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Electronic Supplementary Information

Intense Redox-Driven Chiroptical Switching with a 580 mV Hysteresis Actuated Through Reversible Dimerization of an Azoniahelicene

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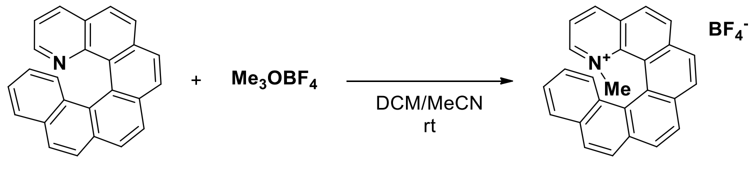
Synthetic Methods

Materials and Methods

Flash chromatography was performed on Merck or Fluorochem Silica Gel 40–63 µm particle size using a forced flow of eluent at 0.3–0.5 bar pressure.[1] HRMS measurements were obtained on a Waters LCT Premier (ES-ToF)/Acquity i-Class. Unless otherwise reported, NMR spectra were recorded between 20–25 °C on a Bruker Avance III 500 MHz instrument. Chemical shifts were referenced to the residual proton solvent peaks (^{1}H: $CDCl_3$, δ 7.26) and solvent ^{13}C signals ($CDCl_3$, δ 77.16).[2] Signals are listed in ppm, and multiplicity identified as s = singlet, br = broad, d = doublet, t = triplet, q =quartet, quin = quintet, sep = septet, m = multiplet; coupling constants in Hz; integration. Concentration under reduced pressure was performed by rotary evaporation at 25–30 °C at appropriate pressure. Purified compounds were further dried under high vacuum (0.1–0.01 mbar). 1-Aza[6]helicene was obtained according to our previously published procedure[3] and resolved by Chiral Technologies Europe (CHIRALPAK ID 5 µm – 250 x 30 mm, mobile phase CO_2/EtOH 70/30, 120 ml/min, rt 7.1 and 10.2 min for (+)-(*P*) and (−)-(*M*) enantiomers, respectively).

Synthetic procedures

(±)-1-Aza1-methyl[6]helicene tetrafluoroborate ((*rac*)-2^{+} $BF4^{-}$)

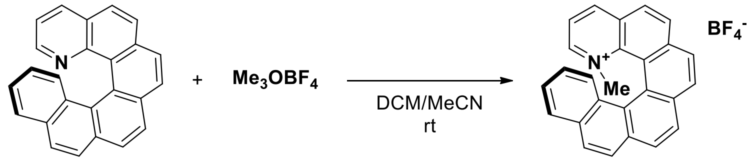


(*rac*)-**1** (*rac*)-$\mathbf{2^{+}}$ BF_4^-

(±)-1-Aza[6]helicene (30.0 mg, 91.1 µmol, 1.00 equiv.) was dissolved in a mixture of DCM (1.5 ml) and MeCN (0.5 ml). Trimethyloxonium tetrafluoroborate (13.5 mg, 91.3 µmol, 1.00 equiv.) was added at room temperature. The mixture was left to stir for 15 h, then diluted with DCM and concentrated *in vacuo*. The orange residue was treated with THF (2 ml) until it solidified, then filtered and washed with more THF (2 ml). The residue was dissolved in DCM, then filtered over a pipette filled with silica gel. The silica gel was washed with DCM until no more UV-absorption was visible on TLC, then the product was eluted with

5 % MeOH in DCM. The mixture was concentrated *in vacuo* to afford **(*rac*)-2$^+$ BF$_4^-$** as an orange powder (25.0 mg, 58.0 µmol, 64 %).

(−)-(*M*)-1-aza-1-methyl[6]helicene tetrafluoroborate ((*M*)-2$^+$ BF$_4^-$)

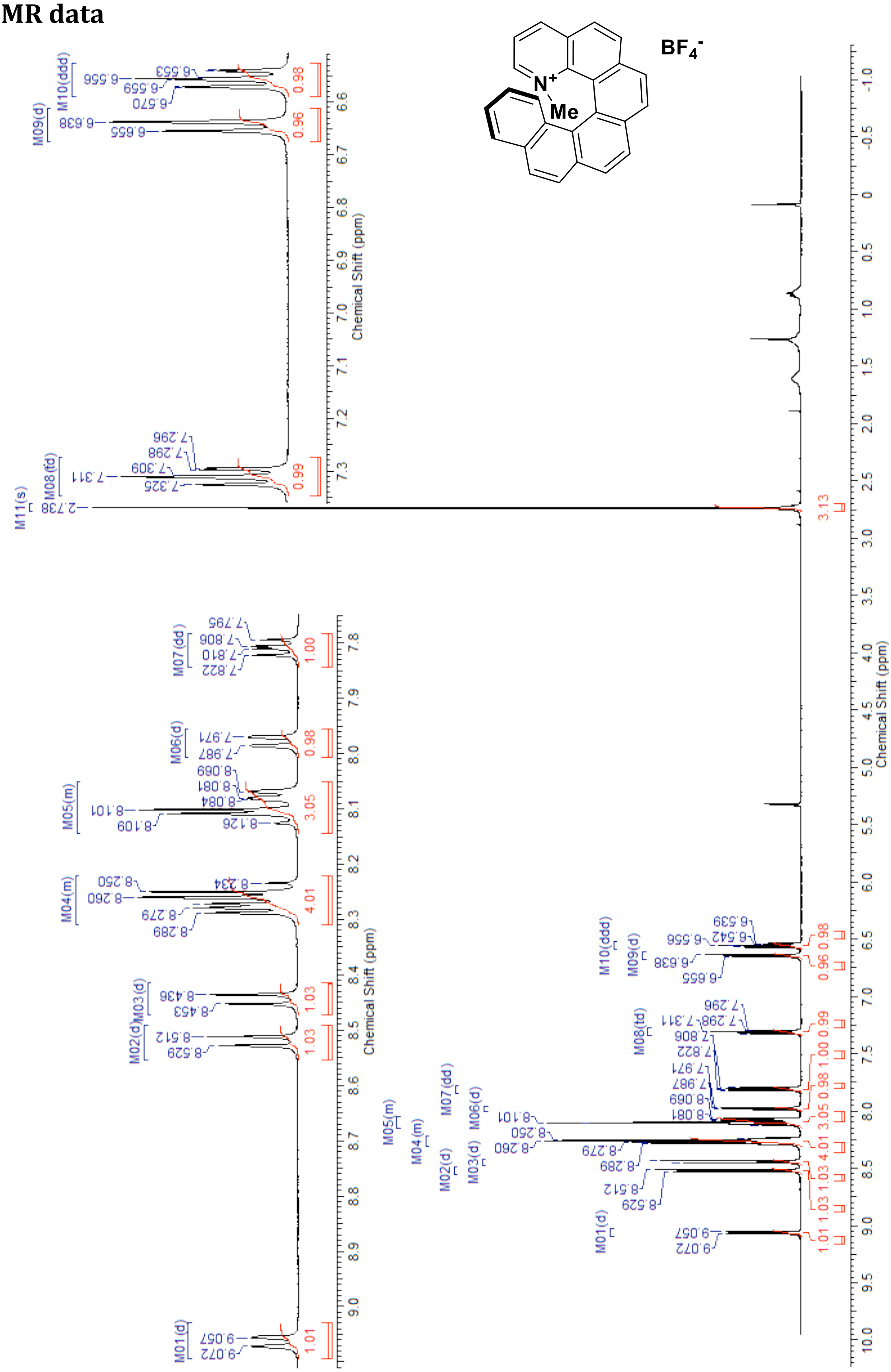


(*M*)-1 **(*M*)-2$^+$ BF$_4^-$**

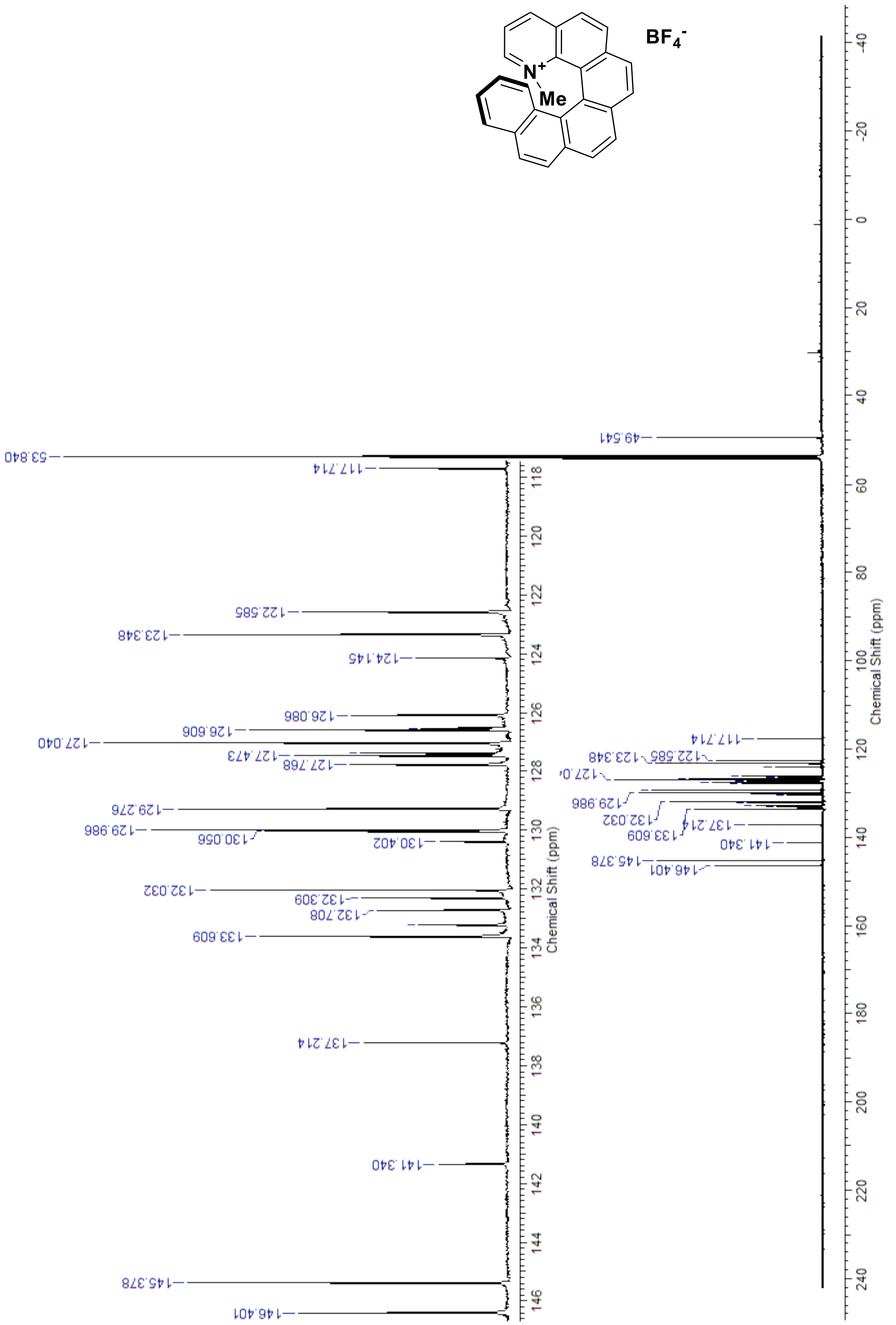
(−)-(*M*)-1-aza[6]helicene (100 mg, 0.304 mmol, 1.00 equiv.) was dissolved in DCM (1.5 ml). Trimethyloxonium tetrafluoroborate (89.8 mg, 0.607 mmol, 2.00 equiv.) and MeCN (0.5 ml) were added at room temperature. The mixture was left to stir overnight, then concentrated *in vacuo* and purified by column chromatography (60 ml silica, 12 ml fractions) using DCM (250 ml) and 2, 3, 4, and 5 % methanol in DCM (250 ml each) as eluent. Fractions 30–90 were combined and concentrated *in vacuo*. Extensive drying under vacuum afforded **(*M*)-2$^+$ BF$_4^-$** as a brown powder (69.4 mg, 0.161 mmol, 53 %).

NMR spectroscopy: ^{1}H NMR (400 MHz, CD_2Cl_2, 50 mM, δ): 9.06 (d, *J* = 7.7 Hz, 1 H), 8.52 (d, *J* = 8.4 Hz, 1 H), 8.44 (d, *J* = 8.4 Hz, 1 H), 8.22–8.31 (m, 4 H), 8.05–8.14 (m, 3 H), 7.98 (d, *J* = 8.1 Hz, 1 H), 7.81 (dd, *J* = 7.9, 5.9 Hz, 1 H), 7.31 (td, *J* = 7.4, 1.0 Hz, 1 H), 6.65 (d, *J* = 8.4 Hz, 1 H), 6.56 (ddd, *J* = 8.5, 7.0, 1.4 Hz, 1 H), 2.74 (s, 3 H). ^{13}C NMR (100 MHz, CD_2Cl_2, 50 mM, δ): 146.4, 145.4, 141.3, 137.2, 133.6, 133.2, 132.7, 132.3, 132.0, 130.4, 130.1, 130.0, 129.3, 127.8, 127.5, 127.4, 127.0, 126.6, 126.5, 126.1, 124.1, 123.3, 122.6, 117.7, 49.5. ν_{max}/cm^{-1} (neat): 3069, 2963, 2924, 2853, 1725, 1621, 1532, 1359, 1302, 1261, 1047 (s), 1033 (s), 849, 751. HRMS-ESI (m/z): calcd for $C_{26}H_{18}N$ [M−BF$_4$]$^+$, 344.1439; found, 344.1443. Optical rotation: $[\alpha]_D^{24}$ −5364° (*c* 0.44x10^{-3}g/ml, CD_2Cl_2); $[\Phi]_D^{24}$ −23130°.

