Supplementary Information for:

Understanding the Nature of Quinoidal and Zwitterionic State in Carbazole-Based Diradicals

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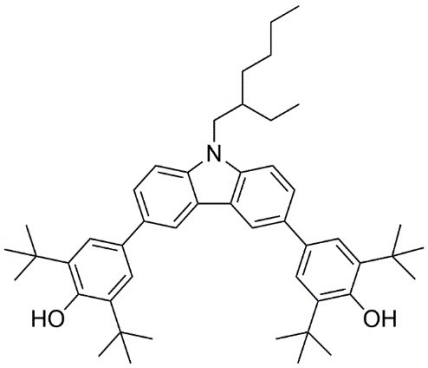
1. General information

All chemicals and reagents were purchased from Alfa, Acros and Adamas without further purifications. Anhydrous tetrahydrofuran (THF) was distilled over sodium under a nitrogen atmosphere. Column chromatography was performed on Haiyang silica gel (200-300 mesh). All reactions were monitored by thin layer chromatography (TLC) using commercial Huanghai glass plates (HSGF 254, 2.5 x 8 cm) visualized under UV radiation at 254 and 365 nm. The acid sensitive compounds were purified with trimethylamine pretreated silica gel and all organic extracts were dried by anhydrous Na_2SO_4. UV/Vis/NIR absorption spectra were performed using a Shimadzu UV-2600 UV-VIS spectrophotometer. MALDI-TOF mass spectra (MS) were measured on a SHIMADZU iD plus Performance using anthracene-1, 8, 9-triol as matrix. High resolution mass spectra (HRMS) were recorded on a Waters-Q-TOF-Premier (ESI). NMR spectra were measured by a Bruker AV III HD 400 MHz. ESR spectroscopy measurement was conducted by a Bruker EMX plus X-band spectrometer with 9.8 GHz microwave frequency. Elemental analysis measurements were performed on a Leeman Labs Euro EA 3000 elemental analyzer. Single Crystal X-Ray Diffraction were measured by a Gemini X-ray Single Crystal Diffractometer. Cyclic voltammograms were measured on a Shanghai Chenhua CHI 660E electrochemical workstation.

2. Preparation of materials

Synthesis of 3,6-bis(2,6-di-*tert*-butylphenol-4-yl)-9-(2-ethylhexyl) carbazole (Cb36OH)

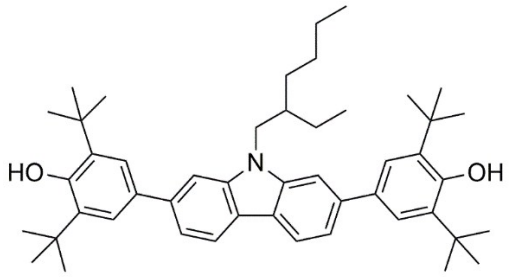


Cb36OH

3,6-dibromo-9-(2-ethylhexyl)-9*H*-carbazole[1] (200.0 mg, 0.5 mmol), tris(dibenzylideneacetone)dipalladium(0) (11.0 mg, 12.0 μmol), 3,5-di-*tert*-butyl-4-hydroxyphenyl boronic acid[2] (386.0 mg, 1.2 mmol), tri(*o*-tolyl)phosphine (13.0 mg, 42.8 μmol) and tetrabutylammonium hydroxide (TBAH) (731.0 mg, 870.0 μmol) were charged in a 50 mL two neck flask with 7.5 mL toluene and 1.5 mL water under nitrogen. The mixture was heated to reflux for 2 h. The reaction was cooled down to room temperature and hydrochloric acid (1 N, 50 mL) was added, and then the mixture was extracted with dichloromethane (3 x 50 mL). The collected organic layers were washed with water, dried over anhydrous Na_2SO_4 and the solvent was removed under reduced pressure. The residue was purified by column chromatography (SiO_2, hexane/DCM, V/V = 5: 1, as eluent) to give **Cb36OH** as a yellow solid (112.0 mg, 35%).

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.33 (s, 2H), 7.73 (d, *J* = 8.0 Hz, 2H), 7.57 (s, 4H), 7.51 (d, *J* = 8.0 Hz, 2H), 5.29 (s, 2H), 4,21-4.32 (m, 2H), 2.16-2.23 (m, 2H), 1.61 (s, 36H), 1.33-1.61 (m, 8H), 1.02 (t, *J* = 8.0 Hz, 3H), 0.96 (t, *J* = 8.0 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 11.0, 14.2, 23.2, 24.5, 29.0, 30.5, 31.1, 34.6, 39.6, 47.7, 109.1, 118.7, 123.4, 124.4, 125.4, 133.6, 133.7, 136.2, 140.5, 153.0. HRMS (ESI^+): calcd. for $C_{48}H_{66}NO_2$ 687.5015, found $[M+H]^+$ 688.5062.

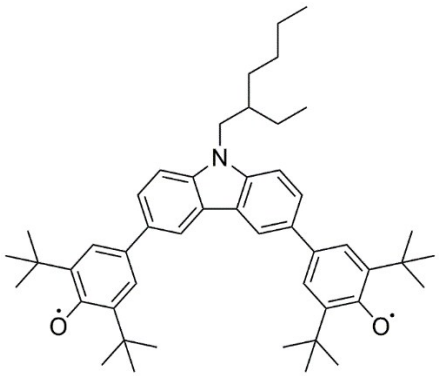
Synthesis of 2,7-bis(2,6-di-*tert*-butylphenol-4-yl)-9-(2-ethylhexyl) carbazole (Cb27OH)



Cb27OH

2,7-dibromo-9-(2-ethylhexyl)-9*H*-carbazole[3] (420.0 mg, 1.0 mmol), tris(dibenzylideneacetone)dipalladium(0) (34.0 mg, 37.2 μmol), 3,5-di-*tert*-butyl-4-hydroxyphenyl boronic acid (832.0 mg, 2.5 mmol), tri(*o*-tolyl)phosphine (28.0 mg, 92.1 μmol) and tetrabutylammonium hydroxide (TBAH) (1.5 g, 1.8 mmol) were charged in a 50 mL two neck flask with 15.0 mL toluene and 2.5 mL water under nitrogen. The mixture was heated to reflux for 2 h. The reaction was cooled down to room temperature and hydrochloric acid (1 M, 50 mL) was added, and then the mixture was extracted with dichloromethane (3 x 50 mL). The collected organic layers were washed with water, dried over anhydrous Na_2SO_4 and the solvent was removed under reduced pressure. The residue was purified by column chromatography (SiO_2, hexane/DCM, V/V = 5: 1, as eluent) to give **Cb27OH** as a yellow solid (145.0 mg, 22%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.09 (d, *J* = 8.0 Hz, 2H), 7.54 (s, 4H), 7.52 (s, 2H), 7.43 (s, 2H), 7.41 (s, 2H), 5.27 (s, 2H), 4.27-4.18 (m, 2H), 2.16-2.13 (m, 1H), 1.54-1.47 (m, 36H), 1.45- 1.26 (m, 8H), 0.97 (t, *J* = 8.0 Hz, 3H), 0.87 (t, *J* = 8.0 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 10.9, 14.2, 23.2, 24.6, 29.4, 30.4, 31.4, 34.6, 39.7, 47.3, 107.2, 118.6, 120.3, 121.4, 124.5, 133.7, 136.3, 139.9, 142.0, 153.4. HRMS (ESI^+): calcd. for $C_{48}H_{66}NO_2$ 687.5015, found $[M+H]^+$ 688.5091.

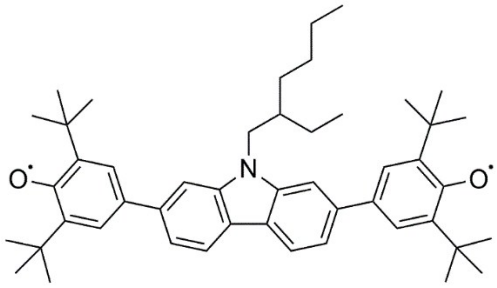
Synthesis of Cb36O



Cb36O

Cb36OH (15.0 mg, 21.8 μmol) and lead (IV) oxide (375.0 mg, 1.6 mmol) were suspended in dry dichloromethane (15.0 mL). The mixture was stirred at room temperature for 2 hours. The excess lead (IV) oxide was removed by suction filtration and the resulting solvent was removed under reduced pressure. The solid was purified by triethylamine pretreated column chromatography (SiO_2, hexane/DCM, V/V = 3: 1) to yield **Cb36O** as a dark green solid (14.1 mg, 94 %). HRMS (ESI^+): calcd. for $C_{48}H_{64}NO_2$ 685.4859, found $[M+H]^+$ 686.4928.

