Supporting Information

Linker-dependent control of the chiroptical properties of polymethylene-vaulted *trans*-Bis[(β-iminomethyl)naphthoxy]platinum(II) complexes

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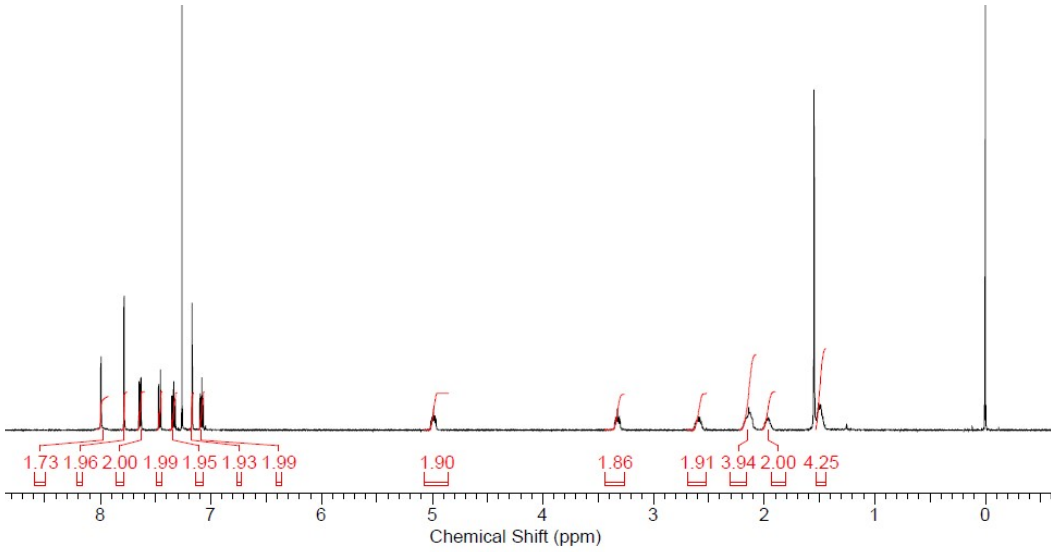
Contents

(a)



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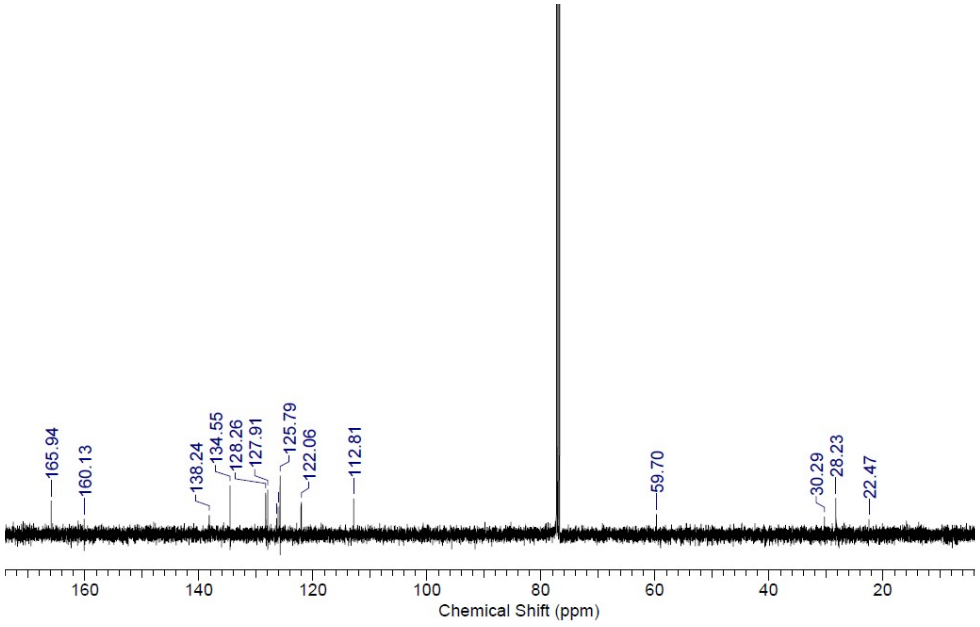
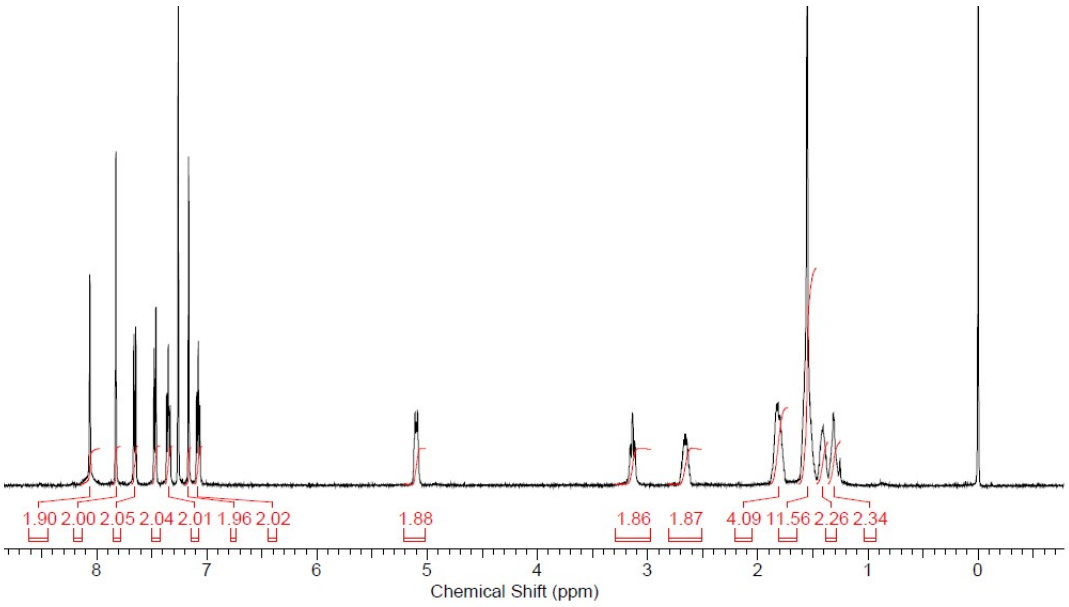


Fig. S1. (a) ^{1}H and (b) ^{13}C NMR spectra of (*R*)-**1a** in $CDCl_3$.

(a)



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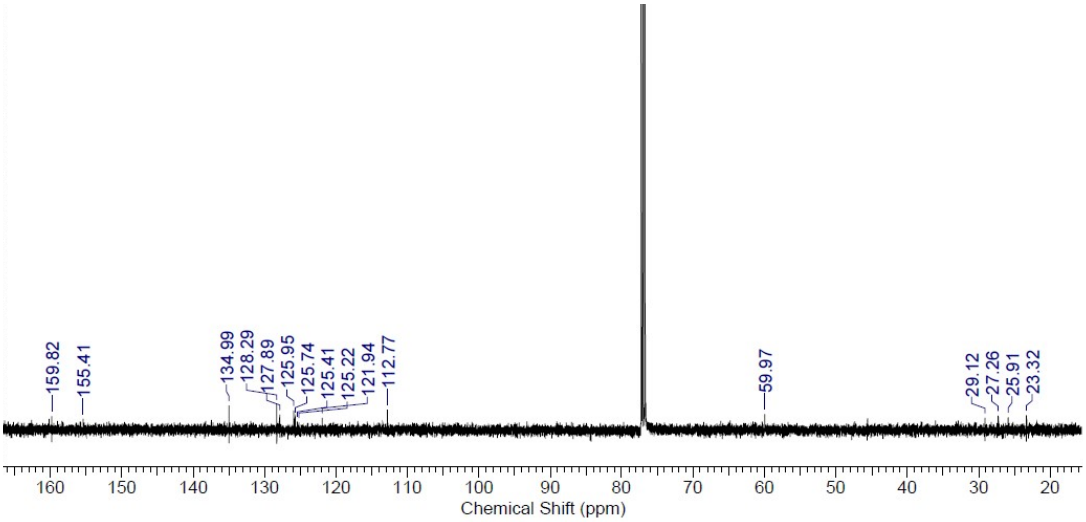
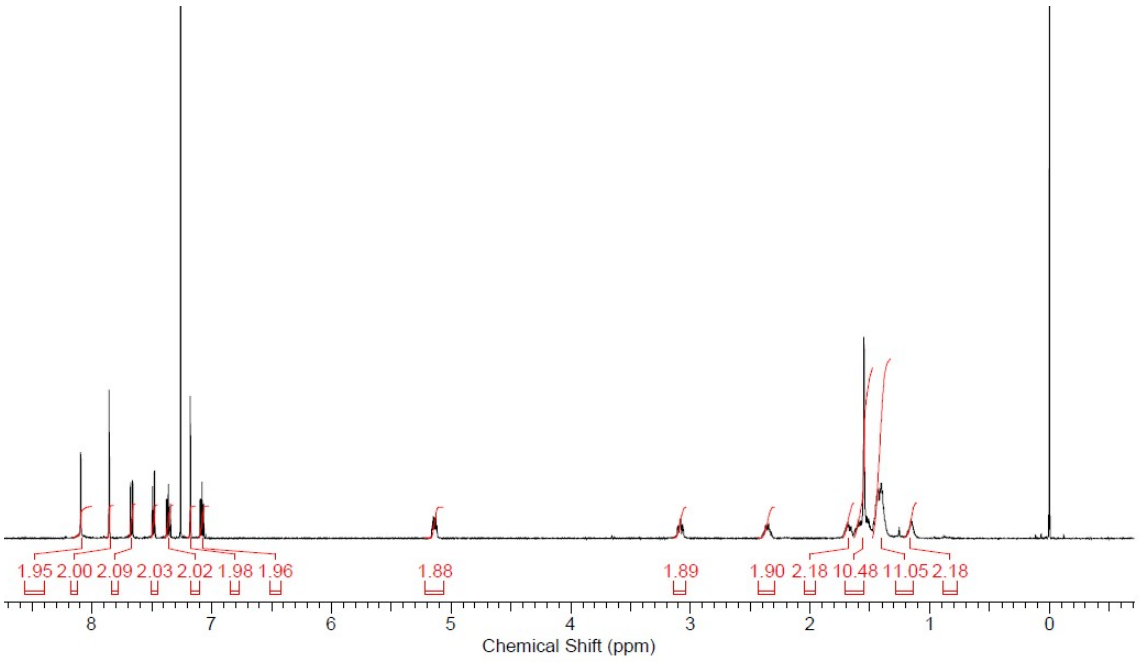


Fig. S2. (a) ^{1}H and (b) ^{13}C NMR spectra of (*R*)-**1b** in $CDCl_3$.

(a)



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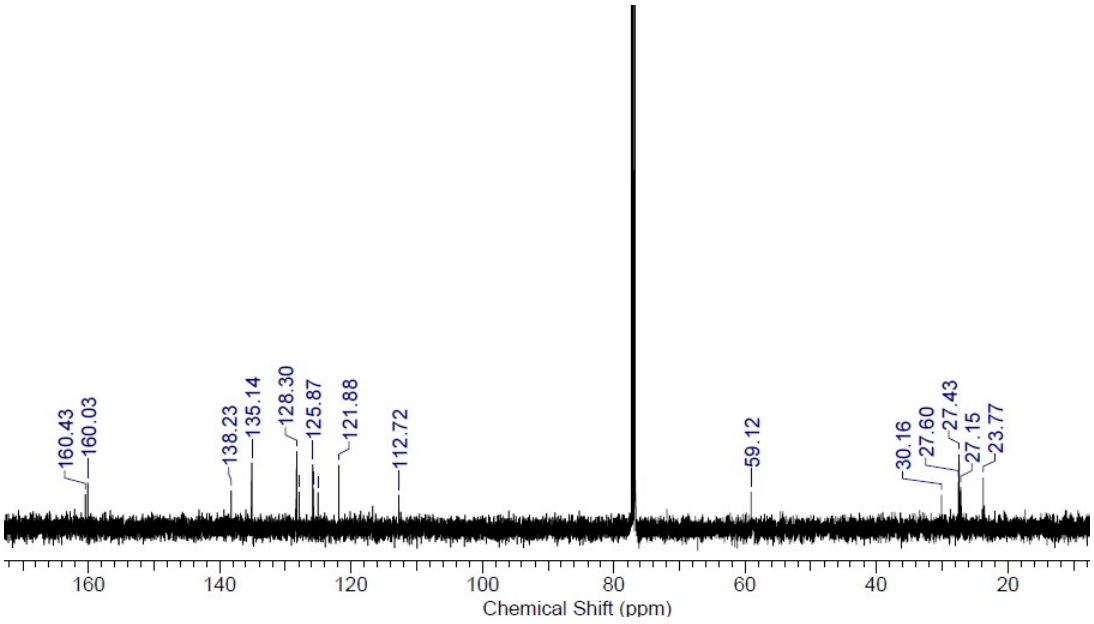
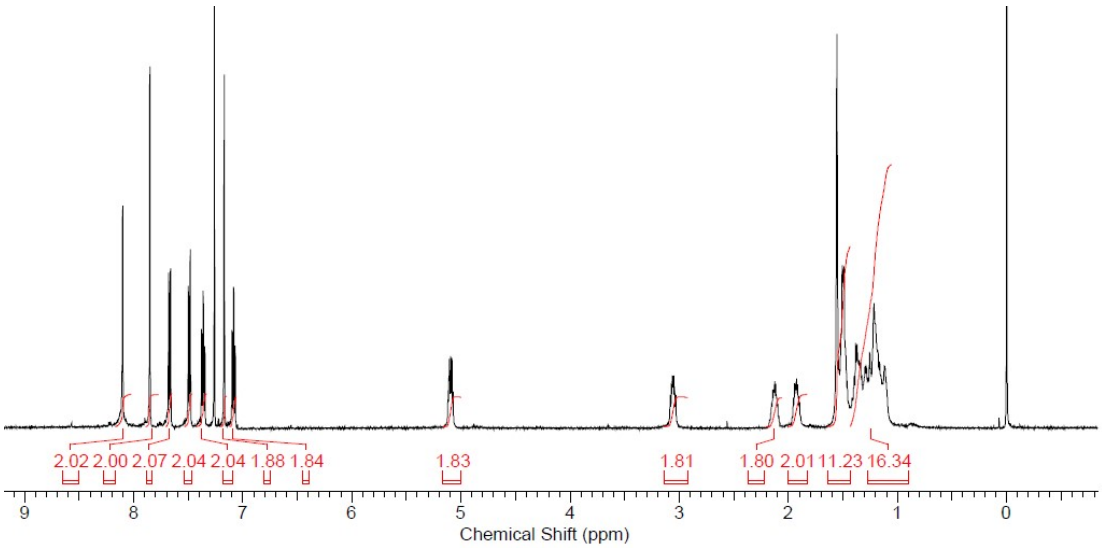


Fig. S3. (a) ^{1}H and (b) ^{13}C NMR spectra of (*R*)-**1c** in $CDCl_3$.