NMR data



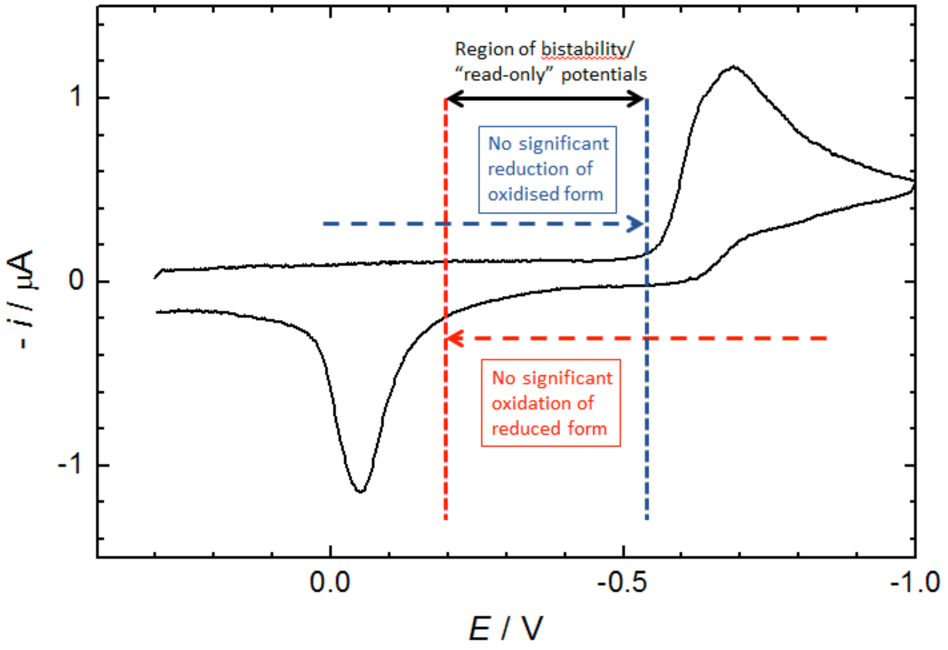
^{1}H NMR (CD_2Cl_2, 24 °C, 50 mM) of (*M*)-2$^+$BF$_4^-$



^{13}C NMR (CD_2Cl_2, 24 °C, 50 mM) of (*M*)-2$^+$BF$_4^-$

Electrochemical Measurements

Explanation of Bistable/"Read-Only" Potential Range



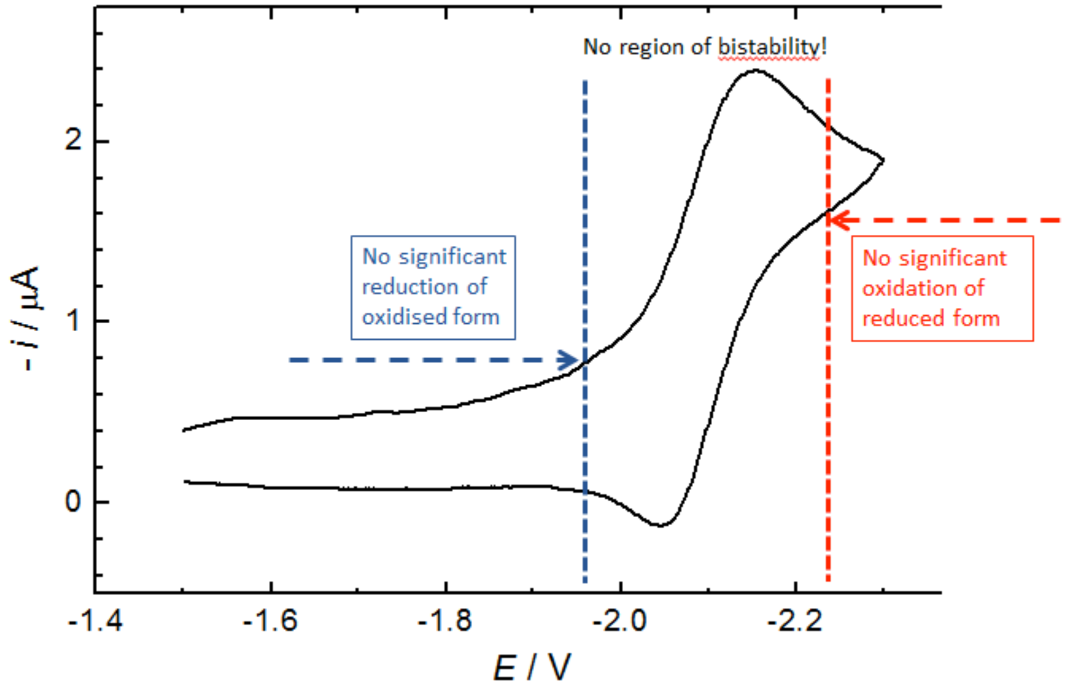


Figure S1 Top: the 580 mV hysteresis between reduction and oxidation leads to a large potential range where both the oxidised and the reduced states are stable and do not interconvert. In this "read-only" potential range, the state of the system (and thus the chiroptical read-out) only depends on its redox history, not the applied potential. Bottom: for reversible redox reactions, no such bistable region exists; the redox state (and thus the chiroptical readout) is always influenced by the applied potential. The positions of the vertical lines are for illustrative purposes only.

General Electrochemical Procedures

Redox properties were investigated by DC polarography, cyclic voltammetry (CV), AC polarography, electrochemical impedance specroscopy (EIS), spectroelectrochemistry and electronic circular dichroism spectra (ECD). Samples for electrochemical measurements were prepared in acetonitrile (AN) using 0.1 M tetra-*n*-butylammonium hexafluorophosphate ($TBAPF_6$) as the indifferent electrolyte. Solvent was dried over activated molecular sieves and $TBAPF_6$ was recrystallized from ethanol and dried in vacuum. Electrochemical measurements were performed using a system for direct current (DC) polarography, cyclic voltammetry (CV), phase–sensitive alternating current (AC) polarography, and electrochemical impedance spectroscopy (EIS). It consisted of a fast rise-time potentiostat, a lock–in amplifier (model SRS830, Stanford Research, USA) and a frequency response analyzer (model SRS760, Stanford Research, USA). The instruments were interfaced to a personal computer via an IEEE–interface card (model PCL–848, PC–Lab, AdvanTech, USA) and a data acquisition card (PCL–818, AdvanTech, USA) using 12–bit precision for A/D and D/A conversion. All data acquisition programs were written in Pascal. A three–electrode electrochemical cell was used. The reference electrode, Ag|AgCl|1 M LiCl, was separated from the test solution by a salt bridge containing 0.1 M $TBAPF_6$ in AN. The redox potential of the ferrocene/ferrocenium couple in acetonitrile against our reference electrode was 0.526 V. The working electrode for polarography was a valve–operated dropping mercury electrode (model SMDE2, Laboratorní Přístroje, Prague) with an area of 6.2×10^{-4} cm^2 and a computer controlled drop time of 1.5 s. The auxiliary electrode was a platinum wire. Oxygen was removed from the solution by passing a stream of argon saturated with vapors of the solvent. All measurements were obtained at room temperature 25°C. Spectroscopic data were measured in an optically transparent electrochemical cell (OTTLE) in combination with the electrochemical system Autolab PGSTAT30 (Metrohm, Switzerland). ECD experiment was carried out on Jasco-815 spectrometer. The reference ECD spectra were measured in acetonitrile in the spectral range from 200 nm to 600 nm in the 0.02 cm quartz cell with following parameters (concentration 0.6 mM, 2 scans, 0.1 nm steps, 50 nm/min scanning speed, 2 s time constant, 1 nm spectral bandwidth). Spectroelectrochemical ECD data were collected in the OTTLE cell placed into the ECD spectrometer and directly connected to the external electrochemical apparatus potentiostat/galvanostat Autolab PGSTAT30 (Metrohm, Switzerland). When the potential reached a value corresponding to generation of reduced form (at -1.16 V resp. -1.3 V), the potential scan was stopped and the registration of ECD spectrum started. The ECD spectrum was also recorded at the potential +0.23 V to verify reproducibility. All spectra were recorded with the following parameters (sample of concentration 0.612 mM in acetonitrile/0.2 M $TBAPF_6$, spectral range 200 nm - 600 nm, 0.019 cm OTTLE CaF_2 cell 1 scan, 0.1 nm steps, 100 nm/min scanning speed, 1 s time constant, 1 nm spectral bandwidth). Electrolysis in the OTTLE cell leads to the complete conversion to the individual redox forms within a few seconds. This is confirmed from the fast time decay of the faradaic current recorded by the electrochemical instrument. Hence the ECD spectra are not influenced by the time dependence of concentrations inside the cell. The optical switching was registered for two chosen wavelengths at 267 and 292 nm with the following parameters: the potential switched between -1.3 V and +0.30 V each potential kept during 100 s, time dependent spectrum registered with 1 s time constant, 1 nm spectral bandwidth in the scale of 800 s.

DC Polarography of (*M*)-2^+

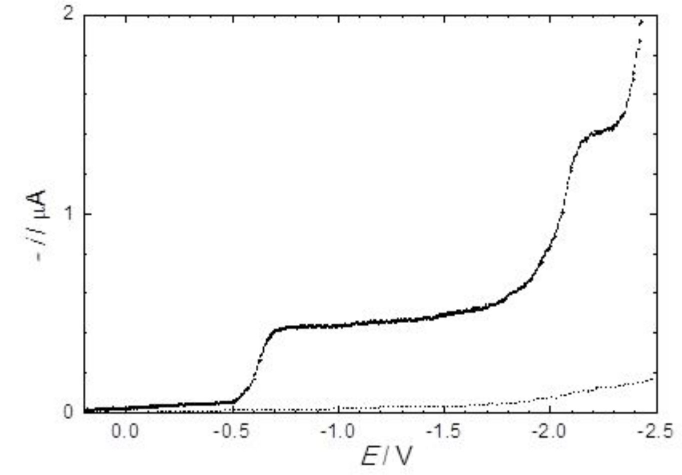


Figure S2 DC polarogram of 0.23 mM $\mathbf{2}^+$ and 0.1 M $TBAPF_6$ in acetonitrile. The dashed line is the blank.

In addition to the one-electron reduction wave of **(*M*)-2^+** ($E_{1/2}$ at -0.63 V) illustrated in DC polarogram in Figure S2, further reduction occurs at very negative potential at $E_{1/2}$ = -2.01 V and involves transfer of two electrons (see also Figure S7 for the corresponding voltammogram). The number of electrons was estimated by comparison of observed limiting currents with those of ferrocene.

The log-plot analysis of the first polarographic reduction suggests a quasi-reversible character with the limiting slope corresponding to RT/F, as expected for a one-electron wave (Figure S3). Oxidation was not detected.

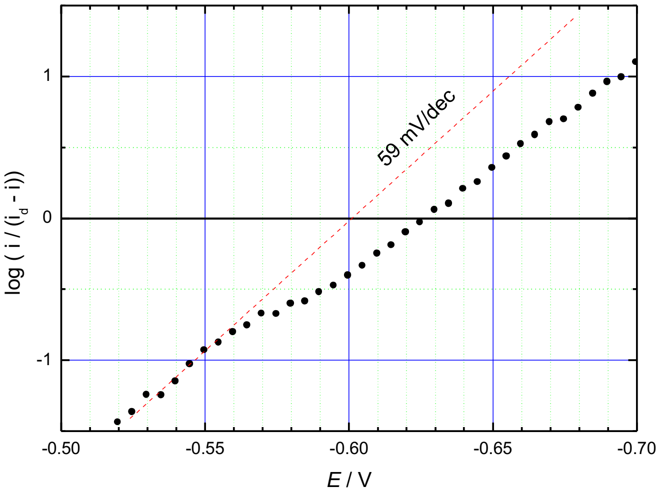


Figure S3 The log-plot analysis of the first polarographic reduction wave given in Figure S2.

Electrochemical Impedance Spectroscopy (EIS)

AC polarography with a mercury drop electrode provides additional evidence supporting the redox triggered dimerization (Figure S4).

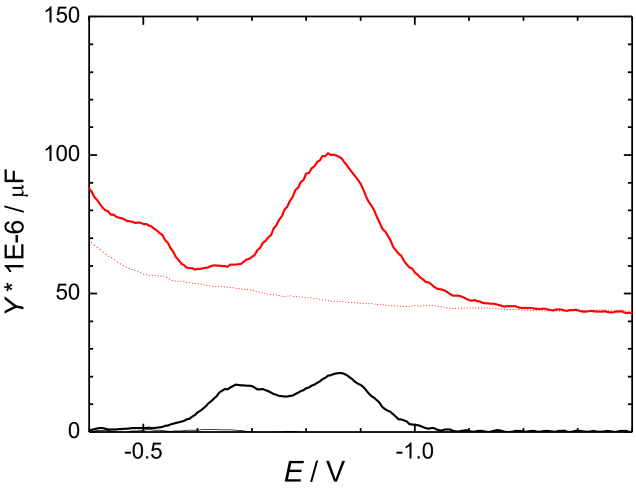


Figure S4 AC polarogram of 0.30 mM **(*M*)-2**$^{+}$ and 0.1 M TBAPF$_6$ in acetonitrile. The applied frequency was 160 Hz. The black and red curves correspond to the real and imaginary admittance components, respectively. The dashed line is the blank.

Two maxima are observed on the real admittance component *Y'*. The imaginary admittance component *Y''* yields a large maximum at -0.89 V, which is shifted to potentials more negative than $E_{1/2}$. The ratio of faradaic admittance maxima at −0.89 V is larger than unity. This suggests that the kinetics is influenced by the adsorption of a redox active form. The adsorption is further evidenced by the difference of imaginary curves in the absence (blank, dotted line in Figure S4) and in the presence of **(*M*)-2**$^+$ at potentials around -0.5 V. The mechanistic analysis of impedance or admittance data is better achieved from their dependence on the frequency ω of applied sine wave perturbation. The frequency dependence was measured in the range from 100 kHz to 1 Hz at several constant DC potentials, corresponding to peak potentials observed on AC polarograms. Vector analysis of impedance data[4] at the peak potential of the admittance yielded the solution resistance, the double layer capacitance and finally the faradaic phase angle ϕ, which contains information on the rate of the electron transfer (Figure S5).

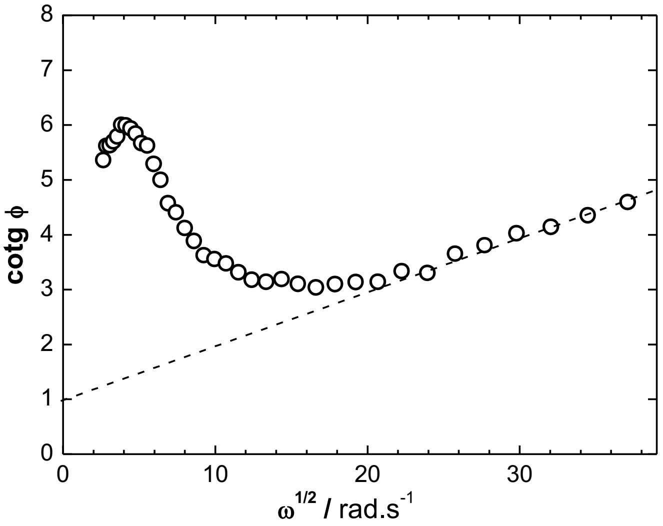


Figure S5 The dependence of the faradaic phase angle on the frequency of the sine wave signal at the DC potential -0.675 V. The slope of the linear asymptote yields the heterogeneous rate constant $k^0 = 3.08 \cdot 10^{-2}$.

The frequency dependence of cotgϕ is linear at higher frequencies and yields the heterogeneous rate constant $k^0 = 3.08 \cdot 10^{-2}$ cm·s^{-1}. However, the low frequency part passes through a maximum, which indicates the coupling of a fast electron transfer and a homogeneous chemical reaction.[5] This could be redox induced bond cleavage, radical recombination, protonation and other processes. The frequency dependence at -0.89 V (the second maximum on AC polarogram) confirmed the participation of an adsorption process related to the product (Figure S6). An analogous analysis of EIS for the reversible reduction at -2.1 V yielded the standard heterogeneous rate constant k^0 = $1.92 \cdot 10^{-2}$ cm·s^{-1} with no indication of a coupled chemical reaction. Hence both electron transfer rates are very similar.

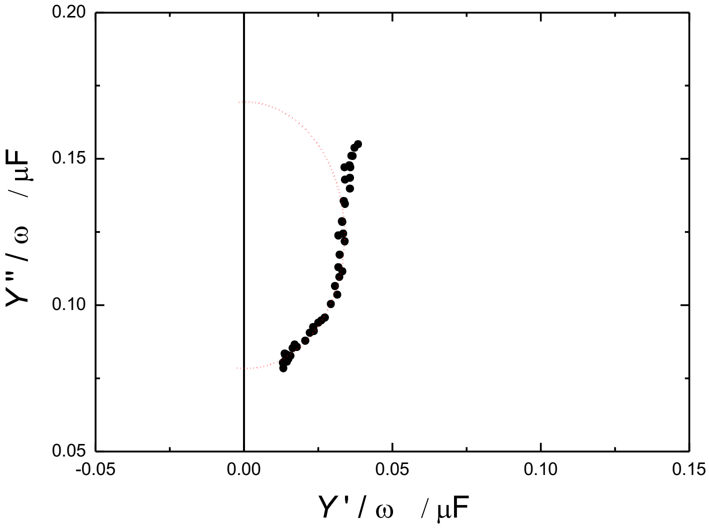


Figure S6 The complex capacitance plot of electrochemical impedance spectrum measured at applied DC potential -0.890 V corresponding to an adsorption maximum observed on AC polarogram. The shape of data plot in a form of a quarter-circle confirms the strong adsorption of a product on the electrode surface.