Synthesis of Cb27O



Cb27O

Cb27OH (20.0 mg, 29.0 μmol) and lead (IV) oxide (0.5 g, 2.1 mmol) were suspended in dry dichloromethane (15 mL). The mixture was stirred at room temperature for 1 hour. The excess lead (IV) oxide was removed by suction filtration and the resulting solvent was removed under reduced pressure. The solid was purified by triethylamine pretreated column chromatography (SiO_2, hexane/DCM, V/V = 3: 1) to yield **Cb27O** as a dark green solid (18.6 mg, 93%). HRMS (ESI^+): calcd. for $C_{48}H_{64}NO_2$ 685.4859, found $[M+H]^+$ 686.4846.

Methods to grow single crystals

Three common methods have been used to grow single crystals for X-ray diffraction. Method A: slow evaporation of compounds in pure or mixed solutions (e.g. DCM, toluene, THF, MeOH, DCM/MeOH, DCM/toluene, DCM/hexane, DCM/EA, DCM/acetone) in 4 mL glass vials (with cap).

Method B: slow diffusion of poor solvents e.g. hexane, toluene and MeOH to saturated DCM solution of compounds in NMR tubes (with cap) and 4 mL glass vials (with cap) at room temperature and -20 °C (in refrigerator).

Method C: slow cooling the hot solutions of compounds in pure or mixed solvents (e.g. toluene, THF, EA, MeOH, acetone, DCM/toluene, DCM/hexane, DCM/EA, DCM/MeOH, DCM/acetone).

The single crystal of **Cb27OH** suitable for X-ray crystallographic analysis was grown by method A using pure methanol solution. Unfortunately, only amorphous powders were obtained for **Cb36OH** using above methods. **Cb36O** and **Cb27O** were not stable in solutions so we failed to obtain suitable single crystal of both diradicals for X-ray diffraction.

3. NMR and Mass spectra

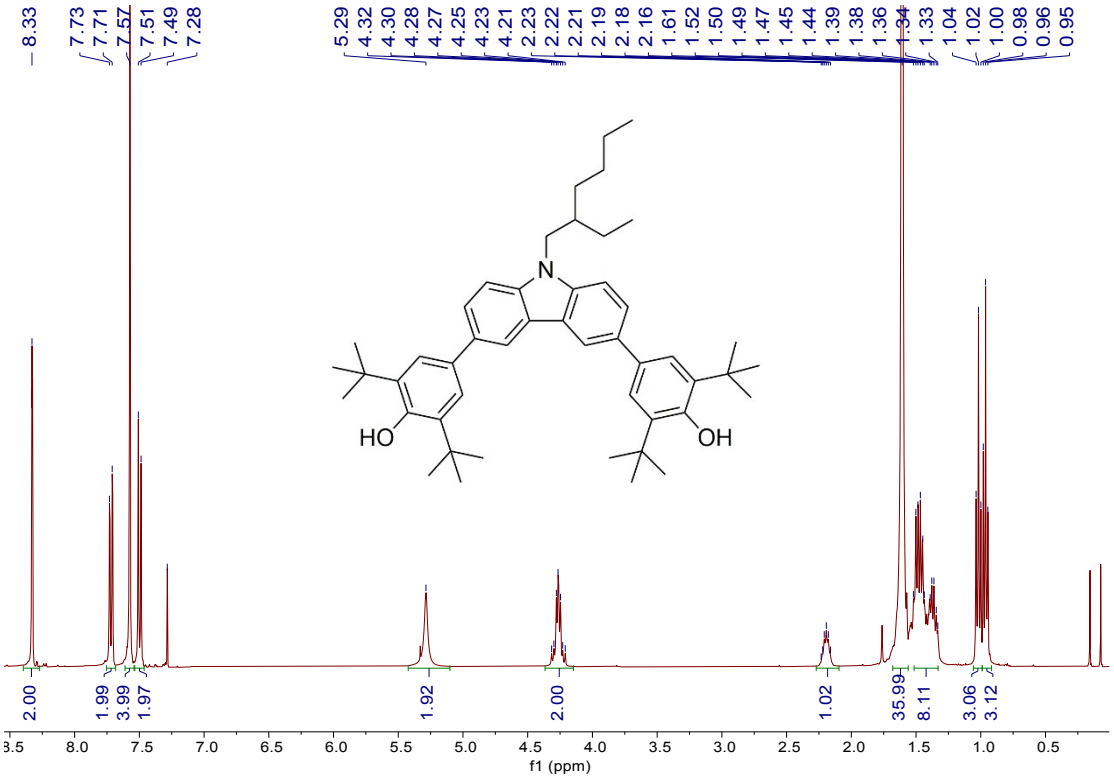


Figure S1. [1]H NMR spectrum of **Cb36OH**.

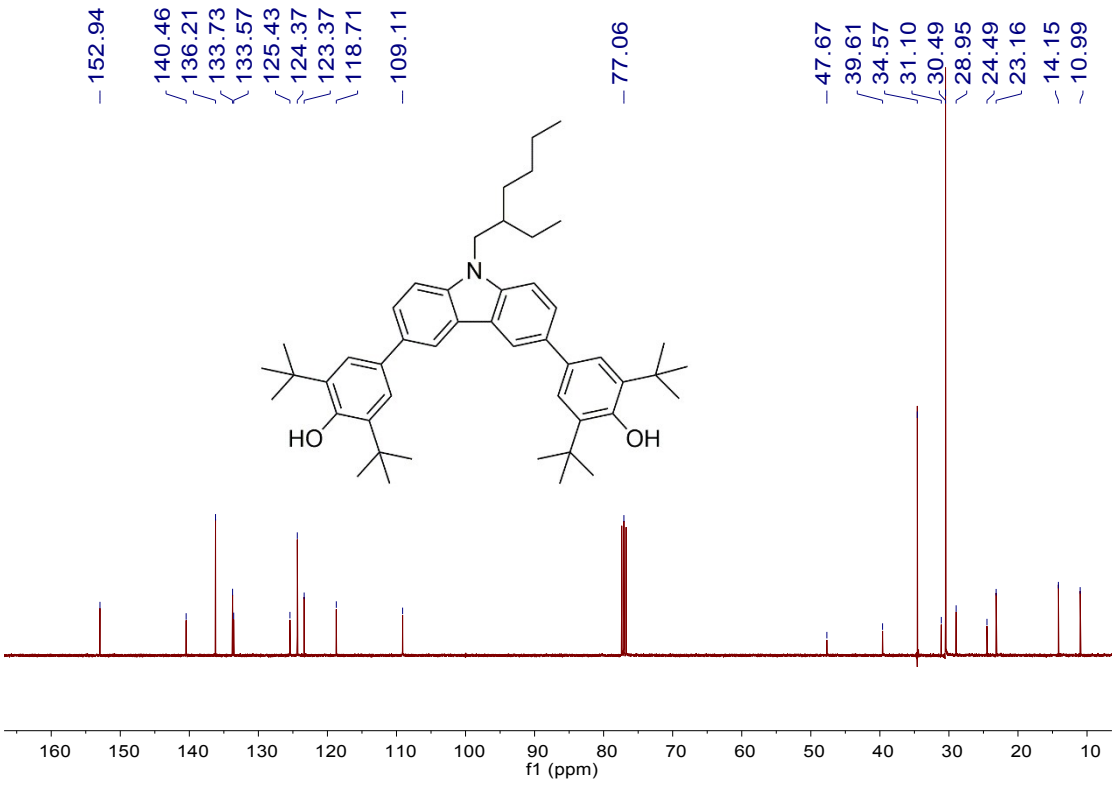


Figure S2. [13]C NMR spectrum of **Cb36OH**.