(a)



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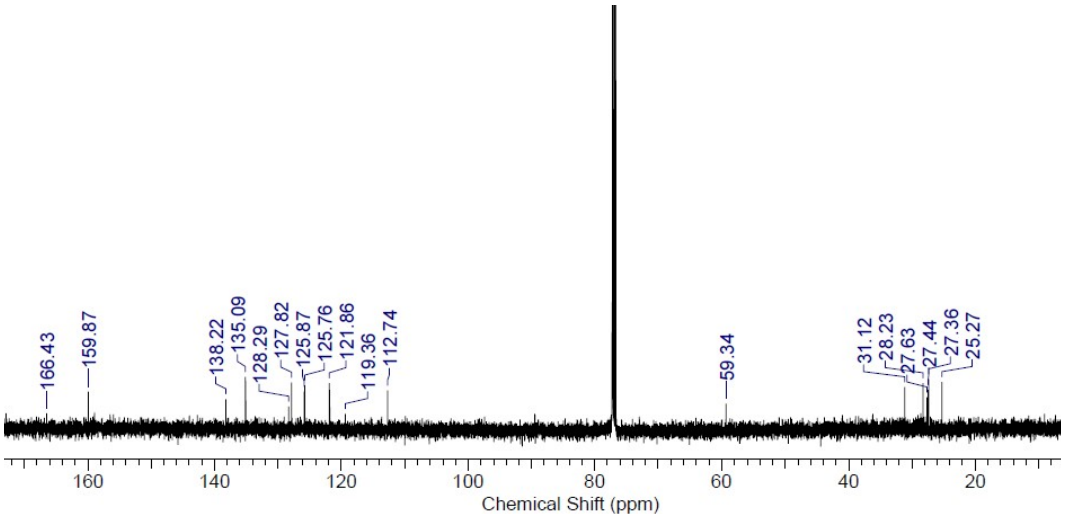
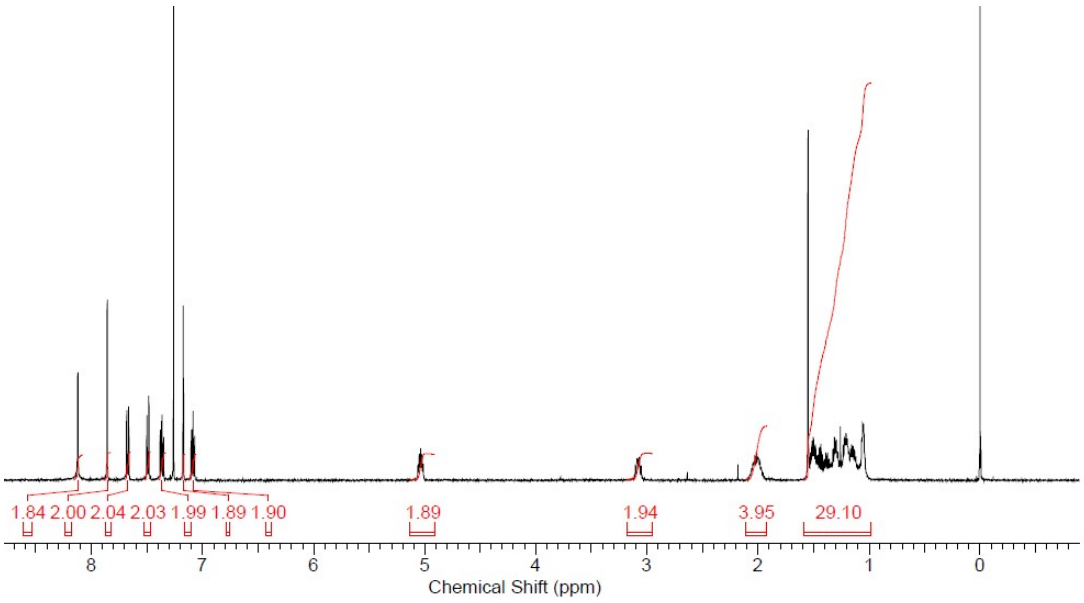


Fig. S4. (a) ^{1}H and (b) ^{13}C NMR spectra of (*R*)-**1d** in $CDCl_3$.

(a)



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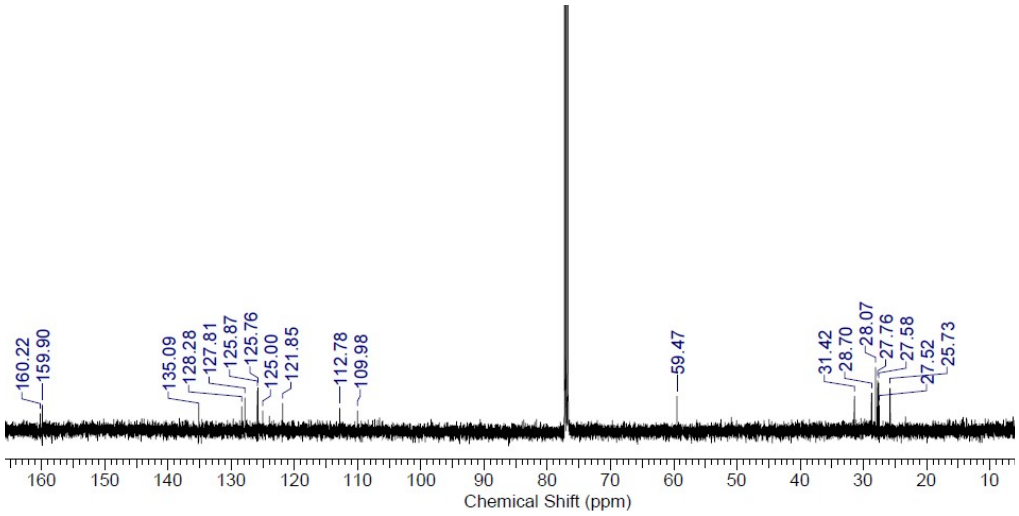
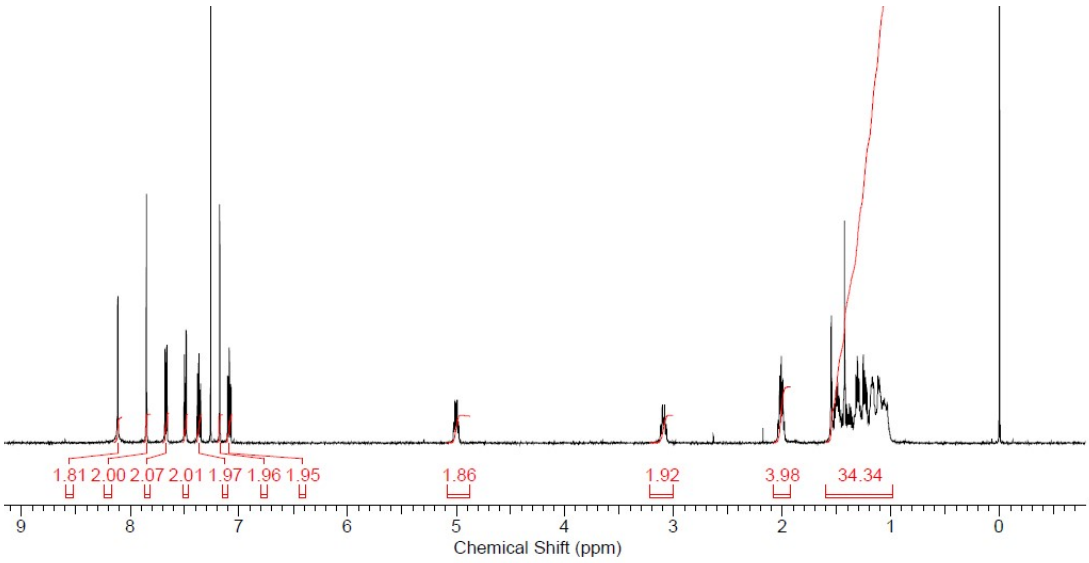


Fig. S5. (a) ^{1}H and (b) ^{13}C NMR spectra of (*R*)-**1e** in $CDCl_3$.

(a)



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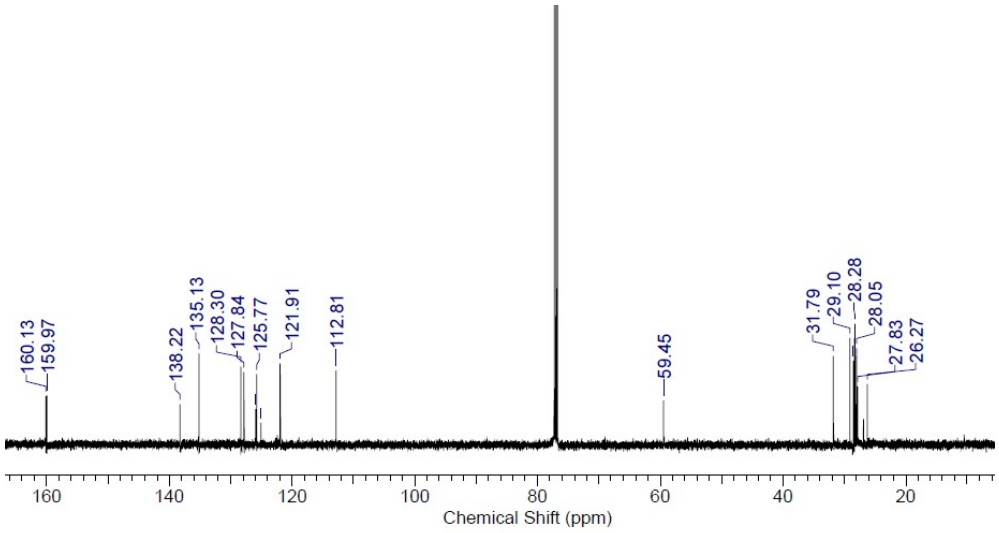

Fig. S6. (a) ^{1}H and (b) ^{13}C NMR spectra of (*R*)-**1f** in $CDCl_3$.

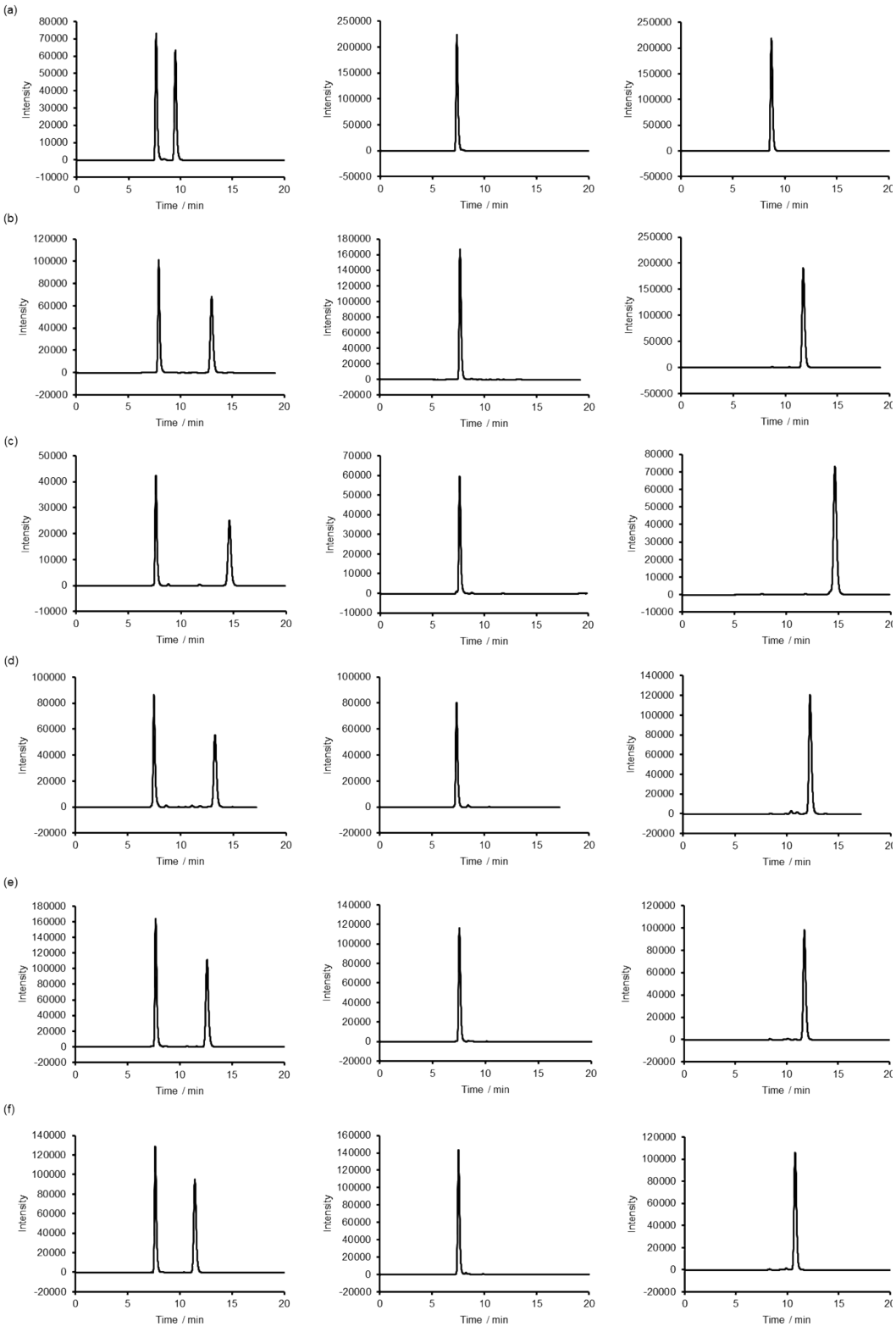

Fig. S7. Time-dependent UV absorption intensity of before (left) and after (middle and right) optical resolution of (a) **1a**, (b) **1b**, (c) **1c**, (d) **1d**, (e) **1e** and (f) **1f** on CHIRAL ART Cellulose-SC (CH_2Cl_2, flow = 0.5 mL/min, abs. at 250 nm).

