Supplementary Information

Pivotal Role of Transition Density in Circularly Polarized Luminescence

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Step-by-step tutorial on the nuclear ensemble approach

Step 1. Perform geometry optimization and vibrational analysis of the first singlet or triplet excited state of a molecule using Gaussian 16.

Keywords:

#p opt td(singlet) freq cam-b3lyp def2svp em(gd3bj)

#p opt td(triplet) freq cam-b3lyp def2svp em(gd3bj)

Step 2. Prepare a template file for NewtonX. The 'name.log' file refers to the Gaussian output file that is normally terminated in step 1.

obabel -i g09 **name**.log -o xyz -O **name**.xyz

xyz2nx < **name**.xyz

cp **name**.log gaussian.log

mkdir JOB_AD

echo 'def2svp' > JOB_AD/basis

cp **name**.gjf JOB_AD/gaussian.com

Step 3. Generate the input files for NewtonX.

nxinp

select “1. GENERATE INITIAL CONDITIONS”

nact= 2

numat = ‘the number of atoms’

npoints =1000

file_geom = geom

iprog = 4

file_nmodes = gaussian.log

anh_f = 0.953

temp= 300

ics_flg = n

chk_e = 0

nis= 1

nfs= 2

kvert = 1

de =100

prog= 6.5

iseed = -1

lvprt = 1

Step 4. Generate a bunch of Gaussian input file.

echo 0 \n 100 | finaloutput2dynmld.pl

obabel -i xyz dyn.mld -m -o gjf -O osc

Step 5. Perform excited-state calculations using Gaussian 16.

Keywords:

#p td(singlet) cam-b3lyp def2svp

Step 6. Collect the relevant information from Gaussian output files and then calculate the average values.

For Oscillator strengths ($\bar{f}$), angles ($\bar{\theta}_{E,M}$) between the electric and magnetic transition dipole moments, and rotatory strengths ($\bar{R}$), we calculate the arithmetic mean, i.e., $\bar{R} = \frac{\sum_{i=1}^{n} R_i}{n}$.

For the dissymmetry factor ($\bar{g}$), we calculate the weighted average, i.e., $\bar{g} = \frac{\sum_{i=1}^{n} (g_i \times f_i)}{\sum_{i=1}^{n} f_i}$, starting from the experimental formula[1] for the *g*-factor ($g = \frac{I_L - I_R}{\frac{1}{2}(I_L + I_R)} = \frac{2\sum_{i=1}^{n}(I_{Li} - I_{Ri})}{\sum_{i=1}^{n}(I_{Li} + I_{Ri})} = \frac{\sum_{i=1}^{n}\left[\frac{2(I_{Li} - I_{Ri})}{I_{Li} + I_{Ri}} \times (I_{Li} + I_{Ri})\right]}{\sum_{i=1}^{n}(I_{Li} + I_{Ri})}$) and considering the correlation between oscillator strength and observed emission intensity.

Data analysis of the Dalton output files

Dalton provides implementations of the calculation of the radiative $T_1 \rightarrow S_0$ transition process. Considering T_1 has three degenerate sub-states (m = 0, ±1), the transition velocity dipole moment and orbital angular momentum of the three sub-states are given by the matrices:

$$DIPVEL = \begin{bmatrix} u_{1x} & u_{1y} & u_{1z} \\ u_{2x} & u_{2y} & u_{2z} \\ u_{3x} & u_{3y} & u_{3z} \end{bmatrix} \text{a.u.} \quad (1)$$

$$ANGMOM = \begin{bmatrix} L_{1x} & L_{1y} & L_{1z} \\ L_{2x} & L_{2y} & L_{2z} \\ L_{3x} & L_{3y} & L_{3z} \end{bmatrix} \text{a.u.} \quad (2)$$

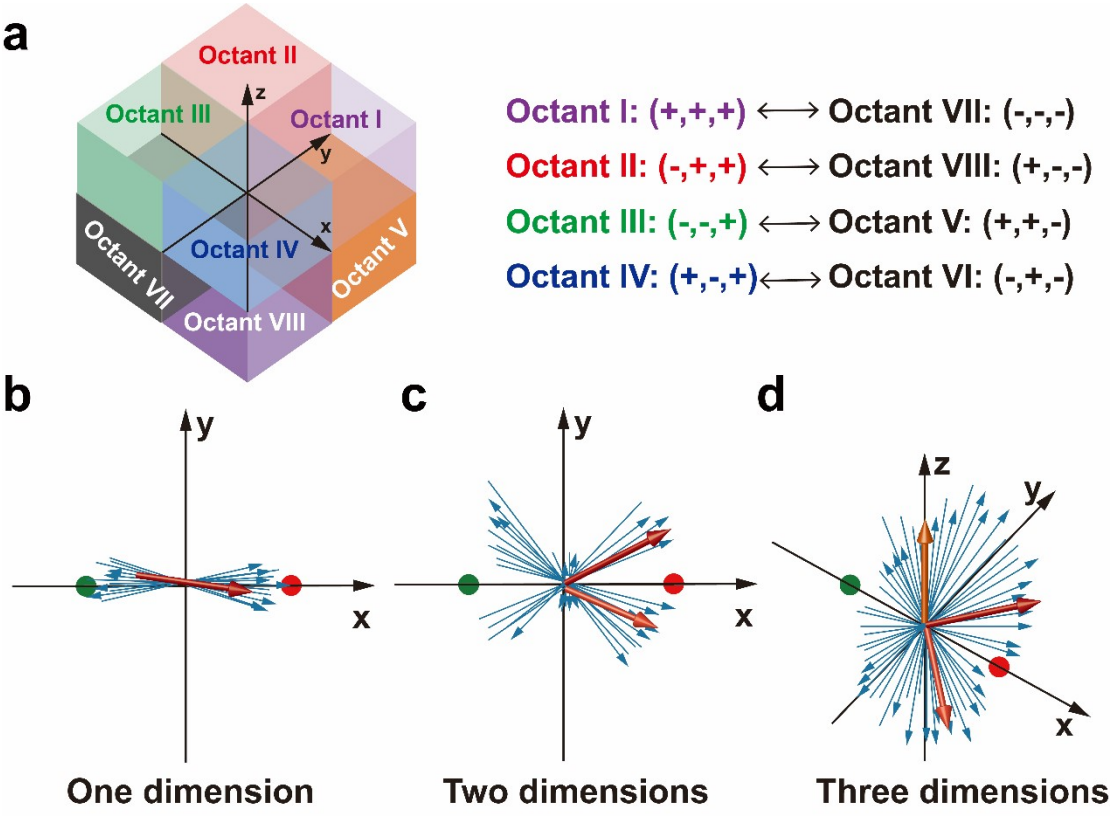
Equations (1) and (2) allow for accurate simulation of rotatory strength (R) and dissymmetry factor (g) of circularly polarized phosphorescence:

$$R = -\frac{1}{2c}\left[\left(u_{1x} \bullet L_{1x} + u_{1y} \bullet L_{1y} + u_{1z} \bullet L_{1z}\right) + \left(u_{2x} \bullet L_{2x} + u_{2y} \bullet L_{2y} + u_{2z} \bullet L_{2z}\right) + \left(u_{3x} \bullet L_{3x} + u_{3y} \bullet \right.\right. \quad (3)$$

$$g = \frac{4R}{\left[\left({u_{1x}}^2 + {u_{2x}}^2 + {u_{3x}}^2\right) + \left({u_{1y}}^2 + {u_{2y}}^2 + {u_{3y}}^2\right) + \left({u_{1z}}^2 + {u_{2z}}^2 + {u_{3z}}^2\right)\right]} \quad (4)$$

Singular value decomposition (SVD)

The SVD implemented in NumPy was used on the electric and magnetic dipole transition moments (EDTMs and MDTMs) from the ensemble to obtain principal components, which represent the main directions of the EDTMs and MDTMs. We know that, in three-dimensional space, a plane can be defined by the three points it contains, as long as those points are not on the same line. First, the geometry center (the center of three atoms) of the donor plane (green point) and the acceptor plane (red point) were placed on the X-axis (Y=0). Then, the midpoint of the donor-acceptor line (two-point one line) was set as the origin of the three-dimensional coordinates. Finally, SVD was used to reduce the data sets (n × 3 matrices) of EDTMs and MDTMs into three mutually orthogonal vectors (3 × 3 matrices) (EDTM 1, EDTM 2, and EDTM 3; MDTM 1, MDTM 2, and MDTM 3), respectively (see Scheme S1).



Scheme S1. (a) Eight-octant representation of 3D space. (b) One vector of one-dimensional space obtained via the singular value decomposition (SVD) method. (c) Two vectors of two-dimensional space obtained via the SVD method. (d) Three vectors of three-dimensional space obtained via the SVD method.

Table S1. Oscillator strengths, supplementary angles between the electric and magnetic transition dipole moments, rotatory strengths, and optical *g*-factors for absolute configurations (*S* or *M*), as evaluated from stationary-point calculations and the nuclear ensemble approach.

Molecule	stationary point calculation				nuclear ensemble approach				exptl	
	f	$\theta_{E,M}$	R	g	$\bar{f}$	$\bar{\theta}_{E,M}$	$\bar{R}$	$\bar{g}$	g_{PL}	State of matter
S_p-CzpPhTrz	3.0E-1	77	5.0E-39	8.5E-4	2.8E-1	74	4.2E-39	7.6E-4	1.3E-3	In toluene
(+)-(*S*,*S*)-CAI-Cz	2.0E-2	124	-1.7E-39	-3.7E-3	1.8E-2	114	-1.5E-39	-3.1E-3	-1.1E-3	Film state
(*S*)-OBN-Cz	4.8E-2	75	7.6E-40	6.6E-4	4.2E-2	70	4.4E-40	4.3E-4	5.6E-4	In toluene
(*M*)-Pt(mppy)(acac)	4.1E-6	94	-1.2E-42	-1.1E-3	4.0E-6	98	-2.2E-42	-5.0E-3	-1.2E-2	In CH_2Cl_2
(M)-hetero[6]helicene	3.3E-2	69	8.4E-39	1.0E-2	4.0E-2	70	8.3E-39	7.4E-3	9.0E-3	In $CHCl_3$
(*M*)-methyl[6]helicene	1.8E-3	80	8.5E-41	2.4E-3	1.7E-2	87	4.0E-40	2.9E-5	5.0E-5	-
iso-(*S*)-OBN-CzB1	1.9E-2	113	-1.1E-39	-2.8E-3	2.2E-2	110	-6.9E-40	-1.6E-3	-2.1E-3	In toluene
iso-(*S*)-OBN-CzC1	3.3E-2	91	-7.5E-41	-1.1E-4	2.9E-2	91	-1.1E-42	-3.2E-5	-1.0E-4	In toluene
(-)-(*S*)-Cz-Ax-CN	6.4E-3	115	-1.6E-39	-1.2E-2	1.0E-2	105	-1.2E-39	-4.1E-3	-5.7E-3	Film state
(*S*)-OSFSO	6.6E-3	83	7.1E-40	5.3E-3	6.6E-3	82	9.4E-40	9.7E-4	1.4E-3	In toluene

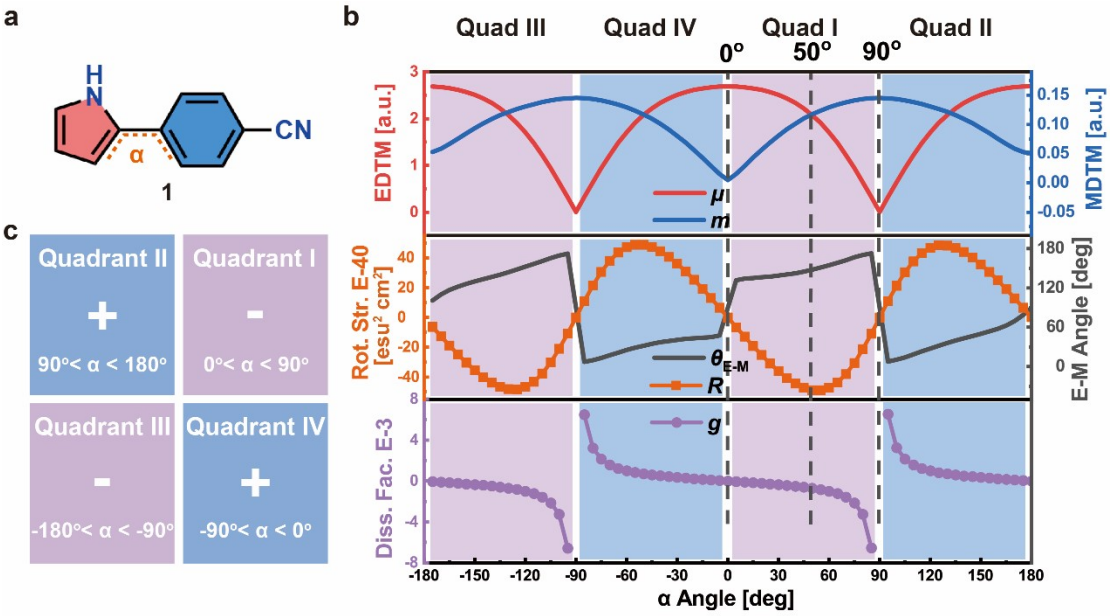
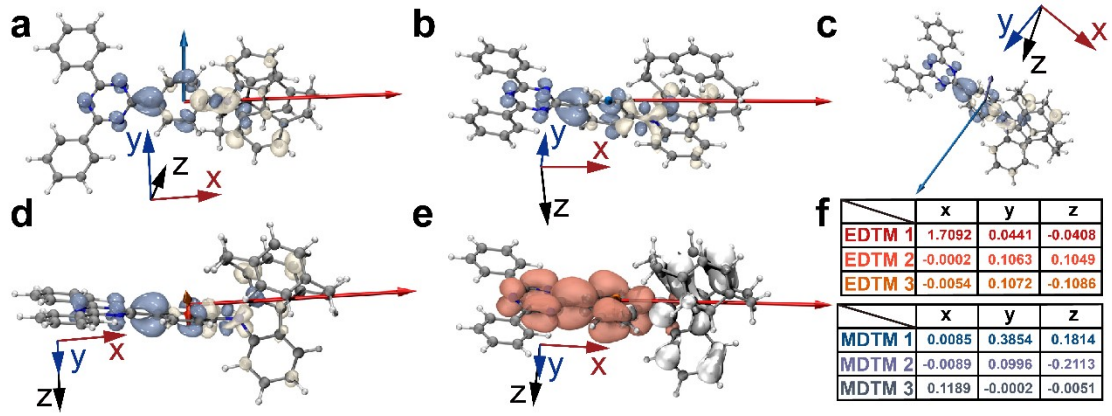


Figure S1 (a) Chemical structure of molecule **1**. (b) EDTM (red, in atomic units), MDTM (blue, in atomic units), E-M angle ($\theta_{E,M}$, grey, in units of deg), rotatory strength (orange, in units of E-40 esu^2·cm^2), and dissymmetry factor (violet, in units of E-3) as a function of α (in units of deg). (c) Four-quadrant diagram.



	x	y	z
EDTM 1	1.7092	0.0441	-0.0408
EDTM 2	-0.0002	0.1063	0.1049
EDTM 3	-0.0054	0.1072	-0.1086

	x	y	z
MDTM 1	0.0085	0.3854	0.1814
MDTM 2	-0.0089	0.0996	-0.2113
MDTM 3	0.1189	-0.0002	-0.0051

Figure S2 R_p-CzpPhTrz. (a) Front view of electric dipole transition moment 1 (EDTM 1), magnetic dipole transition moment 1 (MDTM 1) and transition density (TD) plots. (b) Bird's-eye view of EDTM 1, MDTM 1 and TD plots. (c) MDTM 1, MDTM 2, MDTM 3 and TD plots. (d) EDTM 1, EDTM 2, EDTM 3 and TD plots. (e) EDTM 1, EDTM 2, EDTM 3 and natural transition orbitals. (f) x, y and z components of EDTM 1, EDTM 2, EDTM 3, MDTM 1, MDTM 2, MDTM 3. See the above "SVD" section for the origin of EDTM 1-3 and MDTM 1-3.

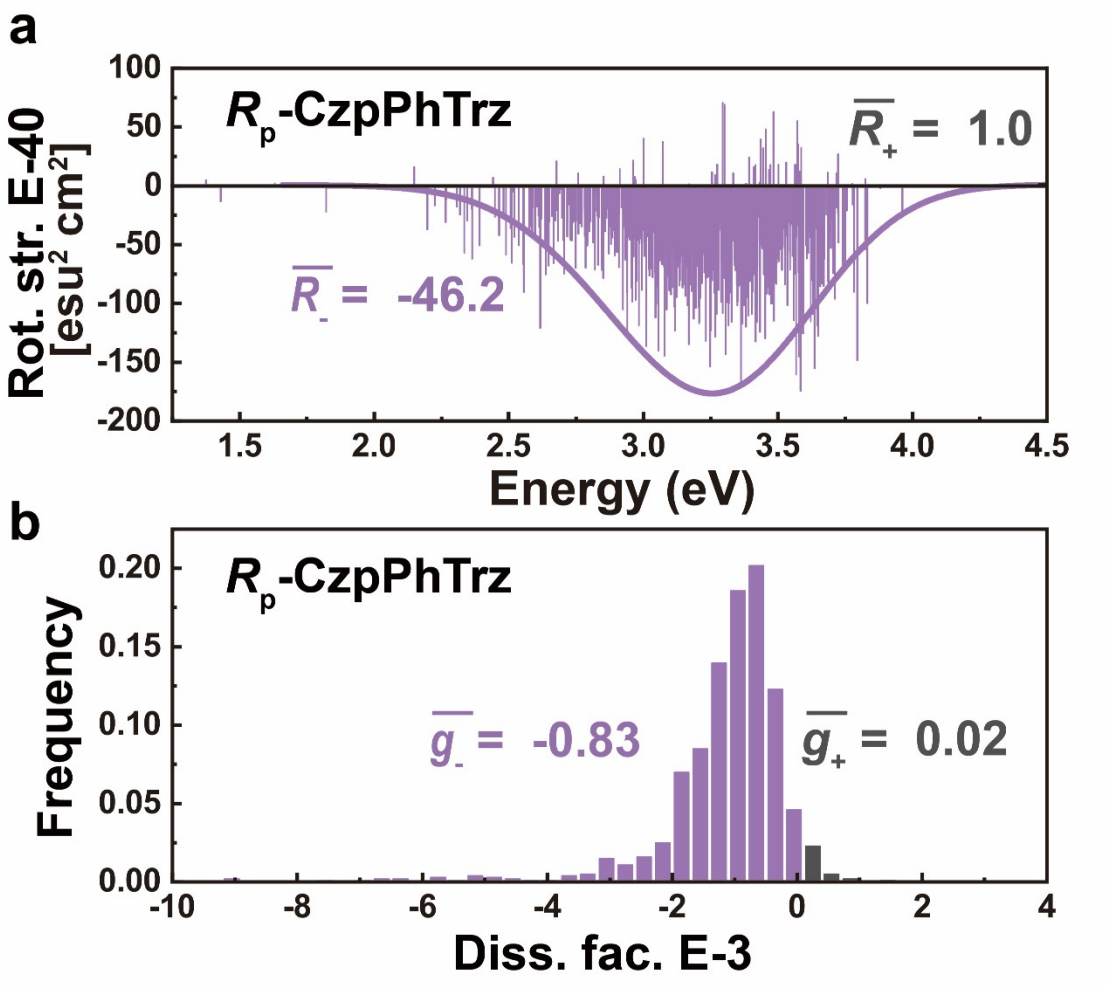


Figure S3 (a) Rotatory strength and simulated CPL spectra based on nuclear ensembles of R_p-CzpPhTrz. (b) Histogram of optical *g*-factor of R_p-CzpPhTrz.