Additional details on Cyclic Voltammetry

The second electron transfer at -2.1 V observed on the Hg electrode is an uncomplicated reversible process (Figure S7). For voltammogram and DC polarogram of **(*M*)-2$^+$**, see Figure 2 and Figure S2, respectively.

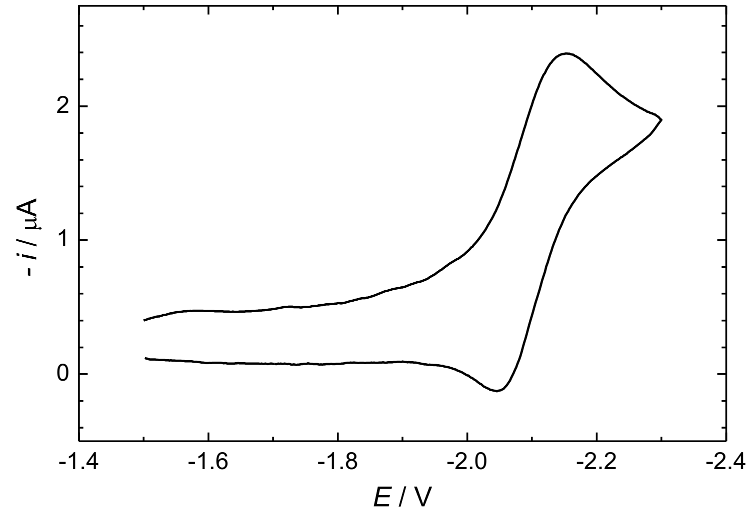


Figure S7 Cyclic voltammetry of 0.30 mM ***(M)*-2**$^+$ and 0.1 M TBAPF$_6$ in acetonitrile using the static mercury drop electrode. The scan rate was 0.5 V/s.

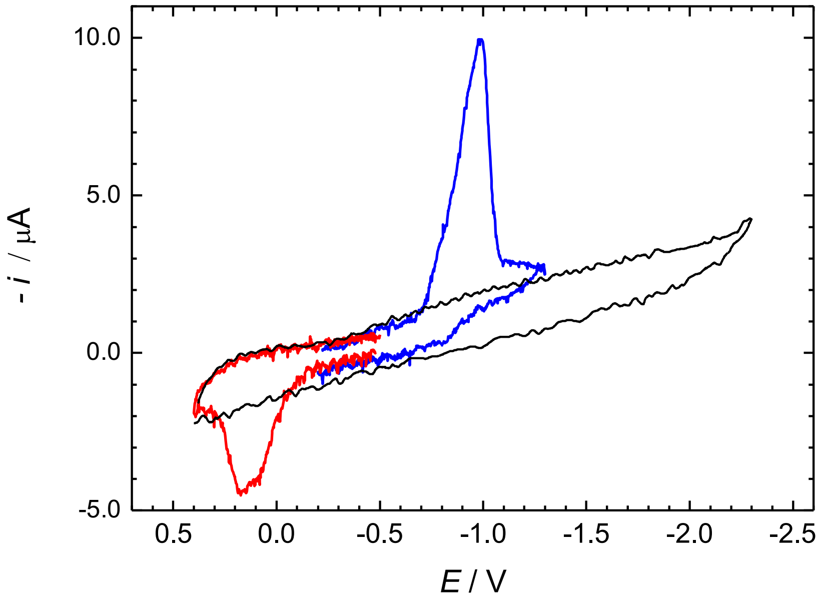


Figure S8 Cyclic voltammetry performed in an OTTLE cell experimental setup (0.67 mM ***(M)*-2**$^+$ and 0.1 M TBAPF$_6$ in acetonitrile). The applied potential was scanned at the rate of 0.005 V/s from -0.2 V to -1.2 V (blue curve) and from -0.5 V to 0.4 V (red curve). The black curve corresponds to a blank sample.

The cyclic voltammogram obtained in the OTTLE cell (Figure S8) is in agreement with the voltammogram given in Figure S7 and Figure 2 of the manuscript.

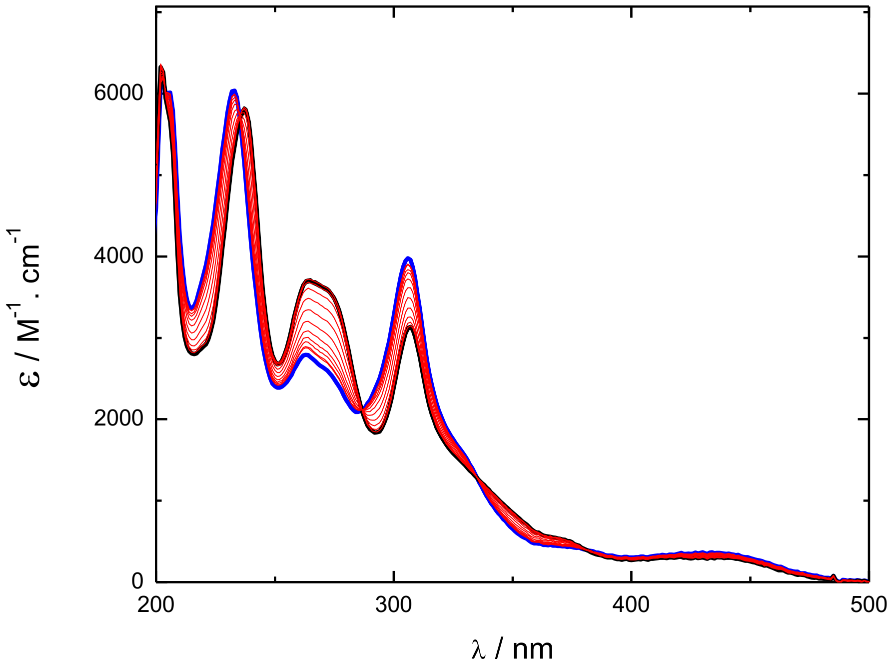


Figure S9 Cyclic voltammetry of 0.67 mM **(*M*)-2**$^+$ and 0.1 M TBAPF$_6$ in acetonitrile. The applied potential was scanned at the rate of 0.005 V/s from -0.5 V to +0.4 V. The blue curve is the spectrum after the reduction. The black curve is recorded after re-oxidation and matches with the starting curve Ox in Figure 4 of the main text.

Our results also show that the electron transfer is not coupled with the cleavage of the methyl substituent. If the methyl group would be cleaved off the compound would be changed to azahelicene. Our previous study reported the redox potential of such azahelicene,[6] which yields three redox couples at -1.80, -2.05 and -2.36 V. This is evidently not the case in the present study. Instead, the second reduction observed only on renewable Hg electrode is located at -2.09 V, which is close to the reduction of helicene core at -2.17 V reported earlier by us.[7]

Computational Methods

Analysis of ECD and dimer identity.

Time-dependent approximate coupled cluster calculations (RI-CC2)[8–10] calculations were performed to infer the nature of the electrochemical reduction product from comparison of the experimental ECD data with computationally simulated spectra, a technique that has been highly successful in the past,[11–14] for example in the investigation of chiroptical switching.[15,16] The simulation of ECD spectra of dimer **3** is complicated by the fact that numerous different isomers (regio- and stereo-) and rotamers are possible upon the dimerization event depicted in Scheme 1. Specifically, recombination of the neutral radical

$\mathbf{2}^{\bullet}$ to dimer **3** can occur to form 2,2’, 2,4’ and 4,4’ regioisomers,[17] with the newly formed C-C bond creating two new stereocentres (see below for optimised structures).

Nine different isomers were optimized at the DFT-D3(BJ)-TPSS/def2-TZVP level.[18,19] All of these isomers showed comparable energies and their ECD spectra were simply averaged for comparison. The strong coincidence between the averaged spectrum and the experimental data (see Figure 5) is fully consistent with the proposed reductive dimerization; however, based on our data it is not possible to unambiguously determine whether a single isomer or a mixture is present. *We emphasise, however, that the output of the chiroptical switching is highly robust and reproducible (Figure 6)—any negative impact caused by the putative formation of an isomeric mixture is therefore likely to be negligible. As supported by the relatively constant magnitude of the RI-CC2 results, stereoselective dimer formation would be unlikely to give a significant improvement of the chiroptical readout: The two dihydrohelicene units in* ***3*** *are electronically decoupled, hence the chiroptical response of* ***3*** *is dominated by its constituent monomers, not by their connectivity*.

General Computational Details

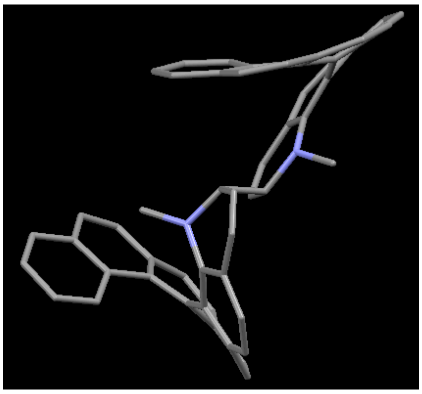
All calculations were performed on Linux-PCs by using Turbomole 7.0 program suite. Geometries were fully optimized at the dispersion-corrected density functional theory (3rd generation, DFT-D3 with BJ dumping), with AO basis-set of valence triple-ξ quality at the TPSS-D3/def2-TZVP level. The resolution of identity (RI) approximation was employed and the corresponding auxiliary basis-sets were taken from the Turbomole basis-set library. The numerical quadrature grid m5 was employed and the convergence criterion for the optimization regarding the change of total energy between two subsequent optimization cycles was set to 10^{-7} E_h.

Subsequently, the ECD spectra were calculated by the time-dependent, second-order approximate coupled-cluster singles and doubles model (RI-CC2 method), employing the def2-SVP basis-set, thus corresponding to the vertical transition approximation. The ECD spectra were simulated by expanding the calculated transitions by Gaussian function(s) where the bandwidth at 1/e height was fixed at 0.4 eV. The calculated transition energy was shifted by 0.2 eV and intensity was scaled to one third. These values are empirical without any rigorous ground but are able to successfully reproduce and match to the experimental spectra, which facilitates the direct comparison and the interpretation. Spectra were only calculated for >250 nm due to the prohibitively high cost for accurately calculating the oscillator/rotatory strength at shorter wavelengths.

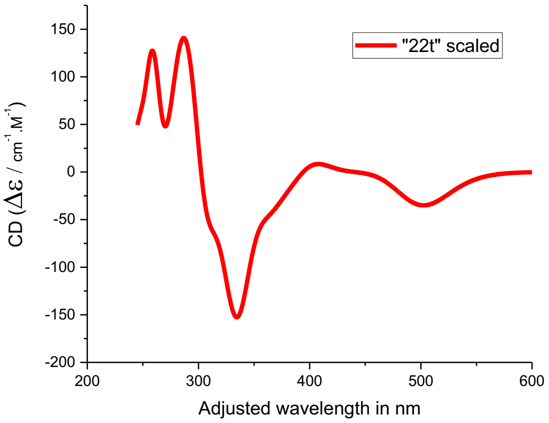
Optimized Dimer Structures and calculated ECD spectra

Only dimers having both helices of (*M*) configuration are analysed in this section.

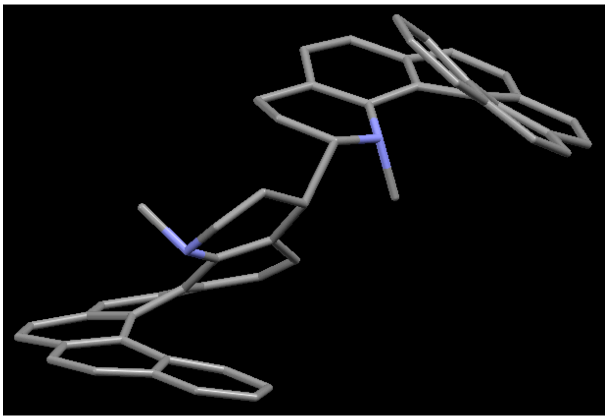
Structure of dimer (*M*),(*M*),2(*S*),2´(*R*)-trans



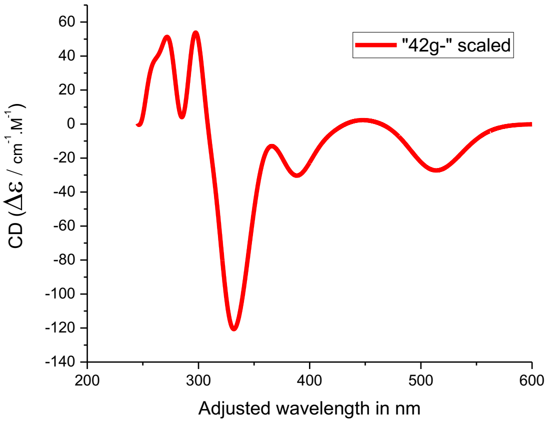
ECD spectrum of dimer (*M*),(*M*),2(*S*),2´(*R*)-trans



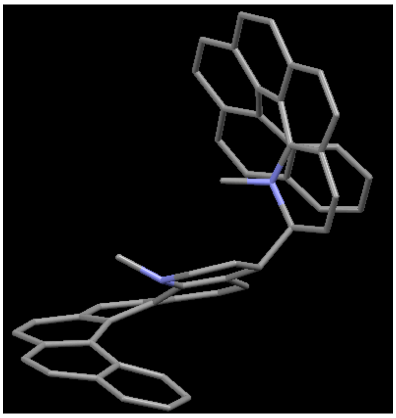
Structure of dimer (*M*),(*M*),4(*S*),2´(*S*)-gauche(−)



Calculated ECD spectrum of dimer (*M*),(*M*),4(*S*),2´(*S*)-gauche(−)



Structure of dimer (*M*),(*M*),4(*S*),2´(*S*)-gauche(+)



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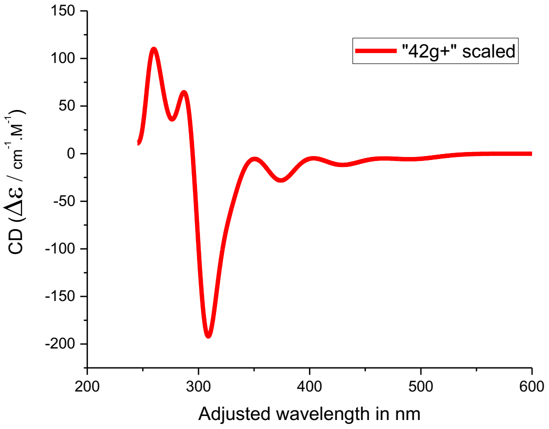