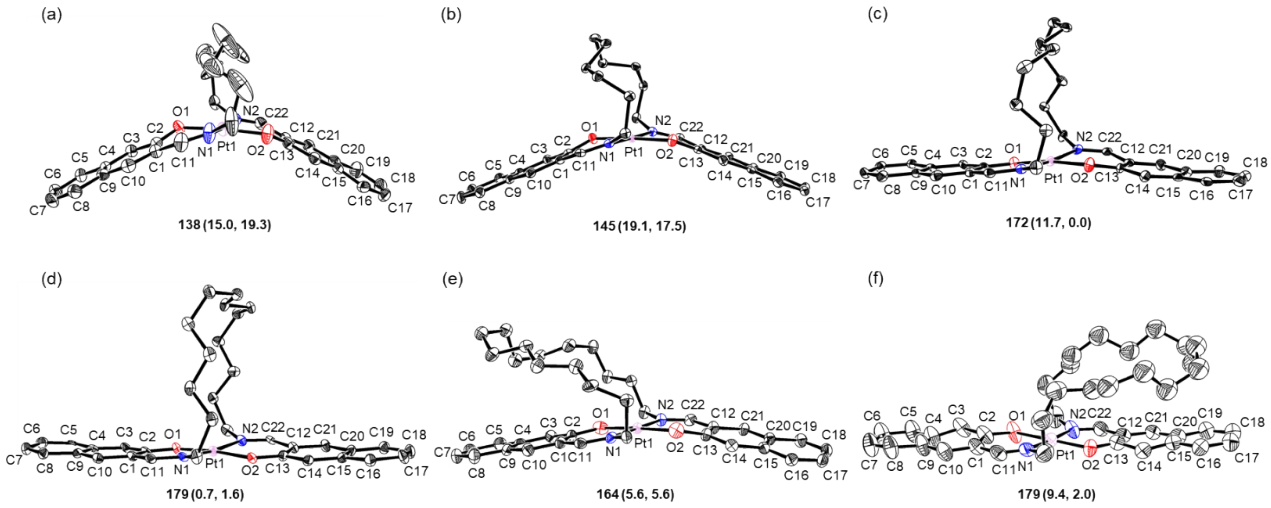

Fig. S8. ORTEP representation of (a) (*R*)-**1a**, (b) (*R*)-**1b**, (c) (*R*)-**1c**, (d) (*R*)-**1d**, (e) (*R*)-**1e** and (f) (*R*)-**1f** as their optically pure crystals. Thermal ellipsoids are shown at 50% probability level and hydrogen atoms are omitted for clarity. The angles of C(7)–Pt(1)–C(18) and dihedral angles of C(11)–N(1)–Pt(1)–O(1)/C(22)–N(2)–Pt(1)–O(2) (in parentheses) are given under the structure.

Table S1. Crystal data and structural refinement details for complexes (–)-**1a**–**e** and (+)-**1f**. [a]

	(–)-**1a**	(–)-**1b**	(–)-**1c**	(–)-**1d**	(–)-**1e**	(+)-**1f**
Formula	$C_{30}H_{30}N_2O_2Pt$	$C_{32}H_{34}N_2O_2Pt$ •1/3CH_2Cl_2	$C_{34}H_{38}N_2O_2Pt$	$C_{36}H_{42}N_2O_2Pt$	$C_{36}H_{42}N_2O_2Pt$	$C_{40}H_{50}N_2O_2Pt$
M_F	645.67	702.12	701.78	729.83	757.88	785.94
T [K]	113	113	113	113	113	113
Crystal color, habit	red, block	red, block	red, chip	red, chip	red, block	red, chip
Crystal size [mm]	0.20×0.20×0.20	0.20×0.20×0.10	0.20×0.20×0.05	0.20×0.20×0.20	0.20×0.20×0.20	0.10×0.10×0.05
Crystal system	orthorhombic	orthorhombic	orthorhombic	orthorhombic	orthorhombic	monoclinic
Space group	$P2_12_12$ (#18)	$P2_12_12_1$ (#19)	$P2_12_12_1$ (#19)	$P2_12_12_1$ (#19)	$P2_12_12_1$ (#19)	$P2_1$ (#4)
a [Å]	17.04673(16)	17.07120(16)	12.075(3)	22.1932(6)	30.3209(7)	9.1109(3)
b [Å]	17.16019(18)	17.85690(17)	10.511(2)	32.7977(7)	9.4282(3)	10.0604(4)
c [Å]	13.07172(12)	26.8416(2)	22.225(5)	32.8261(9)	11.2103(3)	18.7421(6)
α [°]	90	90	90	90	90	90
β [°]	90	90	90	90	90	91.389(3)
γ [°]	90	90	90	90	90	90
V [Å^3]	3823.81(6)	8182.36(13)	2820.8(11)	23893.7(11)	3204.71(15)	1717.38(10)
Z	6	12	4	32	4	2
D_{calcd} [gcm^{-3}]	1.682	1.710	1.652	1.623	1.571	1.520
μ(MoKα) [cm^{-1}]	55.120	52.226	49.884	47.148	43.973	41.057
F(000)	1908.00	4176.48	1400.00	11712.00	1528.00	796.00
$2\theta_{max}$ [°]	55.0	55.0	55.1	55.0	55.0	55.0
No. of reflections measured	69614	148976	26918	120429	60703	30832
No. observed reflections	8767	18755	6425	52747	7362	7216
No. variables	474	1027	346	2953	388	406
R_1 (I > 2σ(I))[a]	0.0220	0.0152	0.0341	0.0579	0.0341	0.1229
wR_2 (all reflections)[b]	0.0572	0.0358	0.0684	0.1049	0.0906	0.3273
Goodness of fit	1.082	1.025	0.991	0.969	1.018	1.068
Flack parameter	–0.004(3)	–0.0170(10)	–0.013(9)	–0.024(5)	–0.025(4)	0.126(12)

[a] $R_1 = \Sigma(|F_o|-|F_c|)/ \Sigma(|F_o|)$. [b] $wR_2 = [w(F_o^2-F_c^2)^2]/wF_o^2)^2]^{1/2}$.

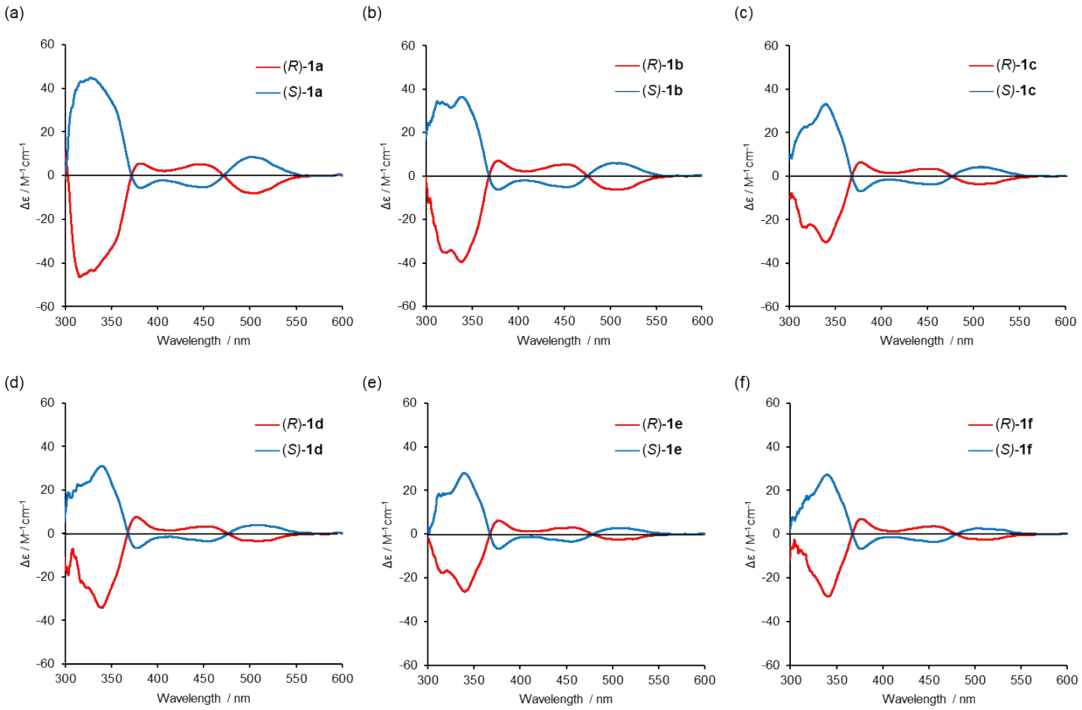

Fig. S9. CD spectra of 2.00×10^{-4} M solutions of (a) **1a**, (b) **1b**, (c) **1c**, (d) **1d**, (e) **1e**, and (f) **1f** in 2-MeTHF.

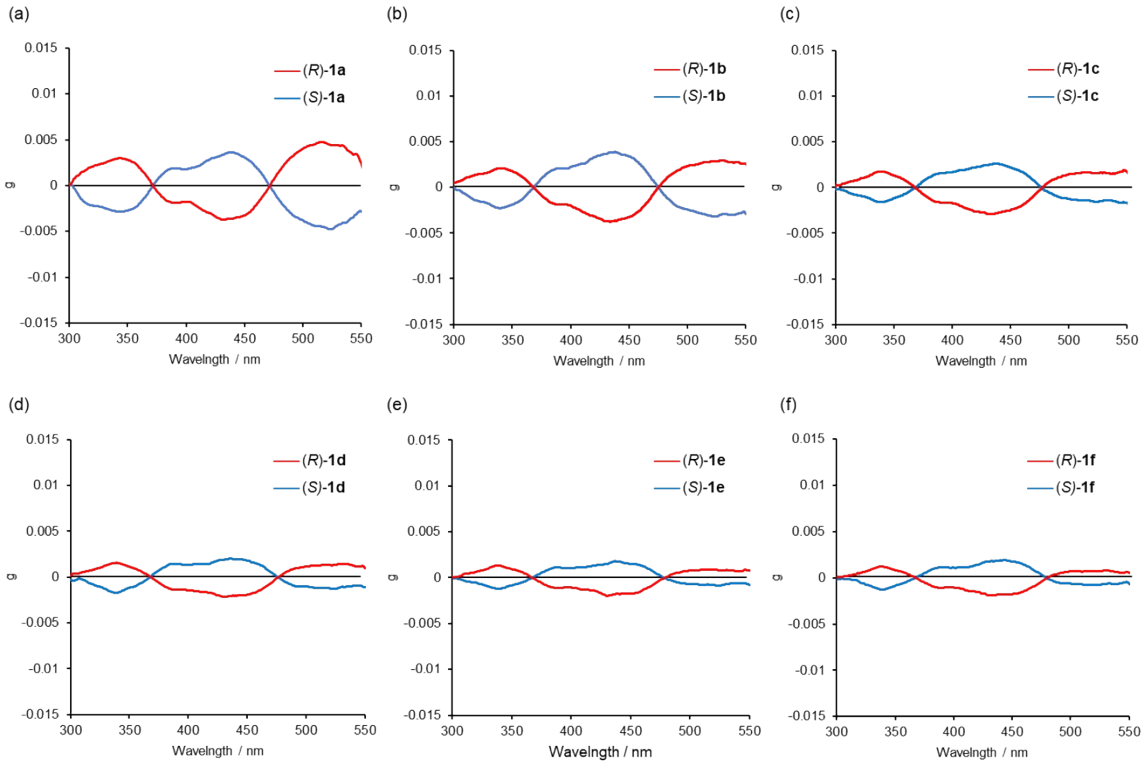

Fig. S10. Anisotropy factor *g* values of CD spectra for (a) **1a**, (b) **1b**, (c) **1c**, (d) **1d**, (e) **1e**, (f) **1f** in 2-MeTHF.

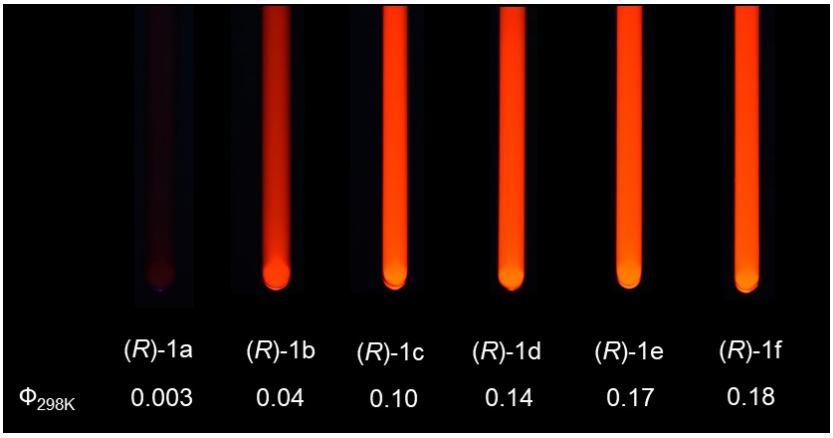

Fig. S11. Photographs of 2.00×10^{-4} M solutions of (*R*)-**1a**-**f** in 2-MeTHF under UV irradiation (365 nm) at room temperature.

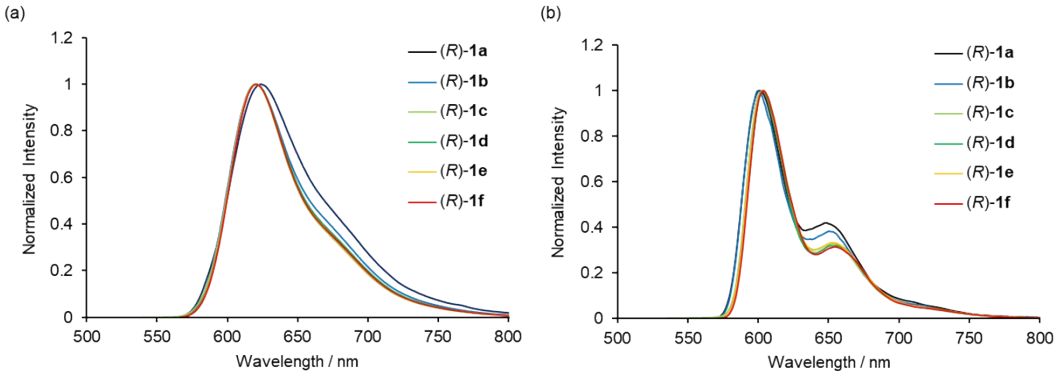

Fig. S12. Normalized emission spectra for (*R*)-**1a**–**f** in 2-MeTHF solution state (2.0×10^{-4} M) at a) 298 K and b) 77 K (λ_{ex} = 500 nm).

Table S2. Photophysical data for (*R*)-**1a**–**f**.[a]

Compound	λ_{abs} [nm]	λ_{em} [nm][b]	Φ[b,c,d]	τ [μs][b,c]	$k_r \times 10^4$ [s^{-1}][b,d]	$k_{nr} \times 10^5$ [s^{-1}][b,e]	CIE (x, y)[f]
1a	487	624 (601, 648)	0.003 (0.36)	0.16 (27.2)	1.8 (1.3)	62 (0.24)	0.67, 0.33
1b	493	620 (600, 650)	0.05 (0.41)	2.7 (24.5)	1.9 (1.7)	3.5 (0.24)	0.67, 0.33
1c	497	620 (603, 657)	0.10 (0.45)	5.1 (22.1)	2.0 (2.0)	1.8 (0.25)	0.67, 0.33
1d	498	620 (603, 651)	0.14 (0.43)	5.3 (21.4)	2.6 (2.0)	1.6 (0.27)	0.67, 0.33
1e	498	620 (603, 652)	0.17 (0.41)	5.7 (21.8)	3.0 (1.9)	1.5 (0.27)	0.67, 0.33
1f	499	621 (604, 654)	0.18 (0.42)	5.8 (20.1)	3.1 (2.1)	1.4 (0.29)	0.67, 0.33

[a] Data were obtained from a 2.0×10^{-4} M in 2-MeTHF at 298 K unless otherwise stated. [b] Values in parentheses are those measured at 77 K. [c] λ_{ex} = 500 nm. [d] Luminescent quantum efficiencies measured using the absolute method with an integrating sphere. [e] $k_r = \Phi_{298K}/\tau$. [f] $k_{nr} = (1-\Phi_{298K})/\tau$. [g] CIE color coordinates for the emission at 298 K.