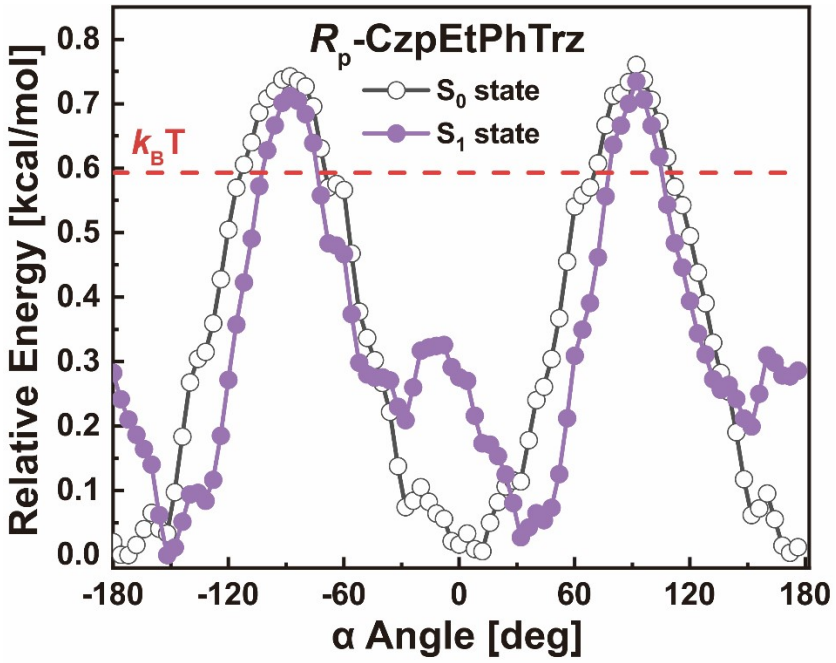
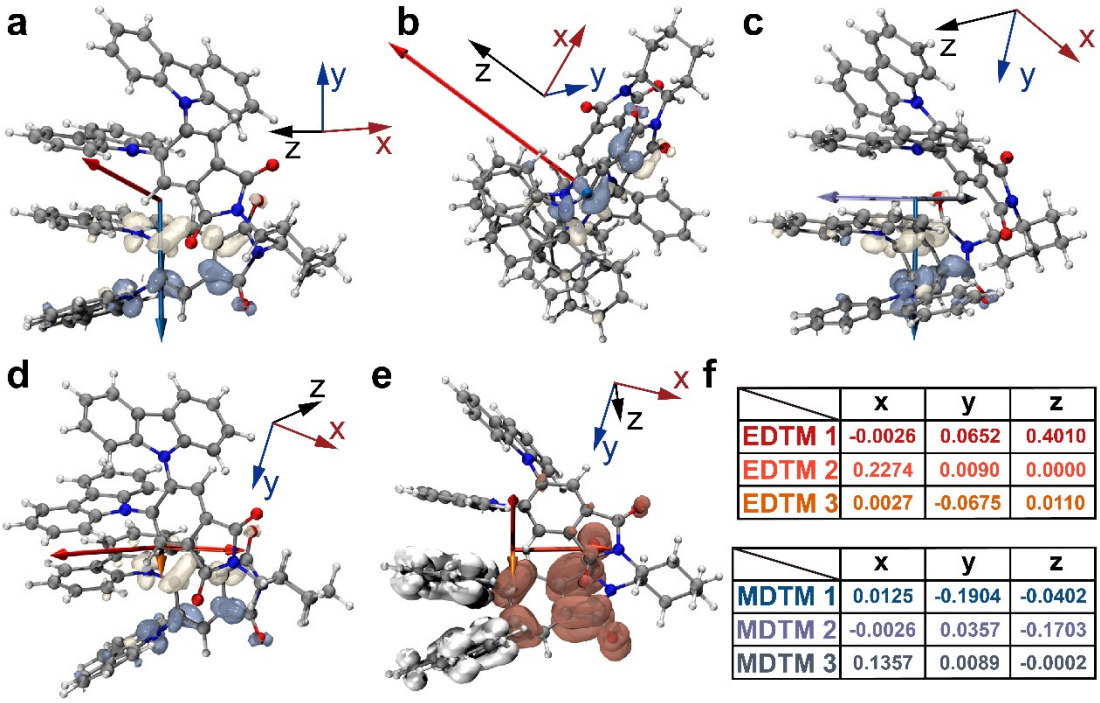


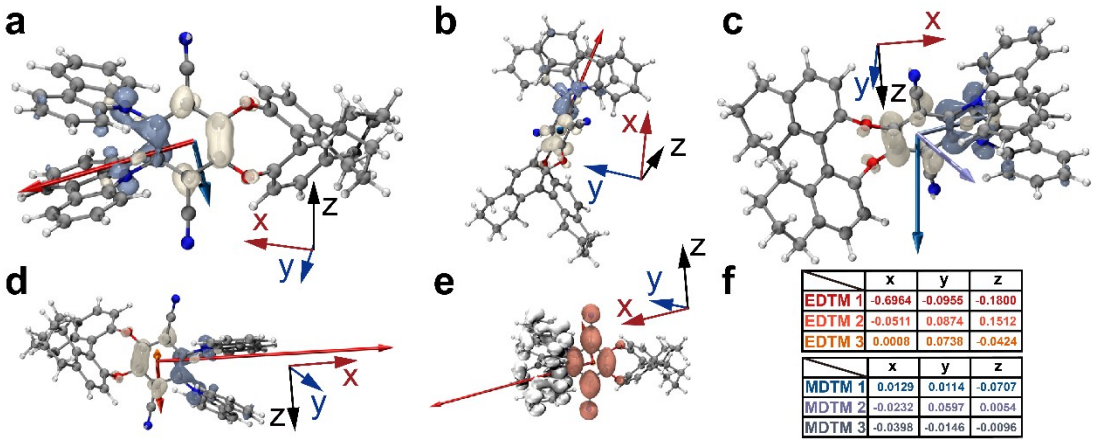
Figure S4 Potential energy surface (in units of kcal/mol) as a function of dihedral angle α (in units of deg) between the donor-acceptor planes of R_p-CzpEtPhTrz in the optimized S_0 and S_1 states.



	x	y	z
EDTM 1	-0.0026	0.0652	0.4010
EDTM 2	0.2274	0.0090	0.0000
EDTM 3	0.0027	-0.0675	0.0110

	x	y	z
MDTM 1	0.0125	-0.1904	-0.0402
MDTM 2	-0.0026	0.0357	-0.1703
MDTM 3	0.1357	0.0089	-0.0002

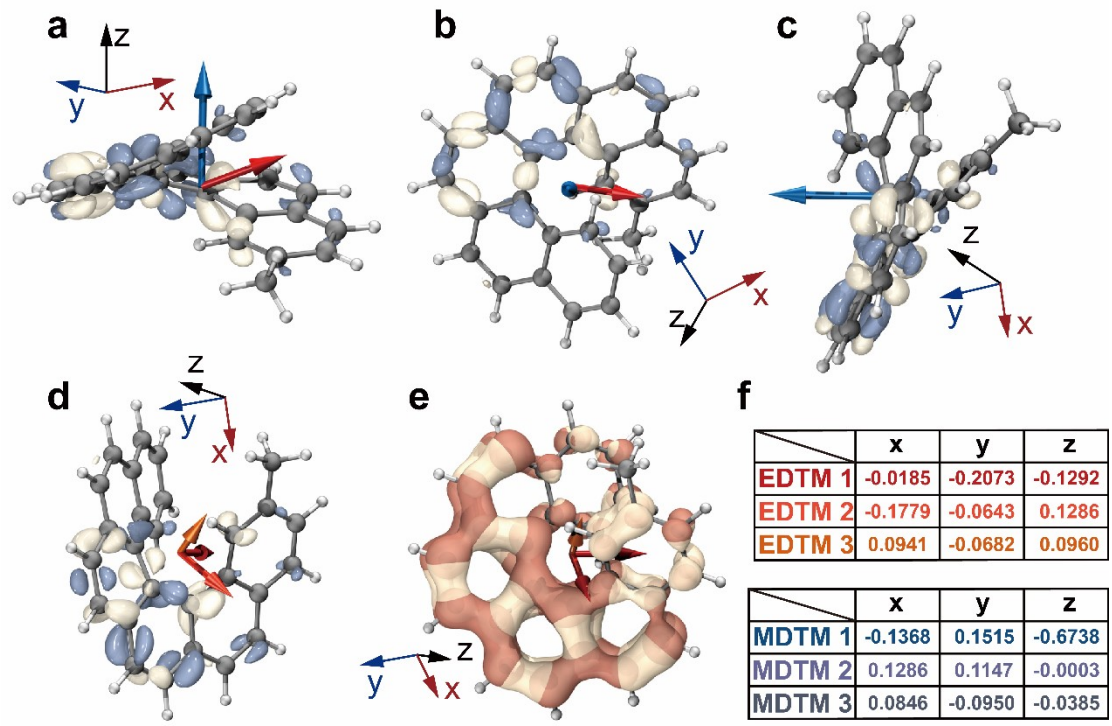
Figure S5 (-)-(*R*,*R*)-CAI-Cz. (a) Front view of electric dipole transition moment 1 (EDTM 1), magnetic dipole transition moment 1 (MDTM 1) and transition density (TD) plots. (b) Bird's-eye view of EDTM 1, MDTM 1 and TD plots. (c) MDTM 1, MDTM 2, MDTM 3 and TD plots. (d) EDTM 1, EDTM 2, EDTM 3 and TD plots. (e) EDTM 1, EDTM 2, EDTM 3 and natural transition orbitals. (f) x, y and z components of EDTM 1, EDTM 2, EDTM 3, MDTM 1, MDTM 2, MDTM 3. See the above "SVD" section for the origin of EDTM 1-3 and MDTM 1-3.



	x	y	z
EDTM 1	-0.6964	-0.0955	-0.1800
EDTM 2	-0.0511	0.0874	0.1512
EDTM 3	0.0008	0.0738	-0.0424

	x	y	z
MDTM 1	0.0129	0.0114	-0.0707
MDTM 2	-0.0232	0.0597	0.0054
MDTM 3	-0.0398	-0.0146	-0.0096

Figure S6 (*R*)-OBN-Cz. (a) Front view of electric dipole transition moment 1 (EDTM 1), magnetic dipole transition moment 1 (MDTM 1) and transition density (TD) plots. (b) Bird's-eye view of EDTM 1, MDTM 1 and TD plots. (c) MDTM 1, MDTM 2, MDTM 3 and TD plots. (d) EDTM 1, EDTM 2, EDTM 3 and TD plots. (e) EDTM 1, EDTM 2, EDTM 3 and natural transition orbitals. (f) x, y and z components of EDTM 1, EDTM 2, EDTM 3, MDTM 1, MDTM 2, MDTM 3. See the above "SVD" section for the origin of EDTM 1-3 and MDTM 1-3.



	x	y	z
EDTM 1	-0.0185	-0.2073	-0.1292
EDTM 2	-0.1779	-0.0643	0.1286
EDTM 3	0.0941	-0.0682	0.0960

	x	y	z
MDTM 1	-0.1368	0.1515	-0.6738
MDTM 2	0.1286	0.1147	-0.0003
MDTM 3	0.0846	-0.0950	-0.0385

Figure S7 (*P*)-methyl[6]helicene. (a) Front view of electric dipole transition moment 1 (EDTM 1), magnetic dipole transition moment 1 (MDTM 1) and transition density (TD) plots. (b) Bird's-eye view of EDTM 1, MDTM 1 and TD plots. (c) MDTM 1, MDTM 2, MDTM 3 and TD plots. (d) EDTM 1, EDTM 2, EDTM 3 and TD plots. (e) EDTM 1, EDTM 2, EDTM 3 and natural transition orbitals. (f) x, y and z components of EDTM 1, EDTM 2, EDTM 3, MDTM 1, MDTM 2, MDTM 3. See the above “SVD” section for the origin of EDTM 1-3 and MDTM 1-3.

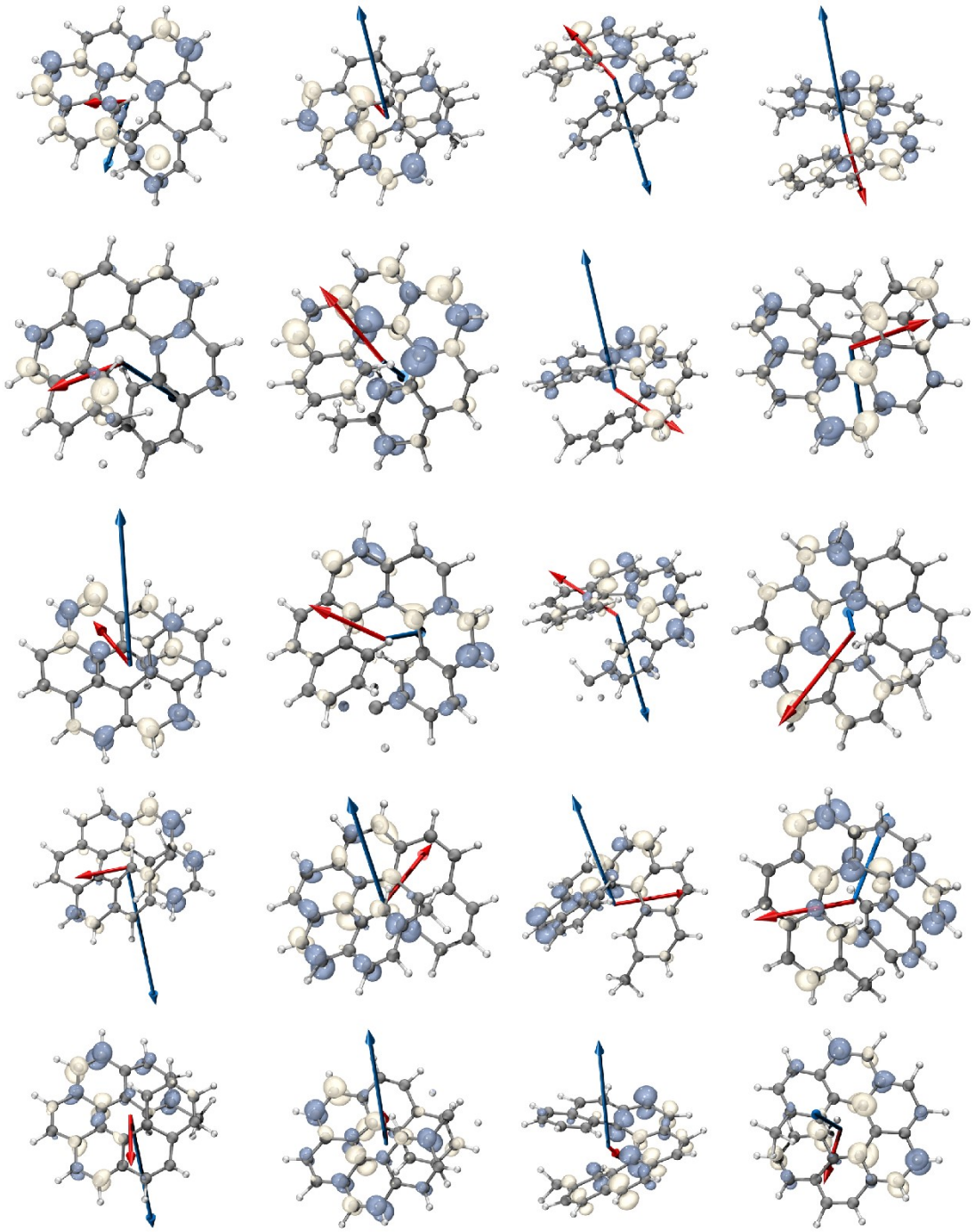


Figure S8 Transition density plots of some representative conformations of (*P*)-methyl[6]helicene showing CPL with a positive sign, (+)-CPL.

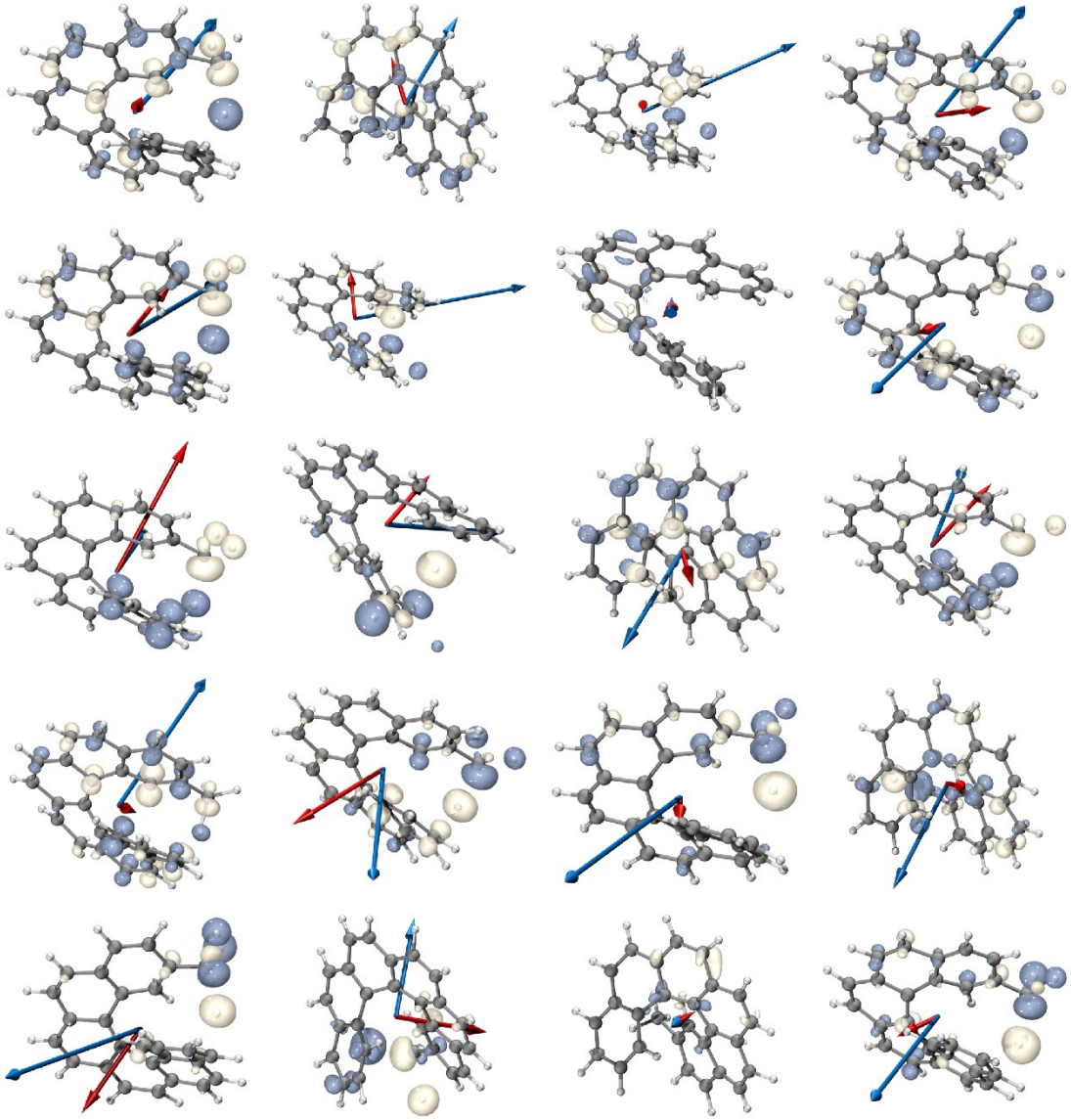
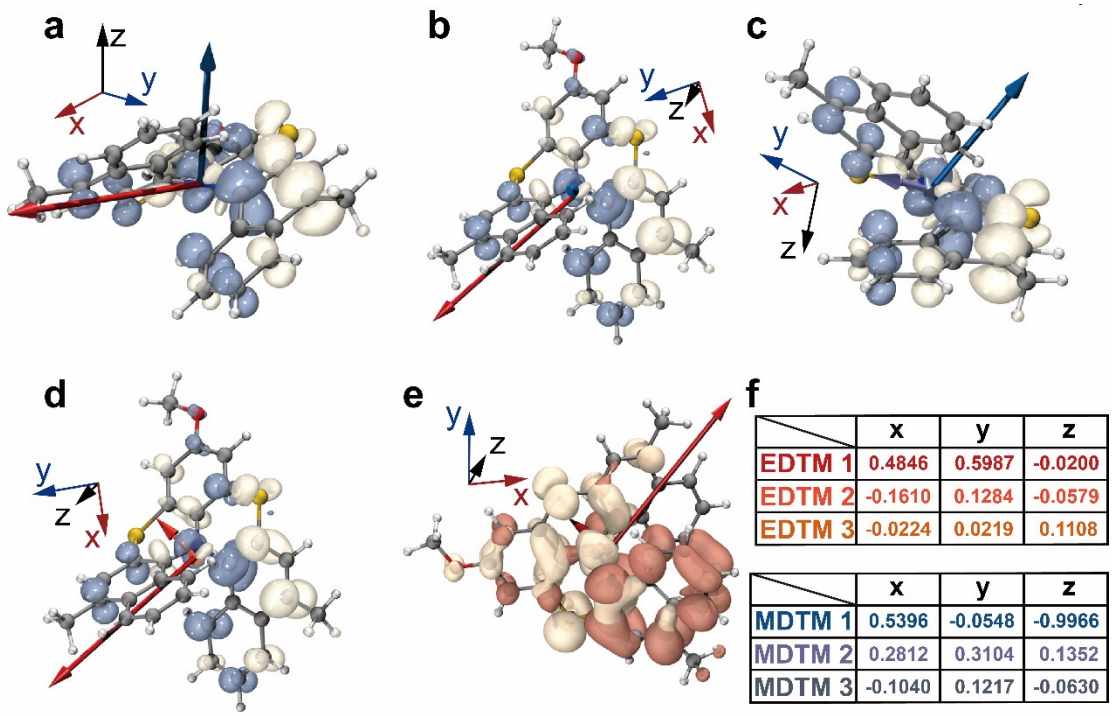


