spectra of Ag(I)-(R3)-1(M) using the TD-B3LYP and TD-BHLYP functionals with a TZVP basis set. The B3LYP spectra was shifted by -0.15 eV and the BHLYP spectra was shifted by -0.85 eV and a 0.3 eV Gaussian line-broadening was applied to each excitation. The B3LYP spectrum was normalized to the experimental peak at 260 nm and the BHLYP spectrum was normalized to 220 nm.
Figure S28. Electron density difference plots of (R)-2(Conformer A) as calculated by TD-BHLYP/TZVP. The contour values are ±0.002 au. Excitation energies in wavelengths are provided for each excited state before and after (in parentheses) a -0.85 eV shift was applied. Excited states with large oscillator or rotatory strengths were chosen for presenting these plots.
**Figure S29.** Electron density difference plots of (R)-2(Conformer A) as calculated by TD-B3LYP/TZVP. The contour values are ±0.002 au. Excitation energies in wavelengths are provided for each excited state before and after (in parentheses) a -0.15 eV shift was applied. Excited states with large oscillator or rotatory strengths were chosen for presenting these plots.
**Figure S30.** Electron density difference plots of \((R)\)-2 (Conformer A) as calculated by RI-CC2/TZVP. The contour values are ±0.002 au. Excitation energies in wavelengths are provided for each excited state before and after (in parentheses) a -0.6 eV shift was applied. Excited states with large oscillator or rotatory strengths were chosen for presenting these plots.

S2 Excited State
267 (306) nm

S4 Excited State
255 (292) nm

S7 Excited State
229 (258) nm

S8 Excited State
215 (240) nm

S10 Excited State
208 (231) nm

S12 Excited State
198 (219) nm
Figure S31. Electron density difference plots of Ag(I)-(R$_3$)-1(P) as calculated by TD-BHLYP/TZVP. The contour values are ±0.002 au. Excitation energies in wavelengths are provided for each excited state before and after (in parentheses) a -0.85 eV shift was applied. Excited states with large oscillator or rotatory strengths chosen for presenting these plots.
**Figure S32.** DFT (RI-BP86/TZVP) calculations for relaxed potential energy scan along the N-C-C-C dihedral angle (shown in red).

<table>
<thead>
<tr>
<th>N-C-C-C Dihedral Angle (in degrees)</th>
<th>RI-BP86/TZVP energies (in hartrees)</th>
<th>$E_{bw}$ Relative Energies (in kcal/mol)</th>
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<tr>
<td>79 (Conformer B)</td>
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**Figure S33.** Monte Carlo/Molecular Mechanics (MC/MM) conformational search on (R)-2 using the MM3 force field. Bolded entries are the starting geometries for DFT optimization of conformations A and B, respectively. Dihedral angle is measured along the N-C-C-C torsion depicted (in red) on the structure below.

<table>
<thead>
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<th>Entry ID</th>
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<th>Relative PE (kJ/mol)</th>
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**Figure S34.** Monte Carlo/Molecular Mechanics (MC/MM) conformational search on Ag(I)-(R,R)-1 using the MM3 force field. The first table is the gas phase calculation and the second table is the calculation with water included as an implicit solvent. Bolded entries are the starting geometries for DFT optimization of $I_{\text{three in}}$, $I_{\text{two in}}$, $I_{\text{one in}}$ and $I_{\text{none in}}$ respectively. Dihedral is measured along the C-N-C-H torsion for each ‘arm’ as depicted (in red) on the structure below.

![Diagram of molecular structure](image)

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### Energies and Thermochemistry

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**Energies and Thermochemistry**

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ln(qrot) = 15.29 \\
ln(qvib) = 12.26 \\
chem. pot. (kJ/mol) = 517.27 \\
energy (kJ/mol) = 672.23 \\
entropy (kJ/mol/K) = 0.52807 \\
Cv (kJ/mol-K) = 0.2476201 \\
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**RI-CC2/TZVP//BLYP/TZVP**

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BHLYP/TZVP

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![Structure](image)

**BHLYP/SV(P),TZVP**

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ln(qvib) 55.5
chem. pot. (kJ/mol) 2213.85
energy (kJ/mol) 2589.78
entropy (kJ/mol/K) 1.26922
Cv (kJ/mol-K) 0.9064513
Cp (kJ/mol-K) 0.9147656
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B3LYP/SV(P),TZVP

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BHLYP/SV(P),TZVP

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Energies and Thermochemistry

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\[ \ln(q\text{trans}) \quad 21.04 \]
\[ \ln(q\text{rot}) \quad 18.01 \]
\[ \ln(q\text{vib}) \quad 56.79 \]
\[ \text{chem. pot. (kJ/mol)} \quad 2210.1 \]
\[ \text{energy (kJ/mol)} \quad 2589.74 \]
\[ \text{entropy (kJ/mol/K)} \quad 1.28164 \]
\[ \text{Cv (kJ/mol-K)} \quad 0.9071422 \]
\[ \text{Cp (kJ/mol-K)} \quad 0.9154565 \]
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$G_{298} = -3233.374734$

**B3LYP/SV(P),TZVP**

**Excited State Data (before shifting)**

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