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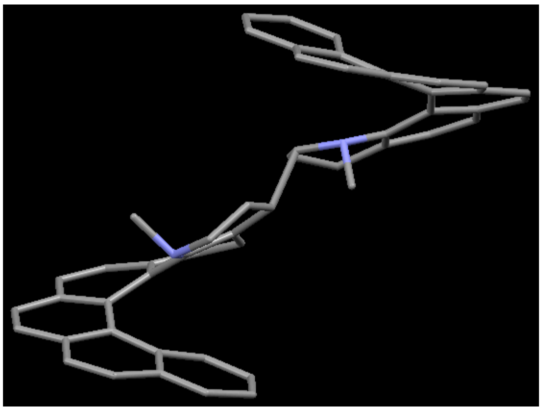
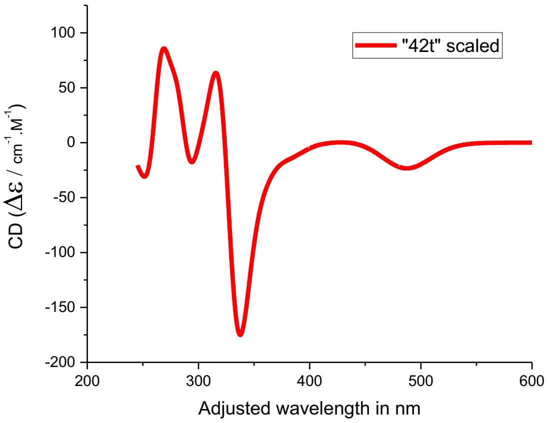
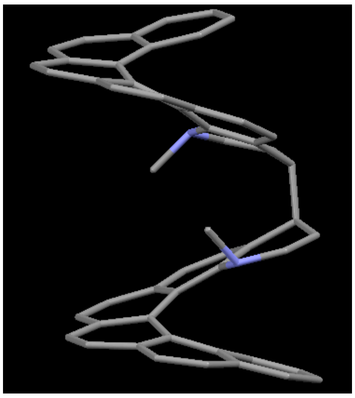


Calculated ECD spectrum of dimer (*M*),(*M*),4(*S*),2´(*S*)-trans



Structure of dimer (*M*),(*M*),4(*R*),4´(*R*)-gauche(-)



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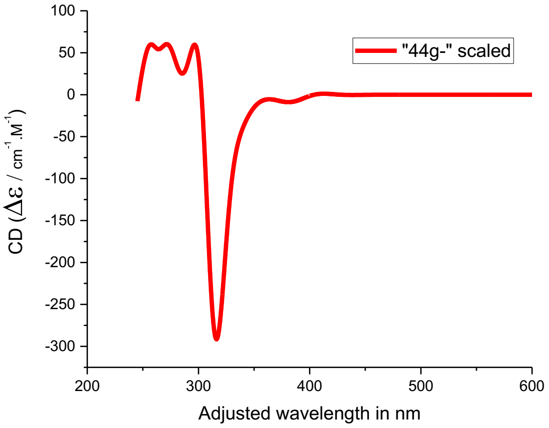

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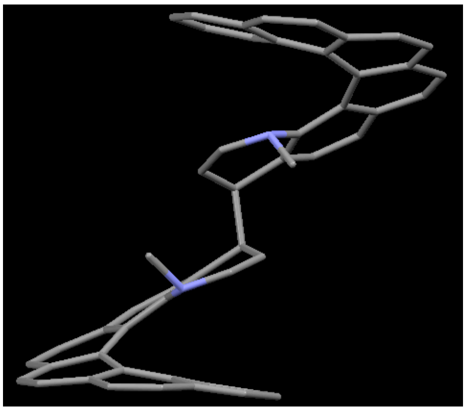
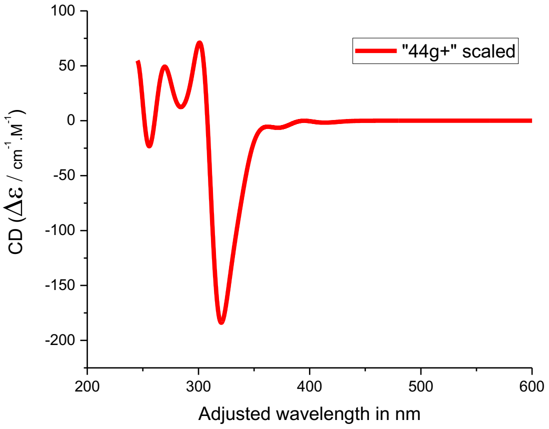
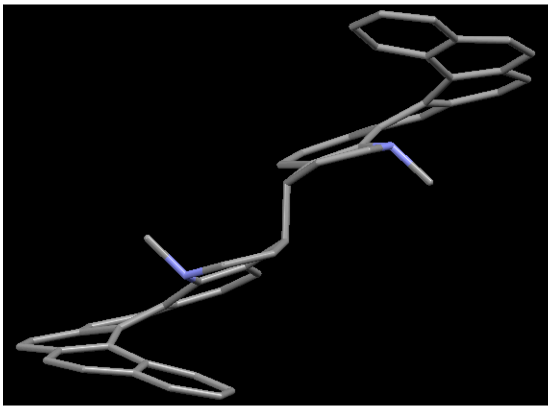


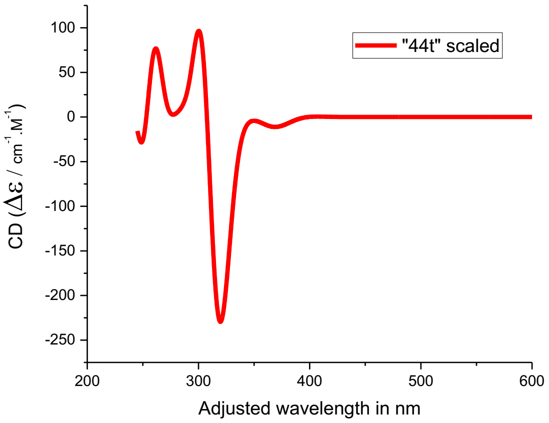
Calculated ECD spectrum of dimer (*M*),(*M*),4(*R*),4´(*R*)-gauche(+)



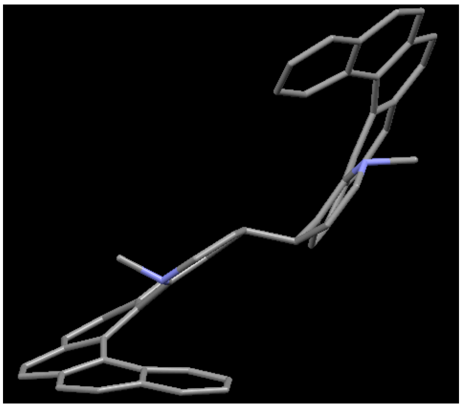
Structure of dimer (*M*),(*M*),4(*R*),4´(*R*)-trans



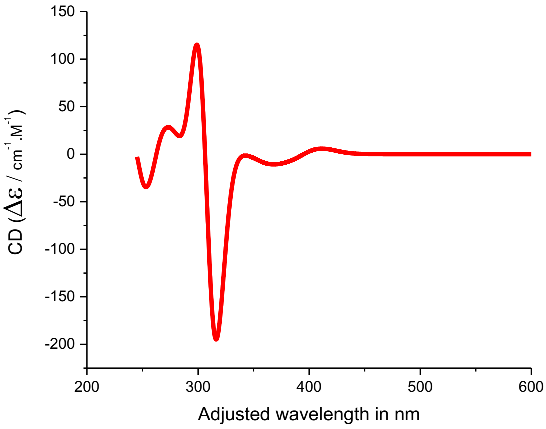
Calculated ECD spectrum of dimer (*M*),(*M*),4(*R*),4´(*R*)-trans



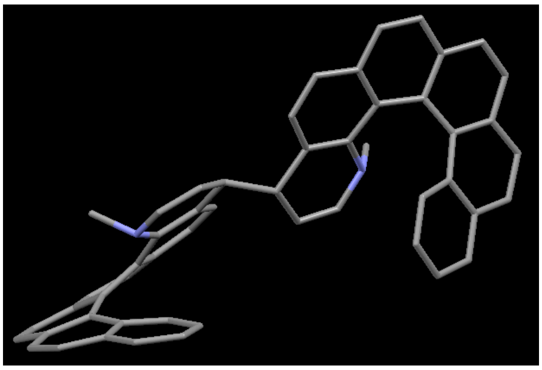
Structure of dimer (*M*),(*M*),4(*S*),4´(*S*)-trans



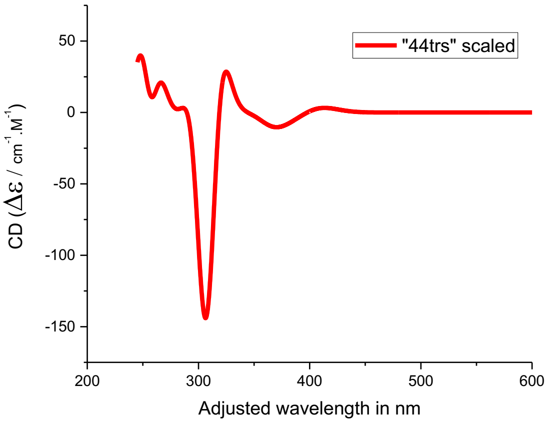
Calculated ECD spectrum of dimer (*M*),(*M*),4(*S*),4´(*S*)-trans



Structure of dimer (*M*),(*M*),4(*S*),4´(*R*)-trans



Calculated ECD spectrum of dimer (*M*),(*M*),4(*S*),4´(*R*)-trans



X-ray crystallography

1-Aza[6]helicene (1)

The main difference between the packing of the structures of the racemic[20] (**(*rac*)-1**) and enantiomerically pure ((*P*)-isomer, **(*P*)-1**, Figure S10) forms of 1-aza[6]helicene is the presence in the racemic form of a chain of π-stacked molecules of alternating chirality along the crystallographic *a* axis direction. The centroid···centroid and mean interplanar separations between ring **C** in one molecule and ring **D** in the next are *ca*. 3.94 and 3.45 Å respectively, the two rings being inclined by *ca*. 9°. There are no significant π-π interactions in the packing of the enantiomerically pure (*P*)-isomer (the closest centroid···centroid separation is *ca*. 4.40 Å).

The packing of both structures also involves a number of C–H···π contacts (

Table S1). In the structure of **(*rac*)-1** these form a chain along the crystallographic *b* axis direction. Combined with the π-π stacking, this forms a sheet of molecules in the *ab* plane (Figure S14). In the structure of **(*P*)-1** the C–H···π contacts form a complex three-dimensional network.

The X-ray crystal structure of (*P*)-1

Crystal data for **(*P*)-1**: $C_{25}H_{15}N$, *M* = 329.38, orthorhombic, $P2_12_12_1$ (no. 19), *a* = 7.3037(3), *b* = 13.0339(5), *c* = 17.4036(6) Å, *V* = 1656.75(11) $Å^3$, *Z* = 4, D_c = 1.321 g cm^{-3}, μ(Mo-Kα) = 0.076 mm^{-1}, *T* = 173 K, pale yellow needles, Oxford Diffraction Xcalibur 3 diffractometer; 5596 independent measured reflections (R_{int} = 0.0379), F^2 refinement,[21–23] R_1(obs) = 0.0483, wR_2(all) = 0.1231, 4370 independent observed absorption-corrected reflections [$|F_o| > 4\sigma(|F_o|)$, $2\theta_{\mathrm{full}}$ = 50°], 340 parameters. The absolute structure of **(*P*)-1** could not be determined [Flack parameter x = 0.2(10)], and so was assigned as the *P* enantiomer based on the comparison of the chiroptical data to literature precedent.[20] CCDC 921948.

Due to significant elongation of the thermal ellipsoids along the C–C bond direction of pairs of atoms on the outside of the curve of the helicene, [C(6)–C(7), C(9)–C(10), C(12)–C(13) and C(15)–C(16)], the structure of **(*P*)-1** was modelled using two partial occupancy orientations of the whole molecule (Figure S12 and Figure S13). The geometries of the two orientations were restrained to be similar, as were the thermal parameters of adjacent atoms. Initially both orientations were refined isotropically giving occupancies of *ca*. 51:49; when the 51% occupancy orientation was refined anisotropically this ratio changed to *ca*. 76:24. It is important to note that the two partial occupancy orientations of the molecule have the same chirality.

The position of the nitrogen atom in the initial un-split structure was determined primarily by locating the C(21)–H proton from a Δ*F* map. With just this proton missing from the structure, a difference electron density peak of *ca*. 0.43 eÅ^{-3} was located near C(21) in the right place to be the hydrogen atom, with the next largest peak being *ca*. 0.27 Å. Interestingly, peaks of *ca*. 0.17 and 0.16 eÅ^{-3} were found adjacent to N(1) in potential hydrogen atom positions, suggesting a flipping of the nitrogen position, and this was accounted for in the second orientation when the structure was split (see above).

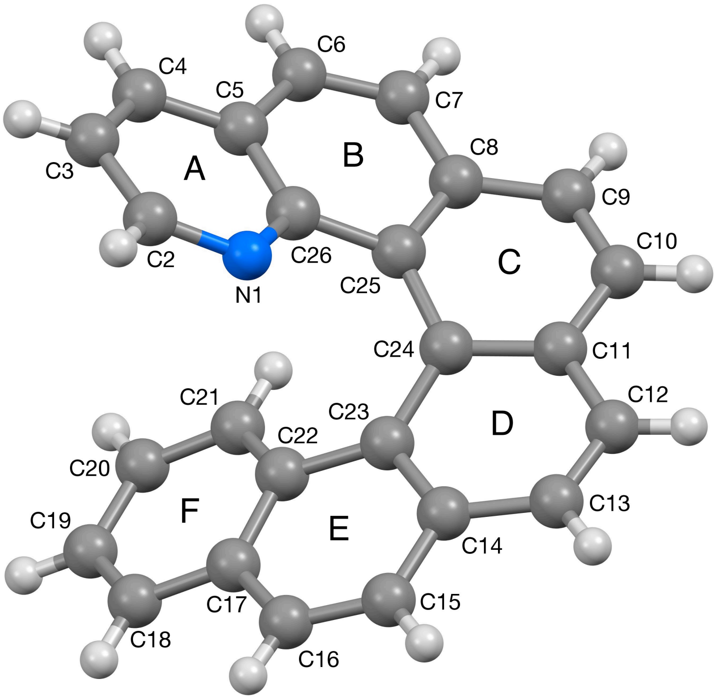


Figure S10 The crystal structure of **(*P*)-1**, showing the labelling of the aryl rings; a similar labelling scheme has been used for (***rac***)**-1**.