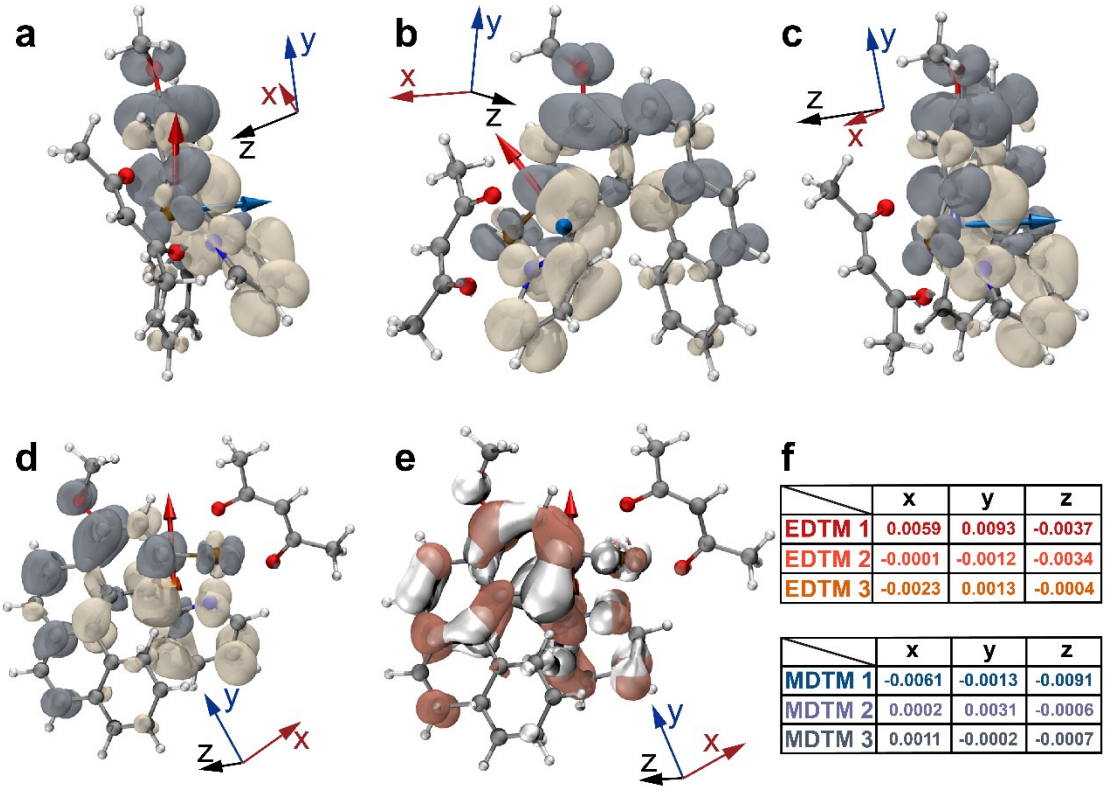
Figure S9 Transition density plots of some representative conformations of (*P*)-methyl[6]helicene showing CPL with a negative sign, (-)-CPL.



	x	y	z
EDTM 1	0.4846	0.5987	-0.0200
EDTM 2	-0.1610	0.1284	-0.0579
EDTM 3	-0.0224	0.0219	0.1108

	x	y	z
MDTM 1	0.5396	-0.0548	-0.9966
MDTM 2	0.2812	0.3104	0.1352
MDTM 3	-0.1040	0.1217	-0.0630

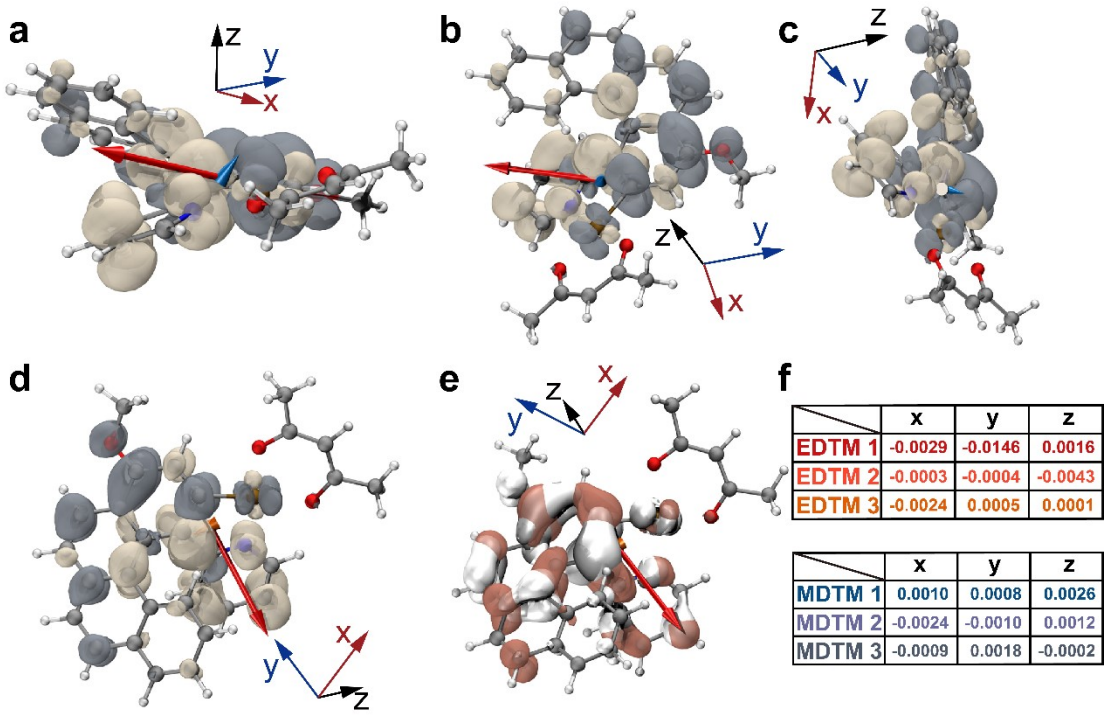
Figure S10 (*P*)-hetero[6]helicene. (a) Front view of electric dipole transition moment 1 (EDTM 1), magnetic dipole transition moment 1 (MDTM 1) and transition density (TD) plots. (b) Bird's-eye view of EDTM 1, MDTM 1 and TD plots. (c) MDTM 1, MDTM 2, MDTM 3 and TD plots. (d) EDTM 1, EDTM 2, EDTM 3 and TD plots. (e) EDTM 1, EDTM 2, EDTM 3 and natural transition orbitals. (f) x, y and z components of EDTM 1, EDTM 2, EDTM 3, MDTM 1, MDTM 2, MDTM 3. See the above "SVD" section for the origin of EDTM 1-3 and MDTM 1-3.



	x	y	z
EDTM 1	0.0059	0.0093	-0.0037
EDTM 2	-0.0001	-0.0012	-0.0034
EDTM 3	-0.0023	0.0013	-0.0004

	x	y	z
MDTM 1	-0.0061	-0.0013	-0.0091
MDTM 2	0.0002	0.0031	-0.0006
MDTM 3	0.0011	-0.0002	-0.0007

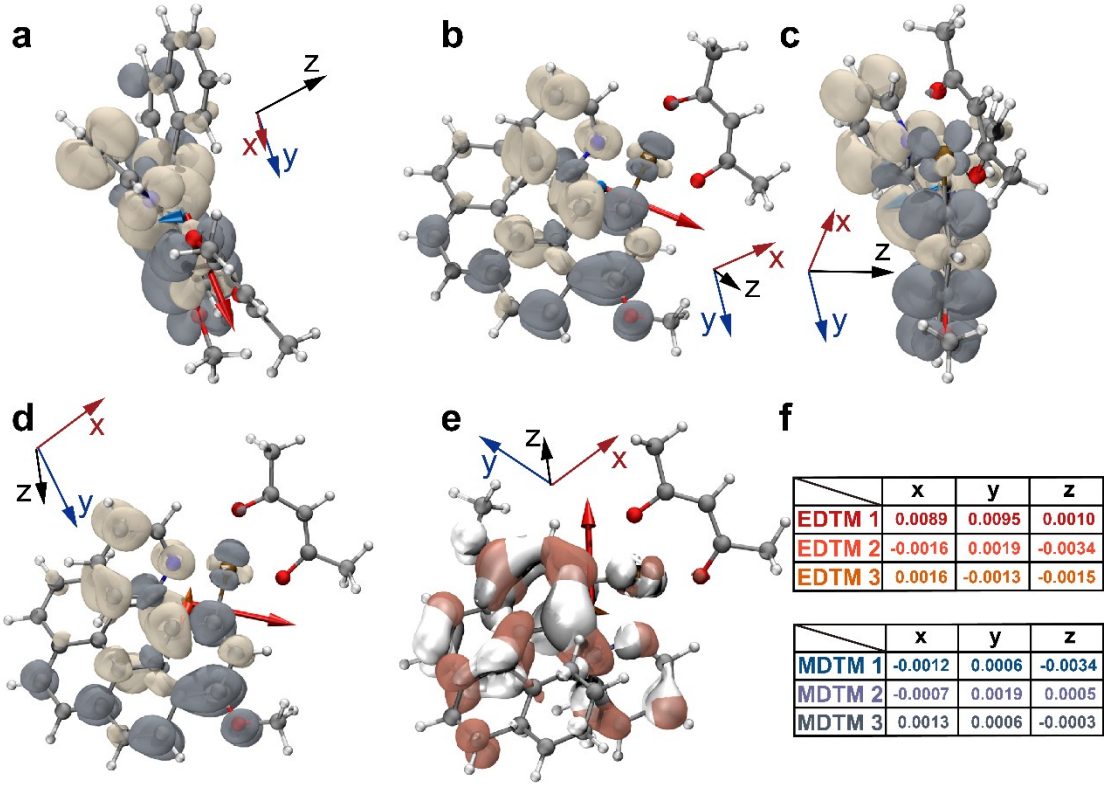
Figure S11 Triplet sub-state-1 of (*P*)-Pt(mppy)(acac). (a) Front view of electric dipole transition moment 1 (EDTM 1), magnetic dipole transition moment 1 (MDTM 1) and transition density (TD) plots. (b) Bird's-eye view of EDTM 1, MDTM 1 and TD plots. (c) MDTM 1, MDTM 2, MDTM 3 and TD plots. (d) EDTM 1, EDTM 2, EDTM 3 and TD plots. (e) EDTM 1, EDTM 2, EDTM 3 and natural transition orbitals. (f) x, y and z components of EDTM 1, EDTM 2, EDTM 3, MDTM 1, MDTM 2, MDTM 3. See the above "SVD" section for the origin of EDTM 1-3 and MDTM 1-3.



	x	y	z
EDTM 1	-0.0029	-0.0146	0.0016
EDTM 2	-0.0003	-0.0004	-0.0043
EDTM 3	-0.0024	0.0005	0.0001

	x	y	z
MDTM 1	0.0010	0.0008	0.0026
MDTM 2	-0.0024	-0.0010	0.0012
MDTM 3	-0.0009	0.0018	-0.0002

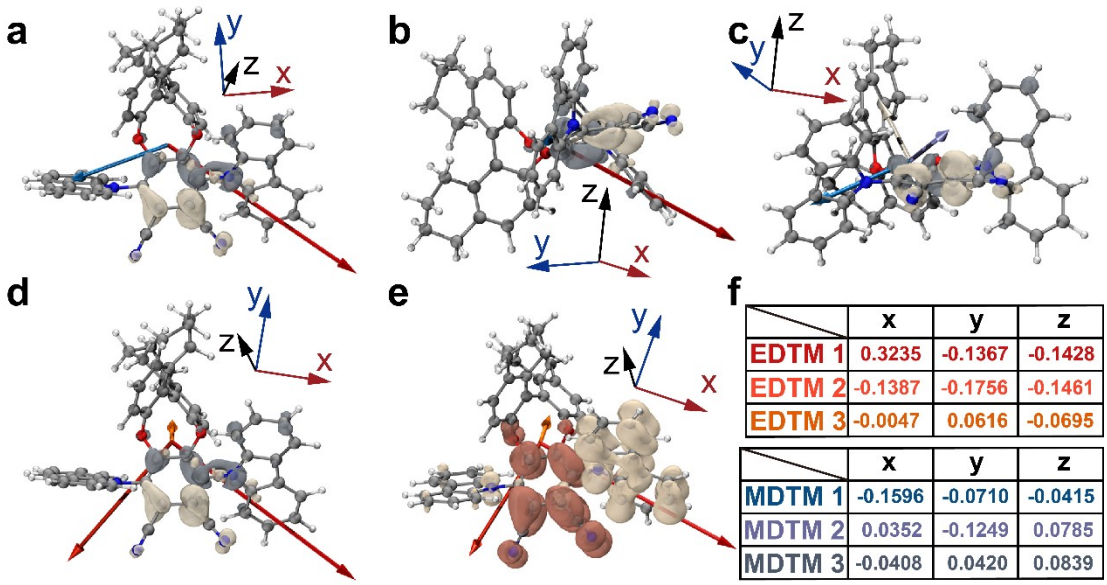
Figure S12 Triplet sub-state-2 of (*P*)-Pt(mppy)(acac). (a) Front view of electric dipole transition moment 1 (EDTM 1), magnetic dipole transition moment 1 (MDTM 1) and transition density (TD) plots. (b) Bird's-eye view of EDTM 1, MDTM 1 and TD plots. (c) MDTM 1, MDTM 2, MDTM 3 and TD plots. (d) EDTM 1, EDTM 2, EDTM 3 and TD plots. (e) EDTM 1, EDTM 2, EDTM 3 and natural transition orbitals. (f) x, y and z components of EDTM 1, EDTM 2, EDTM 3, MDTM 1, MDTM 2, MDTM 3. See the above "SVD" section for the origin of EDTM 1-3 and MDTM 1-3.



	x	y	z
EDTM 1	0.0089	0.0095	0.0010
EDTM 2	-0.0016	0.0019	-0.0034
EDTM 3	0.0016	-0.0013	-0.0015

	x	y	z
MDTM 1	-0.0012	0.0006	-0.0034
MDTM 2	-0.0007	0.0019	0.0005
MDTM 3	0.0013	0.0006	-0.0003

Figure S13 Triplet sub-state-3 of (*P*)-Pt(mppy)(acac). (a) Front view of electric dipole transition moment 1 (EDTM 1), magnetic dipole transition moment 1 (MDTM 1) and transition density (TD) plots. (b) Bird's-eye view of EDTM 1, MDTM 1 and TD plots. (c) MDTM 1, MDTM 2, MDTM 3 and TD plots. (d) EDTM 1, EDTM 2, EDTM 3 and TD plots. (e) EDTM 1, EDTM 2, EDTM 3 and natural transition orbitals. (f) x, y and z components of EDTM 1, EDTM 2, EDTM 3, MDTM 1, MDTM 2, MDTM 3. See the above "SVD" section for the origin of EDTM 1-3 and MDTM 1-3.



	x	y	z
EDTM 1	0.3235	-0.1367	-0.1428
EDTM 2	-0.1387	-0.1756	-0.1461
EDTM 3	-0.0047	0.0616	-0.0695

	x	y	z
MDTM 1	-0.1596	-0.0710	-0.0415
MDTM 2	0.0352	-0.1249	0.0785
MDTM 3	-0.0408	0.0420	0.0839

Figure S14 iso-(*R*)-OBN-CzB1. (a) Front view of electric dipole transition moment 1 (EDTM 1), magnetic dipole transition moment 1 (MDTM 1) and transition density (TD) plots. (b) Bird's-eye view of EDTM 1, MDTM 1 and TD plots. (c) MDTM 1, MDTM 2, MDTM 3 and TD plots. (d) EDTM 1, EDTM 2, EDTM 3 and TD plots. (e) EDTM 1, EDTM 2, EDTM 3 and natural transition orbitals. (f) x, y and z components of EDTM 1, EDTM 2, EDTM 3, MDTM 1, MDTM 2, MDTM 3. See the above "SVD" section for the origin of EDTM 1-3 and MDTM 1-3.

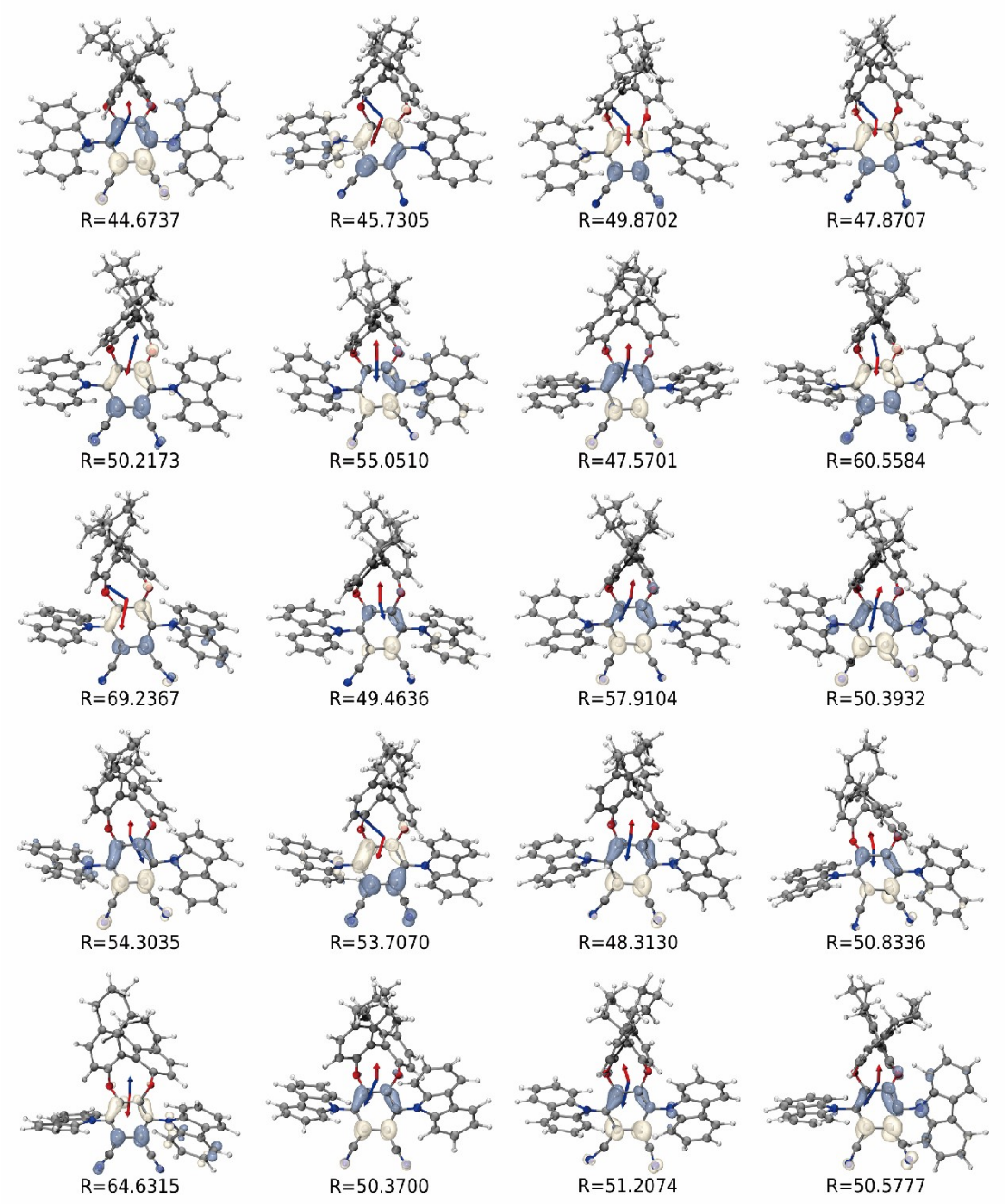


Figure S15 Transition density plots and calculated rotatory strengths (*R*) of some representative conformations of iso-(*R*)-OBN-CzB1 showing CPL with a positive sign, (+)-CPL.

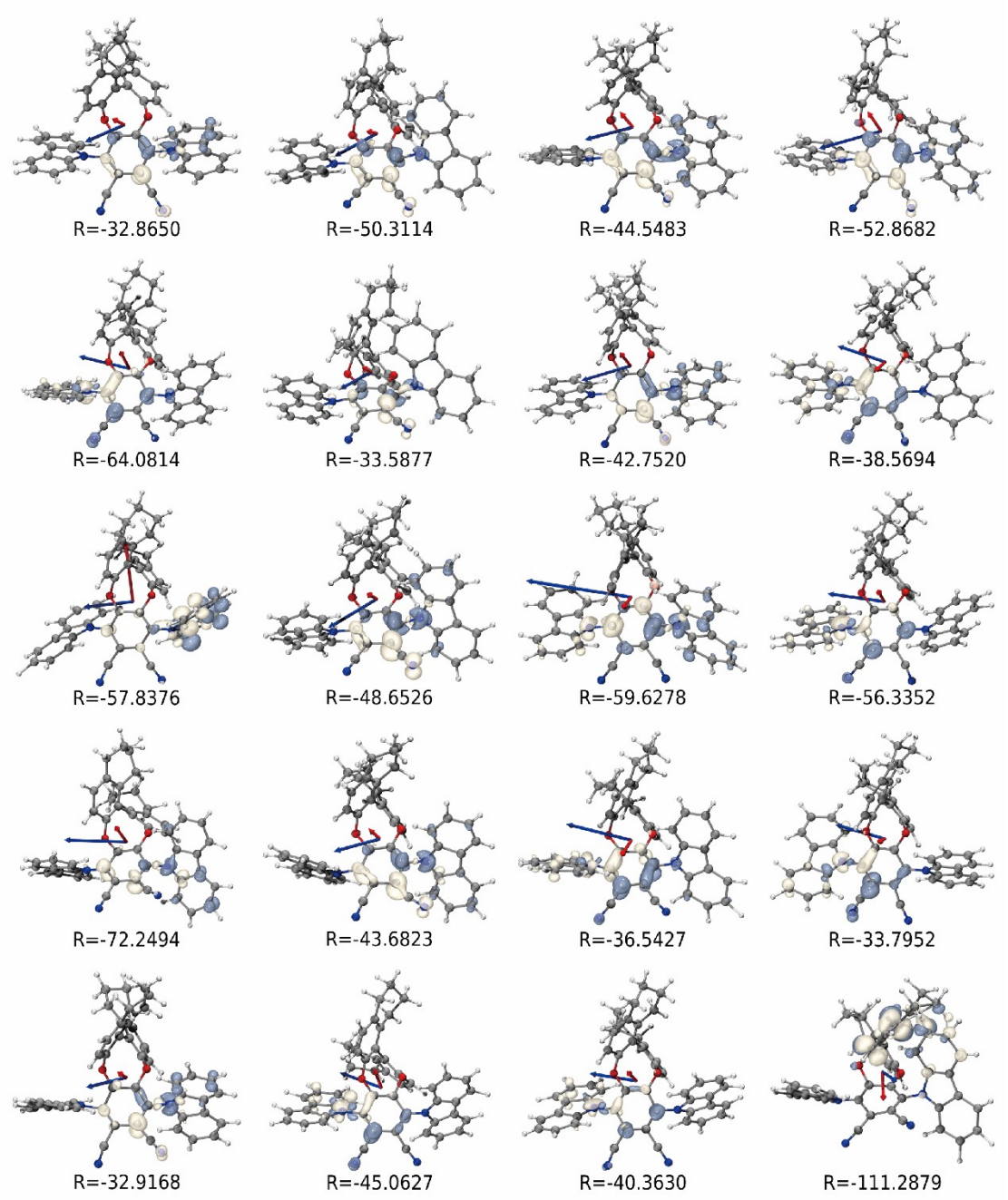


Figure S16 Transition density plots and the calculated rotatory strengths (*R*) of some representative conformations of iso-(*R*)-OBN-CzB1 showing CPL with a negative sign, (-)-CPL.