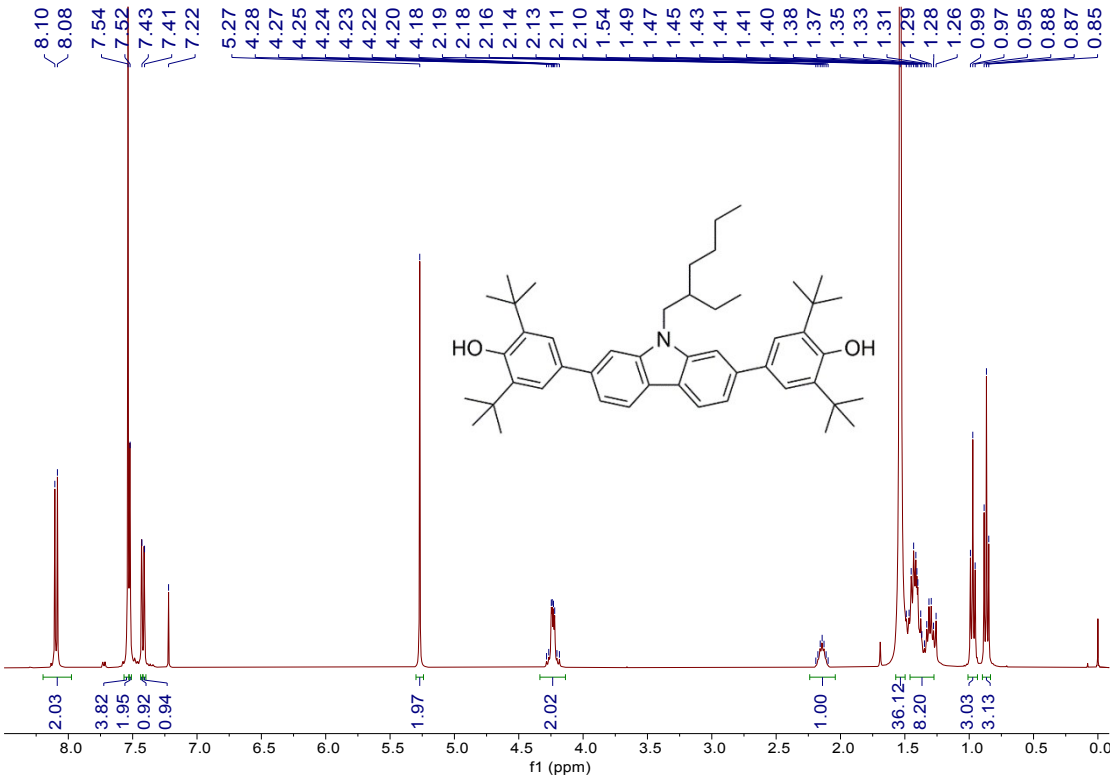


Figure S3. [1]H NMR spectrum of **Cb27OH**.

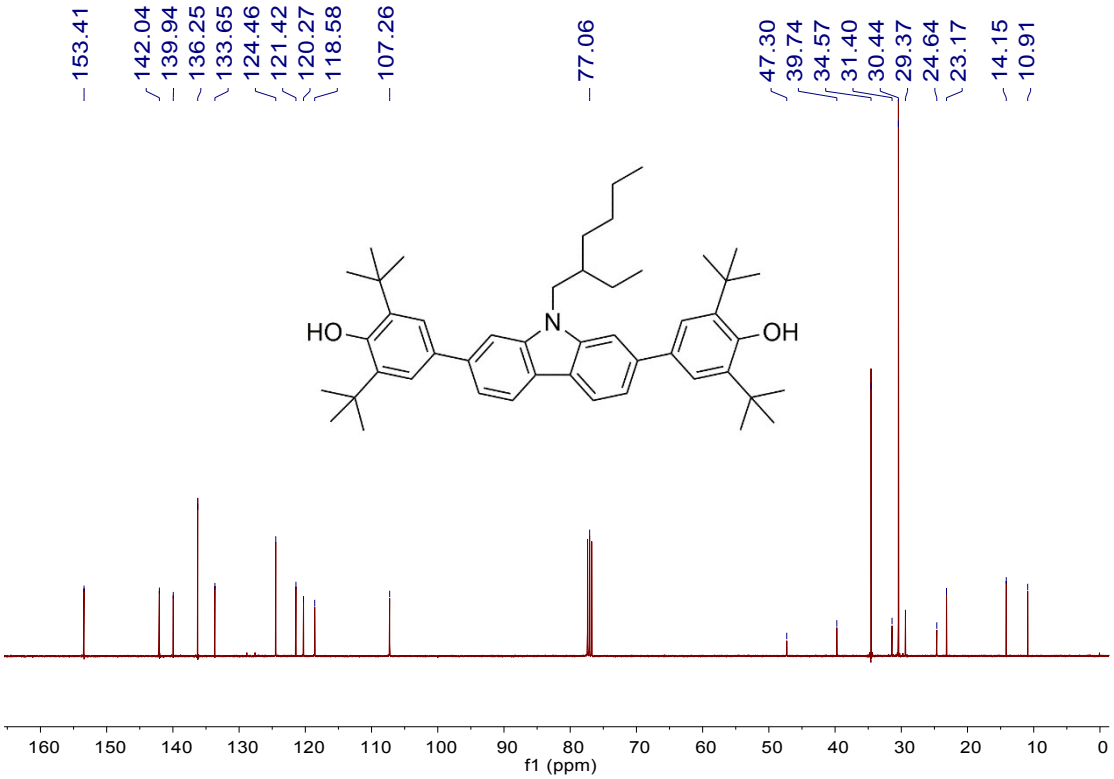


Figure S4. [13]C NMR spectrum of **Cb27OH**.

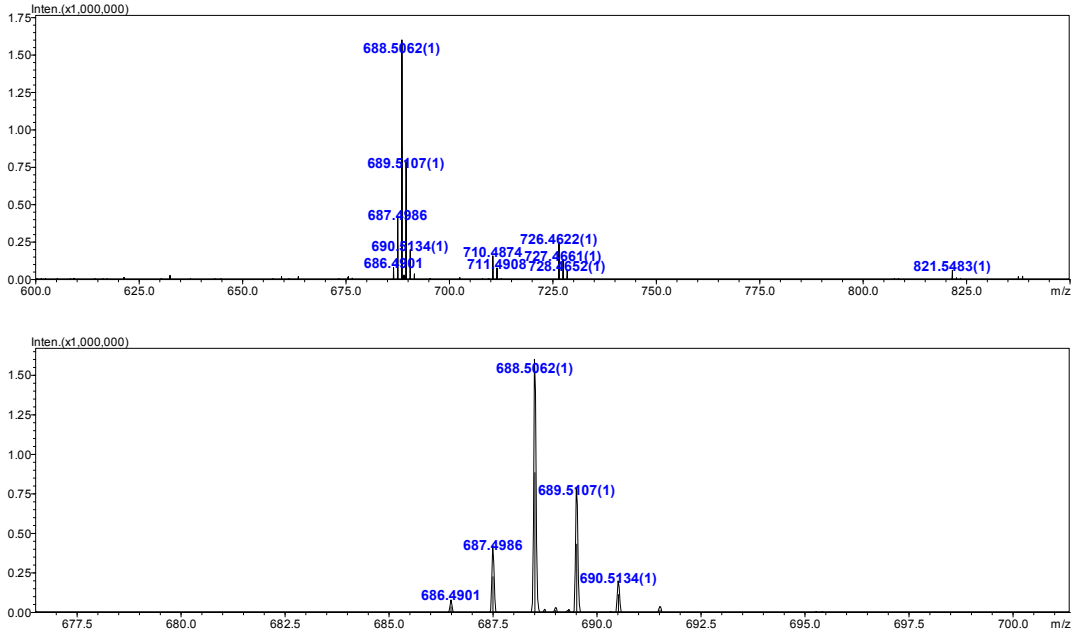


Figure S5. HR mass spectra of **Cb36OH** (ESI+)