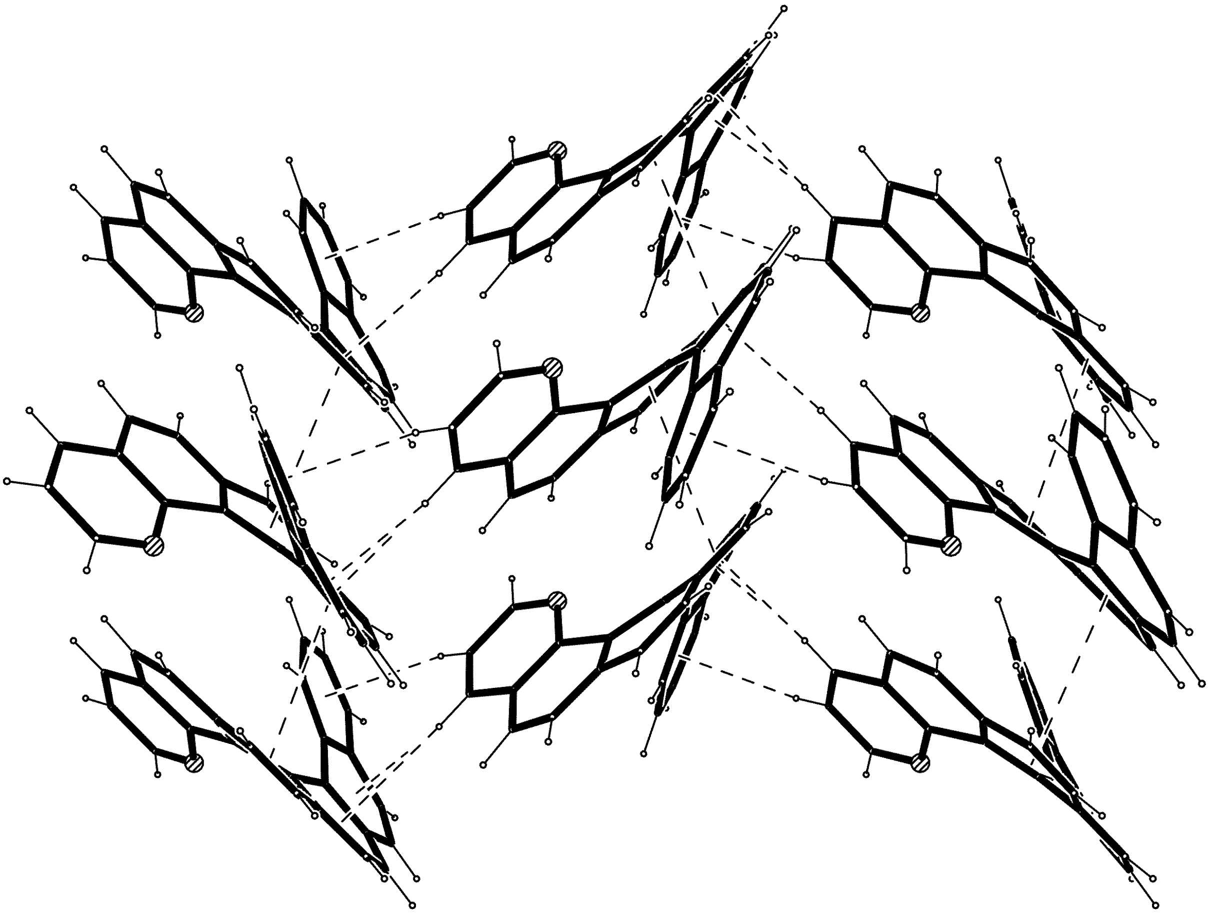


Figure S11 Part of one of the sheets of π-π and C–H···π linked molecules in the structure of (***rac***)**-1**.

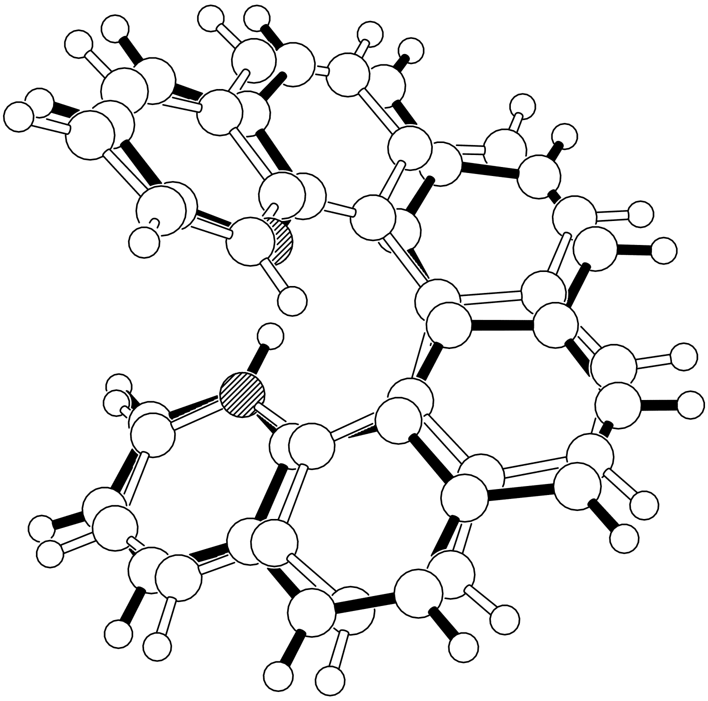


Figure S12 The crystal structure of (***P***)**-1** showing the major (dark bonds, *ca*. 76% occupancy) and minor (open bonds, *ca*. 24% occupancy) occupancy orientations.

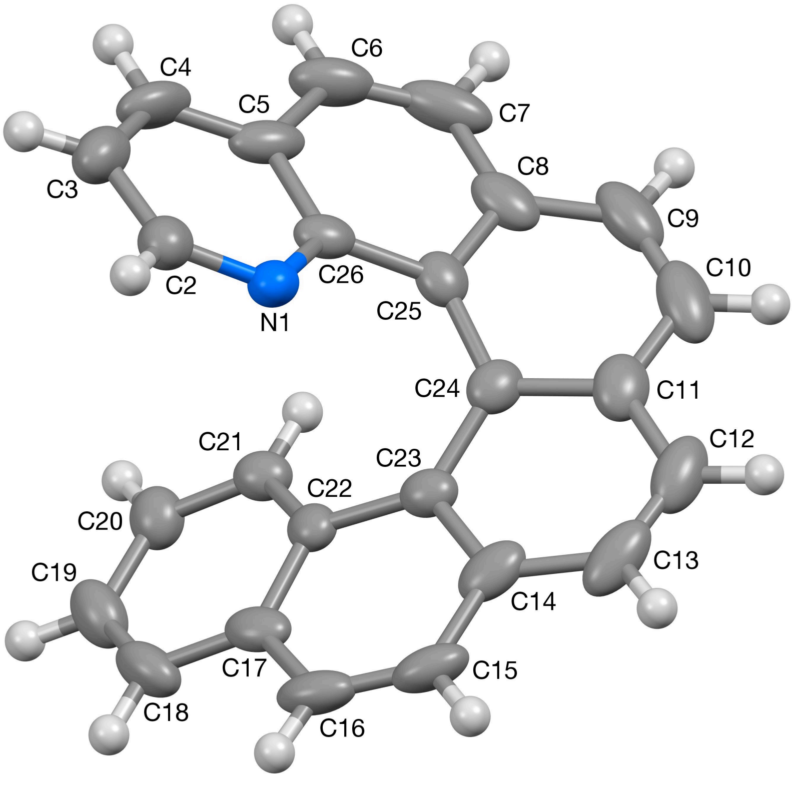


Figure S13 The crystal structure of the major occupancy orientation of **(*P*)-1** (50% probability ellipsoids).

Table S1 C–H···π interactions in the structures of **(*rac*)-1** and **(*P*)-1**.[a]

structure	aryl ring	C–H proton	H···π / Å	C–H···π / °	H···π to ring / °
rac-**1**	D	H4	3.02	162	65
	E	H4	2.74	147	72
	F	H3	2.79	142	88
P-**1**	A	H10	2.72	143	85
	E	H15	3.10	144	74
	F	H4	3.03	137	69
		H13	3.09	137	79

[a] All C–H distances normalised to 0.96 Å. See Figure S10 for the C–H proton and aryl ring labelling scheme.

Pyridinium helicene $2^+BF_4^-$

The helicene cations in the structure of **(*rac*)-$2^+BF_4^-$** form a chain of π-π and C–H···π linked molecules of alternating chirality along the crystallographic *a* axis direction (see Figure S14, Figure S16, Table S2 and Table S3). The structure of **(*P*)-$2^+BF_4^-$** was found to contain two independent cation:anion pairs, and here the dominant feature of the packing is a dimer pair formed by the back-to-back π-π stacking of the two independent cations, **[*P*-2A]**$^+$ and **[*P*-2B]**$^+$ (see Figure S15 and Table S2). These pairs are loosely linked by a couple of C–H···π interactions to form a chain along the (1,–1,1) direction (Table S3).

The X-ray crystal structure of (*rac*)-$2^+BF_4^-$

Crystal data for **(*rac*)-$2^+BF_4^-$**: $[C_{26}H_{18}N](BF_4)$, *M* = 431.22, monoclinic, $P2_1/n$ (no. 14), *a* = 11.3736(2), *b* = 9.77554(19), *c* = 18.3654(4) Å, β = 104.092(2)°, *V* = 1980.46(7) $Å^3$, *Z* = 4, D_c = 1.446 g cm^{-3}, μ(Mo-Kα) = 0.110 mm^{-1}, *T* = 173 K, yellow blocks, Oxford Diffraction Xcalibur 3 diffractometer; 6764 independent measured reflections (R_{int} = 0.0200), F^2 refinement,[21–23] R_1(obs) = 0.0628, wR_2(all) = 0.1730, 5247 independent observed absorption-corrected reflections [$|F_o| > 4\sigma(|F_o|)$, $2\theta_{full}$ = 50°], 354 parameters. CCDC 921949.

The BF$_4$ anion in the structure of **(*rac*)-2$^+$BF$_4^-$** was found to be disordered, and four orientations of *ca*. 47, 24, 17 and 12% occupancy were identified. The geometries of all four orientations were optimised, the thermal parameters of adjacent atoms were restrained to be similar, and only the atoms of the major occupancy orientation were refined anisotropically (the remainder were refined isotropically).

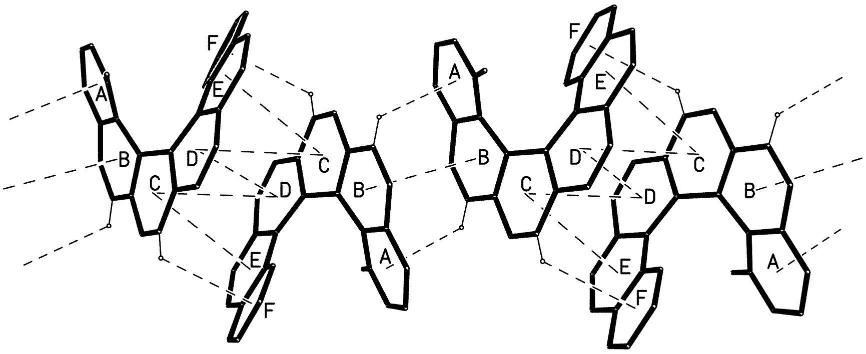


Figure S14 Part of one of the chains of π-π and C–H···π linked cations in the structure of **(*rac*)-2$^+$ BF$_4^-$**.

The X-ray crystal structure of (*P*)-2$^+$BF$_4^-$

Crystal data for **(*P*)-2$^+$BF$_4^-$**: [$C_{26}H_{18}N$](BF_4), *M* = 431.22, monoclinic, *P*2$_1$ (no. 4), a = 11.6327(3), b = 15.2299(3), c = 11.7369(3) Å, β = 105.682(3)°, V = 2001.98(9) Å^3, Z = 4 (two independent molecules), D_c = 1.431 g cm^{-3}, μ(Cu-Kα) = 0.910 mm^{-1}, T = 173 K, yellow blocks, Oxford Diffraction Xcalibur PX Ultra diffractometer; 7181 independent measured reflections (R_{int} = 0.0348), F^2 refinement,[21–23] R_1(obs) = 0.0684, wR_2(all) = 0.1997, 6599 independent observed absorption-corrected reflections [$|F_o| > 4\sigma(|F_o|)$, $2\theta_{\text{full}}$ = 135°], 622 parameters. The absolute structure of **(*P*)-2$^+$BF$_4^-$** was determined by use of the Flack parameter [x^+ = –0.05(13)]. CCDC 921950.

The structure of **(*P*)-2$^+$BF$_4^-$** was found to contain two crystallographically independent cations, **[*P*-2A]$^+$** and **[*P*-2B]$^+$**, in the asymmetric unit. One of the two associated BF$_4$ anions [that based on B(2)] was found to be disordered, and three orientations of *ca*. 68, 24 and 8% occupancy were identified. The geometries of all three orientations were optimised, the thermal parameters of adjacent atoms were restrained to be similar, and only the atoms of the major occupancy orientation were refined anisotropically (the remainder were refined isotropically).

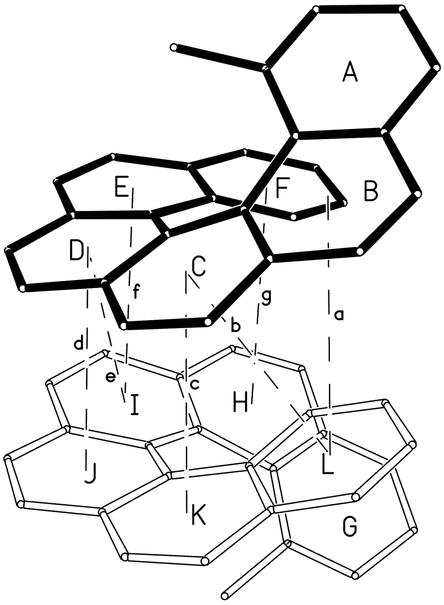


Figure S15 The back-to-back π-π stacking of the two independent cations present in the crystals of **(*P*)-2**$^+$**BF**$_4^-$; **[(*P*)-2A]**$^+$ has been drawn with dark bonds and **[(*P*)-2B]**$^+$ with open bonds.

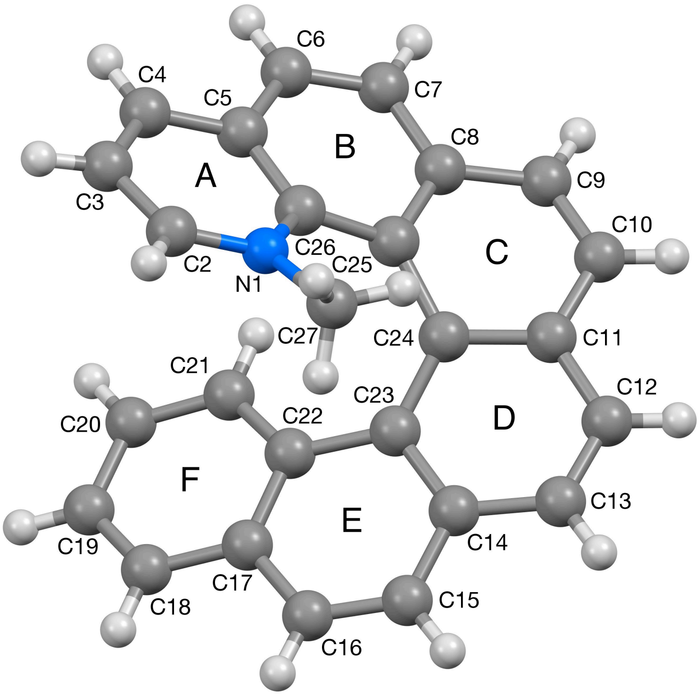


Figure S16 The crystal structure of the cation present in the crystals of **(*rac*)-2**, showing the labelling of the aryl rings; a similar labelling scheme has been used for **(*P*)-2**.

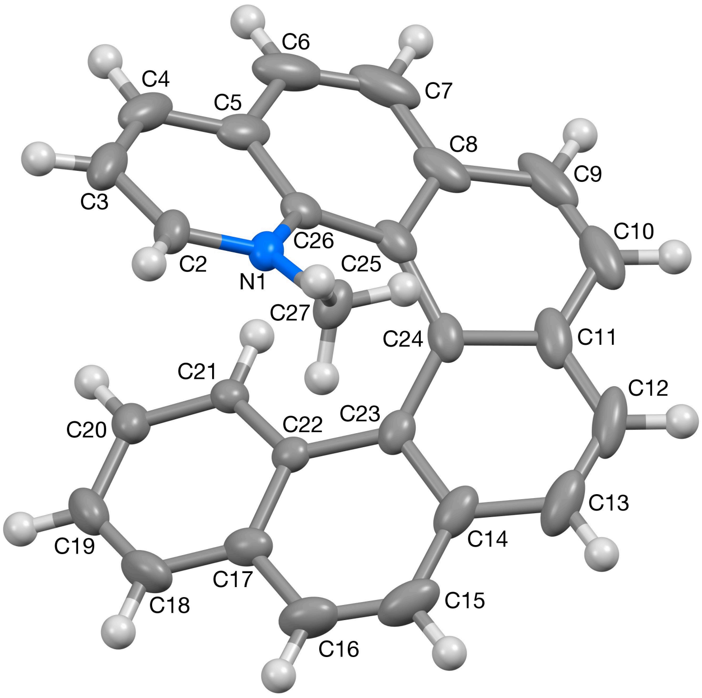


Figure S17 The crystal structure of the cation present in the crystals of **(*rac*)-2** (50% probability ellipsoids).