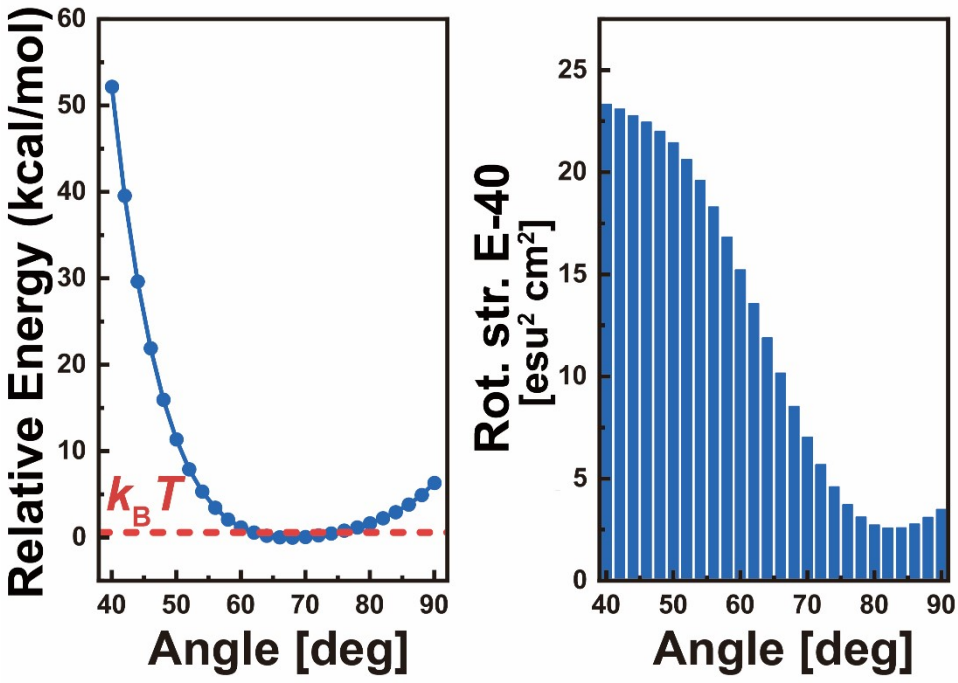
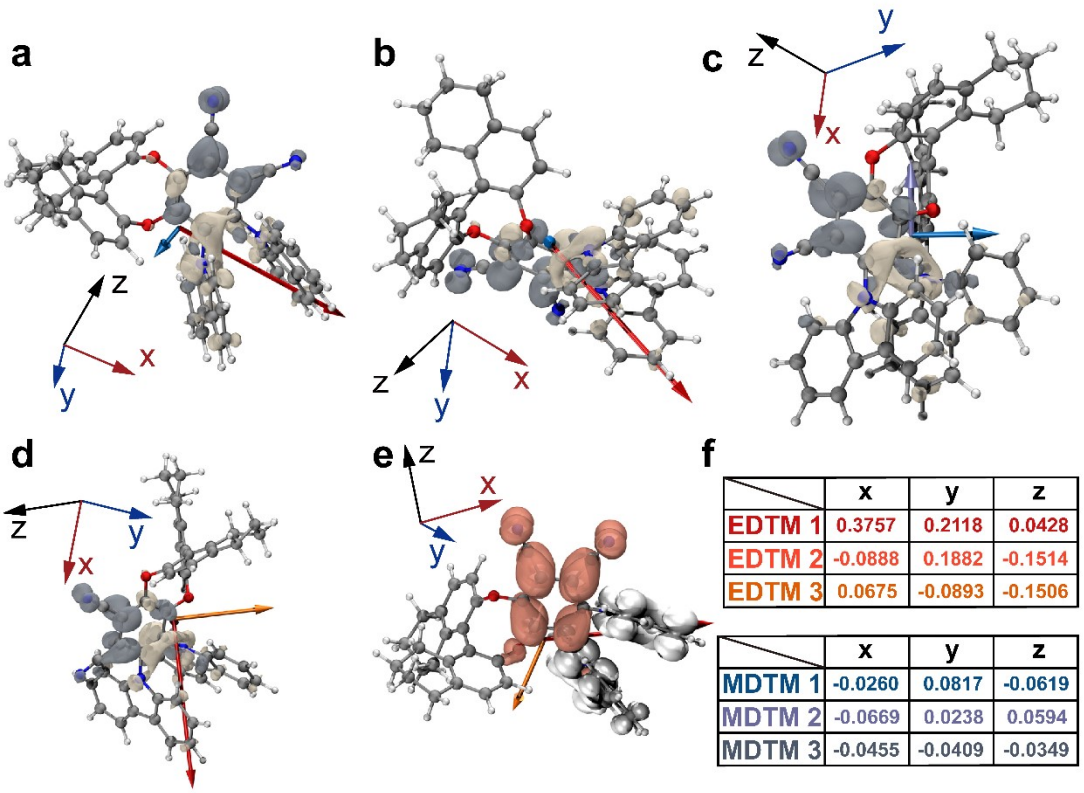


Figure S17 Potential energy surface (in units of kcal/mol) and rotatory strength (in units of E-40 $esu^2 \cdot cm^2$) as a function of the dihedral angle α (in units of deg) between the aryl groups and carbazole units of iso-(*R*)-OBN-CzB1. The red line represents k_BT at 298 K (0.6 $kcal \cdot mol^{-1}$), where k_B is the Boltzmann constant and T is the temperature (in units of K).



	x	y	z
EDTM 1	0.3757	0.2118	0.0428
EDTM 2	-0.0888	0.1882	-0.1514
EDTM 3	0.0675	-0.0893	-0.1506

	x	y	z
MDTM 1	-0.0260	0.0817	-0.0619
MDTM 2	-0.0669	0.0238	0.0594
MDTM 3	-0.0455	-0.0409	-0.0349

Figure S18 iso-(*R*)-OBN-CzC1. (a) Front view of electric dipole transition moment 1 (EDTM 1), magnetic dipole transition moment 1 (MDTM 1) and transition density (TD) plots. (b) Bird's-eye view of EDTM 1, MDTM 1 and TD plots. (c) MDTM 1, MDTM 2, MDTM 3 and TD plots. (d) EDTM 1, EDTM 2, EDTM 3 and TD plots. (e) EDTM 1, EDTM 2, EDTM 3 and natural transition orbitals. (f) x, y and z components of EDTM 1, EDTM 2, EDTM 3, MDTM 1, MDTM 2, MDTM 3. See the above “SVD” section for the origin of EDTM 1-3 and MDTM 1-3.

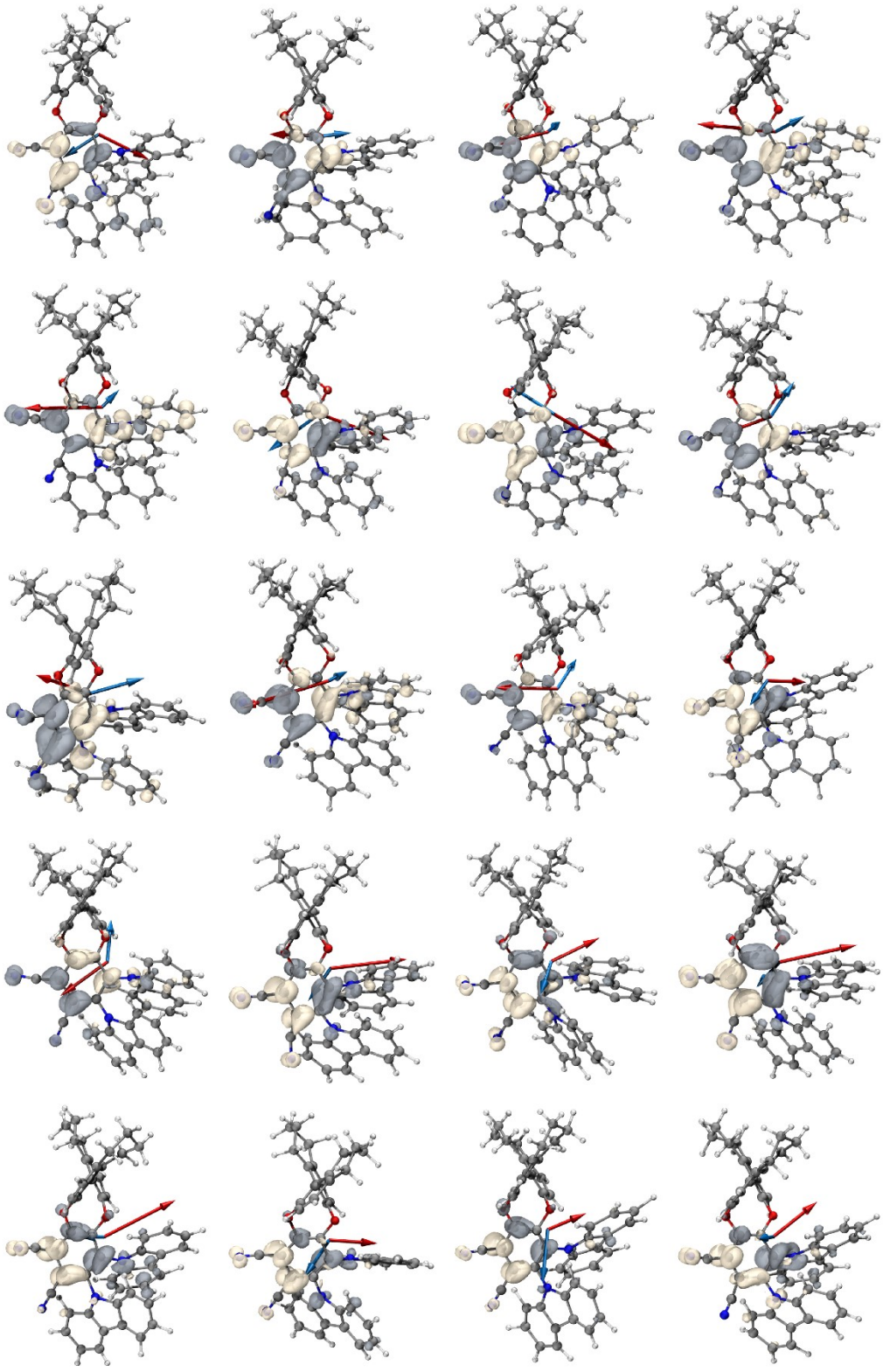


Figure S19 Transition density plots and calculated rotatory strengths (*R*) of some representative conformations of iso-(*R*)-OBN-CzC1 showing CPL with a positive sign, (+)-CPL.

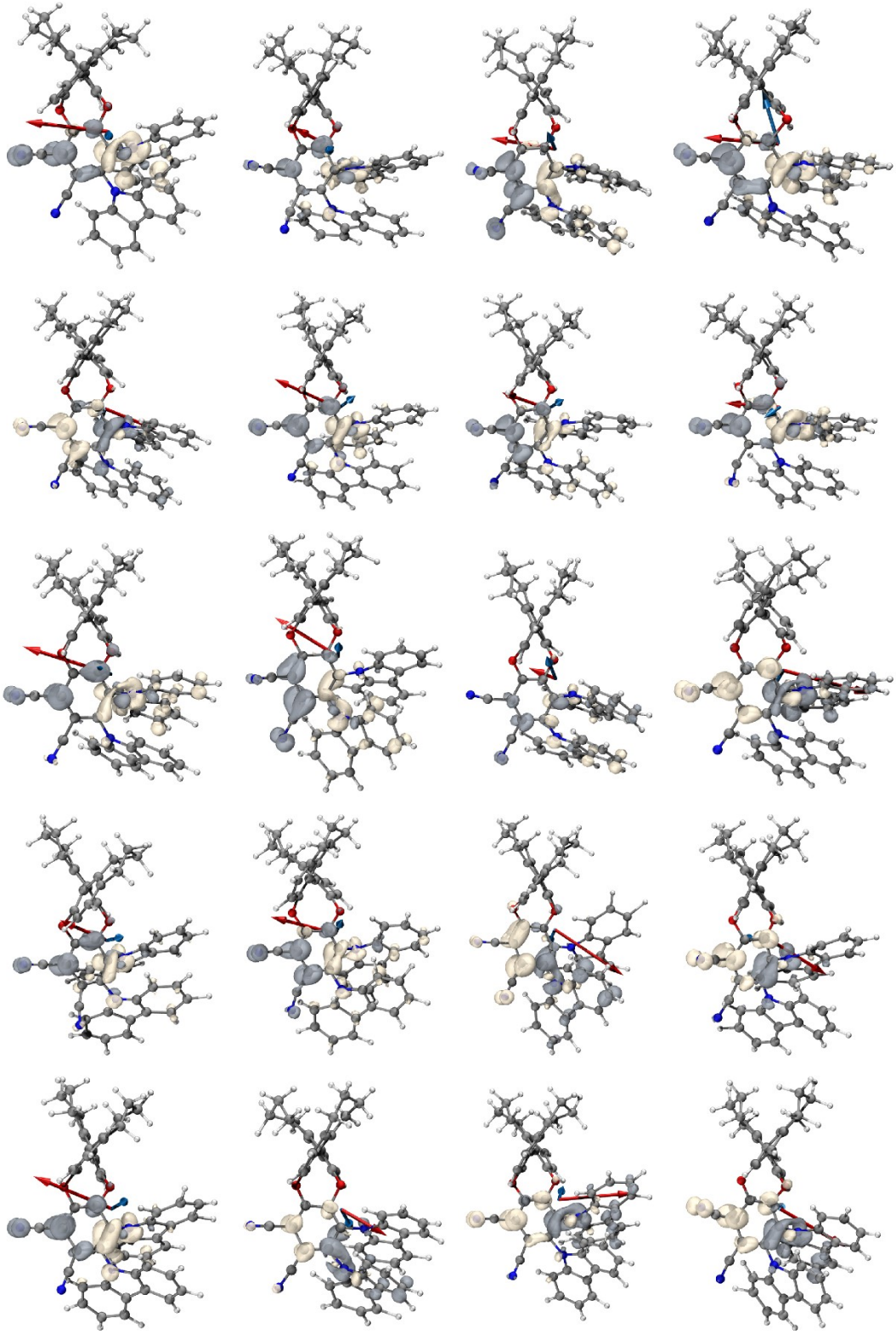
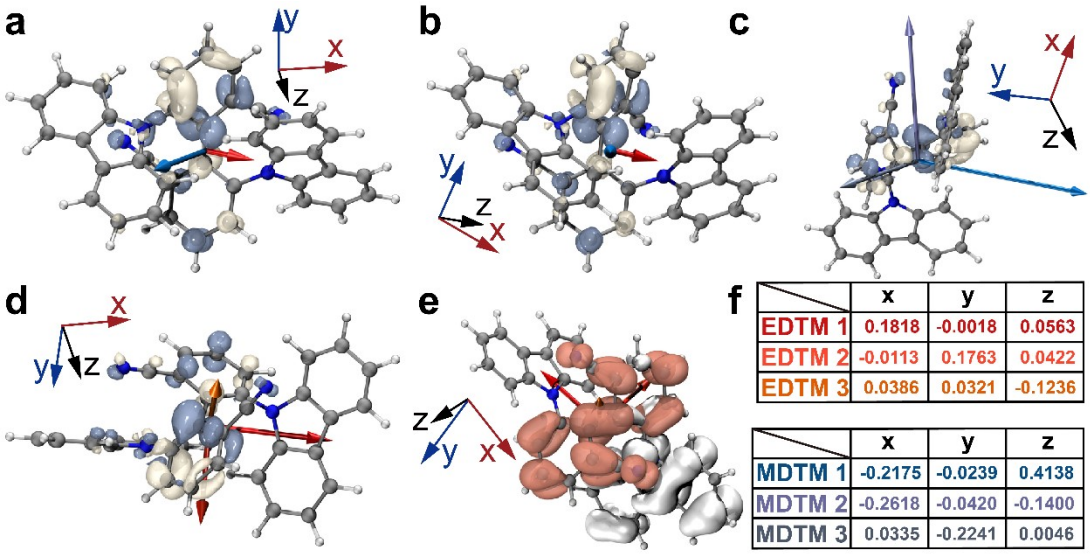


Figure S20 Transition density plots and calculated rotatory strengths (*R*) of some representative conformations of iso-(*R*)-OBN-CzC1 showing CPL with a negative sign, (-)-CPL.



	x	y	z
EDTM 1	0.1818	-0.0018	0.0563
EDTM 2	-0.0113	0.1763	0.0422
EDTM 3	0.0386	0.0321	-0.1236

	x	y	z
MDTM 1	-0.2175	-0.0239	0.4138
MDTM 2	-0.2618	-0.0420	-0.1400
MDTM 3	0.0335	-0.2241	0.0046

Figure S21 (+)-(*R*)-Cz-Ax-CN. (a) Front view of electric dipole transition moment 1 (EDTM 1), magnetic dipole transition moment 1 (MDTM 1) and transition density (TD) plots. (b) Bird's-eye view of EDTM 1, MDTM 1 and TD plots. (c) MDTM 1, MDTM 2, MDTM 3 and TD plots. (d) EDTM 1, EDTM 2, EDTM 3 and TD plots. (e) EDTM 1, EDTM 2, EDTM 3 and natural transition orbitals. (f) x, y and z components of EDTM 1, EDTM 2, EDTM 3, MDTM 1, MDTM 2, MDTM 3. See the above "SVD" section for the origin of EDTM 1-3 and MDTM 1-3.