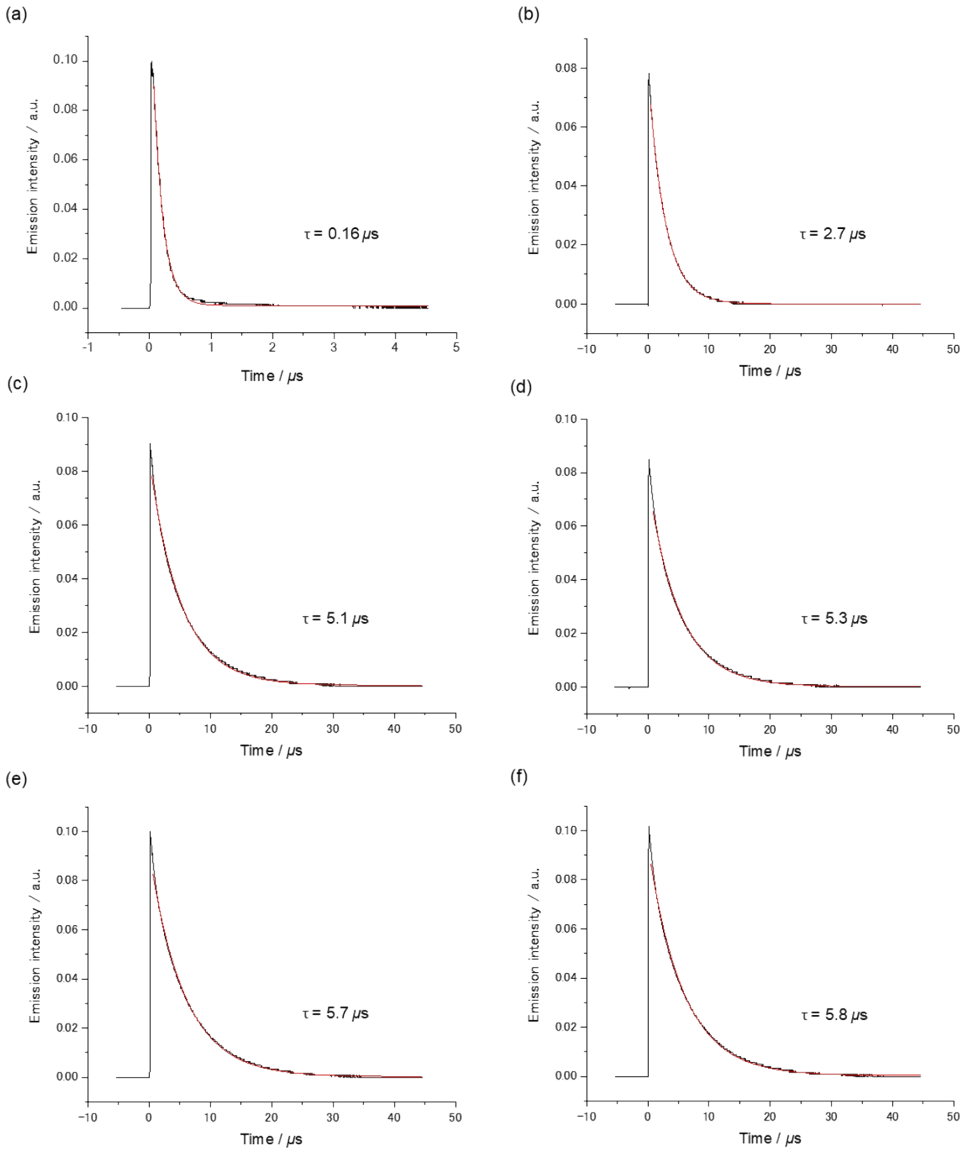

Fig. S13. Emission decay curves (black line) for (a) (*R*)-**1a**, (b) (*R*)-**1b**, (c) (*R*)-**1c** (d) (*R*)-**1d**, (e) (*R*)-**1e**, and (f) (*R*)-**1f** in 2-MeTHF solution state (2.0×10^{-4} M) at 298 K [λ_{ex} = 355 nm, λ_{em} = 620 nm]. The red curves are those estimated by single-exponential fitting analysis.

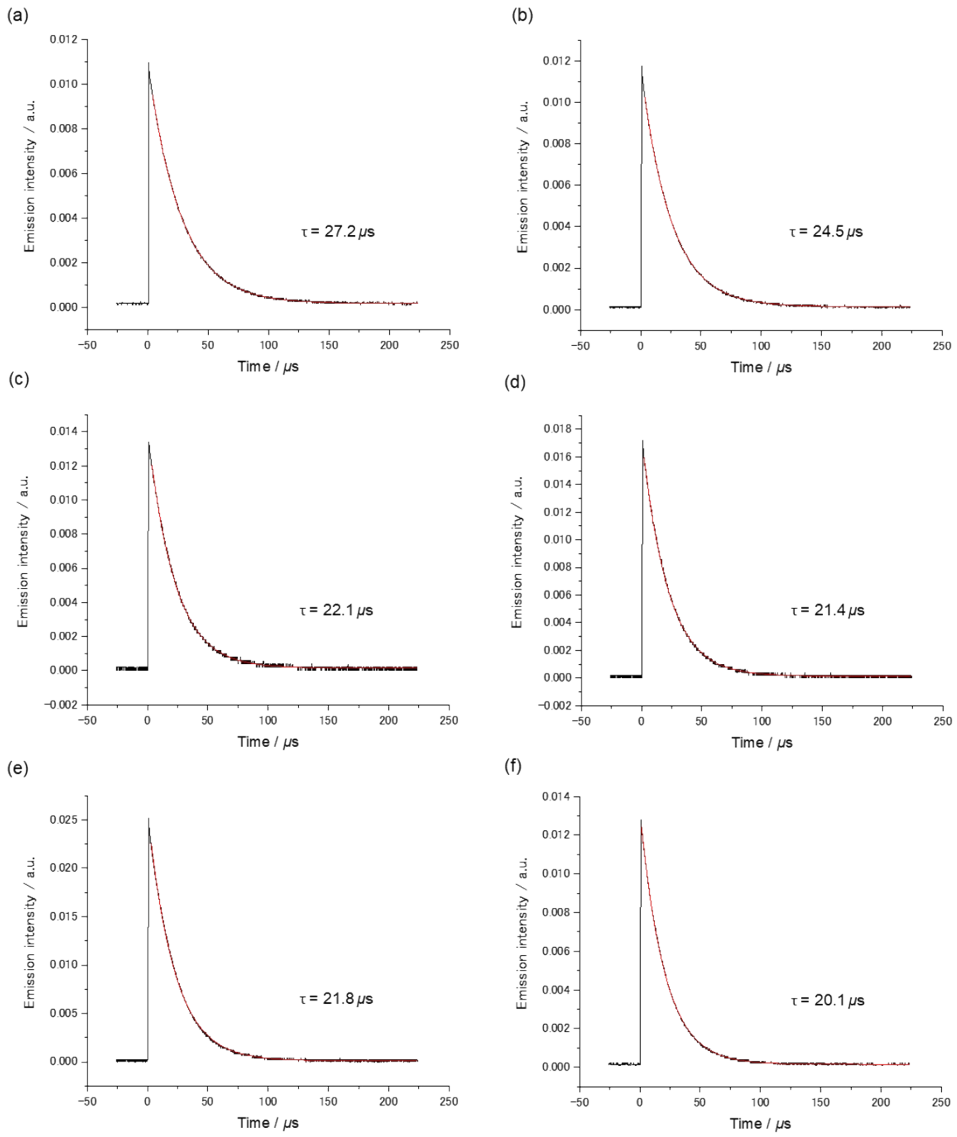

Fig. S14. Emission decay curves (black line) for (a) (*R*)-**1a**, (b) (*R*)-**1b**, (c) (*R*)-**1c** (d) (*R*)-**1d**, (e) (*R*)-**1e**, and (f) (*R*)-**1f** in 2-MeTHF solution state (2.0×10^{-4} M) at 77 K [λ_{ex} = 355 nm, λ_{em} = 620 nm]. The red curves are those estimated by single-exponential fitting analysis.

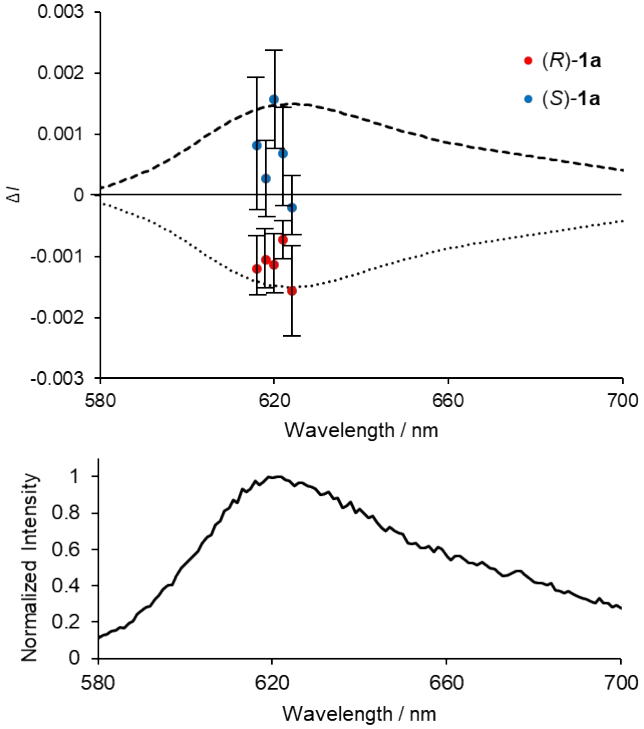

Fig. S15. CPL (upper figure) and total emission (lower figure) spectra of 2.0×10^{-4} M solutions of **1a** in 2-MeTHF at 298 K (λ_{ex} = 420 nm). Red and blue circles in the CPL spectra correspond to optically pure (100% *ee*) (*R*)- and (*S*)-compounds, respectively, and each point is plotted with a standard error bar. The dashed lines in the upper figure are presented to show the luminescence spectral line shape. The average g_{lum} value was calculated to be -3.4×10^{-3} for (*R*)-**1a** and $+2.7 \times 10^{-3}$ for (*S*)-**1a**, respectively. Although the number of measured data is limited due to the weak luminescence intensity, the (*R*)-form tends to show (–)-CPL and the (*S*)-form (+)-CPL, as in **1b**–**f**.

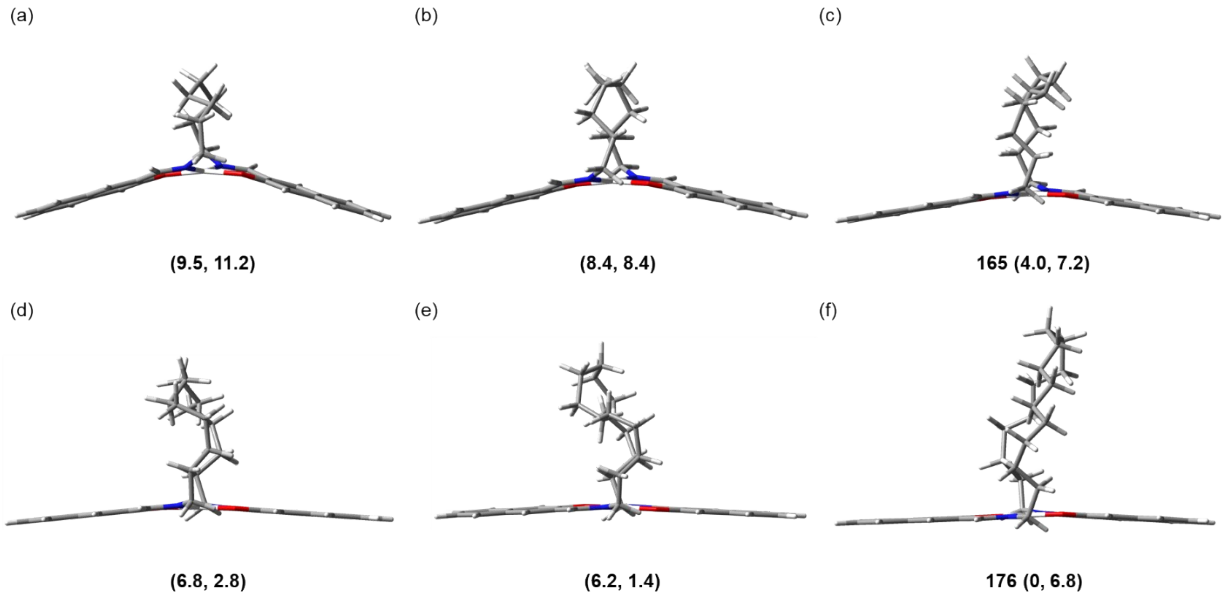

Fig. S16. Optimized molecular structures of (a) (*R*)-**1a**, (b) (*R*)-**1b**, (c) (*R*)-**1c**, (d) (*R*)-**1d**, (e) (*R*)-**1e** and (f) (*R*)-**1f** in the excited state (T_1) as obtained from DFT calculations (UB3LYP/6-31G*, LanL2DZ). The C(11)–N(1)–Pt(1)–O(1) and C(22)–N(2)–Pt(1)–O(2) dihedral angles are provided in parentheses under each structure.

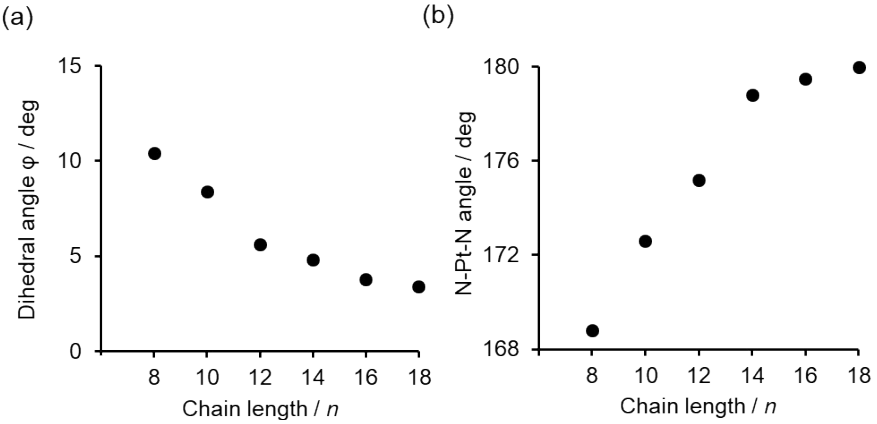

Fig. S17. Relationship between linker length and distortion of coordination site for (*R*)-**1a**–**f**. (a) The average C(11)–N(1)–Pt(1)–O(1)/C(22)–N(2)–Pt(1)–O(2) dihedral angles and (b) N(1)–Pt(1)–N(2) angles as functions of chain length. Values were estimated based on optimized structures in the excited state (T_1) estimated using DFT calculations (UB3LYP/6-31G*, LanL2DZ).