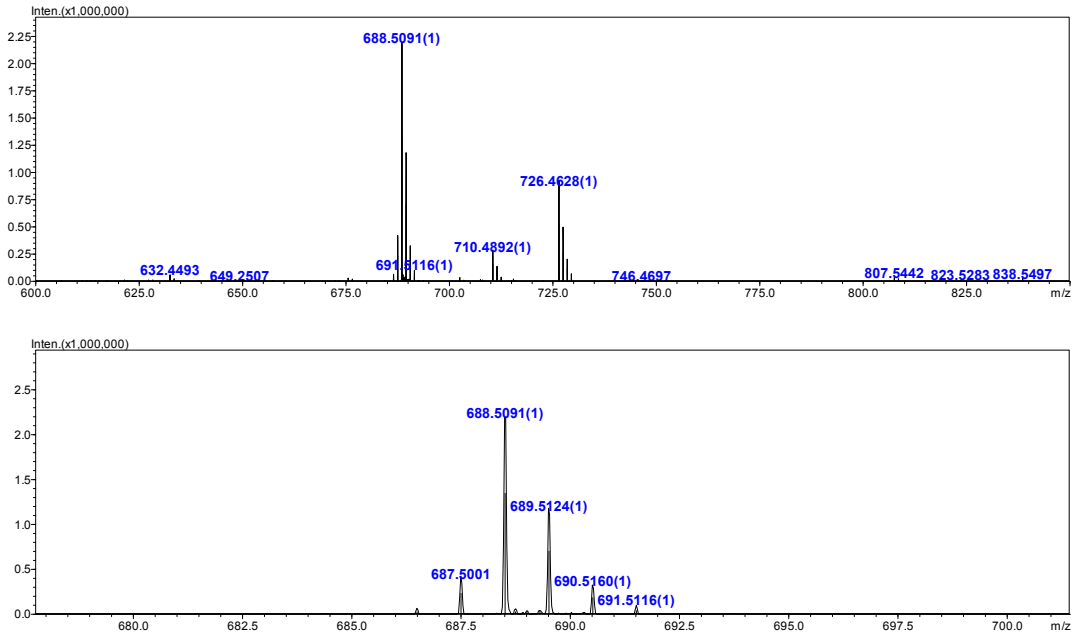


Figure S6. HR mass spectra of **Cb27OH** (ESI+)

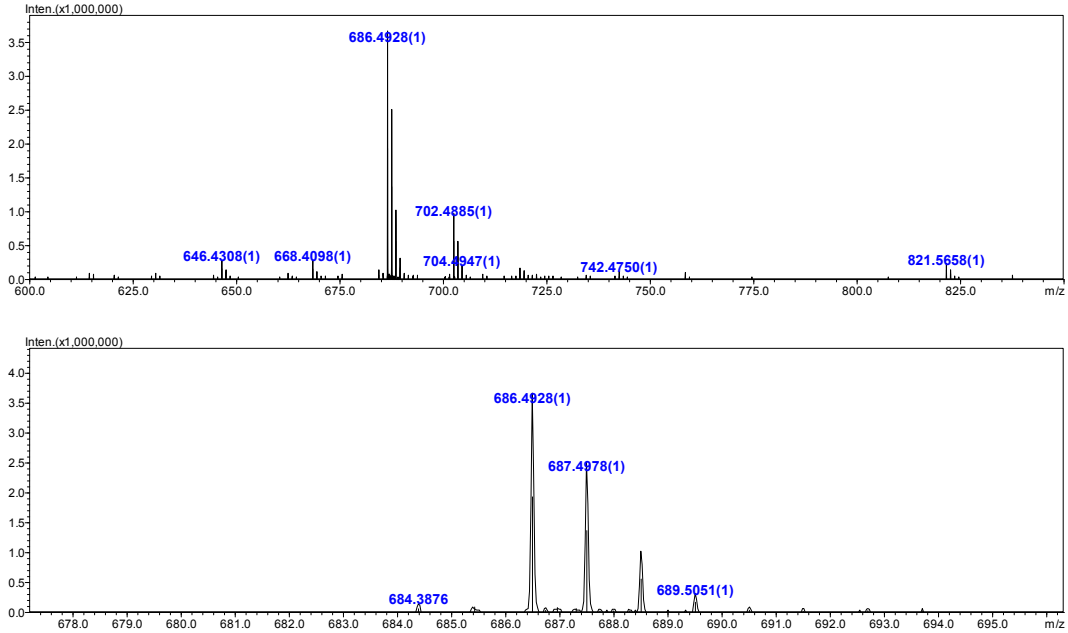


Figure S7. HR mass spectra of **Cb36O** (ESI+)

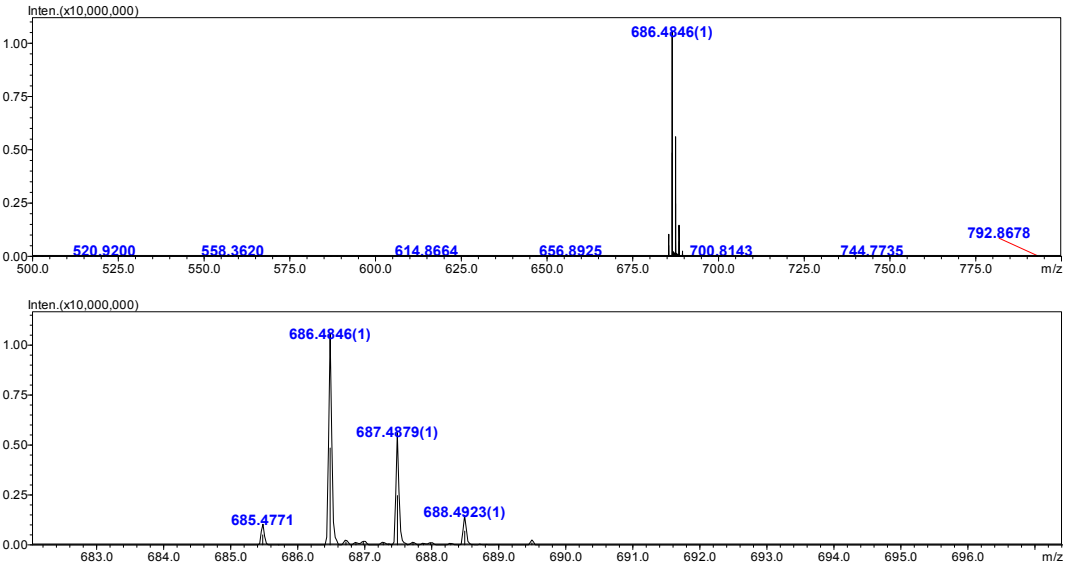


Figure S8. HR mass spectra of **Cb27O** (ESI+)

4. Optical energy gaps

UV/vis/NIR absorption spectra (Figure S9) revealed that the absorption onsets were 728 nm, and 948 nm for **Cb36O** and **Cb27O**, respectively. The corresponding optical energy gaps Eg^{Opt} are 1.70 and 1.31 eV for **Cb36O** and **Cb27O**, respectively.

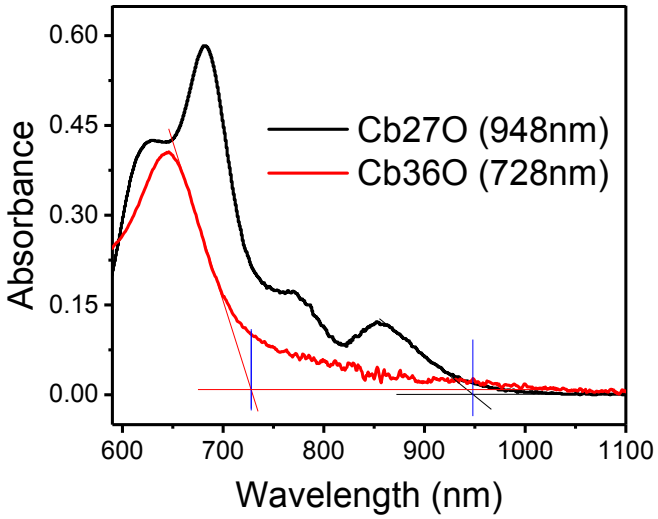


Figure S9. The partial UV/vis/NIR absorption spectra of **Cb36O** and **Cb27O** in dry DCM. The cross indicates the onset of each compound.