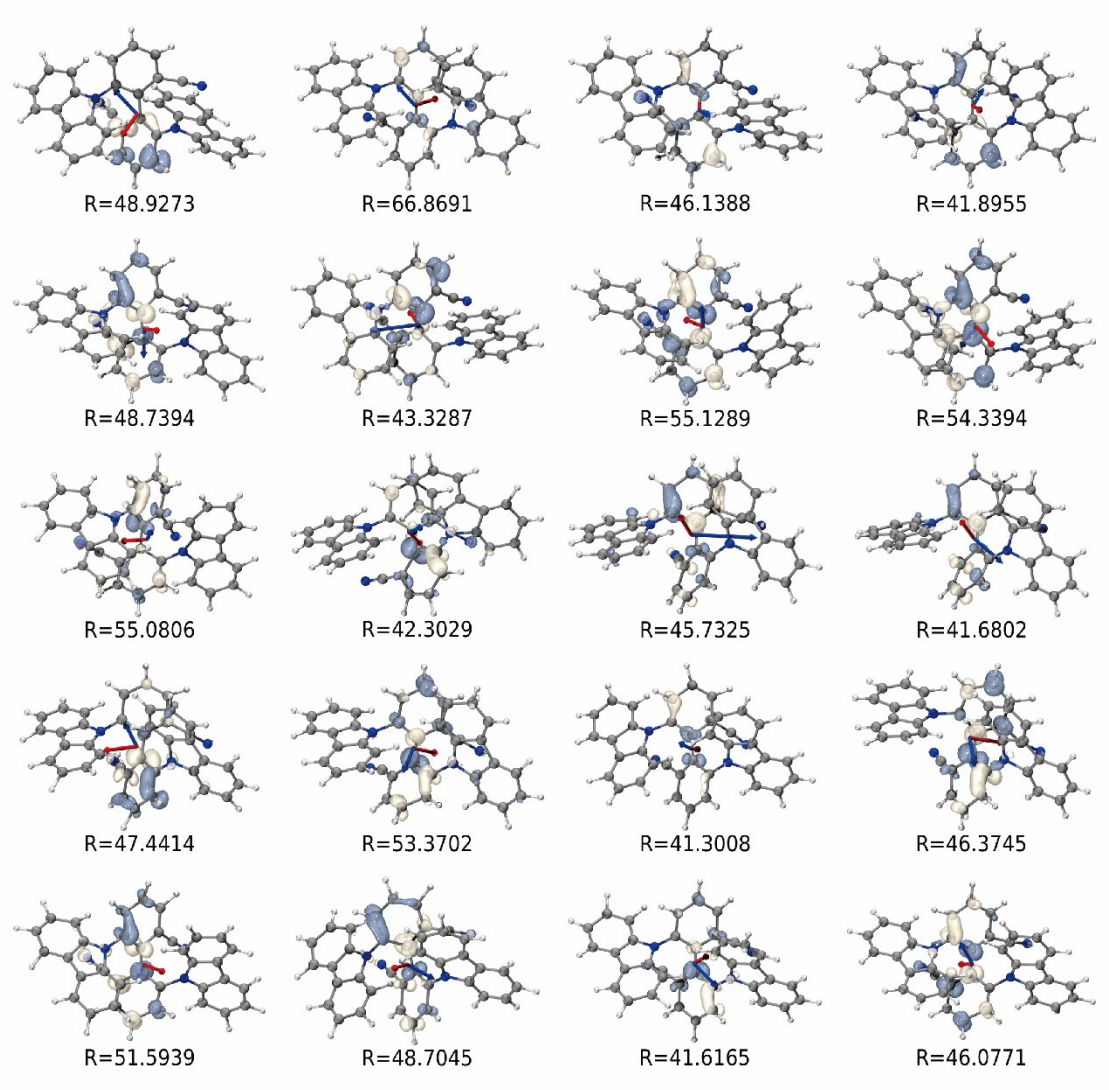


Figure S22 Transition density plots and calculated rotatory strengths (*R*) of some representative conformations of (+)-(*R*)-Cz-Ax-CN showing CPL with a positive sign, (+)-CPL.

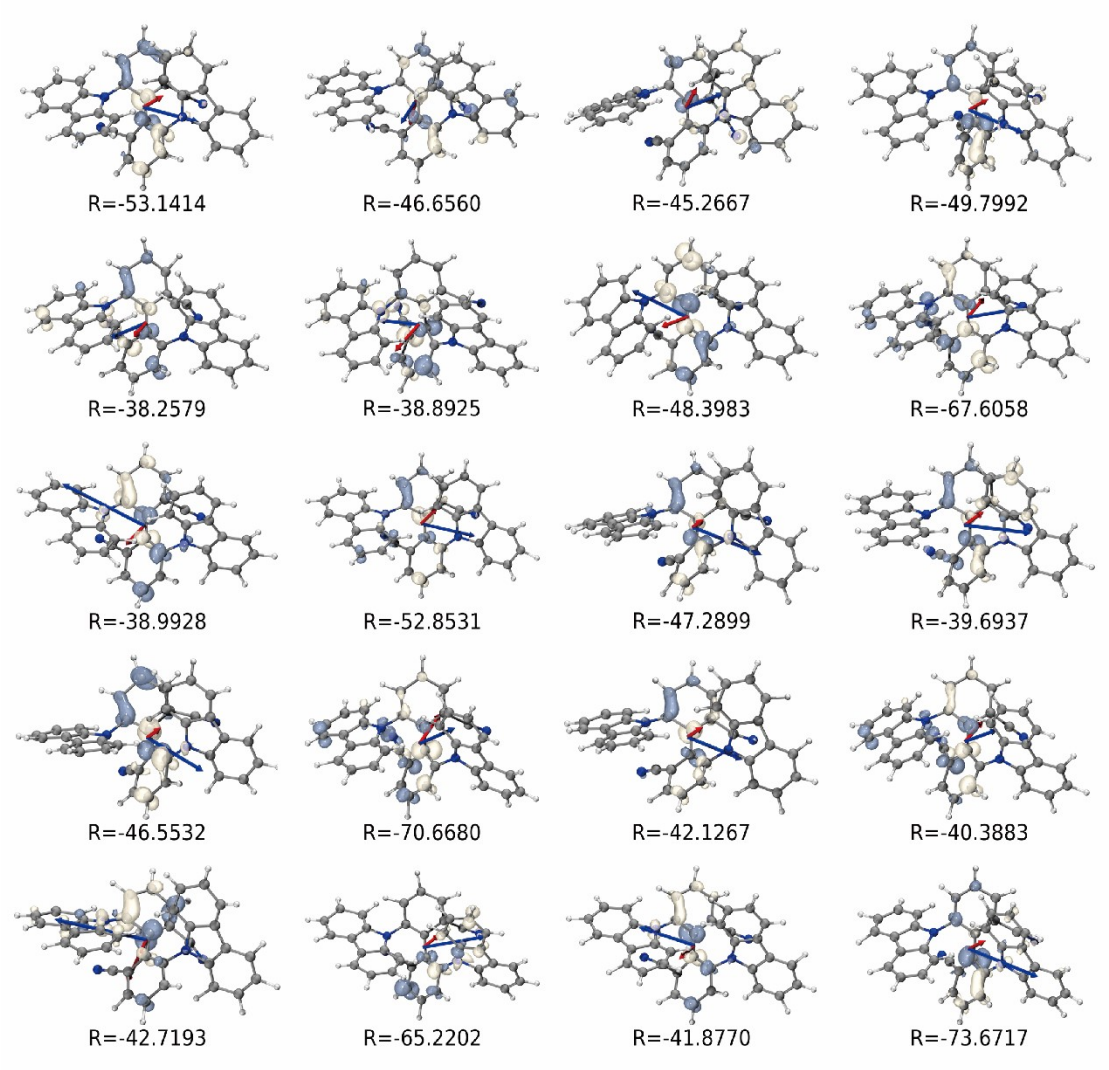
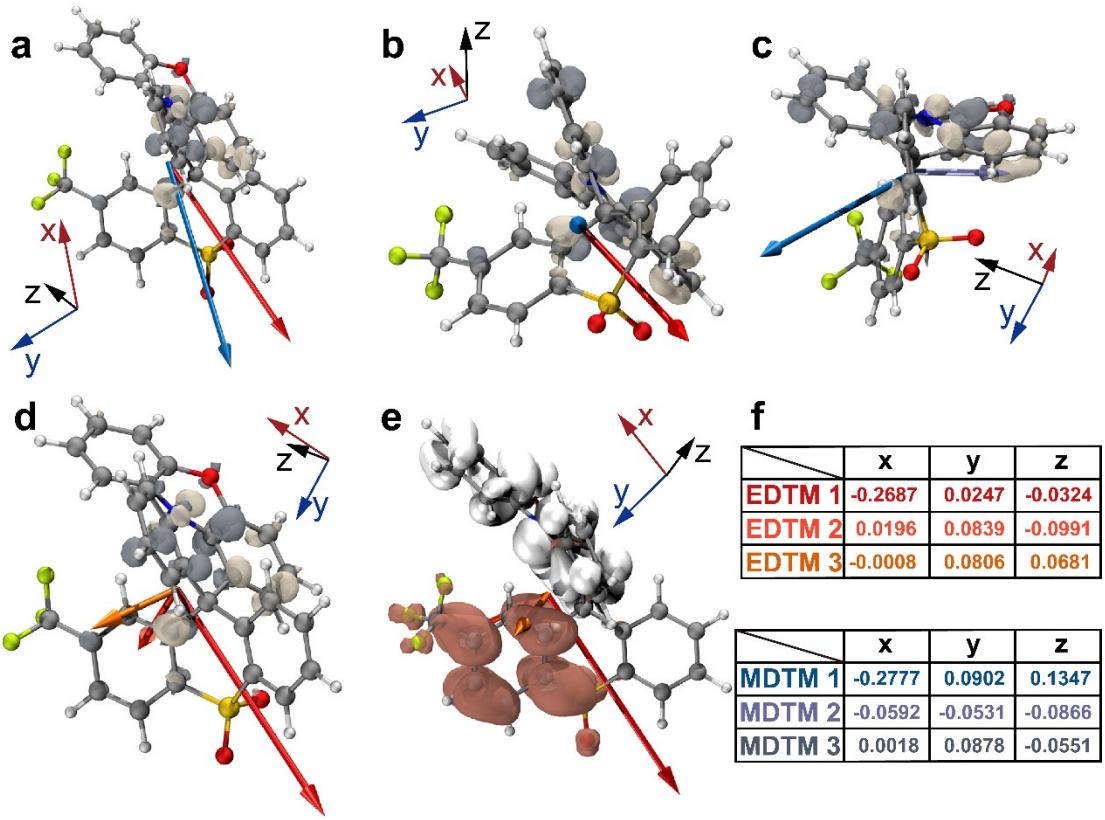


Figure S23 Transition density plots and calculated rotatory strengths (*R*) of some representative conformations of (+)-(*R*)-Cz-Ax-CN showing CPL with a negative sign, (-)-CPL.



	x	y	z
EDTM 1	-0.2687	0.0247	-0.0324
EDTM 2	0.0196	0.0839	-0.0991
EDTM 3	-0.0008	0.0806	0.0681

	x	y	z
MDTM 1	-0.2777	0.0902	0.1347
MDTM 2	-0.0592	-0.0531	-0.0866
MDTM 3	0.0018	0.0878	-0.0551

Figure S24 (*R*)-OSFSO. (a) Front view of electric dipole transition moment 1 (EDTM 1), magnetic dipole transition moment 1 (MDTM 1) and transition density (TD) plots. (b) Bird's-eye view of EDTM 1, MDTM 1 and TD plots. (c) MDTM 1, MDTM 2, MDTM 3 and TD plots. (d) EDTM 1, EDTM 2, EDTM 3 and TD plots. (e) EDTM 1, EDTM 2, EDTM 3 and natural transition orbitals. (f) x, y and z components of EDTM 1, EDTM 2, EDTM 3, MDTM 1, MDTM 2, MDTM 3. See the above "SVD" section for the origin of EDTM 1-3 and MDTM 1-3.

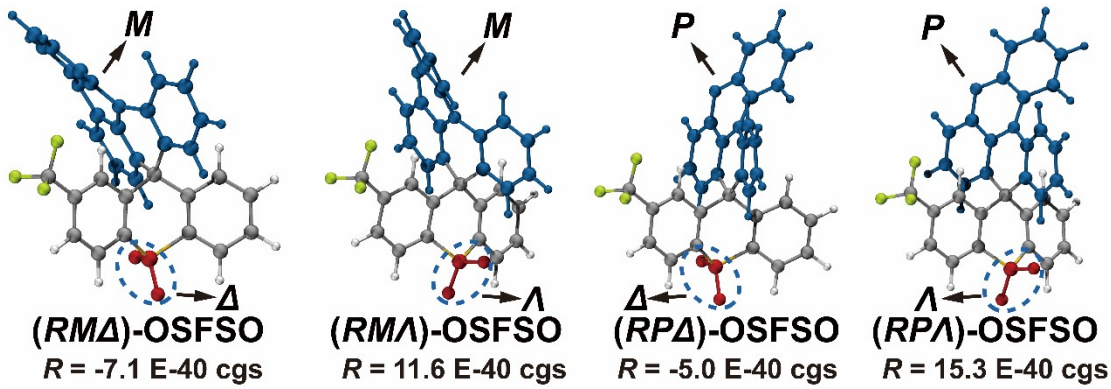


Figure S25 Calculated rotatory strengths (in units of E-40 cgs) based on the optimized S_1-state structure of (*RM*Δ)-OSFSO, (*RM*Λ)-OSFSO, (*RP*Δ)-OSFSO, and (*RP*Λ)-OSFSO.

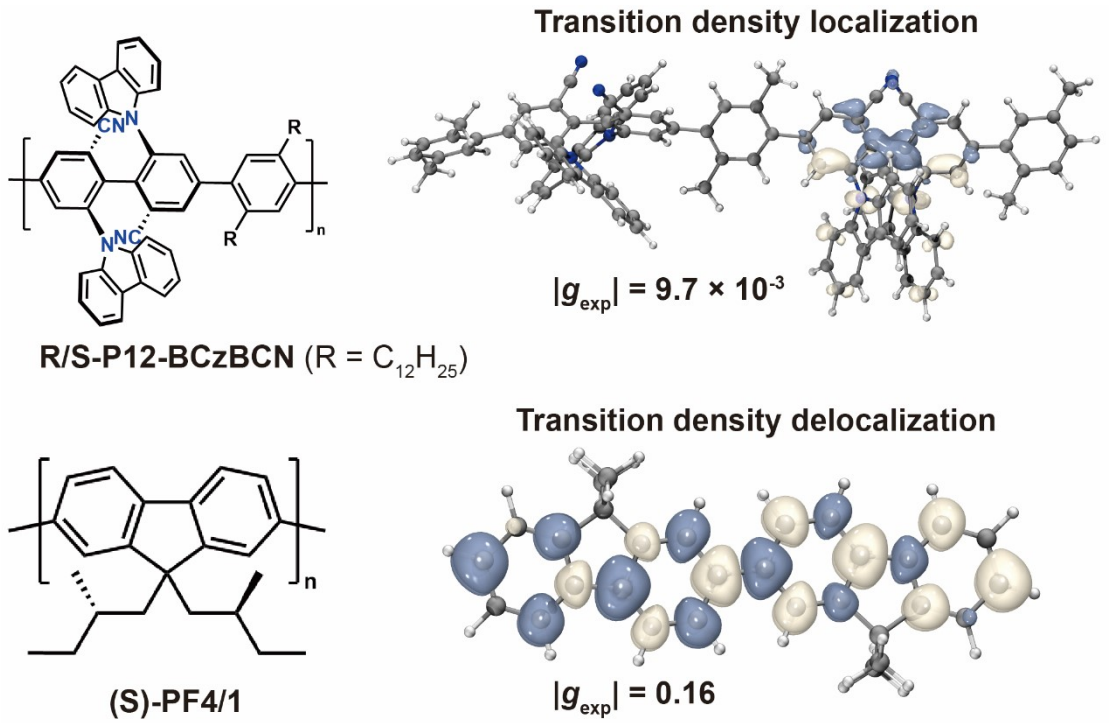


Figure S26 Chemical structures, transition densities, and experimental (absolute) *g*-factors of two typical chiral conjugated polymers [R/S-P12-BCzBCN, (S)-PF4/1].

Table S2. Atomic coordinates and total electronic energies (E) at the first excited-state geometry.

(*P*)-hetero[6]helicene

E = -2042.26147378 a.u.

C	3.012766	0.438293	-2.412201
C	3.694778	1.667750	-2.369414
C	1.401511	3.686727	-0.208196
C	0.184648	3.529358	0.406930
H	-0.296688	4.382872	0.889332
C	-2.705944	0.795255	0.443370
C	-2.456325	-1.435521	-0.483989
C	1.042753	-3.414689	-0.576100
H	0.816537	-4.312749	-1.157108
C	2.284713	-3.286096	0.015788
C	3.761892	-2.027089	1.576731
H	4.539274	-2.777606	1.435573
C	3.996045	-0.965224	2.443030
H	4.952500	-0.890734	2.964554
C	3.005838	-0.008478	2.649806
H	3.171288	0.817887	3.343802
C	1.969066	2.569714	-0.906472
C	-0.471302	2.282967	0.438329
C	0.095851	1.156304	-0.140805
C	-1.865202	-0.243121	0.011448
C	0.047796	-2.443197	-0.423283
C	0.321093	-1.248078	0.310566
C	2.544877	-2.159044	0.880662
C	1.545951	-1.149289	1.061633
C	1.308543	1.305256	-0.907108
C	1.853583	0.262433	-1.696301
H	1.349626	-0.699415	-1.747142
C	1.797417	-0.103308	1.969225
H	1.026336	0.643404	2.153356
H	3.404458	-0.385804	-3.011118
H	4.625513	1.798470	-2.924797
C	3.176606	2.707353	-1.637434
H	3.696718	3.664700	-1.625677
N	-0.480769	-0.116757	0.092513
S	-2.015566	2.188709	1.263025
S	-1.496558	-2.710006	-1.153192
C	-4.091620	0.688311	0.365698

C	-3.854649	-1.542420	-0.551821
H	-4.704211	1.519956	0.706191
C	-4.664506	-0.494811	-0.136160
H	-4.326920	-2.453726	-0.918518
C	3.331278	-4.340686	-0.179423
H	4.255815	-3.924569	-0.614826
H	3.621386	-4.813289	0.774744
H	2.972820	-5.133046	-0.850633
C	2.095389	5.017890	-0.185528
H	3.095004	4.943263	0.270442
H	2.233944	5.422312	-1.200553
H	1.516351	5.750319	0.391996
O	-5.993150	-0.688964	-0.235611
C	-6.873826	0.318156	0.190971
H	-7.888833	-0.060731	0.021032
H	-6.751019	0.540539	1.264437
H	-6.739451	1.249412	-0.384838

(*M*)-hetero[6]helicene

E = -2042.26297204 a.u.

C	-3.084700	0.342567	-2.584070
C	-3.935456	1.414406	-2.331574
C	-1.836060	3.485189	0.020361
C	-0.563491	3.451363	0.554387
H	-0.199013	4.310532	1.124120
C	2.635765	1.017522	0.352993
C	2.553337	-1.232916	-0.564280
C	-0.667863	-3.546688	-0.416515
H	-0.320488	-4.458487	-0.907045
C	-1.865917	-3.540555	0.250892
C	-3.434392	-2.329505	1.742920
H	-4.073767	-3.211446	1.766081
C	-3.779375	-1.227115	2.483385
H	-4.692789	-1.231482	3.081223
C	-2.940965	-0.096402	2.481385
H	-3.194317	0.774557	3.088478
C	-2.277512	2.405163	-0.834677
C	0.292804	2.361355	0.356842
C	-0.169756	1.210873	-0.358073
C	1.872102	-0.079574	-0.118526
C	0.139870	-2.393269	-0.495614
C	-0.253699	-1.201981	0.087703
C	-2.253175	-2.354348	0.957540

C	-1.435488	-1.186639	0.911830
C	-1.424243	1.277465	-1.059905
C	-1.843827	0.279326	-1.959102
H	-1.179507	-0.554587	-2.181334
C	-1.803082	-0.076536	1.713950
H	-1.175937	0.811011	1.732515
H	-3.383615	-0.450659	-3.272120
H	-4.915913	1.465165	-2.809482
C	-3.529549	2.433648	-1.475336
H	-4.198730	3.275459	-1.298812
N	0.484037	-0.015003	-0.171041
S	1.892217	2.431825	1.000812
S	1.650691	-2.503810	-1.383756
C	4.046576	0.926809	0.403813
C	3.929832	-1.318865	-0.505435
H	4.609357	1.787251	0.760793
C	4.682174	-0.227407	-0.015003
H	4.458248	-2.206239	-0.852088
C	-2.725660	-4.771418	0.275568
H	-3.726177	-4.571204	-0.138164
H	-2.869484	-5.146422	1.300876
H	-2.271521	-5.576560	-0.316533
C	-2.730651	4.662763	0.262085
H	-3.680215	4.364648	0.738596
H	-3.001027	5.173061	-0.678400
H	-2.245249	5.399975	0.916202
O	6.015932	-0.405752	-0.011229
C	6.840662	0.626526	0.462574
H	7.873509	0.266478	0.384846
H	6.622162	0.868658	1.516647
H	6.732630	1.542537	-0.142883

(*P*)-methyl[6]helicene

E = -1038.34760901 a.u.

C	0.688054	-2.499990	1.506915
C	0.051289	-3.680929	1.058905
H	0.500920	-4.651549	1.281551
C	-1.143371	-3.614989	0.378697
H	-1.655423	-4.531289	0.075532
C	-3.022108	-2.301048	-0.545289
H	-3.529807	-3.229253	-0.815840
C	-3.639585	-1.089227	-0.735257
H	-4.653977	-1.045831	-1.138103

C	-3.672407	1.363089	-0.504519
H	-4.721554	1.363118	-0.806644
C	-3.049062	2.541453	-0.136481
H	-3.610973	3.477132	-0.102807
C	-1.035955	3.738859	0.628736
H	-1.642481	4.627714	0.814418
C	0.325497	3.758575	0.867349
H	0.800634	4.649954	1.281954
C	2.543045	2.694858	0.703370
H	2.971986	3.554672	1.223036
C	3.352626	1.681797	0.257864
H	4.429217	1.712389	0.437608
C	3.659216	-0.366850	-1.087058
H	4.728785	-0.325922	-0.867983
C	3.155544	-1.338545	-1.924680
H	3.819488	-2.086262	-2.362837
C	1.784148	-1.338431	-2.242386
H	1.386569	-2.074838	-2.943253
C	-1.744499	-2.374225	0.072848
C	-2.989725	0.128104	-0.419408
C	-1.610969	0.103573	0.013378
C	-1.674546	2.566836	0.174688
C	-0.888054	1.342324	0.027712
C	1.140206	2.659366	0.508897
C	0.535420	1.488390	-0.077868
C	2.817402	0.613344	-0.516205
C	1.406349	0.554907	-0.754530
C	-1.064198	-1.165719	0.430228
C	0.114858	-1.280841	1.200646
H	0.593231	-0.373836	1.565649
C	0.936693	-0.412653	-1.673602
H	-0.118134	-0.420213	-1.941186
C	1.978758	-2.578274	2.271002
H	1.918772	-3.307956	3.093042
H	2.800170	-2.898095	1.609384
H	2.254820	-1.602459	2.692756

(*M*)-methyl[6]helicene

E = -1038.34760901 a.u.