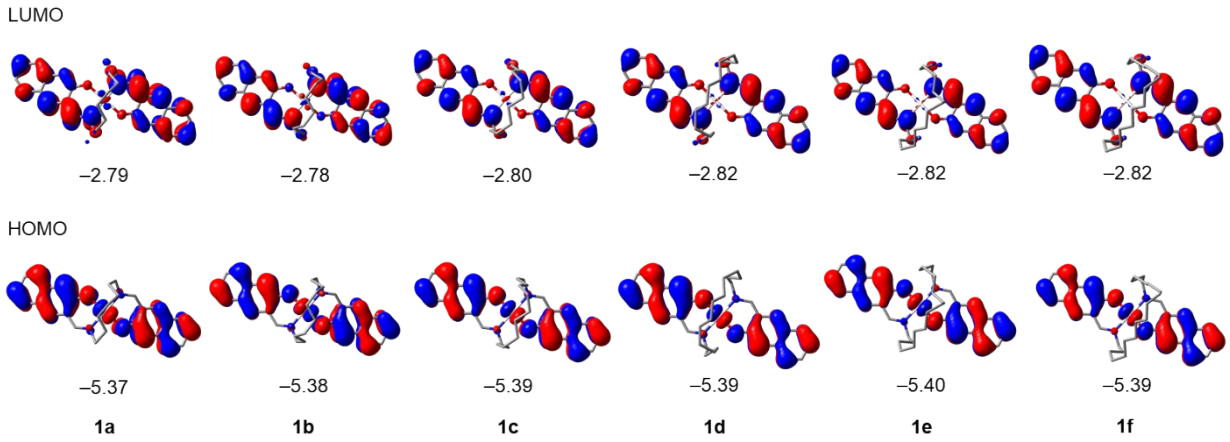

Fig. S18. Frontier orbitals and their eigenvalues [eV] for **1a**–**f** as estimated from DFT calculations (UB3LYP/6-31G*, LanL2DZ) on the basis of the optimized geometries in the T_1 state.

Table S3. Selected data for excitation energy, major configuration, coefficient, oscillator strength, and the character of charge transfer for (*R*)-**1a–f** (for the geometries optimized in the S_0 state).[a]

Compound	State	Excitation energy (eV)	Major configuration[b]	Coefficient	Oscillator strength	Character
(*R*)-**1a**	S_1	2.38 (521 nm)	H→L	0.693	0.0212	^{1}MLCT/^{1}LC
	T_1	1.95 (636 nm)	H→L	0.550	—	^{3}MLCT/^{3}LC
(*R*)-**1b**	S_1	2.37 (522 nm)	H→L	0.696	0.0229	^{1}MLCT/^{1}LC
	T_1	1.95 (637 nm)	H→L	0.601	—	^{3}MLCT/^{3}LC
(*R*)-**1c**	S_1	2.37 (522 nm)	H→L	0.697	0.0244	^{1}MLCT/^{1}LC
	T_1	1.93 (642 nm)	H→L	0.603	—	^{3}MLCT/^{3}LC
(*R*)-**1d**	S_1	2.34 (530 nm)	H→L	0.698	0.0259	^{1}MLCT/^{1}LC
	T_1	1.91 (650 nm)	H→L	0.609	—	^{3}MLCT/^{3}LC
(*R*)-**1e**	S_1	2.33 (531 nm)	H→L	0.698	0.0263	^{1}MLCT/^{1}LC
	T_1	1.90 (652 nm)	H→L	0.611	—	^{3}MLCT/^{3}LC
(*R*)-**1f**	S_1	2.33 (532 nm)	H→L	0.698	0.0270	^{1}MLCT/^{1}LC
	T_1	1.90 (652 nm)	H→L	0.613	—	^{3}MLCT/^{3}LC

[a] Estimated by TD-DFT (B3LYP/6-31G*, LanL2DZ) calculations based on the optimized geometries. [b] Molecular orbitals are shown in Fig. 7.

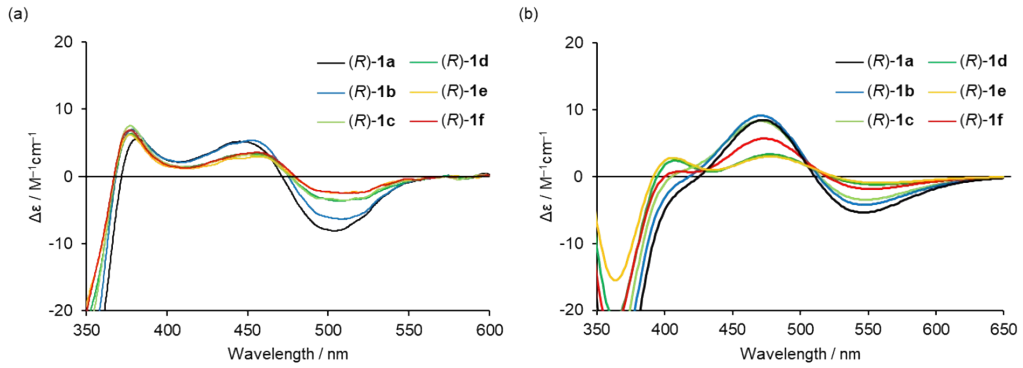

Fig. S19. (a) Experimental (2.0×10^{-4} M in 2-MeTHF) and (b) theoretical CD spectra of (*R*)-**1a**–**f**. Theoretical spectra were estimated by DFT (B3LYP/6-31G*, LanL2DZ) calculation.

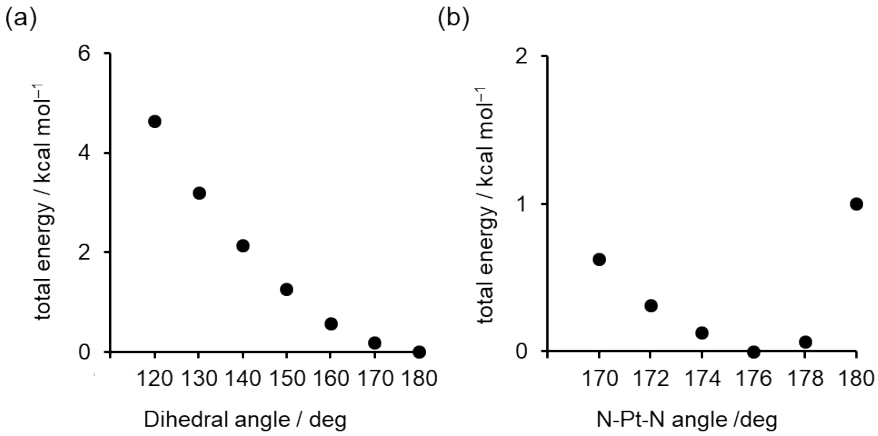

Fig. S20 Effects of (a) the C(23)–N(1)–N(2)–C(24) dihedral angles and (b) N(1)–Pt(1)–N(2) angles on total energies of **2** estimated using DFT calculations (B3LYP/6-31G*, LanL2DZ).

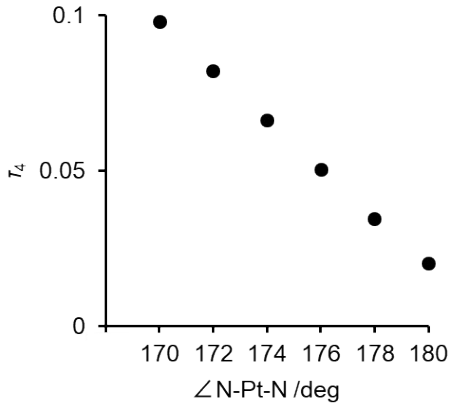

Fig. S21 Effects of N(1)–Pt(1)–N(2) angles on geometry index (τ_4) of **2** estimated using DFT calculations (B3LYP/6-31G*, LanL2DZ).

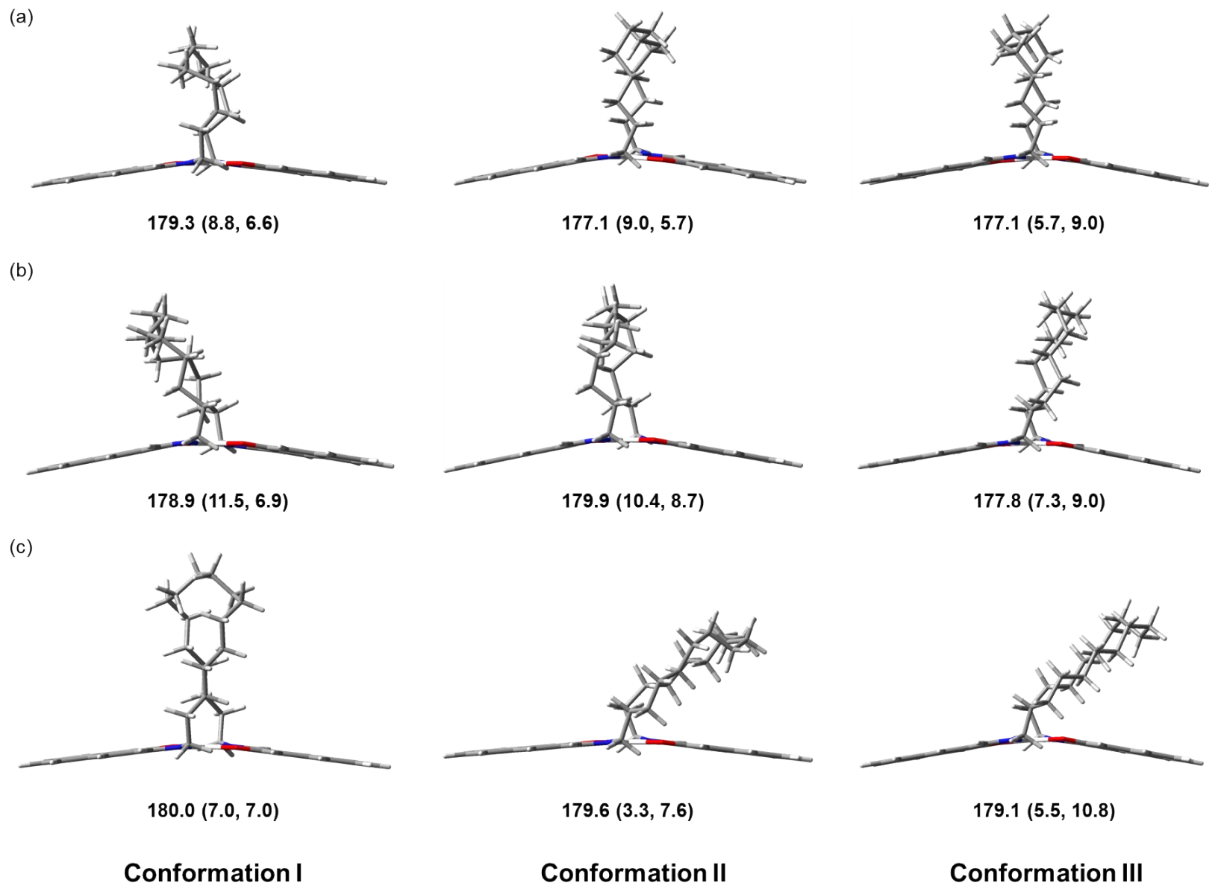

Fig. S22. Optimized structures of (a) (*R*)-**1d**, (b) (*R*)-**1e**, and (c) (*R*)-**1f** in the S_0 state estimated by DFT calculations from different initial structures (B3LYP/6-31G*, LanL2DZ). The N(1)–Pt(1)–N(2) angles and the C(11)–N(1)–Pt(1)–O(1)/C(22)–N(2)–Pt(1)–O(2) dihedral angles (in parentheses) and are provided under each structure.

Table S4. Relative energies of various conformations of (*R*)-**1d**–**f** and transition dipole moments in the $S_0 \rightarrow S_1$ transition.[a]

Compound	Structure	Relative energy (kcal/mol)	$\lvert\boldsymbol{\mu}_e\rvert$ / 10^{-20} [b] (esu·cm)	$\lvert\boldsymbol{\mu}_m\rvert$ / 10^{-20} [c] (erg·G^{-1})	$\cos(\theta_{e,m})$ [d]	g_{abs}[e]
(*R*)-**1d**	Optimized	0	170.8	0.367	–0.110	-9.5×10^{-4}
	Conformation I	0.02	170.9	0.367	–0.106	-9.1×10^{-4}
	Conformation II	1.63	168.0	0.386	–0.306	-2.8×10^{-3}
	Conformation III	1.63	168.0	0.385	–0.306	-2.8×10^{-3}
(*R*)-**1e**	Optimized	0	172.3	0.357	–0.0890	-7.4×10^{-4}
	Conformation I	6.66	171.2	0.398	–0.0239	-2.2×10^{-4}
	Conformation II	5.33	170.2	0.422	–0.0875	-8.7×10^{-4}
	Conformation III	6.40	170.8	0.422	–0.216	-2.1×10^{-3}
(*R*)-**1f**	Optimized	0	174.7	0.377	–0.0600	-5.2×10^{-4}
	Conformation I	1.26	175.6	0.427	–0.142	-1.4×10^{-3}
	Conformation II	3.70	174.4	0.328	–0.102	-7.7×10^{-4}
	Conformation III	3.26	170.4	0.406	–0.149	-1.5×10^{-3}

[a] Estimated by TD-DFT (B3LYP/6-31G*, LanL2DZ) calculations. [b] Transition electric dipole moment (TEDM). [c] Transition magnetic dipole moment (TMDM). [d] $\cos(\theta_{e,m})$ represents the angle of TEDM and TMDM. [e] Dissymmetry factor (g_{abs}) was calculated follows: $g_{abs} = 4R/(D + G)$, where R, D, and G represent the rotatory, electric dipole, magnetic dipole strength ($R = \lvert\boldsymbol{\mu}_e\rvert\lvert\boldsymbol{\mu}_m\rvert\cos\theta$, $D = \lvert\boldsymbol{\mu}_e\rvert^2$, $G = \lvert\boldsymbol{\mu}_m\rvert^2$)

Table S5. Cartesian coordinates (in angstrom) of (*R*)-**1a** in the S_0 state[a].

atom	x	y	z
Pt	0.02439	0.14294	-0.02232
O	1.84087	0.22508	0.90696
O	-1.75518	-0.08291	-0.98361
N	0.95782	0.29181	-1.8362
N	-0.91171	0.32869	1.77648
C	3.14075	-0.48605	-1.03071
C	2.91875	-0.3369	0.39268
C	3.93822	-0.74985	1.25353
H	3.77512	-0.63166	2.32102
C	5.14739	-1.30235	0.78796
C	6.18096	-1.73369	1.67123
H	6.02689	-1.63183	2.74266
C	7.34959	-2.26834	1.18328
H	8.12523	-2.59109	1.87312
C	7.56109	-2.40577	-0.21608
H	8.49194	-2.83032	-0.58112
C	6.58808	-2.00157	-1.09753
H	6.73706	-2.10175	-2.17053
C	5.36429	-1.44476	-0.62739
C	4.34679	-1.01075	-1.49464
H	4.5059	-1.09059	-2.5689
C	2.20467	-0.00039	-2.01821
H	2.6122	0.1608	-3.02009
C	-3.09374	-0.51404	1.01464
C	-2.86021	-0.5151	-0.41521
C	-3.89642	-0.96575	-1.24081
H	-3.72037	-0.96111	-2.31275
C	-5.12907	-1.41657	-0.73604
C	-6.17955	-1.88209	-1.583
H	-6.01772	-1.88813	-2.65809
C	-7.3723	-2.31416	-1.05553
H	-8.16033	-2.66419	-1.7175
C	-7.59429	-2.3102	0.35004
H	-8.54495	-2.65601	0.74583
C	-6.60711	-1.87025	1.19675
H	-6.7638	-1.86254	2.27329
C	-5.35672	-1.41535	0.68561
C	-4.32413	-0.95029	1.51439

H	-4.48868	-0.9274	2.5905
C	-2.15019	0.00329	1.97383
H	-2.54354	0.15828	2.98277
C	0.22213	0.97697	-2.91577
H	-0.60489	0.3291	-3.21871
H	0.9007	1.1072	-3.76886
C	-0.35886	2.33147	-2.45306
H	-1.21436	2.10909	-1.81142
H	-0.76475	2.82783	-3.34528
C	0.6195	3.27753	-1.72589
H	1.34317	2.69509	-1.14508
H	1.20664	3.83945	-2.46548
C	-0.08801	4.2754	-0.78231
H	-0.88062	4.79077	-1.34356
H	0.62918	5.05564	-0.48976
C	-0.70384	3.66306	0.49525
H	-1.40517	4.39262	0.92583
H	-1.308	2.78733	0.2311
C	0.31597	3.28077	1.58642
H	0.79901	4.20447	1.93422
H	1.11494	2.65772	1.17091
C	-0.30263	2.55959	2.81224
H	0.19774	2.90959	3.72505
H	-1.35938	2.84375	2.92016
C	-0.19084	1.01845	2.8637
H	0.85436	0.716	2.79441
H	-0.5959	0.66819	3.82257

[a] The geometry was optimized by DFT calculation (B3LYP/6-31G*, LanL2DZ).