5. UV/vis/NIR absorption spectra of precursors

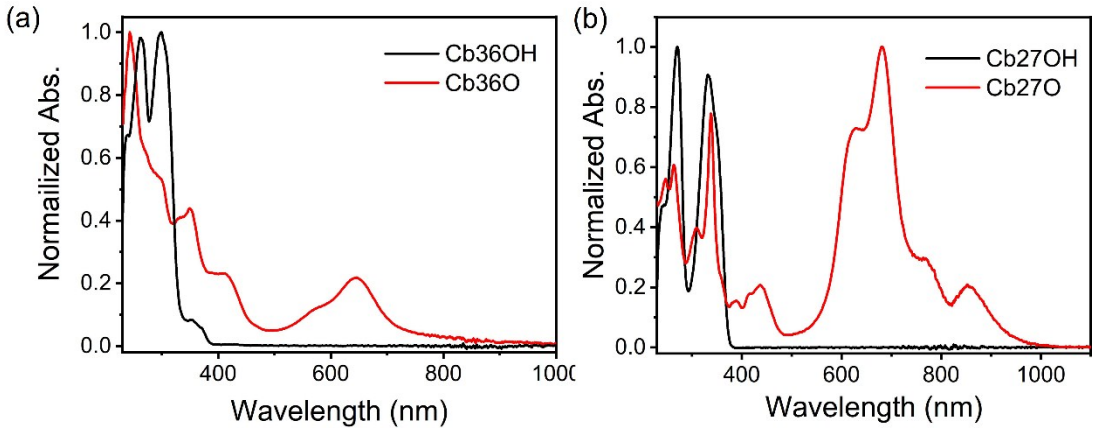


Figure S10. The UV/vis/NIR absorption spectra of **Cb36O** and **Cb36OH** (a), **Cb27O** and **Cb27OH** (b) in dry DCM.

6. Photostability Test

The photostability test indicates that the half-life is 18.3 and 10.7 min for **Cb36O** (changes of the optical density at 649 nm) and **Cb27O** (changes of the optical density at 679 nm), respectively. The concentration of both samples is around 5×10^{-5} M in DCM.

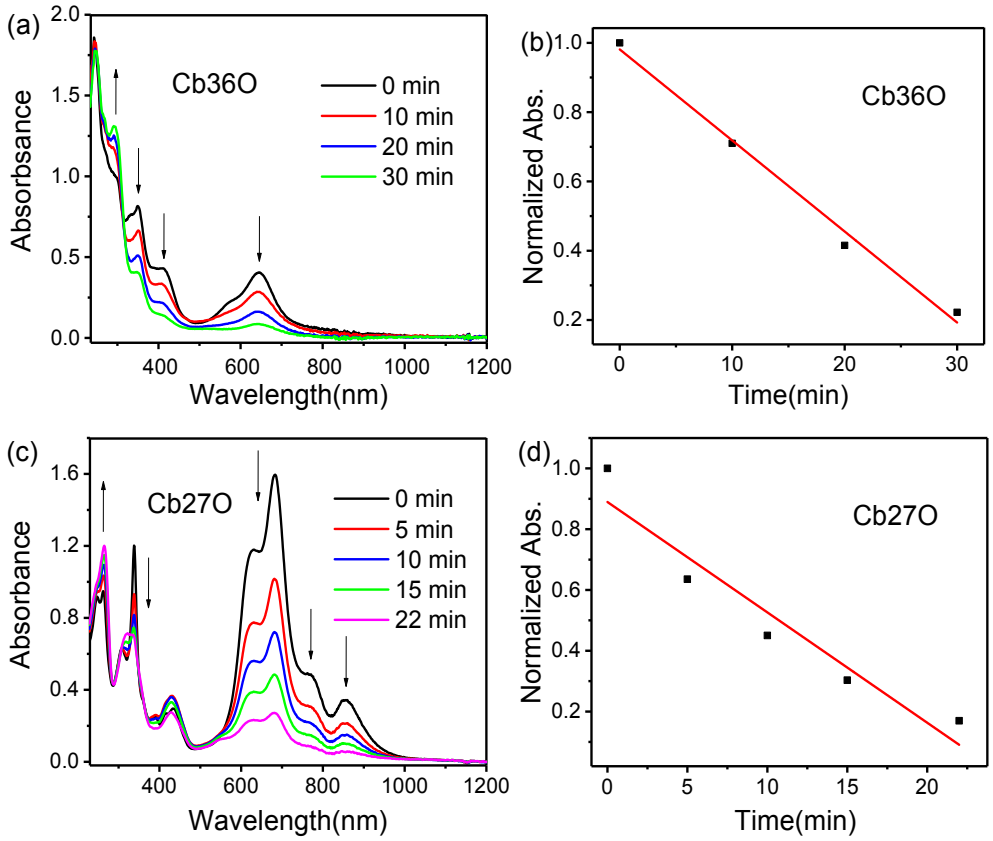


Figure S11. UV/vis/NIR absorption spectra of **Cb27O** (a) and **Cb36O** (c) in DCM (ca. 5×10^{-5} M). The change of the optical density at the absorption maximum with the irradiation time (b) and (d) under a 400 W white light lamp. The distance between sample and lamp is 20 cm.

In addition, nitrogen-centered diradicals have good stability due to efficient electron delocalization and steric effect, the half-life ($t_{1/2}$) of **CDR1** upon irradiation with 400 W white light in the ambient environment is estimated to be 10 hours. The stability of oxygen-centered diradicals **Cb36O** and **Cb27O** decrease with smaller $t_{1/2}$ value of 18.3

and 10.7 min, respectively. While carbon-centered ***m*-Cz-ph** and ***p*-Cz-alky** become active and oligomerize quickly.

7. Chemical stability Test

The freshly prepared solution samples gradually decomposed in dark at room temperature. The yield half-life ($t_{1/2}$) was 423 min (649 nm) for **Cb36O**, and 593 min (679 nm) for **Cb27O**. The concentration of both samples is around 5×10^{-5} M in DCM.

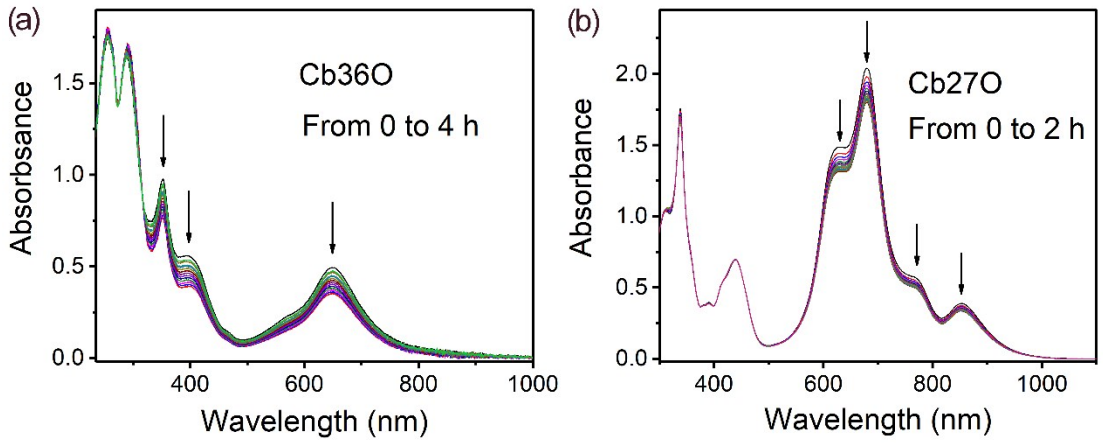


Figure S12. UV-Vis-NIR absorption spectra of **Cb36O** (a) and **Cb27O** (b) in DCM (ca. 5×10^{-5} M) for different time.

8. Crystallographic data

Single crystals of **Cb27OH** suitable for X-ray crystallographic analysis were grown by slow solvent evaporation method using methanol solution. The structure is shown in Figure S12. **Cb27OH** crystalizes in a monoclinic system, space group $P2_1/n$ with a R-factor of 7.1%. The phenoxyl substituents are rotated out of the carbazole-plane by 44.86°/ 39.68°. In the crystal packing, the molecules adopt an antiparallel packing mode (Figure S13) in which the closest interplanar distance is 3.840 Å (Figure S14).