C	0.688053	-2.499990	-1.506915
C	0.051288	-3.680929	-1.058905
H	0.500918	-4.651549	-1.281551
C	-1.143372	-3.614989	-0.378697

H	-1.655425	-4.531288	-0.075532
C	-3.022109	-2.301047	0.545289
H	-3.529808	-3.229252	0.815840
C	-3.639585	-1.089226	0.735257
H	-4.653977	-1.045829	1.138103
C	-3.672406	1.363090	0.504519
H	-4.721553	1.363120	0.806644
C	-3.049061	2.541454	0.136481
H	-3.610972	3.477133	0.102807
C	-1.035954	3.738859	-0.628736
H	-1.642479	4.627715	-0.814418
C	0.325498	3.758575	-0.867349
H	0.800636	4.649954	-1.281954
C	2.543046	2.694857	-0.703370
H	2.971987	3.554671	-1.223036
C	3.352627	1.681796	-0.257864
H	4.429218	1.712387	-0.437608
C	3.659216	-0.366851	1.087058
H	4.728785	-0.325924	0.867983
C	3.155544	-1.338546	1.924680
H	3.819487	-2.086263	2.362837
C	1.784148	-1.338432	2.242386
H	1.386568	-2.074839	2.943253
C	-1.744500	-2.374224	-0.072848
C	-2.989725	0.128105	0.419408
C	-1.610969	0.103574	-0.013378
C	-1.674545	2.566837	-0.174688
C	-0.888053	1.342324	-0.027712
C	1.140207	2.659366	-0.508897
C	0.535421	1.488390	0.077868
C	2.817402	0.613343	0.516205
C	1.406349	0.554906	0.754530
C	-1.064198	-1.165719	-0.430228
C	0.114858	-1.280841	-1.200646
H	0.593231	-0.373836	-1.565649
C	0.936693	-0.412653	1.673602
H	-0.118134	-0.420213	1.941186
C	1.978757	-2.578275	-2.271002
H	1.918771	-3.307957	-3.093042
H	2.800169	-2.898096	-1.609384
H	2.254819	-1.602460	-2.692756

(*P*)-Pt(mppy)(acac)

E = -1517.02004198 a.u.

C	4.608721	-1.455519	0.200584
C	5.132710	-0.239581	0.674726
C	4.427184	0.958610	0.852052
Pt	1.868761	-0.220976	-0.082623
O	3.408693	-1.662512	-0.139084
O	3.194150	1.156188	0.622277
C	5.521012	-2.645853	0.067482
H	6.549754	-2.433585	0.381445
H	5.117063	-3.473547	0.669099
H	5.519951	-2.979654	-0.980930
C	5.154830	2.173344	1.362437
H	4.649112	2.538510	2.268347
H	6.209335	1.974053	1.586002
H	5.087251	2.972978	0.609552
C	0.387483	1.031451	-0.136935
C	0.456647	2.416374	-0.044568
C	-0.897897	0.390877	-0.388995
C	-0.704118	3.171183	-0.209903
H	1.425844	2.880281	0.129524
C	-2.105518	1.125734	-0.135675
C	-0.782485	-0.917113	-0.947415
C	-1.993256	2.549064	-0.262991
C	-3.391308	0.559153	0.131274
C	-1.776274	-1.660255	-1.617849
N	0.494058	-1.460583	-0.813310
C	-3.163252	3.318563	-0.442157
C	-4.547938	1.341398	-0.150291
C	-3.595195	-0.748512	0.737100
C	-1.509680	-2.932356	-2.064199
H	-2.751427	-1.204096	-1.779671
C	0.738070	-2.715732	-1.232069
C	-4.397854	2.715271	-0.452734
H	-3.061491	4.390164	-0.609818
C	-5.842870	0.737465	-0.120318
C	-4.893617	-1.324983	0.723721
C	-2.567907	-1.446399	1.412606
C	-0.225940	-3.487329	-1.840480
H	-2.276831	-3.503735	-2.588853
H	1.757104	-3.069755	-1.064399
H	-5.293869	3.306645	-0.654335
C	-6.006815	-0.561930	0.240144
H	-6.701893	1.348317	-0.406999

C	-5.082202	-2.620823	1.251622
C	-2.781174	-2.697535	1.947827
H	-1.592519	-0.978025	1.532205
H	0.018915	-4.500213	-2.160384
H	-6.995541	-1.025159	0.232826
C	-4.042966	-3.306927	1.840041
H	-6.080879	-3.061744	1.208369
H	-1.967132	-3.210574	2.463203
H	-4.206409	-4.305120	2.251434
H	6.191443	-0.225106	0.927126
O	-0.719261	4.515213	-0.268910
C	0.495310	5.219473	-0.221583
H	0.246626	6.281714	-0.334079
H	1.012248	5.070133	0.740892
H	1.170733	4.913976	-1.037815

(*M*)-Pt(mppy)(acac)

E = -1517.01646673 a.u.

C	-4.608721	-1.455519	0.200584
C	-5.132710	-0.239581	0.674726
C	-4.427184	0.958610	0.852052
Pt	-1.868761	-0.220976	-0.082623
O	-3.408693	-1.662512	-0.139084
O	-3.194150	1.156188	0.622277
C	-5.521012	-2.645853	0.067482
H	-6.549754	-2.433585	0.381445
H	-5.117063	-3.473547	0.669099
H	-5.519951	-2.979654	-0.980930
C	-5.154830	2.173344	1.362437
H	-4.649112	2.538510	2.268347
H	-6.209335	1.974053	1.586002
H	-5.087251	2.972978	0.609552
C	-0.387483	1.031451	-0.136935
C	-0.456647	2.416374	-0.044568
C	0.897897	0.390877	-0.388995
C	0.704118	3.171183	-0.209903
H	-1.425844	2.880281	0.129524
C	2.105518	1.125734	-0.135675
C	0.782485	-0.917113	-0.947415
C	1.993256	2.549064	-0.262991
C	3.391308	0.559153	0.131274
C	1.776274	-1.660255	-1.617849
N	-0.494058	-1.460583	-0.813310

C	3.163252	3.318563	-0.442157
C	4.547938	1.341398	-0.150291
C	3.595195	-0.748512	0.737100
C	1.509680	-2.932356	-2.064199
H	2.751427	-1.204096	-1.779671
C	-0.738070	-2.715732	-1.232069
C	4.397854	2.715271	-0.452734
H	3.061491	4.390164	-0.609818
C	5.842870	0.737465	-0.120318
C	4.893617	-1.324983	0.723721
C	2.567907	-1.446399	1.412606
C	0.225940	-3.487329	-1.840480
H	2.276831	-3.503735	-2.588853
H	-1.757104	-3.069755	-1.064399
H	5.293869	3.306645	-0.654335
C	6.006815	-0.561930	0.240144
H	6.701893	1.348317	-0.406999
C	5.082202	-2.620823	1.251622
C	2.781174	-2.697535	1.947827
H	1.592519	-0.978025	1.532205
H	-0.018915	-4.500213	-2.160384
H	6.995541	-1.025159	0.232826
C	4.042966	-3.306927	1.840041
H	6.080879	-3.061744	1.208369
H	1.967132	-3.210574	2.463203
H	4.206409	-4.305120	2.251434
H	-6.191443	-0.225106	0.927126
O	0.719261	4.515213	-0.268910
C	-0.495310	5.219473	-0.221583
H	-0.246626	6.281714	-0.334079
H	-1.012248	5.070133	0.740892
H	-1.170733	4.913976	-1.037815

(*R*)-OSFSO

E = -2205.91316369 a.u.

C	-5.150469	-1.889792	1.123050
C	-4.941469	-0.713022	0.419520
C	-3.641399	-0.294052	0.141310
C	-2.526479	-1.005771	0.584980
C	-2.763339	-2.207472	1.261820
C	-4.053829	-2.650052	1.525850
C	-0.920970	0.949849	-0.000640
C	-2.003910	1.760939	-0.489200

C	-1.800271	3.151509	-0.729120
H	-2.654581	3.739988	-1.066980
C	-0.582941	3.734269	-0.528940
C	0.513049	2.933410	-0.063270
C	0.293160	1.579360	0.201470
H	-6.165909	-2.222923	1.345990
H	-5.769530	-0.096393	0.065310
H	-1.918009	-2.808291	1.600700
H	-4.202918	-3.591842	2.057480
H	-0.447501	4.802759	-0.699220
H	1.131550	1.032890	0.614490
S	-3.475330	1.059718	-1.003710
O	-3.379910	0.394098	-2.320160
O	-4.595230	1.987198	-0.823450
C	-1.078239	-0.547981	0.332960
C	-0.501369	-1.351741	-0.836700
C	-0.255179	-0.801971	1.589790
C	0.878551	-1.629790	-0.858620
C	-1.246939	-1.711541	-1.948860
C	1.083591	-1.217180	1.509720
C	-0.780049	-0.560711	2.860420
C	1.481151	-2.201720	-1.998300
C	-0.643949	-2.321431	-3.057420
H	-2.302649	-1.452861	-2.000560
C	1.824011	-1.507810	2.669050
C	-0.038969	-0.795131	4.007970
H	-1.798570	-0.182661	2.940260
C	0.719841	-2.572920	-3.095530
H	-1.263189	-2.580331	-3.917430
H	2.830851	-1.913240	2.584810
C	1.261631	-1.301830	3.912790
H	-0.480569	-0.599511	4.986330
H	1.212222	-3.026360	-3.955160
H	1.833151	-1.535200	4.812220
C	3.043471	-1.170129	0.008460
C	3.868601	-0.375659	0.823680
C	3.599711	-1.763829	-1.141650
C	5.214841	-0.264229	0.537900
H	3.433810	0.182721	1.649500
C	4.962421	-1.673649	-1.408230
C	5.769951	-0.934468	-0.561260
H	5.842040	0.371292	1.163610
H	5.349661	-2.166189	-2.300210

H	6.836101	-0.844248	-0.773530
O	2.818171	-2.420980	-2.024400
N	1.677941	-1.353170	0.236350
C	1.850879	3.522800	0.124810
F	2.492599	3.802170	-1.034190
F	1.825049	4.688440	0.797330
F	2.686679	2.699950	0.807360

(*S*)-OSFSO

E = -2205.91316369 a.u.

C	5.150469	-1.889792	1.123050
C	4.941469	-0.713022	0.419520
C	3.641399	-0.294052	0.141310
C	2.526479	-1.005771	0.584980
C	2.763339	-2.207472	1.261820
C	4.053829	-2.650052	1.525850
C	0.920970	0.949849	-0.000640
C	2.003910	1.760939	-0.489200
C	1.800271	3.151509	-0.729120
H	2.654581	3.739988	-1.066980
C	0.582941	3.734269	-0.528940
C	-0.513049	2.933410	-0.063270
C	-0.293160	1.579360	0.201470
H	6.165909	-2.222923	1.345990
H	5.769530	-0.096393	0.065310
H	1.918009	-2.808291	1.600700
H	4.202918	-3.591842	2.057480
H	0.447501	4.802759	-0.699220
H	-1.131550	1.032890	0.614490
S	3.475330	1.059718	-1.003710
O	3.379910	0.394098	-2.320160
O	4.595230	1.987198	-0.823450
C	1.078239	-0.547981	0.332960
C	0.501369	-1.351741	-0.836700
C	0.255179	-0.801971	1.589790
C	-0.878551	-1.629790	-0.858620
C	1.246939	-1.711541	-1.948860
C	-1.083591	-1.217180	1.509720
C	0.780049	-0.560711	2.860420
C	-1.481151	-2.201720	-1.998300
C	0.643949	-2.321431	-3.057420
H	2.302649	-1.452861	-2.000560
C	-1.824011	-1.507810	2.669050

C	0.038969	-0.795131	4.007970
H	1.798570	-0.182661	2.940260
C	-0.719841	-2.572920	-3.095530
H	1.263189	-2.580331	-3.917430
H	-2.830851	-1.913240	2.584810
C	-1.261631	-1.301830	3.912790
H	0.480569	-0.599511	4.986330
H	-1.212222	-3.026360	-3.955160
H	-1.833151	-1.535200	4.812220
C	-3.043471	-1.170129	0.008460
C	-3.868601	-0.375659	0.823680
C	-3.599711	-1.763829	-1.141650
C	-5.214841	-0.264229	0.537900
H	-3.433810	0.182721	1.649500
C	-4.962421	-1.673649	-1.408230
C	-5.769951	-0.934468	-0.561260
H	-5.842040	0.371292	1.163610
H	-5.349661	-2.166189	-2.300210
H	-6.836101	-0.844248	-0.773530
O	-2.818171	-2.420980	-2.024400
N	-1.677941	-1.353170	0.236350
C	-1.850879	3.522800	0.124810
F	-2.492599	3.802170	-1.034190
F	-1.825049	4.688440	0.797330
F	-2.686679	2.699950	0.807360

(-)-(*R*,*R*)-CAI-Cz

E = -3320.72471979 a.u.

C	6.889858	-1.967548	-1.236000
C	8.242311	-1.495913	-0.710554
C	8.255473	-1.466581	0.816551
C	7.169046	-0.539586	1.354224
C	5.796098	-0.957137	0.833913
C	5.761415	-1.082888	-0.709441
H	9.238847	-1.140249	1.188601
H	8.461121	-0.483779	-1.093355
H	9.038919	-2.154993	-1.088612
H	6.702450	-3.003498	-0.923684
H	6.864989	-1.951150	-2.336402
H	7.371447	0.493253	1.039137
H	7.151316	-0.546542	2.455104
H	5.529000	-1.937909	1.253636
H	5.870093	-0.072507	-1.130244

H	8.095394	-2.489471	1.199209
N	4.724075	-0.053202	1.250119
C	4.677204	1.305816	0.894650
C	3.464534	-0.533639	1.634643
C	3.248268	1.706405	1.029347
O	5.607090	1.982990	0.544107
C	2.527538	0.612953	1.485002
O	3.209061	-1.665292	1.967517
C	2.621532	2.872765	0.648554
C	1.149408	0.649627	1.572601
C	1.224843	2.919235	0.685280
H	3.190583	3.724376	0.275623
C	0.483810	1.800955	1.144882
H	0.584584	-0.222343	1.892726
N	4.436612	-1.528291	-1.109493
C	3.423626	-0.594645	-1.432583
C	3.922248	-2.807381	-0.818320
C	2.180169	-1.325581	-1.332638
O	3.629722	0.593922	-1.660703
C	2.478562	-2.676146	-0.971856
O	4.579022	-3.772446	-0.465443
C	0.863593	-0.872027	-1.359897
C	1.476940	-3.584755	-0.686582
C	-0.136425	-1.765689	-1.026970
H	0.633369	0.170989	-1.573109
C	0.162474	-3.140411	-0.723502
H	1.718519	-4.612839	-0.411327
N	-0.930904	1.818855	1.158890
C	-1.772431	2.094168	0.078726
C	-1.710689	1.727659	2.310914
C	-1.468772	2.218154	-1.275575
C	-3.098304	2.215311	0.547305
C	-1.320451	1.469587	3.624689
C	-3.059928	1.975000	1.976256
C	-2.505264	2.515184	-2.150498
H	-0.451711	2.108528	-1.644978
C	-4.125924	2.509581	-0.350089
C	-2.309949	1.450036	4.601474
H	-0.275512	1.293477	3.881084
C	-4.033501	1.954973	2.973998
C	-3.821984	2.667763	-1.695618
H	-2.281458	2.633763	-3.211941
H	-5.153293	2.615183	0.004717

C	-3.654491	1.688573	4.284205
H	-2.029610	1.250102	5.637763
H	-5.079360	2.149138	2.727272
H	-4.613527	2.904554	-2.408605
H	-4.406085	1.670590	5.075565
N	0.581645	4.054481	0.155708
C	0.706064	4.455426	-1.178280
C	-0.397455	4.835708	0.766051
C	1.509164	3.918913	-2.186578
C	-0.208728	5.500251	-1.426649
C	-0.842727	4.821144	2.086181
C	-0.917678	5.741875	-0.183110
C	1.392295	4.473984	-3.455839
H	2.187968	3.082798	-2.004140
C	-0.302085	6.041021	-2.710220
C	-1.857159	5.703267	2.434814
H	-0.416394	4.140852	2.822192
C	-1.931624	6.624362	0.193030
C	0.503319	5.526895	-3.718330
H	2.009610	4.076508	-4.264021
H	-1.005879	6.849551	-2.918943
C	-2.403358	6.593217	1.498974
H	-2.233875	5.699826	3.459572
H	-2.348294	7.327115	-0.531478
H	0.442149	5.940769	-4.726598
H	-3.200773	7.273040	1.804672
N	-1.500749	-1.361685	-0.944430
C	-2.287469	-1.393839	0.204657
C	-2.303075	-1.057948	-2.022385
C	-1.898788	-1.588580	1.526978
C	-3.635760	-1.163841	-0.149303
C	-1.942523	-0.915409	-3.366213
C	-3.648545	-0.939856	-1.587721
C	-2.896675	-1.596873	2.502304
H	-0.852475	-1.714946	1.791349
C	-4.612108	-1.172527	0.834338
C	-2.956181	-0.639219	-4.273969
H	-0.902820	-1.007963	-3.678519
C	-4.642550	-0.670523	-2.513933
C	-4.232987	-1.400388	2.163422
H	-2.617480	-1.746273	3.545449
H	-5.659020	-0.995835	0.581180
C	-4.288075	-0.518575	-3.856848

H	-2.709940	-0.512832	-5.329478
H	-5.684257	-0.577243	-2.203050
H	-4.991199	-1.400762	2.947287
H	-5.061915	-0.301029	-4.595016
N	-0.922008	-3.993067	-0.380913
C	-1.188200	-4.436148	0.897882
C	-2.008783	-4.302838	-1.196246
C	-0.390690	-4.323082	2.044213
C	-2.486858	-5.006948	0.936403
C	-2.159289	-4.095659	-2.564600
C	-3.016163	-4.912680	-0.416035
C	-0.916330	-4.806183	3.234799
H	0.599627	-3.867397	1.999895
C	-2.988775	-5.477730	2.142581
C	-3.372172	-4.468273	-3.142002
H	-1.351977	-3.671038	-3.159461
C	-4.215201	-5.283262	-1.014276
C	-2.196062	-5.376958	3.286706
H	-0.320182	-4.739011	4.146418
H	-3.988498	-5.912211	2.199289
C	-4.389901	-5.046934	-2.379471
H	-3.524618	-4.303964	-4.210105
H	-5.008570	-5.751167	-0.428166
H	-2.578854	-5.746048	4.239824
H	-5.328508	-5.328113	-2.859806

(+)-(*S*,*S*)-CAI-Cz

E = -3320.72471996 a.u.