Table S6. Cartesian coordinates (in angstrom) of (*R*)-**1b** in the S_0 state[a].

atom	x	y	z
Pt	0.00003	-0.20376	0
O	1.79761	-0.26887	0.94864
O	-1.79752	-0.26922	-0.94868
N	0.90924	-0.1003	-1.82865
N	-0.9092	-0.09996	1.82863
C	2.92612	-0.66388	0.4005
C	-2.16643	-0.35573	2.0091
H	-2.54529	-0.25689	3.02964
C	-0.13081	0.41014	2.9738
H	-0.76347	0.36417	3.87003
H	0.72538	-0.25373	3.11044
C	3.1501	-0.73884	-1.0269
C	4.40336	-1.12385	-1.511
H	4.55994	-1.15884	-2.58795
C	0.6902	2.89213	-2.43044
H	1.36014	2.51647	-1.6474
H	1.31767	3.04884	-3.31987
C	0.38538	1.84225	2.74438
H	0.92891	2.13446	3.65437
H	1.12655	1.799	1.94284
C	0.13081	0.40957	-2.97389
H	0.76343	0.36348	-3.87013
H	-0.72537	-0.25435	-3.1104
C	-2.92606	-0.66408	-0.40044
C	2.16649	-0.35601	-2.00909
H	2.54534	-0.25729	-3.02964
C	5.46886	-1.46825	-0.66473
C	-0.51695	4.26181	-0.56999
H	-1.14065	5.16172	-0.47029
H	-1.19953	3.40984	-0.45709
C	6.74267	-1.87423	-1.15861
H	6.89235	-1.92469	-2.23498
C	0.5165	4.26222	0.5694
H	1.13967	5.16247	0.46948
H	1.19956	3.41061	0.45663
C	-6.7426	-1.8741	1.15892
H	-6.89227	-1.92435	2.2353
C	-3.99333	-0.99284	-1.24348
H	-3.82404	-0.93104	-2.31473

C	-0.38545	1.84171	-2.74471
H	-0.92882	2.1338	-3.65483
H	-1.12675	1.79851	-1.94328
C	-4.40328	-1.12364	1.51115
H	-4.55988	-1.1584	2.58811
C	5.25004	-1.39402	0.75624
C	3.99338	-0.99253	1.2436
H	3.82409	-0.93054	2.31485
C	-6.33301	-1.73707	-1.62013
H	-6.17823	-1.68556	-2.69505
C	-5.4688	-1.4682	0.66496
C	0.09921	4.24597	-1.9851
H	-0.66675	4.55178	-2.71214
H	0.88527	5.01279	-2.03461
C	-0.09949	4.24641	1.98457
H	-0.88557	5.01322	2.03412
H	0.66659	4.55234	2.71145
C	7.76098	-2.19606	-0.29566
H	8.72948	-2.50521	-0.67826
C	-7.54791	-2.12511	-1.10902
H	-8.36046	-2.38202	-1.78389
C	6.33307	-1.73669	1.62041
H	6.17826	-1.68501	2.69532
C	-5.24999	-1.39423	-0.75603
C	-7.76091	-2.19612	0.29603
H	-8.72938	-2.50524	0.67871
C	-0.69036	2.89261	2.43018
H	-1.31764	3.04944	3.31972
H	-1.36046	2.51682	1.64735
C	7.54797	-2.12481	1.10939
H	8.36052	-2.38159	1.78431
C	-3.15002	-0.73874	1.02697

[a] The geometry was optimized by DFT calculation (B3LYP/6-31G*, LanL2DZ).

Table S7. Cartesian coordinates (in angstrom) of (*R*)-**1c** in the S_0 state[a].

atom	x	y	z
Pt	0.07362	-0.54033	0.0081
O	-1.72547	-0.57477	-0.93526
O	1.86841	-0.62193	0.95291
N	-0.82025	-0.56354	1.85233
N	0.96227	-0.40056	-1.83146
C	-2.08302	-0.80437	2.01904
H	-2.45005	-0.79526	3.04841
C	-2.8692	-0.93811	-0.3989
C	-3.95361	-1.17808	-1.25073
H	-3.78682	-1.07023	-2.31873
C	0.14011	-0.05209	-3.00748
H	-0.69167	-0.75758	-3.04348
H	0.75492	-0.183	-3.90776
C	2.23666	-0.55629	-2.01359
H	2.59626	-0.4657	-3.0415
C	3.03587	-0.83566	0.38934
C	-0.02659	-0.22204	3.05043
H	0.81336	-0.91834	3.09772
H	-0.66037	-0.37409	3.93371
C	-0.51369	2.31409	2.75017
H	-1.03135	2.08293	1.81207
H	-1.28482	2.3254	3.53578
C	-5.22342	-1.55068	-0.77572
C	0.52098	1.21522	3.02231
H	1.01108	1.38813	3.99132
H	1.30513	1.25967	2.26114
C	3.26182	-0.82622	-1.03852
C	-3.08859	-1.0751	1.0234
C	-4.35476	-1.43343	1.49603
H	-4.5065	-1.5201	2.57071
C	-0.42212	1.3776	-2.94936
H	-1.02586	1.51417	-3.85872
H	-1.1134	1.43034	-2.10453
C	0.14089	3.70036	2.6419
H	0.53327	3.99402	3.62584
H	1.01698	3.62337	1.98389
C	5.65368	-1.28472	-0.70125
C	5.43224	-1.29099	0.72153
C	-6.32408	-1.80464	-1.64848

H	-6.17272	-1.70516	-2.72051
C	0.63224	2.48788	-2.8621
H	1.34784	2.37879	-3.6912
H	1.2154	2.36576	-1.94097
C	4.1383	-1.06481	1.22157
H	3.96535	-1.06743	2.294
C	-0.31817	4.33706	-0.38713
H	0.45849	5.1169	-0.36301
H	0.19258	3.38931	-0.17516
C	7.80314	-1.74963	1.04972
H	8.64331	-1.93065	1.71533
C	-6.72531	-2.06594	1.12311
H	-6.87152	-2.16482	2.19659
C	-1.35989	4.60884	0.70987
H	-2.08293	3.78155	0.72093
H	-1.93929	5.504	0.44142
C	6.55227	-1.53121	1.57366
H	6.39614	-1.53852	2.6496
C	-5.43817	-1.68779	0.64135
C	8.01845	-1.74247	-0.35717
H	9.01604	-1.91735	-0.74977
C	-0.93879	4.28228	-1.7915
H	-1.37604	5.26405	-2.0229
H	-1.78149	3.5772	-1.78536
C	0.04052	3.91041	-2.92135
H	0.86878	4.63342	-2.92703
H	-0.47593	4.03413	-3.8843
C	4.55141	-1.04371	-1.5348
H	4.70639	-1.02574	-2.61233
C	-0.781	4.81886	2.12323
H	-0.21487	5.76124	2.13585
H	-1.61538	4.95778	2.82577
C	6.96595	-1.51482	-1.20855
H	7.11687	-1.50687	-2.28589
C	-7.55112	-2.1685	-1.14908
H	-8.37679	-2.35788	-1.83031
C	-7.76002	-2.30209	0.25223
H	-8.73846	-2.59069	0.62544

[a] The geometry was optimized by DFT calculation (B3LYP/6-31G*, LanL2DZ).

Table S8. Cartesian coordinates (in angstrom) of (*R*)-**1d** in the S_0 state[a].

atom	x	y	z
Pt	-0.18294	-0.86576	-0.00517
O	1.61682	-0.9362	0.93516
O	-1.98317	-0.89275	-0.94313
N	0.70122	-1.07273	-1.844
N	-1.05405	-0.56895	1.824
C	1.94039	-1.42278	-1.99138
H	2.30392	-1.51333	-3.01813
C	2.72658	-1.42761	0.43012
C	3.79635	-1.67725	1.29756
H	3.6461	-1.46993	2.35326
C	-0.20815	-0.20393	2.97796
H	0.6082	-0.92587	3.02266
H	-0.81217	-0.29338	3.89062
C	-2.334	-0.64526	2.01663
H	-2.68327	-0.48307	3.03934
C	-3.15832	-1.00829	-0.36697
C	-0.0648	-0.73897	-3.06194
H	-0.9614	-1.36215	-3.06876
H	0.55031	-0.995	-3.93431
C	0.64774	1.75394	-2.91076
H	1.23419	1.46	-2.03098
H	1.33974	1.73513	-3.76606
C	5.03258	-2.17877	0.85318
C	-0.48679	0.74007	-3.10862
H	-0.98429	0.90398	-4.07496
H	-1.24576	0.8899	-2.33552
C	-3.37693	-0.90795	1.05881
C	2.92637	-1.69525	-0.97668
C	4.15946	-2.18272	-1.4197
H	4.2972	-2.36622	-2.48405
C	0.38193	1.21162	2.86746
H	1.03361	1.34943	3.74281
H	1.03059	1.23948	1.98788
C	0.12534	3.17984	-2.67614
H	-0.32457	3.57995	-3.59641
H	-0.68993	3.12689	-1.93969
C	-5.79275	-1.24574	0.75171
C	-5.5787	-1.34332	-0.66888
C	6.11831	-2.43959	1.74243

H	5.98216	-2.24234	2.80292
C	-0.65522	2.3411	2.81972
H	-1.32254	2.25722	3.69091
H	-1.29025	2.21713	1.93194
C	-4.27637	-1.21972	-1.18306
H	-4.1096	-1.29159	-2.25405
C	-7.97371	-1.68239	-0.96662
H	-8.82618	-1.8514	-1.61964
C	6.48069	-2.95288	-0.99912
H	6.61179	-3.14876	-2.06117
C	-6.71499	-1.5657	-1.50422
H	-6.5651	-1.6415	-2.5784
C	5.22736	-2.44557	-0.5482
C	-8.18151	-1.58478	0.43804
H	-9.18556	-1.67999	0.84148
C	-0.04476	3.75525	2.80222
H	-0.86117	4.48687	2.8858
H	0.57995	3.89452	3.69746
C	-4.67431	-1.02359	1.56863
H	-4.82246	-0.93806	2.64389
C	-7.11344	-1.3713	1.27352
H	-7.258	-1.29501	2.34907
C	7.31284	-2.92964	1.27287
H	8.12775	-3.12148	1.96628
C	7.5021	-3.19094	-0.11312
H	8.45495	-3.57795	-0.46277
C	1.29429	5.52963	1.51979
H	0.43893	6.22212	1.51746
H	1.82216	5.7148	2.46617
C	0.6048	5.48178	-1.66257
H	0.18853	6.0224	-2.52482
H	-0.25009	5.28125	-1.00183
C	2.2488	5.87885	0.35441
H	2.87959	5.00702	0.1327
H	2.94185	6.65856	0.69804
C	1.59981	6.4079	-0.94163
H	1.08393	7.35045	-0.70775
H	2.40693	6.67325	-1.6402
C	1.19222	4.14649	-2.14234
H	1.71216	3.65579	-1.30929
H	1.95768	4.33242	-2.91015
C	0.78412	4.07785	1.54896

H	1.64923	3.40322	1.49303
H	0.17656	3.8658	0.65995

[a] The geometry was optimized by DFT calculation (B3LYP/6-31G*, LanL2DZ).