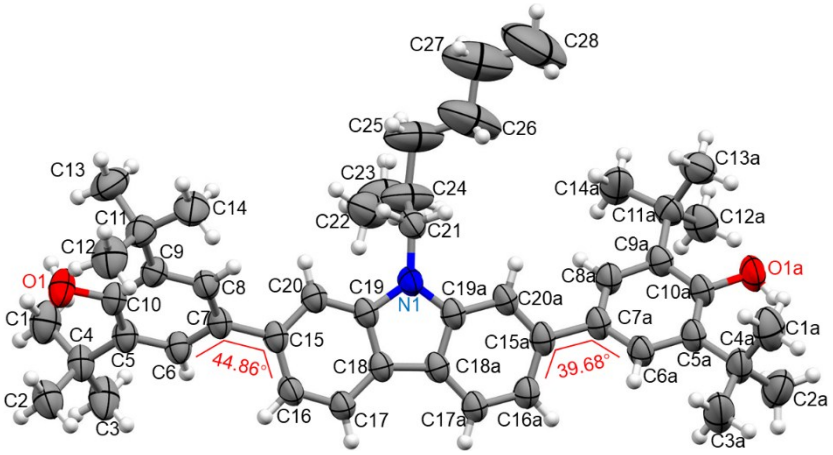


Figure S13. Single-crystal X-ray structure of **Cb27OH** with thermal ellipsoids shown at the 50% probability level.

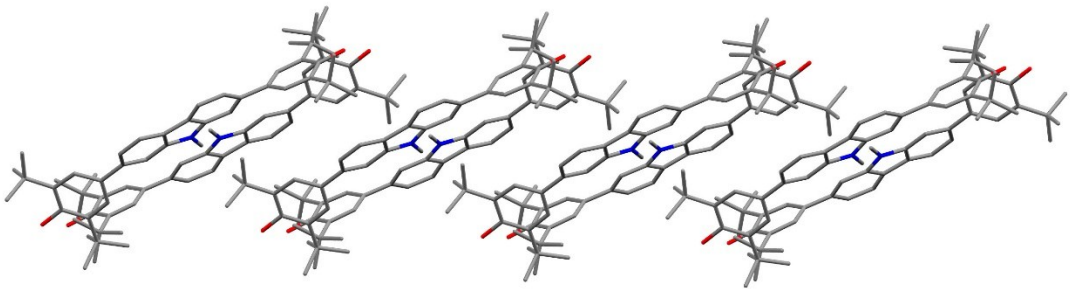


Figure S14. Partial solid-state packing of **Cb27OH** (hydrogen atoms and alkyl chains were omitted for clarity).

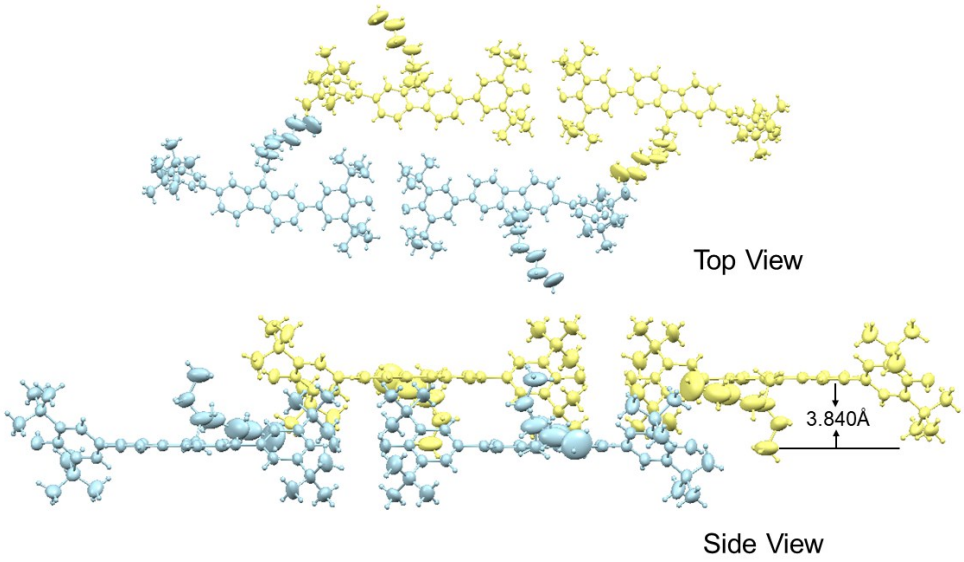


Figure S15. Crystal structure of **Cb27OH** (thermal ellipsoids at 50% probability level) with top view and side view.

Table S1. Crystal data and structure refinement for **Cb27OH**.

Identification code	Cb27OH
Chemical formula	$C_{48}H_{65}NO_2$
Formula weight	688.01 g/mol
Temperature	293.32 K
Crystal size	0.65 x 0.6 x 0.3 mm
Crystal system	monoclinic
Space group	$P2_1/n$
Unit cell dimensions	a = 12.1364(3) Å
	b = 17.5731(4) Å
	c = 22.0778(4) Å
Volume	4703.14(17) $Å^3$
Z	4
Density (calculated)	0.972 g/cm^3
Absorption coefficient	0.437 mm^{-1}
F(000)	1504.0

Table S2. Data collection and structure refinement for **Cb27OH**.

Identification code	Cb27OH
Theta range for data collection	8.018 to 145.792°
Index ranges	-14<=h<=15, -21<=k<=13, -20<=l<=27
Reflections collected	26933
Independent reflections	9218 [R_{int} = 0.0313, R_{sigma} = 0.0265]
Structure solution technique	Intrinsic Phasing
Structure solution program	ShelXL
Refinement method	Least Squares minimisation

Refinement program	ShelXL
Data / restraints / parameters	9218 / 30 / 486
Goodness-of-fit on F^2	1.027
Final R indexes	I>2σ(I)
	all data
Largest diff. peak and hole	0.25 / -0.28 eÅ^{-3}

Table S3. Bond lengths (Å) for **Cb27OH**.

Atom	Atom	Lengths (Å)	Atom	Atom	Lengths (Å)
N1	C19	1.384(3)	C10	C9	1.411(3)
N1	C21	1.446(3)	C10	C5	1.401(3)
O1	C10	1.375(3)	C9	C8	1.386(3)
O1	H1	0.820	C5	C6	1.391(3)
C1	C4	1.534(4)	C6	C7	1.391(3)
C2	C4	1.524(4)	C8	C7	1.389(3)
C3	C4	1.536(4)	C7	C15	1.488(3)
C4	C5	1.538(3)	C15	C20	1.384(3)
C12	C11	1.525(4)	C15	C16	1.405(3)
C13	C11	1.541(4)	C20	C19	1.386(3)
C14	C11	1.527(4)	C16	C17	1.375(3)
C11	C9	1.540(3)	C19	C18	1.412(3)
C21	C24	1.511(5)	C17	C18	1.390(3)
C24	C22	1.385(8)	C18	C18a	1.446(3)
C22	C23	1.573(8)	C6	H2	0.930
C24	C25	1.546(5)	C8	H3	0.930
C25	C26	1.491(8)	C20	H4	0.931

C26	C27	1.486(8)	C16	H5	0.931
C27	C28	1.480(1)	C17	H6	0.930

Table S4. Bond angles (°) for **Cb27OH**.

Atom	Atom	Atom	Angles (°)	Atom	Atom	Atom	Angles (°)
C19a	N1	C19	108.5(2)	C9	C10	C5	122.4(2)
C19a	N1	C21	125.0(2)	C19	C20	C15	118.9(2)
C19	N1	C21	126.4(2)	C9	C8	C7	122.9(2)
H1	O1	C10	109.4	C18	C17	C16	119.5(2)
N1	C19	C18	108.8(2)	C15	C16	C17	121.9(2)
N1	C19	C20	129.3(2)	C7	C6	C5	122.6(2)
C18	C19	C20	121.9(2)	C10	C5	C6	117.2(2)
C10	C9	C8	116.9(2)	C10	C5	C4	121.9(2)
C10	C9	C11	121.8(2)	C6	C5	C4	120.9(2)
C8	C9	C11	121.3(2)	C9	C11	C14	111.2(2)
C18a	C18	C19	106.9(2)	C9	C11	C12	110.4(2)
C18a	C18	C17	134.6(2)	C9	C11	C13	110.2(2)
C19	C18	C17	118.5(2)	C14	C11	C12	107.0(2)
C7	C15	C20	120.9(2)	C14	C11	C13	107.3(2)
C7	C15	C16	119.8(2)	C12	C11	C13	110.6(2)
C20	C15	C16	119.2(2)	C5	C4	C1	111.5(2)
C15	C7	C8	121.3(2)	C5	C4	C3	111.2(2)
C15	C7	C6	120.8(2)	C5	C4	C2	110.1(2)
C8	C7	C6	117.9(2)	C1	C4	C3	106.4(2)
O1	C10	C9	118.2(2)	C1	C4	C2	110.7(2)
O1	C10	C5	119.4(2)	C3	C4	C2	106.9(2)

Table S5. Torsion angles (°) for **Cb27OH**.