C	-6.889220	-1.969001	-1.236140
C	-8.241816	-1.497717	-0.710754
C	-8.255077	-1.468487	0.816350
C	-7.168921	-0.541245	1.354139
C	-5.795827	-0.958406	0.833897
C	-5.761010	-1.084110	-0.709469
H	-9.238556	-1.142429	1.188361
H	-8.460843	-0.485610	-1.093506
H	-9.038244	-2.156963	-1.088902
H	-6.701590	-3.004924	-0.923865
H	-6.864291	-1.952544	-2.336540
H	-7.371569	0.491559	1.039095
H	-7.151261	-0.548253	2.455020
H	-5.528491	-1.939118	1.253609
H	-5.869881	-0.073741	-1.130252

H	-8.094759	-2.491360	1.198954
N	-4.724097	-0.054179	1.250238
C	-4.677600	1.304880	0.894873
C	-3.464456	-0.534261	1.634875
C	-3.248763	1.705831	1.029539
O	-5.607643	1.981780	0.544217
C	-2.527747	0.612556	1.485175
O	-3.208682	-1.665861	1.967703
C	-2.622327	2.872343	0.648714
C	-1.149620	0.649562	1.572708
C	-1.225648	2.919132	0.685356
H	-3.191593	3.723801	0.275762
C	-0.484328	1.801046	1.144938
H	-0.584568	-0.222263	1.892824
N	-4.436095	-1.529231	-1.109478
C	-3.423278	-0.595382	-1.432512
C	-3.921494	-2.808235	-0.818349
C	-2.179685	-1.326090	-1.332570
O	-3.629593	0.593151	-1.660611
C	-2.477833	-2.676736	-0.971898
O	-4.578102	-3.773467	-0.465619
C	-0.863193	-0.872289	-1.359767
C	-1.476049	-3.585186	-0.686700
C	0.136984	-1.765782	-1.026867
H	-0.633160	0.170788	-1.572887
C	-0.161663	-3.140592	-0.723537
H	-1.717445	-4.613334	-0.411519
N	0.930379	1.819345	1.158885
C	1.771759	2.095080	0.078717
C	1.710251	1.728253	2.310858
C	1.467973	2.219225	-1.275541
C	3.097627	2.216526	0.547232
C	1.320160	1.469901	3.624621
C	3.059404	1.975998	1.976151
C	2.504326	2.516684	-2.150483
H	0.450913	2.109399	-1.644891
C	4.125109	2.511216	-0.350183
C	2.309722	1.450482	4.601343
H	0.275285	1.293465	3.881053
C	4.033042	1.956097	2.973832
C	3.821037	2.669529	-1.695667
H	2.280416	2.635385	-3.211892
H	5.152472	2.617044	0.004572

C	3.654183	1.689419	4.284025
H	2.029500	1.250330	5.637621
H	5.078834	2.150580	2.727071
H	4.612469	2.906652	-2.408668
H	4.405828	1.671531	5.075338
N	-0.582698	4.054451	0.155641
C	-0.707443	4.455375	-1.178320
C	0.396493	4.835738	0.765756
C	-1.510757	3.918815	-2.186421
C	0.207217	5.500263	-1.426903
C	0.842110	4.821160	2.085769
C	0.916430	5.741946	-0.183524
C	-1.394221	4.473887	-3.455713
H	-2.189491	3.082680	-2.003806
C	0.300244	6.041029	-2.710500
C	1.856560	5.703355	2.434169
H	0.416023	4.140803	2.821864
C	1.930398	6.624505	0.192385
C	-0.505363	5.526845	-3.718419
H	-2.011710	4.076379	-4.263744
H	1.003936	6.849603	-2.919392
C	2.402451	6.593375	1.498215
H	2.233538	5.699914	3.458832
H	2.346845	7.327298	-0.532214
H	-0.444456	5.940719	-4.726703
H	3.199891	7.273251	1.803730
N	1.501221	-1.361495	-0.944222
C	2.287899	-1.393586	0.204895
C	2.303516	-1.057427	-2.022106
C	1.899209	-1.588541	1.527182
C	3.636154	-1.163253	-0.148985
C	1.942980	-0.914773	-3.365925
C	3.648944	-0.939096	-1.587377
C	2.897058	-1.596712	2.502548
H	0.852913	-1.715161	1.791498
C	4.612464	-1.171824	0.834694
C	2.956610	-0.638238	-4.273608
H	0.903308	-1.007509	-3.678281
C	4.642923	-0.669423	-2.513517
C	4.233340	-1.399902	2.163740
H	2.617853	-1.746272	3.545667
H	5.659346	-0.994868	0.581598
C	4.288463	-0.517368	-3.856424

H	2.710378	-0.511756	-5.329108
H	5.684598	-0.575950	-2.202582
H	4.991520	-1.400182	2.947636
H	5.062282	-0.299550	-4.594533
N	0.922954	-3.993082	-0.380958
C	1.189146	-4.436226	0.897815
C	2.009818	-4.302625	-1.196258
C	0.391534	-4.323418	2.044100
C	2.487915	-5.006767	0.936375
C	2.160347	-4.095367	-2.564598
C	3.017276	-4.912313	-0.416028
C	0.917194	-4.806503	3.234683
H	-0.598876	-3.867935	1.999749
C	2.989851	-5.477535	2.142551
C	3.373329	-4.467721	-3.141959
H	1.352980	-3.670881	-3.159480
C	4.216416	-5.282636	-1.014227
C	2.197042	-5.377011	3.286632
H	0.320971	-4.739525	4.146268
H	3.989657	-5.911822	2.199290
C	4.391135	-5.046214	-2.379403
H	3.525794	-4.303339	-4.210048
H	5.009844	-5.750420	-0.428101
H	2.579848	-5.746096	4.239747
H	5.329820	-5.327192	-2.859706

R_p-CzpPhTrz

E = -1874.47709412 a.u.

N	2.586669	-0.362283	0.958189
N	-3.759446	-1.202830	0.310652
N	-5.698065	0.085625	-0.057893
N	-3.605751	1.157875	0.101818
C	3.140497	-1.555728	-1.175266
C	4.185165	-2.306552	-1.729425
H	4.009627	-2.823335	-2.674722
C	5.479783	-2.238550	-1.236554
H	6.280820	-2.732933	-1.790222
C	5.828816	-1.405200	-0.142582
C	5.615801	0.379066	2.729823
H	6.681213	0.175365	2.625030
C	5.155582	1.136119	3.813800
H	5.874687	1.519700	4.539500
C	3.795343	1.402209	3.989029

H	3.466540	1.986399	4.849834
C	2.850456	0.926397	3.083024
H	1.784219	1.113254	3.205182
C	3.429685	-1.023638	0.108323
C	4.771375	-0.923698	0.604869
C	4.694003	-0.100594	1.809780
C	3.325608	0.194217	1.998060
C	2.005640	-1.107499	-2.060569
H	1.973805	-1.792067	-2.919074
H	1.035513	-1.171333	-1.558024
C	2.192896	0.373515	-2.594932
H	1.476797	1.020118	-2.071927
H	1.916381	0.378924	-3.658965
C	3.592984	0.902526	-2.391733
C	4.670085	0.421471	-3.141132
H	4.480404	-0.130332	-4.065591
C	5.966612	0.479548	-2.638900
H	6.770567	-0.029046	-3.178129
C	6.220432	1.030120	-1.379340
C	5.192367	1.762289	-0.781451
H	5.375401	2.280997	0.162125
C	3.894746	1.695789	-1.280127
H	3.082594	2.167481	-0.723324
C	7.412147	0.585996	-0.565375
H	8.338812	0.620023	-1.156418
H	7.549425	1.272706	0.281605
C	7.241453	-0.891171	-0.014428
H	7.587298	-0.927635	1.027940
H	7.904030	-1.560787	-0.579507
C	1.178424	-0.278413	0.845015
C	0.394295	-1.459375	0.882063
H	0.881575	-2.420670	1.057847
C	-0.962667	-1.384272	0.705509
H	-1.580149	-2.281015	0.739054
C	-1.614705	-0.131615	0.485226
C	-0.807702	1.045745	0.476154
H	-1.304078	2.003085	0.322551
C	0.550359	0.980039	0.656793
H	1.153324	1.889972	0.638959
C	-3.030770	-0.057305	0.293747
C	-5.058807	-1.078371	0.130226
C	-4.913207	1.173228	-0.059943
C	-5.884846	-2.317649	0.136237

C	-5.287098	-3.567284	0.324476
H	-4.207346	-3.606612	0.466141
C	-6.059456	-4.722879	0.329411
H	-5.583097	-5.694686	0.477641
C	-7.439143	-4.643507	0.146368
H	-8.046038	-5.551870	0.150627
C	-8.040664	-3.401328	-0.041529
H	-9.121385	-3.333490	-0.185048
C	-7.268322	-2.244419	-0.046815
H	-7.718573	-1.263000	-0.192103
C	-5.574726	2.492620	-0.260116
C	-6.959613	2.569206	-0.430417
H	-7.533448	1.643230	-0.414169
C	-7.578462	3.801412	-0.614100
H	-8.661689	3.850880	-0.745703
C	-6.820412	4.969857	-0.630023
H	-7.306894	5.937354	-0.774043
C	-5.438419	4.899734	-0.461149
H	-4.839690	5.813356	-0.472752
C	-4.819467	3.668907	-0.277229
H	-3.740891	3.591473	-0.142483

S_p-CzpPhTrz

E = -1874.47709416 a.u.

N	-2.586669	-0.362283	0.958189
N	3.759446	-1.202830	0.310652
N	5.698065	0.085625	-0.057893
N	3.605751	1.157875	0.101818
C	-3.140497	-1.555728	-1.175266
C	-4.185165	-2.306552	-1.729425
H	-4.009627	-2.823335	-2.674722
C	-5.479783	-2.238550	-1.236554
H	-6.280820	-2.732933	-1.790222
C	-5.828816	-1.405200	-0.142582
C	-5.615801	0.379066	2.729823
H	-6.681213	0.175365	2.625030
C	-5.155582	1.136119	3.813800
H	-5.874687	1.519700	4.539500
C	-3.795343	1.402209	3.989029
H	-3.466540	1.986399	4.849834
C	-2.850456	0.926397	3.083024
H	-1.784219	1.113254	3.205182
C	-3.429685	-1.023638	0.108323

C	-4.771375	-0.923698	0.604869
C	-4.694003	-0.100594	1.809780
C	-3.325608	0.194217	1.998060
C	-2.005640	-1.107499	-2.060569
H	-1.973805	-1.792067	-2.919074
H	-1.035513	-1.171333	-1.558024
C	-2.192896	0.373515	-2.594932
H	-1.476797	1.020118	-2.071927
H	-1.916381	0.378924	-3.658965
C	-3.592984	0.902526	-2.391733
C	-4.670085	0.421471	-3.141132
H	-4.480404	-0.130332	-4.065591
C	-5.966612	0.479548	-2.638900
H	-6.770567	-0.029046	-3.178129
C	-6.220432	1.030120	-1.379340
C	-5.192367	1.762289	-0.781451
H	-5.375401	2.280997	0.162125
C	-3.894746	1.695789	-1.280127
H	-3.082594	2.167481	-0.723324
C	-7.412147	0.585996	-0.565375
H	-8.338812	0.620023	-1.156418
H	-7.549425	1.272706	0.281605
C	-7.241453	-0.891171	-0.014428
H	-7.587298	-0.927635	1.027940
H	-7.904030	-1.560787	-0.579507
C	-1.178424	-0.278413	0.845015
C	-0.394295	-1.459375	0.882063
H	-0.881575	-2.420670	1.057847
C	0.962667	-1.384272	0.705509
H	1.580149	-2.281015	0.739054
C	1.614705	-0.131615	0.485226
C	0.807702	1.045745	0.476154
H	1.304078	2.003085	0.322551
C	-0.550359	0.980039	0.656793
H	-1.153324	1.889972	0.638959
C	3.030770	-0.057305	0.293747
C	5.058807	-1.078371	0.130226
C	4.913207	1.173228	-0.059943
C	5.884846	-2.317649	0.136237
C	5.287098	-3.567284	0.324476
H	4.207346	-3.606612	0.466141
C	6.059456	-4.722879	0.329411
H	5.583097	-5.694686	0.477641

C	7.439143	-4.643507	0.146368
H	8.046038	-5.551870	0.150627
C	8.040664	-3.401328	-0.041529
H	9.121385	-3.333490	-0.185048
C	7.268322	-2.244419	-0.046815
H	7.718573	-1.263000	-0.192103
C	5.574726	2.492620	-0.260116
C	6.959613	2.569206	-0.430417
H	7.533448	1.643230	-0.414169
C	7.578462	3.801412	-0.614100
H	8.661689	3.850880	-0.745703
C	6.820412	4.969857	-0.630023
H	7.306894	5.937354	-0.774043
C	5.438419	4.899734	-0.461149
H	4.839690	5.813356	-0.472752
C	4.819467	3.668907	-0.277229
H	3.740891	3.591473	-0.142483

(*R*)-OBN-Cz

E = -2369.73767905 a.u.

N	-2.701558	-0.319887	-1.306880
O	2.133307	0.384207	1.389452
C	-0.234105	-0.414127	-1.373410
C	5.082064	1.596488	-0.498212
C	4.135120	0.557259	-0.483745
C	0.990069	0.164880	0.677829
C	3.085684	0.577960	-1.399802
N	-2.706449	0.308009	1.316513
C	-4.870862	-0.138420	1.893646
C	-1.441207	-0.187843	-0.656179
C	4.147717	-0.550221	0.508823
C	0.992057	-0.208881	-0.646815
C	3.096756	-0.607003	1.419054
C	-3.301382	-1.522463	-1.616865
C	6.100577	1.703764	0.617192
H	5.577705	2.112804	1.499917
H	6.442248	0.708819	0.926362
C	-3.294978	1.517481	1.621491
C	-4.654257	1.301526	1.962325
C	6.033263	3.692636	-1.586312
H	6.751608	3.424270	-2.381717
H	5.546623	4.620690	-1.923464
C	-4.655485	-1.290975	-1.967958

C	-2.751084	-2.806714	-1.577136
H	-1.701951	-2.957948	-1.326537
C	-3.633215	-0.709771	1.521552
C	-3.456353	-2.085749	1.411852
H	-2.480686	-2.508352	1.179156
C	-1.443434	0.161793	0.674000
C	-5.964802	-0.963643	2.114193
H	-6.932638	-0.543787	2.394567
C	-4.856222	0.151376	-1.900269
C	-5.462526	2.388886	2.253792
H	-6.515244	2.251219	2.506798
C	-4.568793	-2.895787	1.636746
H	-4.464660	-3.978214	1.547496
C	5.000056	2.589661	-1.487785
C	3.014232	-1.608352	2.377279
H	2.189993	-1.598114	3.091874
C	2.988906	1.558277	-2.377145
H	2.164153	1.523116	-3.090363
C	-4.931165	-3.657606	-2.226957
H	-5.565023	-4.513163	-2.466258
C	-5.473673	-2.368931	-2.266292
H	-6.522809	-2.219309	-2.527258
C	-4.905338	3.671303	2.217847
H	-5.531335	4.534109	2.451768
C	-3.614931	0.708453	-1.518721
C	3.959279	2.547903	-2.419675
H	3.904760	3.322566	-3.188844
C	-3.589264	-3.869460	-1.893667
H	-3.190693	-4.885127	-1.885614
C	5.111861	-1.576590	0.502152
C	-2.730010	2.795497	1.585319
H	-1.677334	2.934823	1.342800
C	-5.938887	0.989084	-2.128691
H	-6.909372	0.580470	-2.416397
C	-5.807003	-2.346038	1.972242
H	-6.660391	-3.005044	2.139927
C	-0.238473	0.377279	1.398218
C	-3.558571	3.867791	1.894744
H	-3.148519	4.878898	1.889145
C	3.997333	-2.584603	2.399636
H	3.954230	-3.375621	3.152820
C	5.040094	-2.592780	1.467454
C	7.284661	2.599929	0.278643

H	7.900570	2.758329	1.176884
H	7.931193	2.099592	-0.463630
C	-3.423033	2.082295	-1.407337
H	-2.444310	2.493568	-1.167343
C	-4.524425	2.905092	-1.640244
H	-4.408546	3.986227	-1.549908
C	6.799661	3.926704	-0.290337
H	7.642111	4.612088	-0.469535
H	6.143062	4.417732	0.448323
C	6.040446	-3.729511	1.500551
H	6.314469	-3.940831	2.546140
H	5.541937	-4.642970	1.130629
C	-5.766260	2.369633	-1.985124
H	-6.610767	3.038406	-2.158985
C	7.283017	-3.470325	0.658509
H	7.877144	-4.392517	0.569583
H	7.926918	-2.725841	1.158271
C	6.182763	-1.592723	-0.569227
H	6.943381	-0.827257	-0.338926
H	5.737598	-1.282701	-1.525902
C	6.876683	-2.942116	-0.710288
H	6.195721	-3.665219	-1.191152
H	7.749391	-2.842832	-1.373230
O	2.139066	-0.428528	-1.353290
C	-0.235874	-0.733980	-2.743275
N	-0.279559	-0.999591	-3.874851
N	-0.294709	0.966231	3.898636
C	-0.245620	0.698056	2.767942

(*S*)-OBN-Cz

E = -2369.72599242 a.u.

N	2.689177	-0.762793	-1.221897
O	-2.099902	0.766414	1.242208
C	0.256358	-0.712118	-1.187331
C	-5.089728	1.398176	-0.904206
C	-4.123542	0.410575	-0.614180
C	-0.966999	0.366684	0.613075
C	-3.078598	0.198042	-1.516870
N	2.696745	0.764580	1.223565
C	4.916671	0.691106	1.804879
C	1.494065	-0.366284	-0.597960
C	-4.123859	-0.386771	0.640879
C	-0.970674	-0.360497	-0.591490

C	-3.072595	-0.194147	1.537950
C	3.146902	-2.092914	-1.286902
C	-6.105529	1.793807	0.150936
H	-5.582924	2.438871	0.881752
H	-6.428756	0.917695	0.727504
C	3.158074	2.093533	1.286405
C	4.531424	2.081382	1.638996
C	-6.082064	3.107224	-2.520196
H	-6.798066	2.616048	-3.205848
H	-5.614204	3.914608	-3.106188
C	4.518556	-2.084222	-1.646104
C	2.467345	-3.277638	-1.002275
H	1.414765	-3.279221	-0.716893
C	3.761861	-0.091186	1.550471
C	3.770594	-1.480364	1.668072
H	2.871445	-2.071863	1.502342
C	1.497698	0.370641	0.605579
C	6.116937	0.053572	2.140464
H	7.018000	0.639775	2.333715
C	4.906495	-0.694913	-1.813806
C	5.231943	3.290342	1.718848
H	6.291754	3.296137	1.983037
C	4.979810	-2.094897	1.995466
H	5.017631	-3.183572	2.070502
C	-5.026951	2.087901	-2.132993
C	-2.980932	-0.898009	2.735170
H	-2.157985	-0.693023	3.421875
C	-2.995401	0.877444	-2.727956
H	-2.174687	0.662047	-3.414111
C	4.543688	-4.484872	-1.449327
H	5.075524	-5.436760	-1.510523
C	5.215638	-3.294944	-1.729395
H	6.274143	-3.303391	-1.998702
C	4.561621	4.481936	1.441989
H	5.096136	5.432487	1.500584
C	3.754891	0.090291	-1.553870
C	-3.985336	1.808684	-3.030087
H	-3.944758	2.345378	-3.981676
C	3.184857	-4.472565	-1.088412
H	2.675406	-5.414949	-0.874869
C	-5.088238	-1.383793	0.915185
C	2.480087	3.279936	1.005079
H	1.426147	3.284066	0.724786

C	6.106790	-0.060423	-2.155025
H	7.005429	-0.648918	-2.352561
C	6.143509	-1.339019	2.221378
H	7.075645	-1.849597	2.472740
C	0.263634	0.718021	1.201708
C	3.201010	4.473061	1.087715
H	2.692905	5.416731	0.876658
C	-3.964515	-1.839338	3.022035
H	-3.916331	-2.397403	3.960961
C	-5.011377	-2.103409	2.124771
C	-7.310524	2.547124	-0.409652
H	-7.923439	2.936983	0.418399
H	-7.953235	1.851087	-0.978878
C	3.766608	1.479440	-1.671484
H	2.869756	2.073219	-1.501575
C	4.975853	2.090918	-2.004475
H	5.016064	3.179506	-2.079497
C	-6.850610	3.677441	-1.328507
H	-7.706636	4.272943	-1.683524
H	-6.199656	4.364683	-0.759343
C	-6.007834	-3.196216	2.463686
H	-6.279401	-3.121735	3.529577
H	-5.500829	-4.172575	2.351974
C	6.136553	1.332105	-2.235897
H	7.068809	1.840325	-2.491551
C	-7.256205	-3.181738	1.582953
H	-7.842110	-4.099959	1.746330
H	-7.906993	-2.335376	1.867676
C	-6.163780	-1.691026	-0.110296
H	-6.927129	-0.893232	-0.086896
H	-5.724726	-1.642604	-1.118665
C	-6.853643	-3.036184	0.116994
H	-6.169091	-3.858931	-0.156110
H	-7.728694	-3.120414	-0.546473
O	-2.107290	-0.761329	-1.213540
C	0.225825	-1.360608	-2.463474
N	0.193175	-1.862863	-3.508482
N	0.215606	1.870910	3.522152
C	0.241087	1.367278	2.477612

iso-(*R*)-OBN-CzB1

E = -2369.57941252 a.u.