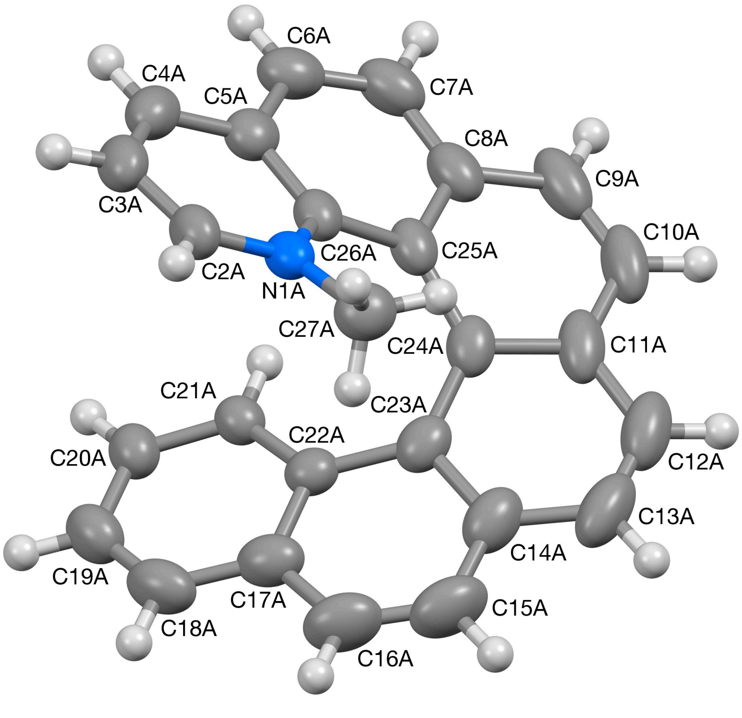


Figure S18 The crystal structure of one, **[*P*-2A]$^+$**, of the two the independent cations present in the crystals of **(*P*)-2$^+$BF$_4$**$^-$ (50% probability ellipsoids).

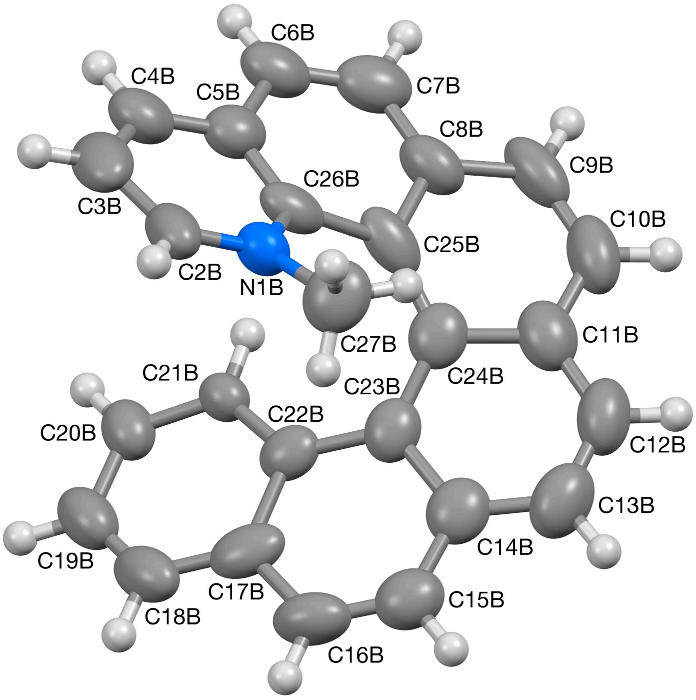


Figure S19 The crystal structure of one **[*P*-2B]**$^+$, of the two the independent cations present in the crystals of **(*P*)-2$^+$BF$_4$**$^-$ (50% probability ellipsoids).

Table S2 π···π interactions in the structures of **(*rac*)-2$^+$BF$_4$**$^-$ and **(*P*)-2$^+$BF$_4$**$^-$.[a]

structure	rings	centroid···centroid separation / Å	mean interplanar separation / Å	inclination between planes / °
(*rac*)-2	B···B	3.59	3.44	0
	C···E	3.89	3.50	23
	C···D	4.06	3.91	14
	D···D	4.14	3.86	0
(*P*)-2	B···L	4.18	3.50	19
	C···L	3.79	3.57	6
	C···K	3.88	3.50	14
	D···J	3.75	3.57	13
	D···I	3.95	3.66	24
	E···I	3.81	3.62	13
	F···H	4.06	3.68	20

[a] See Figure S15, Figure S16 for the aryl ring labelling scheme; the rings labelled G to L in cation **[*P*-2B]**$^+$ correspond to those labelled A to F in cation **[*P*-2A]**$^+$.

Table S3 C–H···π interactions in the structures of **(*rac*)-2$^+$BF$_4$**$^-$ and **(*P*)-2$^+$BF$_4$**$^-$.[a]

structure	aryl ring	C–H proton	H···π / Å	C–H···π / °	H···π to ring / °
(*rac*)-2	A	H7	3.22	103	75

	F	H10	2.99	117	82
(*P*)-2	A	H13A	3.13	142	65
	I	H18B	3.25	121	73

[a] All C–H distances normalised to 0.96 Å. See Figure S15, Figure S16 for the C–H proton and aryl ring labelling scheme; the rings labelled G to L in cation **[*P*-2B]**$^+$ correspond to those labelled A to F in cation **[*P*-2A]**$^+$, and the hydrogen atoms H13A and H18B are in cations **[*P*-2A]**$^+$ and **[*P*-2B]**$^+$ respectively.

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XYZ Coordinates of Calculated Dimer Structures

XYZ coordinates of dimer (*M*),(*M*),2(*S*),2′(*R*)-trans

90

Energy = -2114.035823902

C	-1.3738134	2.3199879	-0.1684612
C	-2.1578227	-0.9439722	2.1994294
C	-0.3369804	1.6717102	0.3750001
C	-2.6960199	1.7299245	-0.2376519
C	-3.7936631	2.4673299	-0.7228208
C	-0.4601943	0.2930789	0.9473834
C	-5.0832706	1.995669	-0.5866727
C	-2.8905037	0.4385657	0.2948059
C	-5.2982202	0.6875809	-0.104739
C	1.5711787	-2.287555	1.7244905
C	-4.1788365	-0.1705157	0.1530415
C	-6.6154749	0.2141909	0.1849362
C	0.5592204	-2.0575216	0.8701888
C	-6.8047572	-1.0205397	0.7349005
C	2.4719474	-1.1950157	2.0792552
C	3.1094489	-1.1878568	3.3387399
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C	-2.4649658	-1.3942679	-1.9839418
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C	-1.6583917	-3.609337	-1.3977904
C	3.291388	3.5865906	3.1128409
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C	2.9642301	3.581887	1.7226714
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C	5.9216753	0.1063993	-1.5147217
C	4.7874448	0.9156148	-3.4842859
C	5.7404242	0.0962705	-2.9117563
H	-1.4853179	-1.8002664	2.2941589
H	-3.1844162	-1.302069	2.2015221
H	-3.6040803	3.4609408	-1.1225895
H	-2.0101969	-0.2812086	3.0664968
H	-5.9415757	2.6210838	-0.816083
H	-7.4482179	0.8951492	0.0278241
H	-0.1846303	-2.8149541	0.6499326
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H	-0.1153178	0.3191608	1.9942292
H	-1.2460949	3.326423	-0.5617483
H	0.0438291	-0.8443564	-0.8079562

C	2.2646835	0.2471246	-1.3774798
H	2.2305807	-0.6329809	-2.0364571
H	1.5858433	1.0255805	-1.755874
H	3.2917312	0.6376776	-1.3260871
H	0.6434304	2.1465361	0.412881

XYZ coordinates of dimer (*M*),(*M*),4(*S*),2´(*S*)-gauche(−)

90

Energy = -2114.57486175

C	0.0326697	-0.8317977	-0.0719719
C	3.0858268	-0.522827	-2.1532359
C	0.7125486	-1.7681243	-1.0228605
C	1.0317521	0.2382774	0.3736436
C	0.7922758	1.2947309	1.2689079
C	2.0588441	-2.0139231	-1.0663583
C	1.6024208	2.4231629	1.3150087
C	2.3427459	0.0867682	-0.0820857
C	2.8346797	2.3549165	0.6839402
C	-0.6014729	1.2958106	-2.2236452
C	3.2497002	1.1040213	0.2404364
C	-1.8215213	0.2839789	1.2516073
C	3.6671847	3.4572594	0.5116171
C	-0.6575116	-0.1657775	-1.8786504
C	4.8798223	3.2786731	-0.1491005
C	-1.8531293	1.9441262	-1.6492801
C	-2.2478516	3.1740608	-2.1733417
C	4.6077565	0.8791075	0.0010957
C	5.3563808	1.9901874	-0.3871576
C	-1.3789869	-0.6024625	-0.7768554
C	-2.6224072	1.3541322	-0.6307745
C	-3.2993423	3.8770613	-1.6009167
C	6.5770178	1.7751065	-1.0217064
C	5.1834223	-0.4020629	0.0650866
C	7.0260211	0.475276	-1.2338451
C	6.3566408	-0.6071341	-0.6661184
C	-4.0474058	3.2942726	-0.580872
C	-3.8105193	1.9728647	-0.1848112
C	4.6920749	-1.4751595	0.8356776
C	-5.0208714	4.0642301	0.0512343
C	6.8721259	-1.8925613	-0.8244462
C	3.7402418	-1.3257943	1.8532519
C	6.2659192	-2.9793487	-0.2055377
C	5.2021114	-2.7685788	0.6679774
C	-5.6988994	3.5308355	1.1394247
C	-4.735484	1.3440088	0.6785998

C	-5.5473295	2.1820887	1.4554561
C	3.2276892	-2.3994031	2.5780511
C	4.6907247	-3.8581107	1.3769413
C	3.6875189	-3.6864146	2.3250594
C	-6.2239121	1.6922771	2.5708577
C	-4.8941469	-0.0491691	0.8489702
C	-6.09824	0.3543606	2.9195916
C	-5.4667467	-0.5208983	2.0386898
C	-4.596314	-1.0269792	-0.1220511
C	-5.4569737	-1.8758877	2.3676582
C	-4.4048944	-0.7175015	-1.4754231
C	-4.5766103	-2.3910598	0.2001878
C	-4.9512859	-2.8112189	1.4741692
C	-4.070994	-1.6769385	-2.4291317
C	-4.2231578	-3.3625083	-0.7393392
C	-3.9478662	-3.01073	-2.0567427
H	3.7117012	-1.2520586	-2.7210153
H	3.6765896	0.4170173	-2.2090907
H	-0.1212482	1.367767	1.85989
H	0.0138642	-1.2364147	0.9632217
H	0.2280179	-2.3245371	-1.8411581
H	-0.833038	0.7991073	1.2914176
H	2.1557392	-0.29556	-2.7302009
H	1.2780777	3.3353022	1.8443978
H	2.4533712	-2.8036264	-1.7350022
H	3.3378331	4.4675681	0.8074711
H	-1.7270371	-0.7131042	1.7398941
H	-2.5224604	0.8664737	1.8888525
H	-0.0070013	-0.876936	-2.4157044
H	-1.6799504	3.6392267	-2.9957469
H	5.4931624	4.1602698	-0.4011647
H	-3.5176888	4.8971341	-1.9604209
H	7.1760084	2.6234478	-1.3940817
H	7.9684261	0.3251646	-1.7876466
H	-5.1899276	5.1184768	-0.2275017
H	3.3679257	-0.3363093	2.1568328
H	7.7743328	-2.0662423	-1.4354095
H	-6.3797465	4.1809044	1.7150789
H	6.6958882	-3.9852993	-0.3494631
H	2.4731101	-2.2301709	3.3650851
H	-6.8226385	2.358586	3.2153672
H	5.0932471	-4.8730851	1.2185193
H	3.2983345	-4.5452956	2.8975116
H	-6.5877869	-0.008488	3.8395335
H	-4.5338805	0.3076932	-1.8540744
H	-5.8681048	-2.2325778	3.3276243

H	-4.9589867	-3.8797016	1.7495695
H	-3.9165845	-1.3837265	-3.4815095
H	-4.1894817	-4.4304464	-0.4642552
H	-3.6897997	-3.7803755	-2.8037118
N	2.8483022	-0.9603058	-0.8159012
N	-2.2793364	0.1421484	-0.0881662
H	-1.9841002	-1.4615123	-1.0667197
H	0.2426252	1.6902625	-2.7892047

XYZ coordinates of dimer (*M*),(*M*),4(*S*),2´(*S*)-gauche(+)

90

Energy = 2114.033846275

C	-0.1753784	-0.5825135	-2.0056221
C	-2.183987	-1.7482237	1.5109073
C	-0.4707866	-1.9912051	-1.5862273
C	-0.9629115	0.4262872	-1.1733404
C	-0.849086	1.7840775	-1.5276199
C	-1.4394652	-2.2691523	-0.705171
C	-1.4504611	2.7636526	-0.7692497
C	-1.9032617	0.044653	-0.2062903
C	-2.3662431	2.4093657	0.2436823
C	2.8577688	-2.0974425	-3.0843608
C	-2.7505354	1.0379156	0.3982302
C	1.4346209	-0.4444772	0.3751565
C	-2.9078895	3.4006652	1.1141777
C	1.8541674	-1.2234301	-3.2396597
C	-3.754095	3.0442084	2.1224762
C	3.746367	-2.0091055	-1.94073
C	4.9212022	-2.7834553	-1.8817069
C	-3.9485566	0.7664587	1.1824315
C	-4.303357	1.7283042	2.1748012
C	1.3749107	-0.3232863	-2.1377375
C	3.4114906	-1.132902	-0.8907981
C	5.7221742	-2.766321	-0.7610549
C	-5.2086499	1.3795786	3.2133921
C	-4.7896164	-0.4022864	1.0622215
C	-5.7697135	0.1330855	3.2601436
C	-5.6074571	-0.76446	2.1710985
C	5.4448093	-1.8594143	0.2834392
C	4.3752139	-0.9095077	0.1528601
C	-4.9047264	-1.2012193	-0.1428687
C	6.2097783	-1.9022493	1.4870037
C	-6.2845357	-2.0209741	2.1826756
C	-4.478743	-0.744048	-1.4125837
C	-6.2224474	-2.868533	1.1159076
C	-5.5795966	-2.4610884	-0.0901962