Atom	Atom	Atom	Atom	Angles (°)	Atom	Atom	Atom	Atom	Angles (°)
C16	C15	C7	C6	45.0(3)	C19	C18	C17	C16	1.7(3)
C20	C15	C7	C8	44.7(3)	C20	C15	C7	C8	44.7(3)
C8a	C7a	C15a	C20a	38.5(3)	C20	C15	C7	C6	135.0(2)
C6a	C7a	C15a	C16a	40.9(3)	C16	C15	C7	C8	135.3(2)
C21	N1	C19	C18	178.5(2)	C7	C15	C20	C19	179.9(2)
C21	N1	C19a	C18a	178.5(2)	C16	C15	C20	C19	0.1(3)
C21	N1	C19	C20	0.2(3)	C7	C15	C16	C17	179.8(2)
C19a	C18a	C18	C19	0.1(2)	C20	C15	C16	C17	0.2(3)
C19a	N1	C19	C18	0.8(2)	C15	C7	C8	C9	177.7(2)
C19a	N1	C19	C20	177.5(2)	C6	C7	C8	C9	2.5(3)
N1	C19	C18	C17	180.0(2)	C15	C7	C6	C5	179.5(2)
C20	C19	C18	C17	1.5(3)	C8	C7	C6	C5	0.8(3)
N1	C19	C20	C15	178.7(2)	C9	C10	C5	C6	2.6(3)
C18	C19	C20	C15	0.6(3)	C9	C10	C5	C4	177.4(2)
C8	C9	C10	C5	1.0(3)	C18	C17	C16	C15	1.1(3)
C11	C9	C10	C5	180.0(2)	C7	C6	C5	C10	1.7(3)
C10	C9	C8	C7	1.7(3)	C7	C6	C5	C4	178.3(2)
C11	C9	C8	C7	177.4(2)	C10	C5	C4	C1	56.7(3)
C10	C9	C11	C14	179.5(2)	C10	C5	C4	C3	175.3(2)
C10	C9	C11	C12	60.8(3)	C10	C5	C4	C2	66.5(3)
C10	C9	C11	C13	61.7(3)	C6	C5	C4	C1	123.2(2)
C8	C9	C11	C14	0.5(3)	C6	C5	C4	C3	4.7(3)
C8	C9	C11	C12	118.1(3)	C6	C5	C4	C2	113.5(2)

C8	C9	C11	C13	119.3(3)

9. ESR measurement

The singlet-triplet energy gap of **Cb27O** and **Cb36O** were estimated by fitting the *I*T* vs. *T* curve with modified Bleaney-Bowers equation:

$$\chi = \frac{Ng^2\mu_\beta^2}{kT}\left[\frac{2}{3 + e^{-2J/kT}}\right](1-\rho) + \frac{Ng^2\mu_\beta^2}{2kT}\rho + TIP(1-\rho) \qquad Equation\ S1$$

The ρ is the fraction of s=1/2 impurity, *TIP* is the temperature independent paramagnetism due to a small energy gap between group singlet state and excited triplet state. The estimated 2*J*= -0.96 kcal/mol for **Cb36O**, with ρ= 0.003, *TIP*= 1.7 x 10^{-3} emu/mol, the Adj. R-Square >0.99. The estimated 2*J*= -6.16 kcal/mol for **Cb27O**, with ρ= 0.0003, *TIP*= 2.9 x 10^{-7} emu/mol, the Adj. R-Square >0.99.

10. Cyclic voltammetry

Cyclic voltammograms were measured in dry DCM with 0.1 M nBu$_4$NPF$_6$ as supporting electrolyte, Ag/AgCl as reference electrode, glassy carbon as working electrode, Pt wire as counter electrode, and a scan rate at 50 mV/s. The LUMO energy levels of these two compounds were estimated from the half-wave potential $E_{1/2}$ in Figure S15 using ferrocene as reference. The energy levels are calculated by:

$$LUMO = -\left(E_{sample}^{red} - E_{Fc/Fc+}^{red} + 4.8\right)$$

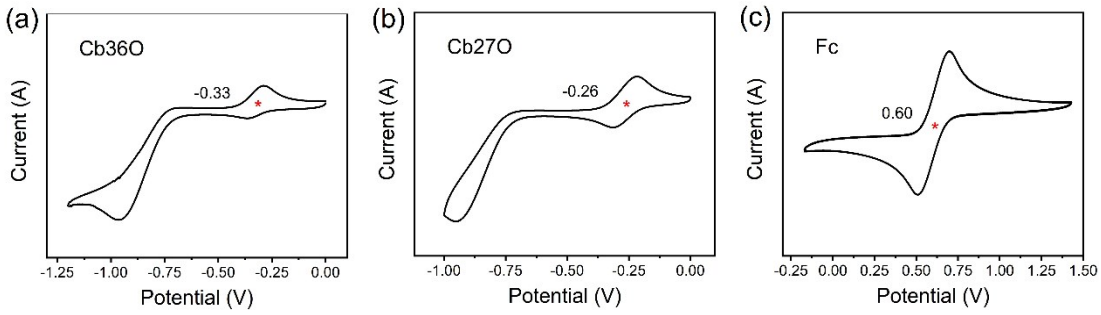


Figure S16. Cyclic voltammograms of **Cb36O** (a), **Cb27O** (b) and ferrocene (c) in dry DCM with 0.1 M nBu$_4$NPF$_6$ as supporting electrolyte, Ag/AgCl as reference electrode,

glassy carbon as working electrode, Pt wire as counter electrode, and a scan rate at 50 mV/s. The red stars indicate the half-wave potential $E_{1/2}$.

11. Computational details

All calculations were performed with the Gaussian 16 program suite[4] using the density functional theory (DFT) with the Becke's three-parameter hybrid exchange functionals[5, 6] and the Lee-Yang-Parr correlation functional (B3LYP)[7] employing the 6-311G(d) basis set[8-10] for all atoms. The alkyl chains were replaced by methyl groups to reduce the computation cost. Full geometry optimizations were carried out at the (U)B3LYP/6–311G(d) level, and the obtained stationary points were characterized by frequency calculations. The diradical character y_0 is calculated based on the occupation number of the lowest unoccupied natural orbital (LUNO). A molecule with $y_0 = 0$ implies a closed-shell structure, whereas a molecule with $y_0 = 1$ indicates a pure diradical structure[11, 12]. Any intermediate value of y_0 refers to diradical structures. The effective electron exchange interaction J_{ab} was determined using following equation:

$$J_{ab} = \frac{(E_{BS} - E_T)}{(\langle S^2 \rangle_T - \langle S^2 \rangle_{BS})}$$

Where E_{BS} and E_T correspond to the energies of the broken-symmetry (BS) singlet and triplet state, with spin expectation values $\langle S^2 \rangle_T$ and $\langle S^2 \rangle_{BS}$ of the triplet state and broken-symmetry singlet, respectively[13]. The spin correction for singlet-triplet energy gap was calculated using the energy difference between BS singlet and open-shell triplet and the correction for spin contamination:

$$\Delta E_{ST} = (E_{BS} - E_T)\frac{\langle S^2 \rangle_T}{(\langle S^2 \rangle_T - \langle S^2 \rangle_{BS})}$$

The time-dependent (TD) DFT calculation was employed with UB3LYP/6-311G(d) level. The spin densities were illustrated using Multiwfn[14] and VMD[15]. The NICS(1)zz[16] value was calculated by standard gauge independent atomic orbital

(GIAO) method based on the optimized geometries at the UB3LYP/6-311(d) level. The typical disjoint SOMO-α and SOMO-β orbitals profile further confirm the open-shell singlet ground state (**Fig. S18**). The NICS(1)zz of the two diradicals were calculated to investigate the aromaticity (**Fig. S17**). **Cb36O** exhibits a larger NICS(1)zz δ value of -18.25 ppm at the central carbazole core, while **Cb27O** owns a smaller δ value of -15.20 ppm. Less aromaticity for **Cb27O** indicated a major contribution of polyenic structure at ground state because of the quinoidal structure. Meanwhile, the aromatic character of the terminal phenoxyl rings shows similar tendency. As a reference, the NICS(1)zz value of benzene is calculated to be δ = -29.12 ppm.