O	1.329600	0.770749	-0.322980

C	-0.953721	-2.136350	-0.273790
C	-0.649058	3.086570	1.758490
C	-0.789339	2.250790	0.638370
C	0.847360	-0.503171	-0.337250
C	-1.438319	1.024311	0.771040
C	-0.037762	-3.193670	-0.191490
C	-0.222809	2.553360	-0.703510
C	-0.544790	-0.800570	-0.361000
C	0.806681	1.738969	-1.166280
C	0.221302	4.322660	1.670370
H	1.273822	3.987299	1.688740
H	0.096593	4.812270	0.696440
C	-1.150928	3.588940	4.202120
H	-2.104968	4.137901	4.295910
H	-1.076578	2.963510	5.104880
C	1.385758	-2.913541	-0.121120
C	-1.228719	2.700681	2.978340
C	1.361151	1.905109	-2.426570
H	2.177321	1.255299	-2.745510
C	-2.009670	0.628071	1.972370
H	-2.516000	-0.335949	2.041060
C	-1.910119	1.482221	3.061280
H	-2.360389	1.190081	4.013380
C	-0.762868	3.530390	-1.559970
C	1.758909	-1.523771	-0.203730
C	0.857192	2.903639	-3.245620
H	1.285612	3.053089	-4.239940
C	-0.203898	3.715580	-2.834970
C	-0.008007	5.313890	2.804160
H	0.763703	6.098059	2.775980
H	-0.978387	5.821330	2.664400
C	-0.008407	4.595570	4.147180
H	-0.095807	5.311490	4.978460
H	0.955732	4.073879	4.278850
C	-0.755227	4.741340	-3.802710
H	0.081163	5.249330	-4.307960
H	-1.305398	4.206831	-4.597080
C	-1.688057	5.753661	-3.150650
H	-2.199287	6.346311	-3.924130
H	-1.103986	6.465200	-2.541390
C	-1.965918	4.333841	-1.112290
H	-1.644367	5.093561	-0.379420
H	-2.653988	3.672981	-0.565450

C	-2.688367	5.032291	-2.258000
H	-3.242198	4.290092	-2.857940
H	-3.436077	5.730792	-1.853530
O	-1.483090	0.202771	-0.337660
C	-0.500993	-4.535170	-0.176850
N	-0.865883	-5.634600	-0.164230
C	2.357278	-3.902121	0.068900
N	3.212587	-4.684852	0.207970
N	-2.336711	-2.392809	-0.237030
C	-3.256941	-1.992368	-1.203310
C	-3.034592	-2.913058	0.854220
C	-3.028351	-1.409698	-2.448480
C	-4.559221	-2.288588	-0.749100
C	-2.547822	-3.375859	2.075880
C	-4.417712	-2.869718	0.574270
C	-4.134251	-1.126978	-3.239000
H	-2.017421	-1.176389	-2.782650
C	-5.655321	-1.998227	-1.562500
C	-3.474862	-3.813858	3.013680
H	-1.478512	-3.403469	2.284120
C	-5.328372	-3.319357	1.530670
C	-5.436301	-1.417257	-2.805280
H	-3.985130	-0.668028	-4.218620
H	-6.669051	-2.225556	-1.226170
C	-4.850882	-3.791967	2.747020
H	-3.119922	-4.189748	3.975350
H	-6.400892	-3.293557	1.327040
H	-6.283821	-1.183977	-3.452530
H	-5.551662	-4.148847	3.503970
N	3.129889	-1.190472	-0.077680
C	3.690990	-0.492672	0.984080
C	4.115359	-1.553052	-0.957540
C	3.048830	0.056218	2.090260
C	5.089160	-0.408573	0.791990
C	3.980829	-2.249752	-2.164340
C	5.370469	-1.100563	-0.468090
C	3.849860	0.709368	3.026700
H	1.968760	-0.014911	2.208050
C	5.865450	0.239857	1.732860
C	5.146519	-2.505853	-2.878970
H	3.003729	-2.580832	-2.511200
C	6.510159	-1.364194	-1.195280
C	5.230750	0.800627	2.853780

H	3.385261	1.155648	3.906970
H	6.947770	0.316026	1.616500
C	6.386799	-2.076234	-2.404640
H	5.089748	-3.056183	-3.818580
H	7.491199	-1.034694	-0.849710
H	5.832061	1.316857	3.603830
H	7.284909	-2.295304	-2.984310

iso-(*S*)-OBN-CzB1

E = -2369.57951126 a.u.

O	-1.330671	0.768738	-0.293031
C	0.956592	-2.134699	-0.266311
C	0.665236	3.098591	1.756839
C	0.794737	2.257481	0.639379
C	-0.847780	-0.504981	-0.314751
C	1.444969	1.031592	0.772029
C	0.042794	-3.194230	-0.183041
C	0.213647	2.553070	-0.697941
C	0.544901	-0.799789	-0.346941
C	-0.819882	1.735179	-1.145681
C	-0.207215	4.333510	1.671749
H	-1.259075	3.996848	1.701839
H	-0.092696	4.819620	0.694759
C	1.188905	3.611721	4.193719
H	2.143015	4.162332	4.276499
H	1.123646	2.989991	5.099719
C	-1.381117	-2.916872	-0.107271
C	1.256327	2.718351	2.973049
C	-1.389192	1.895198	-2.400121
H	-2.207882	1.242717	-2.706971
C	2.027349	0.640862	1.969789
H	2.534280	-0.322917	2.037999
C	1.938108	1.500082	3.055549
H	2.396758	1.212133	4.004909
C	0.742116	3.527381	-1.564771
C	-1.756938	-1.527702	-0.183341
C	-0.896444	2.891049	-3.229051
H	-1.336544	3.035688	-4.218971
C	0.167985	3.706300	-2.833961
C	0.031443	5.329640	2.799339
H	-0.741257	6.112899	2.774819
H	1.000163	5.837151	2.648789
C	0.044544	4.616490	4.144989

H	0.137933	5.335700	4.972789
H	-0.917585	4.093799	4.286829
C	0.706174	4.728691	-3.812291
H	-0.136826	5.231440	-4.311711
H	1.250325	4.192071	-4.609451
C	1.641973	5.747172	-3.174491
H	2.142442	6.338852	-3.955711
H	1.061652	6.458751	-2.561711
C	1.948575	4.335022	-1.134271
H	1.633954	5.095232	-0.399091
H	2.645275	3.677403	-0.594481
C	2.655064	5.033113	-2.290271
H	3.205655	4.291534	-2.893991
H	3.404133	5.736164	-1.896301
O	1.481210	0.205262	-0.333281
C	0.508465	-4.534800	-0.175111
N	0.875586	-5.633579	-0.168121
C	-2.350716	-3.907873	0.080219
N	-3.204475	-4.692594	0.217409
N	2.340213	-2.389067	-0.238731
C	3.253722	-1.985086	-1.209921
C	3.045633	-2.911907	0.846359
C	3.016551	-1.397757	-2.451311
C	4.559193	-2.281785	-0.765241
C	2.567324	-3.378097	2.070089
C	4.426793	-2.866915	0.557309
C	4.117071	-1.110665	-3.247741
H	2.003351	-1.163468	-2.777871
C	5.649732	-1.987173	-1.584571
C	3.500914	-3.817676	3.000619
H	1.499444	-3.406858	2.285399
C	5.344134	-3.318194	1.506489
C	5.422151	-1.401574	-2.823651
H	3.961181	-0.647735	-4.224451
H	6.665892	-2.214492	-1.255591
C	4.875094	-3.794034	2.724889
H	3.152705	-4.195996	3.963819
H	6.415274	-3.291002	1.295849
H	6.265291	-1.164913	-3.475391
H	5.581185	-4.151973	3.476399
N	-3.129309	-1.198514	-0.060971
C	-3.697990	-0.506425	1.000059
C	-4.108838	-1.559495	-0.948391

C	-3.063600	0.039136	2.112369
C	-5.095260	-0.424316	0.799899
C	-3.965368	-2.249925	-2.157711
C	-5.367609	-1.111337	-0.464821
C	-3.871531	0.686555	3.046789
H	-1.984050	-0.030422	2.235689
C	-5.878420	0.218643	1.738759
C	-5.126027	-2.504006	-2.881271
H	-2.985427	-2.577754	-2.499671
C	-6.502199	-1.372918	-1.200741
C	-5.251551	0.775854	2.865849
H	-3.413312	1.129946	3.931849
H	-6.960171	0.293182	1.616179
C	-6.369978	-2.078448	-2.412961
H	-5.062267	-3.049446	-3.823301
H	-7.485919	-1.046359	-0.860021
H	-5.858402	1.287663	3.614469
H	-7.263937	-2.295529	-2.999751

iso-(*R*)-OBN-CzC1

E = -2369.72847675 a.u.

O	2.227449	-0.977166	-1.969850
C	-0.983398	-0.087993	-0.392945
C	4.308670	-1.626117	1.044610
C	3.413669	-0.680272	0.515370
C	0.900796	-0.779049	-1.748572
C	2.110556	-0.623473	1.004412
C	-1.849846	-0.495176	-1.382804
C	3.758392	0.248914	-0.594179
C	0.432340	-0.203292	-0.578479
C	3.106680	0.078481	-1.812328
C	5.655159	-1.838999	0.385925
H	5.478860	-2.420998	-0.535957
H	6.072710	-0.884670	0.042691
C	4.842216	-3.434455	2.755204
H	5.236928	-2.984699	3.684062
H	4.278106	-4.325725	3.070106
C	-1.417560	-1.103733	-2.577978
C	3.896729	-2.442402	2.110866
C	3.351817	0.913181	-2.894658
H	2.842567	0.722296	-3.840326
C	1.688384	-1.432029	2.050133
H	0.662702	-1.351450	2.413186

C	2.594436	-2.323789	2.604635
H	2.282051	-2.962982	3.434423
C	4.632321	1.340753	-0.427260
C	0.022829	-1.235396	-2.763496
C	4.252925	1.953823	-2.737304
H	4.465730	2.613667	-3.582349
C	4.890747	2.188964	-1.514994
C	6.654458	-2.581403	1.263550
H	7.545653	-2.842897	0.673278
H	6.998294	-1.920855	2.078961
C	6.012973	-3.826230	1.862137
H	6.746132	-4.411420	2.437836
H	5.657551	-4.477918	1.045724
C	5.813558	3.383290	-1.390787
H	6.439224	3.452853	-2.294344
H	5.198134	4.300460	-1.381592
C	6.677965	3.355977	-0.136999
H	7.182382	4.325259	-0.005415
H	7.472799	2.597727	-0.245279
C	5.247876	1.606496	0.931352
H	6.053934	0.876378	1.117049
H	4.496104	1.413698	1.710635
C	5.820071	3.012001	1.072756
H	4.998483	3.744523	1.154566
H	6.400163	3.084454	2.005126
O	1.234426	0.276825	0.428137
C	-2.361884	-1.494602	-3.547530
N	-3.182030	-1.819005	-4.305772
N	-1.505581	0.440553	0.815473
C	-1.509484	1.780677	1.150883
C	-2.293300	-0.250248	1.731530
C	-0.825925	2.832998	0.536975
C	-2.373392	1.985127	2.254319
C	-2.516599	-1.621210	1.834779
C	-2.880449	0.672745	2.626811
C	-1.038150	4.110867	1.038995
H	-0.136543	2.645031	-0.285932
C	-2.574256	3.275080	2.732600
C	-3.384560	-2.058881	2.832507
H	-2.013218	-2.321283	1.169287
C	-3.744305	0.211681	3.615579
C	-1.905763	4.333123	2.116935
H	-0.513574	4.955794	0.589120

H	-3.242870	3.459263	3.575708
C	-3.999971	-1.156719	3.705943
H	-3.584107	-3.127337	2.932328
H	-4.213384	0.908937	4.312688
H	-2.052201	5.349765	2.486092
H	-4.676779	-1.530115	4.476259
C	0.566134	-1.749084	-3.960366
N	1.000960	-2.163284	-4.954425
N	-3.242803	-0.294952	-1.141283
C	-3.858365	0.943869	-0.993442
C	-4.134340	-1.286072	-0.810731
C	-3.351644	2.206015	-1.284712
C	-5.163891	0.750883	-0.488813
C	-3.944079	-2.672968	-0.831171
C	-5.348657	-0.692749	-0.373006
C	-4.171396	3.302673	-1.011494
H	-2.363587	2.327001	-1.723475
C	-5.961626	1.851683	-0.227125
C	-5.001944	-3.465674	-0.403518
H	-3.009659	-3.103528	-1.186801
C	-6.380606	-1.503338	0.060141
C	-5.449219	3.131934	-0.483335
H	-3.798980	4.307550	-1.214347
H	-6.970682	1.730628	0.170744
C	-6.198538	-2.893774	0.038846
H	-4.896760	-4.551220	-0.417837
H	-7.319813	-1.075772	0.414660
H	-6.066803	4.007297	-0.276586
H	-7.009686	-3.542812	0.372876

iso-(*S*)-OBN-CzC1

E = -2369.72847653 a.u.

O	2.227449	-0.977166	1.969850
C	-0.983398	-0.087993	0.392945
C	4.308670	-1.626117	-1.044610
C	3.413669	-0.680272	-0.515370
C	0.900796	-0.779049	1.748572
C	2.110556	-0.623473	-1.004412
C	-1.849846	-0.495176	1.382804
C	3.758392	0.248914	0.594179
C	0.432340	-0.203292	0.578479
C	3.106680	0.078481	1.812328
C	5.655159	-1.838999	-0.385925

H	5.478860	-2.420998	0.535957
H	6.072710	-0.884670	-0.042691
C	4.842216	-3.434455	-2.755204
H	5.236928	-2.984699	-3.684062
H	4.278106	-4.325725	-3.070106
C	-1.417560	-1.103733	2.577978
C	3.896729	-2.442402	-2.110866
C	3.351817	0.913181	2.894658
H	2.842567	0.722296	3.840326
C	1.688384	-1.432029	-2.050133
H	0.662702	-1.351450	-2.413186
C	2.594436	-2.323789	-2.604635
H	2.282051	-2.962982	-3.434423
C	4.632321	1.340753	0.427260
C	0.022829	-1.235396	2.763496
C	4.252925	1.953823	2.737304
H	4.465730	2.613667	3.582349
C	4.890747	2.188964	1.514994
C	6.654458	-2.581403	-1.263550
H	7.545653	-2.842897	-0.673278
H	6.998294	-1.920855	-2.078961
C	6.012973	-3.826230	-1.862137
H	6.746132	-4.411420	-2.437836
H	5.657551	-4.477918	-1.045724
C	5.813558	3.383290	1.390787
H	6.439224	3.452853	2.294344
H	5.198134	4.300460	1.381592
C	6.677965	3.355977	0.136999
H	7.182382	4.325259	0.005415
H	7.472799	2.597727	0.245279
C	5.247876	1.606496	-0.931352
H	6.053934	0.876378	-1.117049
H	4.496104	1.413698	-1.710635
C	5.820071	3.012001	-1.072756
H	4.998483	3.744523	-1.154566
H	6.400163	3.084454	-2.005126
O	1.234426	0.276825	-0.428137
C	-2.361884	-1.494602	3.547530
N	-3.182030	-1.819005	4.305772
N	-1.505581	0.440553	-0.815473
C	-1.509484	1.780677	-1.150883
C	-2.293300	-0.250248	-1.731530
C	-0.825925	2.832998	-0.536975

C	-2.373392	1.985127	-2.254319
C	-2.516599	-1.621210	-1.834779
C	-2.880449	0.672745	-2.626811
C	-1.038150	4.110867	-1.038995
H	-0.136543	2.645031	0.285932
C	-2.574256	3.275080	-2.732600
C	-3.384560	-2.058881	-2.832507
H	-2.013218	-2.321283	-1.169287
C	-3.744305	0.211681	-3.615579
C	-1.905763	4.333123	-2.116935
H	-0.513574	4.955794	-0.589120
H	-3.242870	3.459263	-3.575708
C	-3.999971	-1.156719	-3.705943
H	-3.584107	-3.127337	-2.932328
H	-4.213384	0.908937	-4.312688
H	-2.052201	5.349765	-2.486092
H	-4.676779	-1.530115	-4.476259
C	0.566134	-1.749084	3.960366
N	1.000960	-2.163284	4.954425
N	-3.242803	-0.294952	1.141283
C	-3.858365	0.943869	0.993442
C	-4.134340	-1.286072	0.810731
C	-3.351644	2.206015	1.284712
C	-5.163891	0.750883	0.488813
C	-3.944079	-2.672968	0.831171
C	-5.348657	-0.692749	0.373006
C	-4.171396	3.302673	1.011494
H	-2.363587	2.327001	1.723475
C	-5.961626	1.851683	0.227125
C	-5.001944	-3.465674	0.403518
H	-3.009659	-3.103528	1.186801
C	-6.380606	-1.503338	-0.060141
C	-5.449219	3.131934	0.483335
H	-3.798980	4.307550	1.214347
H	-6.970682	1.730628	-0.170744
C	-6.198538	-2.893774	-0.038846
H	-4.896760	-4.551220	0.417837
H	-7.319813	-1.075772	-0.414660
H	-6.066803	4.007297	0.276586
H	-7.009686	-3.542812	-0.372876

(+)-(*R*)-Cz-Ax-CN

E = -1678.14399682 a.u.

C	-0.149649	0.804936	-0.736743
C	-1.340861	1.363513	-0.159726
C	-1.478836	2.721744	0.099416
C	-0.461722	3.623296	-0.216304
C	0.668688	3.139286	-0.870899
C	0.816634	1.784645	-1.159082
C	0.079150	-0.613221	-0.846583
C	-0.940422	-1.497336	-1.364231
C	-0.866770	-2.890102	-1.160952
C	0.220669	-3.445951	-0.530575
C	1.295342	-2.612040	-0.144611
C	1.257240	-1.244363	-0.326547
H	-2.385286	3.069682	0.596832
H	-0.564388	4.681675	0.019560
H	1.449113	3.827671	-1.199149
H	-1.676380	-3.518957	-1.535428
H	0.278025	-4.521790	-0.362276
H	2.183700	-3.044477	0.316770
C	-1.977789	-0.987852	-2.185856
N	-2.830895	-0.573695	-2.857740
C	1.906744	1.406465	-2.003989
N	2.768160	1.159920	-2.735877
N	-2.446111	0.548004	0.217827
C	-2.486836	-0.502772	1.141929
C	-3.724017	0.781168	-0.248964
C	-1.457668	-1.077960	1.882020
C	-3.824457	-0.944572	1.269017
C	-4.135639	1.680082	-1.240381
C	-4.626009	-0.118745	0.370249
C	-1.787732	-2.119394	2.750225
H	-0.427099	-0.760754	1.775693
C	-4.134747	-1.974365	2.134660
C	-5.486377	1.699430	-1.562741
H	-3.417467	2.312142	-1.757258
C	-5.961633	-0.092913	0.027752
C	-3.099356	-2.565968	2.875988
H	-0.993265	-2.593328	3.327536
H	-5.163059	-2.322597	2.244945
C	-6.386824	0.832915	-0.939237
H	-5.842204	2.383106	-2.334005
H	-6.674572	-0.781298	0.483934
H	-3.328344	-3.385856	3.558462
H	-7.440302	0.861747	-1.222196

N	2.418205	-0.514026	0.063991
C	3.686595	-0.816035	-0.441815
C	2.573467	0.406542	1.101023
C	4.035884	-1.654014	-1.500800
C	4.659914	-0.083287	0.264219
C	1.626698	1.026549	1.919183
C	3.949950	0.700272	1.253145
C	5.380833	-1.759853	-1.824161
H	3.276495	-2.192457	-2.066255
C	6.008749	-0.202997	-0.078748
C	2.068121	1.923831	2.883655
H	0.562277	0.860280	1.788613
C	4.371700	1.606508	2.226701
C	6.363636	-1.046806	-1.120549
H	5.677719	-2.404751	-2.653860
H	6.769156	0.363971	0.462592
C	3.428589	2.215279	3.043582
H	1.331557	2.419636	3.519439
H	5.434068	1.832894	2.339716
H	7.412517	-1.151424	-1.404216
H	3.744668	2.927961	3.807526

(-)-(*S*)-Cz-Ax-CN

E = -1678.14399681 a.u.

C	0.149649	0.804936	-0.736743
C	1.340861	1.363513	-0.159726
C	1.478836	2.721744	0.099416
C	0.461722	3.623296	-0.216304
C	-0.668688	3.139286	-0.870899
C	-0.816634	1.784645	-1.159082
C	-0.079150	-0.613221	-0.846583
C	0.940422	-1.497336	-1.364231
C	0.866770	-2.890102	-1.160952
C	-0.220669	-3.445951	-0.530575
C	-1.295342	-2.612040	-0.144611
C	-1.257240	-1.244363	-0.326547
H	2.385286	3.069682	0.596832
H	0.564388	4.681675	0.019560
H	-1.449113	3.827671	-1.199149
H	1.676380	-3.518957	-1.535428
H	-0.278025	-4.521790	-0.362276
H	-2.183700	-3.044477	0.316770
C	1.977789	-0.987852	-2.185856

N	2.830895	-0.573695	-2.857740
C	-1.906744	1.406465	-2.003989
N	-2.768160	1.159920	-2.735877
N	2.446111	0.548004	0.217827
C	2.486836	-0.502772	1.141929
C	3.724017	0.781168	-0.248964
C	1.457668	-1.077960	1.882020
C	3.824457	-0.944572	1.269017
C	4.135639	1.680082	-1.240381
C	4.626009	-0.118745	0.370249
C	1.787732	-2.119394	2.750225
H	0.427099	-0.760754	1.775693
C	4.134747	-1.974365	2.134660
C	5.486377	1.699430	-1.562741
H	3.417467	2.312142	-1.757258
C	5.961633	-0.092913	0.027752
C	3.099356	-2.565968	2.875988
H	0.993265	-2.593328	3.327536
H	5.163059	-2.322597	2.244945
C	6.386824	0.832915	-0.939237
H	5.842204	2.383106	-2.334005
H	6.674572	-0.781298	0.483934
H	3.328344	-3.385856	3.558462
H	7.440302	0.861747	-1.222196
N	-2.418205	-0.514026	0.063991
C	-3.686595	-0.816035	-0.441815
C	-2.573467	0.406542	1.101023
C	-4.035884	-1.654014	-1.500800
C	-4.659914	-0.083287	0.264219
C	-1.626698	1.026549	1.919183
C	-3.949950	0.700272	1.253145
C	-5.380833	-1.759853	-1.824161
H	-3.276495	-2.192457	-2.066255
C	-6.008749	-0.202997	-0.078748
C	-2.068121	1.923831	2.883655
H	-0.562277	0.860280	1.788613
C	-4.371700	1.606508	2.226701
C	-6.363636	-1.046806	-1.120549
H	-5.677719	-2.404751	-2.653860
H	-6.769156	0.363971	0.462592
C	-3.428589	2.215279	3.043582
H	-1.331557	2.419636	3.519439
H	-5.434068	1.832894	2.339716

H	-7.412517	-1.151424	-1.404216
H	-3.744668	2.927961	3.807526

References

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