Table S9. Cartesian coordinates (in angstrom) of (*R*)-**1e** in the S_0 state[a].

atom	x	y	z
Pt	-0.23342	-1.08055	0.19923
O	1.57407	-0.91016	1.10473
O	-2.04435	-1.28579	-0.69198
N	0.61679	-1.73186	-1.55132
N	-1.07737	-0.45754	1.96026
C	2.92107	-1.90226	-0.66671
C	2.72772	-1.34388	0.65191
C	3.84478	-1.25433	1.49193
H	3.69713	-0.83077	2.4813
C	5.12237	-1.69257	1.10348
C	6.25734	-1.60711	1.96552
H	6.12644	-1.18502	2.95889
C	7.49104	-2.04854	1.5533
H	8.34285	-1.97497	2.22464
C	7.67357	-2.60353	0.25528
H	8.65809	-2.94645	-0.04973
C	6.60628	-2.70187	-0.60215
H	6.73189	-3.12393	-1.59692
C	5.31072	-2.25502	-0.20889
C	4.19423	-2.3352	-1.05361
H	4.32394	-2.74976	-2.05196
C	1.87823	-2.0201	-1.65061
H	2.21201	-2.4025	-2.61916
C	-3.42671	-0.68021	1.22094
C	-3.2239	-1.09931	-0.14714
C	-4.36022	-1.32312	-0.93513
H	-4.20545	-1.63871	-1.96297
C	-5.66711	-1.16142	-0.44444
C	-6.82297	-1.39328	-1.25001
H	-6.68451	-1.70527	-2.28225
C	-8.0859	-1.22774	-0.73592
H	-8.95326	-1.40954	-1.36547
C	-8.27881	-0.82028	0.61428
H	-9.28657	-0.69558	1.00003
C	-7.19204	-0.5875	1.41972
H	-7.3253	-0.27552	2.45337
C	-5.86617	-0.74922	0.921
C	-4.7286	-0.52153	1.70871
H	-4.86436	-0.20653	2.74198

C	-2.36042	-0.39814	2.14539
H	-2.69286	-0.09061	3.13951
C	-0.1839	-1.90184	-2.78896
H	-1.20855	-2.11529	-2.48908
H	0.21301	-2.77328	-3.32396
C	-0.12639	-0.66452	-3.70564
H	0.92323	-0.35426	-3.79684
H	-0.43716	-0.98164	-4.71136
C	-1.00417	0.5132	-3.25501
H	-0.89288	0.66556	-2.17733
H	-2.05698	0.23981	-3.40218
C	-0.71903	1.83245	-3.99382
H	-0.84566	1.6859	-5.0767
H	-1.48643	2.56051	-3.69531
C	0.66827	2.45207	-3.72952
H	1.45447	1.83546	-4.18879
H	0.71282	3.42078	-4.24573
C	0.994	4.42866	2.48578
H	1.88394	3.78526	2.53578
H	1.29587	5.38941	2.92785
C	-0.13014	3.84585	3.36052
H	-0.97034	4.55509	3.36461
H	0.22809	3.79536	4.39914
C	-0.67303	2.45898	2.96742
H	-1.48865	2.21814	3.66628
H	-1.13318	2.50188	1.97206
C	0.3721	1.33352	3.00616
H	1.00889	1.45606	3.895
H	1.03628	1.37905	2.13782
C	-0.2171	-0.08338	3.10298
H	0.5962	-0.80735	3.14524
H	-0.81394	-0.17082	4.02025
C	0.98898	2.63684	-2.23822
H	0.14856	3.15103	-1.75165
H	1.04908	1.65194	-1.75953
C	0.6164	4.65812	1.01508
H	0.52042	3.69286	0.5022
H	-0.37666	5.1299	0.96183
C	2.30106	3.38662	-1.94881
H	3.09979	2.95488	-2.56939
H	2.59835	3.18949	-0.9101
C	1.62236	5.55062	0.26712

H	2.63843	5.15562	0.41192
H	1.62022	6.53804	0.74853
C	1.33588	5.70983	-1.24738
H	1.42514	6.7676	-1.52693
H	0.28952	5.44212	-1.44892
C	2.27138	4.90854	-2.17533
H	2.00017	5.12306	-3.21848
H	3.29363	5.29266	-2.04712

[a] The geometry was optimized by DFT calculation (B3LYP/6-31G*, LanL2DZ).

Table S10. Cartesian coordinates (in angstrom) of (*R*)-**1f** in the S_0 state[a].

atom	x	y	z
Pt	-0.55084	-1.43596	-0.15715
O	1.18557	-1.90172	0.78204
N	-2.29516	-1.00009	-1.09771
C	0.3484	-1.48178	-2.00061
C	-1.44912	-1.42026	1.68672
C	2.53966	-2.30507	-1.20298
H	2.31331	-2.27596	0.22375
C	3.36824	-2.66427	1.05911
C	3.19622	-2.6365	2.13134
H	4.61387	-3.08395	0.56172
C	5.68572	-3.48322	1.41628
H	5.53045	-3.46009	2.49211
C	6.89	-3.88897	0.89487
H	7.69391	-4.1888	1.56233
C	7.10385	-3.92335	-0.51198
H	8.06413	-4.24781	-0.90253
C	6.09714	-3.54693	-1.36571
C	6.24753	-3.56824	-2.44295
H	4.83374	-3.12014	-0.86113
C	3.78035	-2.72268	-1.69721
H	3.93616	-2.73539	-2.77469
C	1.56725	-1.88958	-2.17822
H	1.92282	-1.91569	-3.21202
H	-3.72966	-0.92401	0.87012
C	-3.47462	-0.82662	-0.54886
H	-4.5585	-0.53442	-1.38691
H	-4.36581	-0.46667	-2.45384
C	-5.86132	-0.33447	-0.8997
H	-6.96328	-0.03595	-1.75723
H	-6.78539	0.03879	-2.82721
C	-8.22377	0.1542	-1.24572
H	-9.04961	0.38113	-1.91518
H	-8.46798	0.05842	0.15339
C	-9.47286	0.21247	0.53603
H	-7.43401	-0.22794	1.0095
H	-7.60678	-0.3043	2.08087
C	-6.11236	-0.43165	0.51504
H	-5.02787	-0.72703	1.35362
H	-5.20315	-0.80406	2.42539

C	-2.71948	-1.21458	1.85299
H	-3.08816	-1.26567	2.88002
H	-0.36997	-1.04023	-3.2209
C	-1.43459	-1.18029	-3.04191
H	-0.06425	-1.69601	-4.04563
H	-0.06467	0.42294	-3.58995
C	1.02573	0.54768	-3.63468
H	-0.43422	0.58717	-4.61257
H	-0.68831	1.46752	-2.6534
O	-0.45661	1.21032	-1.61225
N	-1.78042	1.40721	-2.73872
C	-0.22448	2.90996	-2.91588
C	-0.40792	3.1866	-3.965
C	-0.8487	3.5833	-2.31167
H	1.23099	2.44864	4.1323
C	1.98873	1.70533	3.8477
C	1.69145	3.05585	4.92506
H	0.00061	1.74594	4.73223
C	-0.72137	2.51347	5.04625
H	0.30925	1.2263	5.65104
C	-0.72664	0.73396	3.82687
H	-1.60071	0.36223	4.38285
C	-1.12614	1.23996	2.93875
H	0.14182	-0.45837	3.39761
C	0.73216	-0.80742	4.25788
C	0.85869	-0.16797	2.62411
H	-0.64751	-1.67991	2.90123
C	0.04802	-2.48417	2.66335
H	-1.32755	-2.02527	3.69101
C	0.93352	3.35711	2.93032
H	0.60909	2.75093	2.07267
H	0.08727	4.01701	3.17474
C	2.1359	4.21884	2.51666
H	3.00342	3.56938	2.32654
H	2.42108	4.86622	3.35967
C	1.24985	3.158	-2.55863
H	1.45942	2.67788	-1.59039
H	1.9088	2.66455	-3.28695
C	1.63185	4.64064	-2.45451
H	1.45666	5.14616	-3.41573
H	0.96027	5.12386	-1.73221
C	1.86993	5.08208	1.27668

H	1.64838	4.42248	0.42793
H	0.96025	5.67984	1.43832
C	3.094	4.83835	-2.02632
H	3.7499	4.50721	-2.84405
H	3.31528	4.16783	-1.18412
C	3.47822	6.27633	-1.64006
H	4.56751	6.31199	-1.4947
H	3.26483	6.94723	-2.48503
C	2.80851	6.85169	-0.37444
H	3.20671	7.86481	-0.23184
H	1.7307	6.98238	-0.54356
C	3.02533	6.0328	0.92133
H	3.96207	5.46108	0.84295
H	3.16931	6.72078	1.7658

[a] The geometry was optimized by DFT calculation (B3LYP/6-31G*, LanL2DZ).

Table S11. Cartesian coordinates (in angstrom) of (*R*)-**1a** in the T_1 state[a].

atom	x	y	z
Pt	0.022934	-0.015046	-0.00453
O	1.796416	-0.068207	0.895033
O	-1.73506	-0.2712	-0.896616
N	0.914314	0.085372	-1.836033
N	-0.883404	0.282221	1.797331
C	3.184881	-0.496315	-1.067976
C	2.943018	-0.448373	0.362079
C	3.972424	-0.773923	1.248917
H	3.754473	-0.724999	2.311842
C	5.263101	-1.148567	0.805291
C	6.307149	-1.481184	1.703069
H	6.108306	-1.445565	2.771595
C	7.557582	-1.846892	1.235735
H	8.348599	-2.101113	1.935392
C	7.806543	-1.89022	-0.153977
H	8.790285	-2.178073	-0.515216
C	6.809161	-1.569311	-1.057444
H	7.005862	-1.603934	-2.126393
C	5.516298	-1.191983	-0.611675
C	4.469618	-0.858536	-1.499781
H	4.670217	-0.884998	-2.568916
C	2.204729	-0.120396	-2.031683
H	2.56998	0.017936	-3.050773
C	-3.144206	-0.412426	1.096646
C	-2.888105	-0.565107	-0.323687
C	-3.911309	-1.010104	-1.163467
H	-3.683839	-1.112912	-2.22051
C	-5.207336	-1.310837	-0.683834
C	-6.247812	-1.758849	-1.536165
H	-6.040257	-1.874384	-2.597321
C	-7.503934	-2.044807	-1.033858
H	-8.29167	-2.387696	-1.698658
C	-7.766839	-1.891121	0.346831
H	-8.756752	-2.11719	0.734044
C	-6.77497	-1.455708	1.205118
H	-6.979994	-1.338684	2.266678
C	-5.474425	-1.154297	0.722396
C	-4.432973	-0.707911	1.564166
H	-4.640753	-0.587176	2.625499

C	-2.168694	0.07575	2.014825
H	-2.534266	0.311869	3.016568
C	0.145261	0.70984	-2.923567
H	-0.679761	0.044443	-3.196383
H	0.803831	0.811239	-3.795701
C	-0.446529	2.083778	-2.528377
H	-1.28861	1.894046	-1.858254
H	-0.8777	2.526007	-3.437439
C	0.531193	3.081955	-1.873252
H	1.28857	2.540216	-1.2959
H	1.081546	3.623733	-2.654706
C	-0.166592	4.106603	-0.950968
H	-0.986585	4.581247	-1.508732
H	0.54289	4.913026	-0.716275
C	-0.731493	3.544127	0.372302
H	-1.425426	4.285239	0.794669
H	-1.337624	2.653542	0.169978
C	0.326393	3.21996	1.446017
H	0.816551	4.161468	1.73014
H	1.116777	2.585592	1.028682
C	-0.243505	2.554146	2.725545
H	0.291269	2.943858	3.602398
H	-1.294769	2.84702	2.857796
C	-0.137938	1.013739	2.832358
H	0.906485	0.707085	2.766229
H	-0.517873	0.706681	3.817096

[a] The geometry was optimized by DFT calculation (UB3LYP/6-31G*, LanL2DZ).

Table S12. Cartesian coordinates (in angstrom) of (*R*)-**1b** in the T_1 state[a].

atom	x	y	z
Pt	0.000041	0.320774	-0.000029
O	1.773495	0.44293	-0.886654
O	-1.773401	0.443049	0.886593
N	0.869727	0.190249	1.841944
N	-0.869669	0.190085	-1.841984
C	2.938732	0.716789	-0.332172
C	-2.161783	0.368646	-2.049541
H	-2.50719	0.249445	-3.077655
C	-0.062906	-0.304835	-2.968004
H	-0.677133	-0.264201	-3.877153
H	0.789004	0.36652	-3.102552
C	3.171486	0.696237	1.098632
C	4.471643	0.966323	1.551959
H	4.663012	0.946417	2.62296
C	0.606664	-2.798727	2.462806
H	1.30955	-2.424171	1.708994
H	1.199297	-2.966716	3.373524
C	0.465535	-1.73598	-2.744942
H	1.034186	-2.016904	-3.643467
H	1.187744	-1.700989	-1.924669
C	0.062918	-0.304496	2.968007
H	0.67714	-0.263864	3.877161
H	-0.788913	0.36697	3.102495
C	-2.938638	0.716885	0.332101
C	2.161845	0.368777	2.049496
H	2.507236	0.249666	3.077626
C	5.545165	1.263485	0.683923
C	-0.539275	-4.150666	0.548914
H	-1.161869	-5.04761	0.41999
H	-1.214464	-3.296105	0.41174
C	6.855532	1.541407	1.151775
H	7.044299	1.525493	2.222605
C	0.538787	-4.150818	-0.548536
H	1.16124	-5.047845	-0.419503
H	1.214112	-3.296347	-0.411467
C	-6.855436	1.541472	-1.151855
H	-7.044215	1.525474	-2.222682
C	-3.993924	1.0107	1.19965
H	-3.781887	1.016638	2.264861

C	-0.465709	-1.735587	2.745034
H	-1.034436	-2.016356	3.643558
H	-1.187881	-1.700565	1.924726
C	-4.471563	0.966304	-1.55203
H	-4.662946	0.946313	-2.623026
C	5.301621	1.286231	-0.735075
C	3.994037	1.010509	-1.199726
H	3.782013	1.016365	-2.264941
C	-6.372753	1.583613	1.613413
H	-6.181726	1.598675	2.683848
C	-5.545067	1.263559	-0.684001
C	0.018687	-4.144038	1.988218
H	-0.779935	-4.444021	2.68183
H	0.793211	-4.920134	2.066891
C	-0.019176	-4.144278	-1.987839
H	-0.793807	-4.920278	-2.066421
H	0.779402	-4.444447	-2.681421
C	7.879273	1.82884	0.267211
H	8.876409	2.039429	0.644559
C	-7.639509	1.851087	1.124858
H	-8.45136	2.078244	1.80986
C	6.372884	1.583335	-1.613506
H	6.181872	1.598316	-2.683944
C	-5.301508	1.286415	0.734993
C	-7.87916	1.828999	-0.2673
H	-8.876297	2.039579	-0.644651
C	-0.606977	-2.798943	-2.462578
H	-1.199647	-2.966957	-3.373268
H	-1.309801	-2.424204	-1.708798
C	7.639637	1.85082	-1.124953
H	8.451501	2.077904	-1.809963
C	-3.171403	0.696222	-1.098699

[a] The geometry was optimized by DFT calculation (UB3LYP/6-31G*, LanL2DZ).