C	5.9016869	-1.0892416	2.5372122
C	4.3269952	0.1803466	1.1188832
C	4.9548552	-0.0327171	2.3805887
C	-4.6010908	-1.5264307	-2.542229
C	-5.6654382	-3.2595203	-1.2560648
C	-5.1720738	-2.811974	-2.4630171
C	4.6413213	0.8078316	3.4825606
C	3.6723735	1.4514507	0.9122358
C	3.7392992	1.8274001	3.3473977
C	3.2654511	2.1920591	2.0588479
C	3.436148	2.0543454	-0.3861876
C	2.385688	3.3072136	1.9171524
C	4.1314773	1.6655173	-1.5560562
C	2.5489938	3.1711981	-0.4914624
C	1.9848614	3.7406935	0.6883337
C	3.8866823	2.2600425	-2.7775089
C	2.2909982	3.7458896	-1.7591399
C	2.9341485	3.2925718	-2.8915715
H	-2.690149	-2.7172838	1.5404898
H	-2.7730503	-1.0416976	2.0904889
H	-0.1416166	2.0725164	-2.300863
H	-0.5148759	-0.4334874	-3.0450678
H	-0.0370031	-2.8160822	-2.1424412
H	0.852576	-1.3643168	0.5102554
H	-1.1914977	-1.8446864	1.9731152
H	-1.2242949	3.8129434	-0.9374077
H	-1.6386183	-3.2924936	-0.3978799
H	-2.5738621	4.4289541	1.003375
H	0.7608403	0.4130929	0.3995649
H	2.1237992	-0.3475391	1.2080292
H	1.2327107	-1.2514144	-4.1326697
H	5.1410172	-3.45956	-2.7047308
H	-4.0823362	3.7738363	2.8583487
H	6.562139	-3.4486474	-0.6650817
H	-5.416763	2.1109012	3.9902647
H	-6.398361	-0.1618186	4.096436
H	6.9927746	-2.65086	1.5759636
H	-4.0519594	0.2469487	-1.5083794
H	-6.8550706	-2.2920908	3.0676139
H	6.4104283	-1.1973883	3.4918511
H	-6.7227754	-3.8333846	1.1470304
H	-4.2649693	-1.1396664	-3.5000728
H	5.0999235	0.5970566	4.4455033
H	-6.1557572	-4.2277371	-1.189308
H	-5.2534267	-3.4302246	-3.3524228
H	3.4336534	2.4157874	4.208657

H	4.8795579	0.8847607	-1.4955462
H	2.039059	3.8085224	2.8175527
H	1.292709	4.573751	0.594661
H	4.4403248	1.9324324	-3.6527123
H	1.5971747	4.5810976	-1.8204948
H	2.7361919	3.7507821	-3.8564936
N	-2.0687655	-1.3170694	0.109498
N	2.1764899	-0.4684339	-0.8916557
H	1.4747844	0.7272533	-2.4603871
H	3.1056181	-2.784388	-3.8904467

XYZ coordinates of dimer (*M*),(*M*),4(*S*),2´(*S*)-trans

90

Energy = -2114.48154027

C	0.2264279	0.5431088	0.302085
C	2.5945867	-1.4965318	-1.6930544
C	0.2080598	-0.8857873	-0.1463016
C	1.6639021	1.0648631	0.2451678
C	2.1080952	2.3518329	0.5935098
C	1.2650283	-1.753087	-0.0726168
C	3.3235073	2.8599306	0.1503067
C	2.6461069	0.132244	-0.093719
C	4.2373972	1.9645566	-0.3830578
C	-0.8387375	3.4329879	0.5714792
C	3.9542639	0.6107455	-0.2391571
C	-2.0811591	-0.1393827	1.1046379
C	5.4153996	2.358248	-1.0117369
C	-0.3932477	2.3660467	-0.3885088
C	6.2572202	1.3745246	-1.52414
C	-2.3109959	3.1868858	0.8693734
C	-3.0567831	4.2463818	1.3836255
C	4.9900366	-0.3203057	-0.3509863
C	6.0538473	0.0391836	-1.1784834
C	-1.0503476	1.1450605	-0.4393516
C	-2.9424642	1.9516204	0.6400215
C	-4.3658664	4.0470793	1.8008687
C	6.8919485	-0.9671705	-1.6514574
C	4.9391322	-1.5835538	0.2642343
C	6.6649018	-2.2881135	-1.2776584
C	5.7202018	-2.595605	-0.3004244
C	-4.9808208	2.8160414	1.5861372
C	-4.3268496	1.8037083	0.8743777
C	4.1960415	-1.8936253	1.4211443
C	-6.2521271	2.6079255	2.1157559
C	5.5687123	-3.9172672	0.1159599
C	3.6430089	-0.9246767	2.2691108

C	4.6878326	-4.2396123	1.1415259
C	4.0343166	-3.2224643	1.8325152
C	-6.8312787	1.3510036	2.0012079
C	-5.0639232	0.6664348	0.4745908
C	-6.2336375	0.3849871	1.1939878
C	2.8716747	-1.2421897	3.3848657
C	3.2536688	-3.5590708	2.9408974
C	2.6512541	-2.5738747	3.716342
C	-6.8317114	-0.8718547	1.1272306
C	-4.7127347	-0.2251117	-0.5631742
C	-6.2665815	-1.861934	0.334892
C	-5.23309	-1.5267968	-0.5371335
C	-3.9334576	0.1049652	-1.6907715
C	-4.7648737	-2.5186135	-1.3981707
C	-3.6778592	1.4284335	-2.0743528
C	-3.4517688	-0.8851426	-2.5582993
C	-3.8223233	-2.2147632	-2.3719064
C	-2.8749254	1.7564959	-3.1648763
C	-2.6284859	-0.5738128	-3.6430255
C	-2.3170957	0.7483763	-3.9429215
H	2.7002703	-2.5908136	-1.8860551
H	3.5140089	-1.0681297	-2.1475454
H	1.4661015	3.0800275	1.0901958
H	0.2462039	0.6278004	1.4102956
H	-0.6307622	-1.3970445	-0.6452706
H	-1.3741875	0.1791618	1.9063621
H	1.7636606	-1.0828631	-2.3159844
H	3.5538191	3.9359898	0.2309454
H	1.1211572	-2.8201722	-0.331457
H	5.6362245	3.4251321	-1.1841332
H	-1.692321	-1.0703488	0.6317392
H	-3.0334432	-0.4284475	1.600918
H	0.5464645	2.4984219	-0.9513185
H	-2.591482	5.233546	1.5393281
H	7.1298187	1.6715948	-2.1301569
H	-4.8954177	4.8711367	2.308778
H	7.7123239	-0.734924	-2.3515872
H	7.3057406	-3.0768314	-1.7073168
H	-6.7610126	3.3857061	2.710569
H	3.8187437	0.149776	2.1124904
H	6.1521781	-4.7265793	-0.3552089
H	-7.7815172	1.1512979	2.5253114
H	4.5882946	-5.2945022	1.4494612
H	2.4516361	-0.441594	4.0173732
H	-7.7227766	-1.114538	1.7313342
H	3.1231805	-4.6131483	3.2395419

H	2.0508536	-2.8408767	4.6023848
H	-6.7125161	-2.8712607	0.3381086
H	-4.1246988	2.2786754	-1.5372666
H	-5.1470807	-3.5521495	-1.3389039
H	-3.4695388	-3.0116465	-3.0487224
H	-2.6907423	2.8137866	-3.4208602
H	-2.2379579	-1.3667663	-4.3033359
H	-1.6845752	0.9954516	-4.8122817
N	2.471771	-1.2160032	-0.299322
N	-2.2533924	0.8816876	0.1287025
H	-1.2412677	0.8879654	-1.4812736
H	-0.1311883	4.1881582	0.9135952

XYZ coordinates of dimer (*M*),(*M*),4(*R*),4´(*R*)-gauche(-)

90

Energy = -2114.63675949

C	-1.2832261	2.194946	-1.990387
C	-1.273246	-1.4733058	-0.9399982
C	-2.0256312	1.1994363	-2.8375586
C	-1.553872	1.8351293	-0.5399653
C	-1.333488	2.8280754	0.4127201
C	-2.3333437	-0.0605682	-2.3434815
C	-1.4044139	2.528121	1.7653331
C	-2.0010769	0.5650789	-0.1346167
C	-1.8140827	1.2599035	2.1680185
C	0.2289364	2.1454281	-2.3770759
C	-2.2525198	0.3126016	1.2340745
C	1.2897098	1.1787347	1.1627255
C	-1.7485208	0.9573976	3.5261365
C	0.9495409	3.1637702	-1.5391021
C	-2.0439791	-0.3331424	3.9429852
C	0.9036728	0.8025649	-2.1360421
C	0.7093066	-0.2025261	-3.0822656
C	-2.8695682	-0.8647988	1.7149001
C	-2.591825	-1.2392284	3.0374489
C	1.630351	2.7786886	-0.3931361
C	1.7127523	0.5424025	-1.0158358
C	1.1855592	-1.4861422	-2.8520763
C	-2.8502276	-2.5311723	3.4912854
C	-3.7202334	-1.7140819	0.9740958
C	-3.3978588	-3.4675827	2.6251134
C	-3.8676788	-3.0471764	1.3828666
C	1.9726543	-1.7416815	-1.7319403
C	2.3655459	-0.7022493	-0.8808717
C	-4.5163708	-1.3100415	-0.1162177

C	2.3405276	-3.0584674	-1.4657686
C	-4.5153136	-3.9886796	0.5838376
C	-4.7954804	0.0351105	-0.3924974
C	-5.1119851	-3.6031441	-0.6096015
C	-5.1654118	-2.248626	-0.9296819
C	3.0335751	-3.3400533	-0.2958178
C	3.3491177	-0.9597245	0.1002697
C	3.5244118	-2.2959275	0.4858248
C	-5.5491201	0.4386536	-1.492577
C	-5.9072509	-1.8603151	-2.0476175
C	-6.0875724	-0.5143688	-2.3495165
C	4.1909889	-2.6204884	1.6656926
C	4.1486153	0.0096802	0.7456636
C	4.6940933	-1.6088875	2.4726423
C	4.7066113	-0.3007494	1.9938295
C	4.5107881	1.2589718	0.2018138
C	5.3204148	0.6718016	2.7824641
C	4.3829162	1.5579273	-1.1613757
C	5.1214355	2.2459311	0.9878203
C	5.4723162	1.9676769	2.3066597
C	4.7026353	2.8053295	-1.6937792
C	5.4282774	3.5081785	0.4739637
C	5.2025717	3.8044451	-0.8663156
H	-1.5830909	-2.3560668	-1.5452365
H	-1.1485758	-1.8489984	0.0989565
H	-1.0152804	3.8382703	0.106405
H	-1.7093645	3.2028318	-2.2101659
H	-2.2046641	1.4211109	-3.9035308
H	0.1813446	1.2604821	1.0683229
H	-0.2702816	-1.1323186	-1.2890321
H	-1.1114414	3.2990877	2.4984548
H	-2.7459149	-0.7976916	-3.0538264
H	-1.3681597	1.687167	4.2613495
H	1.6320189	1.8576028	1.9772847
H	1.5152566	0.1481607	1.5143072
H	0.8167561	4.2377456	-1.7542395
H	0.1072612	-0.010689	-3.9855971
H	0.3668711	2.4380338	-3.4452024
H	-1.8745999	-0.6063876	4.9986448
H	2.011615	3.5791294	0.2641913
H	0.9202582	-2.2889142	-3.5611249
H	-2.5849254	-2.8429421	4.5160809
H	-3.5422912	-4.5039503	2.975627
H	2.0047727	-3.8899598	-2.1088354
H	-4.4475944	0.8429042	0.2688411
H	-4.5864822	-5.0460219	0.8916406

H	3.2172876	-4.3937945	-0.0245571
H	-5.6267348	-4.3609185	-1.224797
H	-5.7319431	1.5107896	-1.6780895
H	4.2864778	-3.6678796	1.9997601
H	-6.3938136	-2.6116784	-2.6926618
H	-6.6917773	-0.2081974	-3.2201539
H	5.164761	-1.8742956	3.4348261
H	4.0411338	0.8029517	-1.885453
H	5.7151756	0.4282443	3.7837688
H	5.9673122	2.7214552	2.942606
H	4.5725581	2.9988516	-2.7721759
H	5.8875648	4.2826765	1.1115967
H	5.4650017	4.7940545	-1.2769598
N	-2.2405326	-0.4343724	-1.0427779
N	1.9400119	1.5006715	-0.0613128

XYZ coordinates of dimer (*M*),(*M*),4(*R*),4´(*R*)-gauche(+)

90

Energy = -2114.60108755

C	-1.1016178	1.8546772	-0.9056387
C	-1.7666418	-1.4237686	0.9298514
C	-0.623556	0.5709027	-1.5247383
C	-2.4840908	1.5871261	-0.3367582
C	-3.2957833	2.6933913	-0.0929275
C	-1.1132257	-0.651687	-1.0866648
C	-4.5039607	2.541878	0.5718402
C	-2.9587995	0.2952953	-0.0483964
C	-4.9591526	1.264892	0.8888051
C	-0.0594397	2.3069955	0.1657571
C	-4.2677148	0.1249332	0.4595417
C	2.3724477	-0.4911176	-0.754252
C	-6.1091499	1.1605207	1.6678464
C	0.1275163	1.1705844	1.131215
C	-6.5226841	-0.0946555	2.092198
C	1.3131953	2.658156	-0.3903069
C	1.4787795	3.9157056	-0.9686458
C	-4.8939974	-1.1333831	0.6099551
C	-5.9096954	-1.2324114	1.5717373
C	1.2095487	0.3111002	1.0066314
C	2.4092062	1.7789942	-0.3356179
C	2.6647888	4.2427921	-1.6119732
C	-6.3387869	-2.4714618	2.0434294
C	-4.5702665	-2.3084566	-0.1028594
C	-5.7583803	-3.6328267	1.5521267
C	-4.9054619	-3.5509656	0.4537287
C	3.7416191	3.3607037	-1.5686083

C	3.6752709	2.1868385	-0.8091748
C	-4.0009252	-2.3415852	-1.3915098
C	4.8771931	3.6624796	-2.3166099
C	-4.4301649	-4.7453305	-0.0865414
C	-3.98029	-1.2258089	-2.2390263
C	-3.6763921	-4.7357456	-1.2530258
C	-3.5137109	-3.5353697	-1.940527
C	5.9142362	2.7403199	-2.3671394
C	4.858104	1.4429478	-0.5997039
C	5.8973356	1.6332104	-1.5209081
C	-3.3826972	-1.2452729	-3.4973978
C	-2.8938056	-3.5667305	-3.1917762
C	-2.8050551	-2.4177102	-3.9709463
C	6.9430748	0.7177729	-1.6216876
C	5.0749659	0.5064447	0.4353845
C	6.9622432	-0.3988612	-0.7968367
C	6.0518145	-0.4827925	0.2542194
C	4.4409614	0.5237347	1.6945153
C	6.1712883	-1.5613024	1.1300602
C	3.7574889	1.6451931	2.1836039
C	4.5487444	-0.5582922	2.579041
C	5.3731321	-1.6358382	2.2641449
C	3.0963474	1.650555	3.4102045
C	3.8747736	-0.5765068	3.8025198
C	3.1267325	0.5199716	4.2187355
H	-1.3113681	-2.4209294	0.7299005
H	-2.6018458	-1.610647	1.639517
H	-2.949717	3.7092869	-0.345461
H	-1.1748182	2.6115331	-1.7226707
H	0.2214163	0.5925201	-2.233994
H	1.4677751	-0.4950262	-1.4066476
H	-1.0199793	-0.7876646	1.4607953
H	-5.0722375	3.4437391	0.8571436
H	-0.6225876	-1.5624609	-1.4712696
H	-6.6361066	2.0557339	2.0402521
H	2.4710762	-1.4901027	-0.2706766
H	3.2577866	-0.3892923	-1.4193614
H	-0.6731624	0.931365	1.8516501
H	0.6432409	4.6344565	-0.9918918
H	-0.4517293	3.1747729	0.7476589
H	-7.3593275	-0.1686882	2.8079609
H	1.2178219	-0.5905472	1.6431142
H	2.7289184	5.1987364	-2.1593627
H	-7.1012103	-2.5503093	2.8373343
H	-6.0616532	-4.6057722	1.9754243
H	4.9256126	4.565852	-2.9484482