Table S13. Cartesian coordinates (in angstrom) of (*R*)-**1c** in the T_1 state[a].

atom	x	y	z
Pt	-0.074366	-0.642068	0.00639
O	1.707033	-0.69943	0.88067
O	-1.853561	-0.776687	-0.860778
N	0.773122	-0.663547	-1.853241
N	-0.920493	-0.450935	1.857793
C	2.066918	-0.84186	-2.055544
H	2.397829	-0.832051	-3.094978
C	2.87866	-0.963381	0.336127
C	3.952188	-1.147746	1.211842
H	3.750497	-1.077626	2.276771
C	-0.073243	-0.114279	3.013512
H	0.748899	-0.832221	3.053089
H	-0.672718	-0.234068	3.925651
C	-2.221703	-0.531271	2.070961
H	-2.549113	-0.404147	3.103723
C	-3.040303	-0.883457	-0.296733
C	-0.050851	-0.359794	-3.035024
H	-0.881129	-1.070084	-3.068348
H	0.565679	-0.518257	-3.929163
C	0.398451	2.191392	-2.802495
H	0.957937	1.967499	-1.887044
H	1.137748	2.216636	-3.617406
C	5.264582	-1.413528	0.754795
C	-0.622788	1.070819	-3.035944
H	-1.132225	1.216446	-3.999745
H	-1.396895	1.128344	-2.264228
C	-3.264742	-0.766457	1.129569
C	3.096937	-1.046625	-1.093619
C	4.401649	-1.308028	-1.539967
H	4.581867	-1.368086	-2.611393
C	0.511735	1.308498	2.954368
H	1.136935	1.435341	3.851018
H	1.186656	1.361499	2.09548
C	-0.276516	3.565414	-2.666322
H	-0.721797	3.848679	-3.630638
H	-1.118152	3.474588	-1.966096
C	-5.687969	-1.091388	0.73805
C	-5.452244	-1.212249	-0.677273
C	6.354041	-1.601496	1.640777

H	6.17401	-1.537165	2.711301
C	-0.526504	2.435278	2.889612
H	-1.207843	2.352045	3.749556
H	-1.150224	2.304377	1.997021
C	-4.123562	-1.106409	-1.151374
H	-3.916172	-1.192323	-2.214004
C	0.317237	4.23636	0.339055
H	-0.464332	5.011629	0.351549
H	-0.198755	3.284907	0.158516
C	-7.839684	-1.53145	-1.044799
H	-8.673729	-1.700441	-1.719885
C	6.8082	-1.765753	-1.124675
H	6.986102	-1.829479	-2.195587
C	1.298654	4.50958	-0.812016
H	2.029382	3.690055	-0.855053
H	1.881076	5.412673	-0.579068
C	-6.552218	-1.432281	-1.54266
H	-6.367147	-1.522376	-2.610444
C	5.493405	-1.496848	-0.6644
C	-8.071685	-1.412702	0.343594
H	-9.085075	-1.491169	0.728129
C	1.010013	4.192628	1.709771
H	1.470082	5.1722	1.903337
H	1.843721	3.477984	1.668578
C	0.088016	3.849336	2.89568
H	-0.728661	4.58451	2.934081
H	0.656762	3.980296	3.827746
C	-4.585155	-0.873164	1.592912
H	-4.769465	-0.783939	2.661618
C	0.647396	4.703441	-2.195698
H	0.063299	5.634861	-2.182856
H	1.4438	4.855907	-2.938352
C	-7.019598	-1.197473	1.215657
H	-7.202307	-1.106539	2.283779
C	7.62498	-1.863311	1.159535
H	8.450908	-2.006271	1.850408
C	7.850124	-1.945376	-0.232621
H	8.85036	-2.151121	-0.604391

[a] The geometry was optimized by DFT calculation (UB3LYP/6-31G*, LanL2DZ).

Table S14. Cartesian coordinates (in angstrom) of (*R*)-**1d** in the T_1 state[a].

atom	x	y	z
Pt	0.084127	-0.909402	-0.112268
O	-1.699281	-0.805679	-0.975088
O	1.871687	-1.084463	0.732646
N	-0.762804	-1.223998	1.722933
N	0.922533	-0.553721	-1.943473
C	-3.10589	-1.376786	0.933133
C	-2.886949	-1.064169	-0.463922
C	-3.973805	-1.023929	-1.341103
H	-3.772914	-0.785349	-2.381491
C	-5.298124	-1.281408	-0.916468
C	-6.40239	-1.240932	-1.804189
H	-6.223717	-1.000334	-2.849517
C	-7.684591	-1.501833	-1.355856
H	-8.52139	-1.467744	-2.047664
C	-7.909132	-1.813726	0.004303
H	-8.91915	-2.017512	0.349694
C	-6.854046	-1.861243	0.896499
H	-7.030416	-2.101373	1.942385
C	-5.526299	-1.599345	0.469235
C	-4.421117	-1.636202	1.346785
H	-4.599558	-1.873012	2.393767
C	-2.059565	-1.412225	1.897744
H	-2.379161	-1.622575	2.92011
C	3.282919	-0.792655	-1.232074
C	3.065277	-1.040702	0.177895
C	4.161103	-1.249799	1.021474
H	3.96016	-1.440319	2.071688
C	5.495334	-1.216917	0.550948
C	6.606804	-1.420833	1.404903
H	6.427148	-1.608486	2.460874
C	7.899694	-1.382879	0.910983
H	8.742794	-1.541031	1.577324
C	8.123822	-1.138375	-0.461468
H	9.140731	-1.109564	-0.843668
C	7.059409	-0.935804	-1.322622
H	7.237022	-0.748123	-2.378906
C	5.723228	-0.968417	-0.848816
C	4.608258	-0.767691	-1.692949
H	4.787415	-0.582557	-2.750094

C	2.226159	-0.572914	-2.160451
H	2.544055	-0.398676	-3.189063
C	0.04499	-1.226782	2.958373
H	1.068363	-1.486551	2.69295
H	-0.343442	-2.014667	3.617716
C	0.009209	0.121143	3.704193
H	-1.041077	0.391657	3.876321
H	0.452792	-0.03713	4.698271
C	0.750374	1.265275	2.99753
H	0.412493	1.330594	1.956836
H	1.817435	1.01161	2.94487
C	0.592932	2.63485	3.684942
H	0.879522	2.540486	4.742618
H	1.315618	3.332895	3.242011
C	-0.819122	3.250553	3.61074
H	-1.539853	2.558368	4.066215
H	-0.840517	4.154419	4.236673
C	-1.306522	3.613702	2.195819
H	-2.389178	3.799538	2.232435
H	-1.178052	2.75129	1.528951
C	-0.631367	4.852251	1.583319
H	-0.912565	5.731	2.180586
H	0.462182	4.771428	1.661292
C	-1.012234	5.084033	0.108355
H	-0.868919	6.142298	-0.150534
H	-2.086866	4.885281	-0.020468
C	-0.206948	4.22767	-0.883192
H	-0.173009	3.186989	-0.533662
H	0.83568	4.579791	-0.886821
C	-0.771102	4.27075	-2.311224
H	-1.733031	3.739469	-2.330743
H	-1.001962	5.313365	-2.573894
C	0.166196	3.7075	-3.395018
H	1.044428	4.364394	-3.472597
H	-0.345007	3.768989	-4.366797
C	0.665576	2.266801	-3.183483
H	1.346242	2.018852	-4.011791
H	1.271002	2.218045	-2.269937
C	-0.443811	1.210243	-3.113375
H	-1.10446	1.308999	-3.988023
H	-1.069794	1.365459	-2.22875
C	0.067118	-0.241303	-3.100536

H	-0.784872	-0.922012	-3.086011
H	0.642249	-0.437095	-4.015501

[a] The geometry was optimized by DFT calculation (UB3LYP/6-31G*, LanL2DZ).

Table S15. Cartesian coordinates (in angstrom) of (*R*)-**1e** in the T_1 state[a].

atom	x	y	z
Pt	0.264848	-1.115039	-0.284541
O	-1.52896	-0.938088	-1.112461
O	2.065303	-1.3337	0.518893
N	-0.540282	-1.865242	1.440876
N	1.060007	-0.349744	-2.006601
C	-2.88476	-1.955108	0.63957
C	-2.698705	-1.344495	-0.660113
C	-3.798762	-1.163433	-1.502434
H	-3.622242	-0.700613	-2.469018
C	-5.105549	-1.56079	-1.135322
C	-6.223384	-1.377611	-1.987358
H	-6.069762	-0.911657	-2.957835
C	-7.487519	-1.781942	-1.597966
H	-8.335077	-1.63567	-2.261475
C	-7.679565	-2.386924	-0.3351
H	-8.675558	-2.702025	-0.035665
C	-6.610498	-2.579953	0.520088
H	-6.76175	-3.045459	1.491186
C	-5.300654	-2.176982	0.151366
C	-4.182391	-2.353494	0.994686
H	-4.336061	-2.815807	1.967692
C	-1.824878	-2.152574	1.569124
H	-2.121923	-2.601736	2.518518
C	3.434819	-0.503604	-1.317358
C	3.24657	-1.054386	0.008477
C	4.359725	-1.322419	0.811671
H	4.180511	-1.740951	1.797671
C	5.682982	-1.066193	0.380749
C	6.811371	-1.331136	1.194876
H	6.653697	-1.744513	2.188243
C	8.093085	-1.071463	0.740399
H	8.949428	-1.279795	1.3753
C	8.288691	-0.535047	-0.551007
H	9.296972	-0.333153	-0.902586
C	7.207251	-0.265025	-1.371478
H	7.362923	0.147916	-2.365337
C	5.881813	-0.519426	-0.936246
C	4.750205	-0.259751	-1.741342
H	4.907657	0.150106	-2.736911

C	2.359934	-0.213381	-2.204825
H	2.658803	0.167612	-3.181842
C	0.278488	-2.117729	2.644537
H	1.306141	-2.289096	2.327483
H	-0.088113	-3.040322	3.113523
C	0.212017	-0.963759	3.665895
H	-0.8426	-0.689913	3.8004
H	0.553261	-1.349416	4.637389
C	1.04856	0.26903	3.289286
H	0.927015	0.483036	2.222891
H	2.111405	0.025254	3.420677
C	0.72019	1.5352	4.100276
H	0.841108	1.329169	5.173936
H	1.468357	2.301516	3.852534
C	-0.682353	2.128089	3.856575
H	-1.453725	1.460406	4.266591
H	-0.762233	3.061153	4.430971
C	-1.138981	4.481797	-2.26285
H	-2.013762	3.819678	-2.331371
H	-1.476742	5.460447	-2.634001
C	-0.02576	3.985647	-3.202532
H	0.792819	4.719684	-3.18926
H	-0.414882	3.985396	-4.231289
C	0.568958	2.595784	-2.908123
H	1.364698	2.4165	-3.646596
H	1.063251	2.595135	-1.928574
C	-0.44505	1.443913	-2.973972
H	-1.098735	1.582481	-3.848671
H	-1.096283	1.447821	-2.093756
C	0.182231	0.046291	-3.121795
H	-0.613489	-0.694869	-3.202328
H	0.771088	0.010161	-4.048167
C	-0.994622	2.395496	2.375827
H	-0.162339	2.955595	1.926531
H	-1.030957	1.438854	1.840611
C	-0.729282	4.626927	-0.789776
H	-0.60161	3.633905	-0.339929
H	0.255147	5.115482	-0.72943
C	-2.321439	3.133461	2.123034
H	-3.112844	2.64827	2.712508
H	-2.61013	2.992394	1.072883
C	-1.735579	5.449563	0.03388

H	-2.747097	5.044854	-0.116661
H	-1.761546	6.465516	-0.383107
C	-1.423077	5.518012	1.54993
H	-1.528938	6.553669	1.898045
H	-0.367799	5.261133	1.715839
C	-2.32473	4.639278	2.440254
H	-2.043716	4.797463	3.490878
H	-3.357473	5.005495	2.348917

[a] The geometry was optimized by DFT calculation (UB3LYP/6-31G*, LanL2DZ).

Table S16. Cartesian coordinates (in angstrom) of (*R*)-**1f** in the T_1 state[a].

atom	x	y	z
Pt	-0.549805	-1.47249	-0.168432
O	1.182008	-1.920039	0.688357
O	-2.293226	-1.067652	-1.024148
N	0.305663	-1.474312	-2.02713
N	-1.395126	-1.462152	1.694379
C	2.549819	-2.237666	-1.30433
C	2.330399	-2.242687	0.126958
C	3.372629	-2.603742	0.98486
H	3.172717	-2.593131	2.052372
C	4.650434	-2.976944	0.506792
C	5.709422	-3.343501	1.374561
H	5.532592	-3.334085	2.447494
C	6.945863	-3.707759	0.872586
H	7.748312	-3.986851	1.549468
C	7.16782	-3.717961	-0.523135
H	8.1416	-4.005303	-0.910657
C	6.156148	-3.365302	-1.397137
H	6.33072	-3.373665	-2.470481
C	4.876186	-2.986529	-0.915262
C	3.81722	-2.616306	-1.772317
H	3.995433	-2.619174	-2.845772
C	1.554152	-1.851211	-2.24533
H	1.873712	-1.866746	-3.288926
C	-3.700307	-0.92878	0.960196
C	-3.469379	-0.864456	-0.467752
C	-4.53437	-0.582341	-1.329212
H	-4.326684	-0.552464	-2.39482
C	-5.845713	-0.338551	-0.856624
C	-6.923848	-0.043777	-1.726751
H	-6.73549	-0.002648	-2.796972
C	-8.195177	0.188742	-1.230552
H	-9.012697	0.413849	-1.909411
C	-8.430951	0.13328	0.16059
H	-9.430943	0.316817	0.544439
C	-7.399358	-0.153075	1.037571
H	-7.58567	-0.194938	2.108109
C	-6.085713	-0.396282	0.561811
C	-5.004747	-0.694003	1.421363
H	-5.193892	-0.741716	2.491817

C	-2.679752	-1.233135	1.905324
H	-3.013056	-1.290267	2.941995
C	-0.437009	-1.04263	-3.228322
H	-1.499827	-1.187657	-3.040694
H	-0.148401	-1.700027	-4.059248
C	-0.152448	0.421547	-3.61668
H	0.93582	0.558494	-3.663876
H	-0.527866	0.576687	-4.638813
C	-0.785333	1.462206	-2.682244
H	-0.556364	1.203175	-1.640747
H	-1.877784	1.399907	-2.774616
C	-0.327995	2.90901	-2.932087
H	-0.510321	3.192725	-3.97938
H	-0.956273	3.575113	-2.323863
C	1.30616	2.361894	4.159114
H	2.06456	1.631374	3.844309
H	1.783028	2.967247	4.94356
C	0.103728	1.637064	4.789171
H	-0.614651	2.392521	5.138798
H	0.449024	1.108352	5.689615
C	-0.644368	0.631108	3.894125
H	-1.495837	0.242534	4.472515
H	-1.078315	1.145235	3.027309
C	0.217842	-0.547429	3.418151
H	0.818347	-0.921681	4.261295
H	0.927221	-0.225675	2.648918
C	-0.577093	-1.752003	2.884987
H	0.117839	-2.551866	2.627631
H	-1.243137	-2.126152	3.67418
C	0.962007	3.278189	2.975665
H	0.619853	2.676244	2.121939
H	0.115182	3.924962	3.251238
C	2.141195	4.158974	2.535796
H	3.01117	3.522271	2.315767
H	2.44195	4.802311	3.376482
C	1.144849	3.159383	-2.570288
H	1.357701	2.665288	-1.609829
H	1.805852	2.680827	-3.306393
C	1.517959	4.642334	-2.4429
H	1.329094	5.163967	-3.392901
H	0.850971	5.107786	-1.704669
C	1.831618	5.030589	1.311864

H	1.598103	4.377099	0.46136
H	0.918363	5.614283	1.502298
C	2.983379	4.842939	-2.027787
H	3.631859	4.526922	-2.857298
H	3.218302	4.162668	-1.197224
C	3.362079	6.278505	-1.627445
H	4.453298	6.322274	-1.499833
H	3.128357	6.959058	-2.45922
C	2.708826	6.829616	-0.342712
H	3.093419	7.847522	-0.196935
H	1.625819	6.944306	-0.488618
C	2.965532	6.000597	0.939164
H	3.907523	5.442046	0.833558
H	3.120067	6.681744	1.787315

[a] The geometry was optimized by DFT calculation (UB3LYP/6-31G*, LanL2DZ).