H	-4.4623684	-0.2782064	-1.955171
H	-4.6604166	-5.7162711	0.3846686
H	6.7578644	2.9227377	-3.0546845
H	-3.3155429	-5.6915736	-1.6699616
H	-3.3786868	-0.3378637	-4.1250181
H	7.7359744	0.8355849	-2.3800925
H	-2.4940175	-4.5098722	-3.6016851
H	-2.3347367	-2.4481305	-4.9682874
H	7.7610124	-1.1489029	-0.9278802
H	3.7316359	2.591813	1.6229492
H	6.9122012	-2.359827	0.9534995
H	5.4875654	-2.4933555	2.9491264
H	2.5595432	2.5533938	3.7478935
H	3.9507632	-1.445705	4.4778626
H	2.6123208	0.5139462	5.1945271
N	-2.1948249	-0.8188302	-0.2851788
N	2.2984458	0.5342708	0.2295713

XYZ coordinates of dimer (*M*),(*M*),4(*R*),4´(*R*)-trans

90

Energy = -2114.59052540

C	0.4777965	-0.506114	0.6662513
C	3.2643586	-1.4208339	-1.7746188
C	1.0757133	-1.8835956	0.7365666
C	1.6235589	0.4661088	0.4461342
C	1.3912337	1.8036373	0.7610358
C	2.2870367	-2.1619254	0.1187975
C	2.3308566	2.7718939	0.4383085
C	2.8764956	0.0746291	-0.0580693
C	3.5591018	2.3882166	-0.0932603
C	-0.5893244	-0.4861176	-0.4736914
C	3.902258	1.0356694	-0.2145833
C	-3.4931383	-0.2864455	1.9997527
C	4.4225899	3.3930469	-0.5233729
C	-1.4689888	-1.6919738	-0.2987828
C	5.6044901	3.0380881	-1.1587218
C	-1.4947465	0.7373415	-0.4762725
C	-0.9954123	1.9152815	-1.0298497
C	5.2388682	0.7114237	-0.5410061
C	6.0021287	1.7028849	-1.1741822
C	-2.7023583	-1.5795164	0.3266621
C	-2.8016562	0.7237071	0.0423385
C	-1.7198928	3.0962113	-0.9403708
C	7.1825489	1.3872227	-1.8441257
C	5.8677375	-0.5317364	-0.3112663
C	7.6193585	0.0701764	-1.8841854

C	6.9839181	-0.8782802	-1.0858779
C	-3.0076671	3.0795498	-0.4103861
C	-3.6171927	1.8727057	-0.0482991
C	5.5152685	-1.4404183	0.70654
C	-3.6658992	4.2934281	-0.2278127
C	7.5183709	-2.165944	-1.0616154
C	4.7136422	-1.0808494	1.7982232
C	7.0049013	-3.121486	-0.1942979
C	6.0411433	-2.73908	0.7357351
C	-4.905532	4.2991313	0.3980214
C	-4.9961842	1.8711682	0.2594761
C	-5.5595521	3.0943113	0.6485225
C	4.3312195	-1.9876091	2.7843948
C	5.6516065	-3.6653774	1.7058511
C	4.7776198	-3.3028279	2.7256234
C	-6.7891851	3.1419983	1.302343
C	-5.8482053	0.7446403	0.2377927
C	-7.4719798	1.9633726	1.5711385
C	-7.0208532	0.7728027	1.0057432
C	-5.6642504	-0.3995404	-0.5651283
C	-7.7927019	-0.3715737	1.2037504
C	-4.7920704	-0.4236119	-1.6618206
C	-6.4297721	-1.5573122	-0.3693579
C	-7.4615143	-1.5601346	0.5662596
C	-4.5789922	-1.5652548	-2.4318434
C	-6.213325	-2.7161603	-1.1188181
C	-5.271939	-2.7353527	-2.142776
H	3.6659163	-2.4352831	-2.000956
H	3.9689187	-0.7046695	-2.2508733
H	0.4253018	2.1193717	1.1886645
H	-0.0014382	-0.3001996	1.6529953
H	0.482919	-2.7110397	1.1625015
H	-2.5048217	-0.273536	2.5166005
H	2.2796526	-1.3019749	-2.2847765
H	2.0750293	3.8345506	0.5899763
H	2.604885	-3.2180427	0.0770325
H	4.1413897	4.4585441	-0.4649065
H	-4.0989687	-1.1298034	2.4038083
H	-4.0316281	0.6404755	2.2954044
H	-1.0728232	-2.6937001	-0.5373961
H	0.0135184	1.9404536	-1.4733509
H	-0.0954267	-0.5782326	-1.4702446
H	6.2289899	3.8292921	-1.6079051
H	-3.2384835	-2.5145709	0.5641274
H	-1.2537506	4.035572	-1.2837222
H	7.7575905	2.1570624	-2.3867724

H	8.5219911	-0.1790842	-2.4680535
H	-3.1802551	5.2530924	-0.4744705
H	4.3649911	-0.0468908	1.9406871
H	8.3679617	-2.4434059	-1.7089105
H	-5.3705219	5.2668926	0.6528266
H	7.4459664	-4.1329226	-0.1837029
H	3.6872197	-1.6623284	3.6191232
H	-7.2125453	4.097526	1.6565752
H	6.0563424	-4.6918045	1.702954
H	4.48759	-4.0288195	3.5038476
H	-8.4139669	2.0079065	2.144239
H	-4.2464957	0.4769808	-1.9817774
H	-8.6883942	-0.3507679	1.8480094
H	-8.0888332	-2.4531039	0.7296832
H	-3.8717603	-1.5402543	-3.2783116
H	-6.8083942	-3.6273274	-0.9370628
H	-5.1164069	-3.6438915	-2.7487398
N	3.1475797	-1.2334504	-0.3686174
N	-3.3403271	-0.412193	0.5906245

XYZ coordinates of dimer (*M*),(*M*),4(*S*),4´(*S*)-trans

90

Energy = -2114.55208719

C	-0.6371007	0.152059	1.2550624
C	-4.5775634	-0.8987141	1.9972914
C	-1.1728535	-0.9981023	2.0625792
C	-1.8954971	0.8446036	0.7201421
C	-1.800258	2.2183415	0.5096192
C	-2.4479083	-1.5162409	1.8900411
C	-2.8370426	2.9282532	-0.0682909
C	-3.159923	0.2379664	0.5429782
C	-3.9849868	2.2517539	-0.4660436
C	0.4122163	-0.3208255	0.193413
C	-4.1593944	0.8773182	-0.2388181
C	4.0900977	-1.2168541	-1.0082349
C	-4.983008	3.0572849	-1.0073605
C	1.2446653	-1.4483504	0.7373224
C	-6.2286442	2.5024324	-1.245046
C	1.3873384	0.7019096	-0.4024612
C	0.8230148	1.7721768	-1.0925182
C	-5.3561624	0.2728556	-0.7098136
C	-6.4098473	1.1337874	-1.0655029
C	2.6281518	-1.4821919	0.6405328
C	2.7955618	0.5926692	-0.4052509
C	1.5990025	2.7361524	-1.7156829
C	-7.718397	0.6878507	-1.2391582

C	-5.6285876	-1.113764	-0.8174246
C	-8.0156487	-0.6487269	-1.030277
C	-6.9660031	-1.5436753	-0.8441709
C	2.9849595	2.6563887	-1.6350012
C	3.6130794	1.6402761	-0.9023797
C	-4.6709994	-2.1405932	-0.9451102
C	3.7031871	3.5817532	-2.3890083
C	-7.3260298	-2.8841445	-0.7110828
C	-3.3470763	-1.8966654	-1.3322397
C	-6.3477369	-3.8631742	-0.6169026
C	-5.0177436	-3.4911457	-0.793964
C	5.0757181	3.4269489	-2.5089797
C	5.0245093	1.6915964	-0.796124
C	5.7226477	2.4669684	-1.7349026
C	-2.3860782	-2.9022169	-1.4123051
C	-4.0638276	-4.5095601	-0.8521404
C	-2.7342959	-4.2198574	-1.139627
C	7.0903421	2.3058276	-1.9503344
C	5.8170398	0.9980077	0.1436249
C	7.7936956	1.3547099	-1.225426
C	7.1620189	0.7320659	-0.1516601
C	5.3817097	0.6036344	1.4222609
C	7.9294957	-0.1317612	0.6289045
C	4.2306528	1.135123	2.0171662
C	6.1441041	-0.2607739	2.2185412
C	7.3997277	-0.68276	1.7883501
C	3.77889	0.7345547	3.2723366
C	5.6936732	-0.6879042	3.4695344
C	4.498965	-0.2082973	3.9970301
N	-3.4374294	-0.9755495	1.1317044
N	3.4128825	-0.5435904	0.0547856
H	-0.051696	0.800841	1.9065861
H	-5.4138685	-0.4696842	1.4453611
H	-4.8327304	-1.9021679	2.3379818
H	-4.3328007	-0.2672289	2.8513508
H	-0.550325	-1.4647617	2.825984
H	-0.8966028	2.7531539	0.8019936
H	-2.73176	-2.4428565	2.3889515
H	-2.7487344	4.0057206	-0.2074504
H	-0.1140243	-0.6628833	-0.6977476
H	4.7407766	-0.5076831	-1.5198923
H	4.6826852	-2.0314382	-0.5918305
H	3.3513732	-1.6130391	-1.7049583
H	-4.7756754	4.1028173	-1.2353409
H	0.7634228	-2.29014	1.2352136
H	-7.0545172	3.1357079	-1.5690764

H	-0.2608138	1.8701175	-1.1543481
H	3.1834154	-2.3214764	1.0593211
H	1.1223615	3.5488701	-2.2637734
H	-8.4980881	1.3889099	-1.5369797
H	-9.0539397	-0.9800781	-1.0142158
H	3.1853858	4.4100897	-2.8725787
H	-8.3787066	-3.1653091	-0.6807879
H	-3.0312376	-0.8849152	-1.5866161
H	-6.6282391	-4.8956693	-0.4086428
H	5.6361482	4.0529399	-3.2033522
H	-1.3609765	-2.6556304	-1.6888215
H	-4.3584963	-5.5432823	-0.6713405
H	-1.9722977	-4.9991186	-1.1541366
H	7.6029637	2.9257386	-2.6858813
H	8.8192604	1.1084639	-1.500525
H	8.9486504	-0.3764598	0.329662
H	3.6484607	1.8945502	1.4952251
H	7.9650013	-1.4311561	2.3437498
H	2.8634614	1.1600988	3.6834357
H	6.2799531	-1.4049174	4.0442238
H	4.1249071	-0.557954	4.9592778

XYZ coordinates of dimer (*M*),(*M*),4(*S*),4´(*R*)-trans

90

Energy = -2114.56297691

C	0.7042455	0.2410893	-1.3446716
C	4.5391838	-0.0645989	-2.2866638
C	1.2812242	-0.8948311	-2.1439657
C	1.818705	0.8254224	-0.4781497
C	1.4893802	1.935087	0.3002383
C	2.6312587	-1.2110937	-2.1185451
C	2.4490674	2.5774905	1.0678424
C	3.1533936	0.3691854	-0.4862528
C	3.7429405	2.0663995	1.1188422
C	-0.6074593	-0.2448827	-0.6508619
C	4.0924417	0.8915313	0.4381047
C	-3.2456888	2.4309763	0.7186027
C	4.6875772	2.810431	1.8221578
C	-0.7365585	0.1178143	0.7942533
C	6.0190413	2.4254437	1.7707465
C	-1.9098141	0.0984062	-1.3778823
C	-1.9676138	-0.1635888	-2.7464232
C	5.3843492	0.3501704	0.652882
C	6.3608847	1.2138801	1.1740885
C	-1.8770941	0.7387374	1.2860708
C	-3.0459581	0.6390737	-0.7409942

C	-3.0912986	0.1426841	-3.4958148
C	7.7190442	0.9080931	1.1103944
C	5.7996668	-0.9705161	0.3615919
C	8.1283482	-0.2770492	0.5171068
C	7.1675107	-1.2268766	0.1784986
C	-4.2303903	0.6051484	-2.8472335
C	-4.271361	0.7355109	-1.4515823
C	4.9577777	-2.1005437	0.3087584
C	-5.3029395	0.9598641	-3.661681
C	7.6324833	-2.4455915	-0.3149379
C	3.6639367	-2.107073	0.8470227
C	6.7457388	-3.4847547	-0.5619605
C	5.41243	-3.3296464	-0.1901909
C	-6.4268155	1.5239141	-3.0789606
C	-5.5320732	1.0052225	-0.8636815
C	-6.5302805	1.547501	-1.6900809
C	2.8178138	-3.2115923	0.7704143
C	4.5713844	-4.4403569	-0.2925814
C	3.2603698	-4.3840006	0.1688817
C	-7.6775202	2.1414951	-1.1678386
C	-5.8817136	0.7932153	0.4901853
C	-7.8498422	2.2025567	0.2068216
C	-6.9694973	1.5001106	1.02653
C	-5.2660264	-0.1325713	1.3576777
C	-7.2394348	1.5125889	2.394583
C	-4.4582754	-1.1859247	0.9073373
C	-5.5103096	-0.1063819	2.7378503
C	-6.4640098	0.7600632	3.2660429
C	-3.7807466	-2.0444138	1.7719304
C	-4.8268936	-0.946698	3.6191939
C	-3.9191465	-1.8820071	3.1437283
N	3.5779711	-0.5937208	-1.3697835
N	-2.9990877	1.0323179	0.5761436
H	0.4414507	1.0551535	-2.0605412
H	5.3684037	0.492296	-1.8012165
H	5.0336608	-0.8860415	-2.8549335
H	4.0670678	0.6418984	-3.0098264
H	0.6362728	-1.4979774	-2.8009694
H	0.4736648	2.362774	0.2618682
H	2.9562649	-2.0485289	-2.7609636
H	2.1689265	3.4975962	1.6090235
H	-0.5802541	-1.3597463	-0.6034711
H	-4.1466265	2.7842923	0.1735726
H	-3.4275055	2.691291	1.7867659
H	-2.3855812	3.0327484	0.3408377
H	4.4225322	3.7563623	2.325089

H	0.0996779	-0.1137491	1.4768677
H	6.7811804	3.0823054	2.2242757
H	-1.1089871	-0.5668542	-3.2966364
H	-1.8752621	0.9828144	2.3626806
H	-3.0631912	-0.0006856	-4.5900041
H	8.4864351	1.6119997	1.4759277
H	9.2079915	-0.4813706	0.4142469
H	-5.2470755	0.8913541	-4.7618121
H	8.7073834	-2.6178334	-0.4962164
H	3.2630153	-1.2370532	1.3885232
H	7.1320148	-4.4455897	-0.9431762
H	-7.2322822	1.9057916	-3.7297091
H	1.8028787	-3.1637749	1.2008654
H	4.939785	-5.3946113	-0.7062588
H	2.6028013	-5.2677466	0.1099731
H	-8.435584	2.6091865	-1.819522
H	-8.7296857	2.728831	0.615343
H	-8.0703115	2.108369	2.8100858
H	-4.3239067	-1.3839432	-0.1667258
H	-6.6836191	0.7881563	4.3471108
H	-3.1193122	-2.8315479	1.371692
H	-4.9907159	-0.877421	4.708294
H	-3.3618267	-2.501456	3.8551555