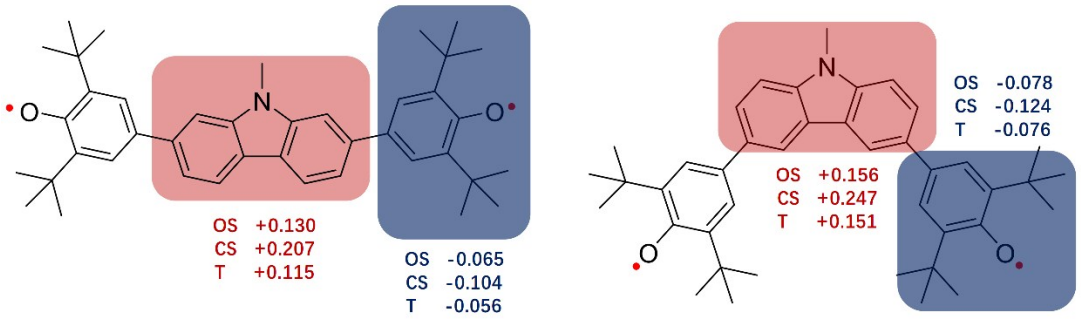


Figure S17. Calculated Hirshfeld charges of **Cb27O** and **Cb36O** (a.u.).

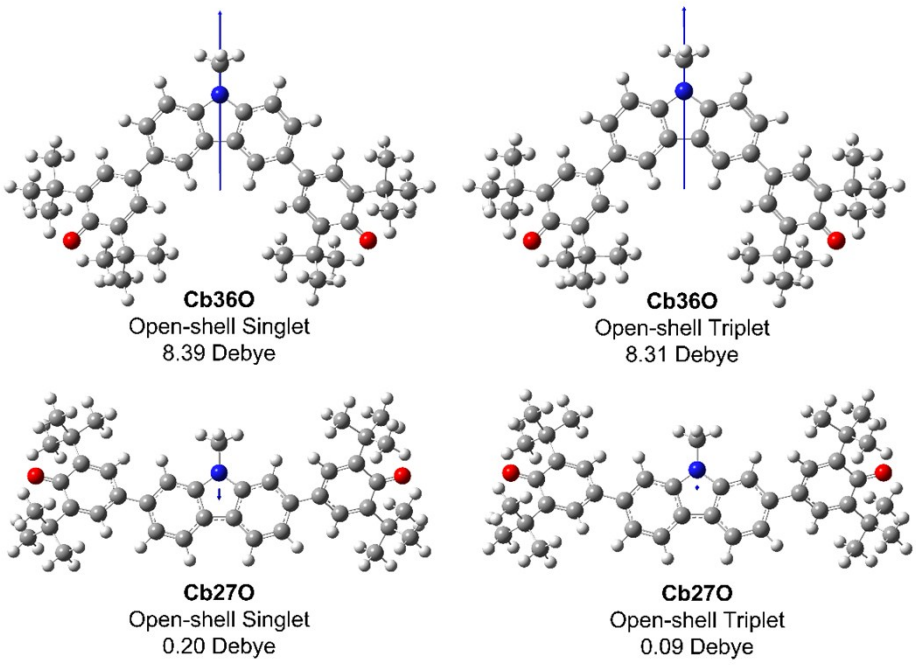


Figure S18. Calculated dipole moments (blue arrow) of **Cb36O** and **Cb27O** at open-singlet ground state and triplet state. (The magnitude of **Cb27O** were 3 times to get insight of vectors)

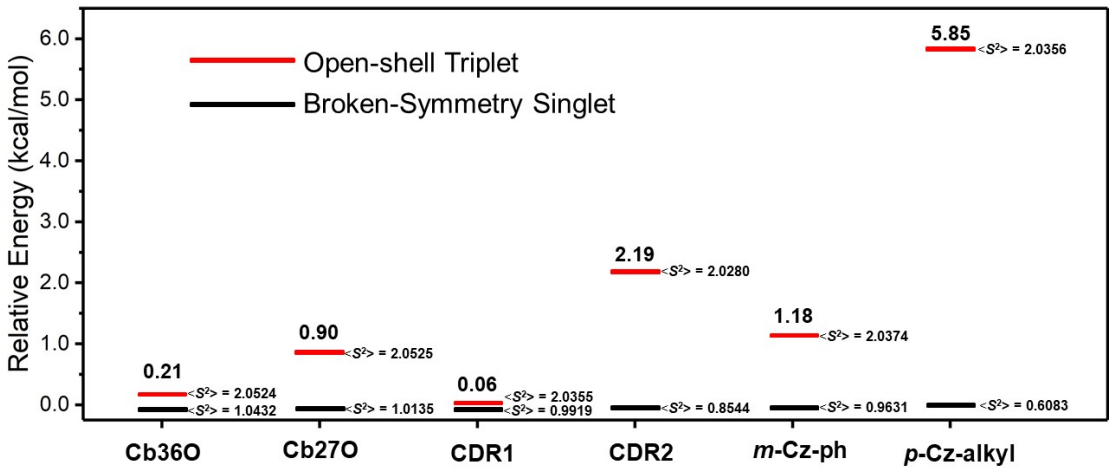


Figure S19. Calculated relative energy (kcal/mol) of triplet and broken-symmetry singlet along with spin contamination for oxygen, nitrogen and carbon-centered diradicals with open-shell singlet ground state.

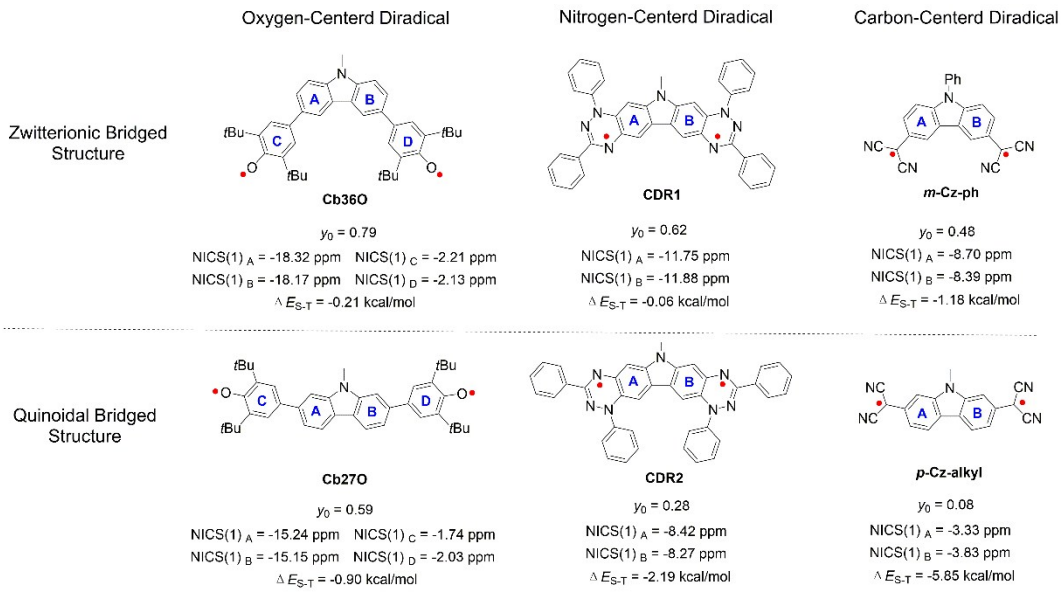


Figure S20. The diradical character y_0, NICS(1)zz value (Ring A and Ring B) and calculated singlet-triplet energy gaps (ΔE_{S-T}) of oxygen-centered diradicals (**Cb36O** and **Cb27O**), nitrogen-centered diradicals (**CDR1** and **CDR2**) and carbon-centered diradicals (***m*-Cz-ph** and ***p*-Cz-alkyl**) at the same level of (U)B3LYP/6-311(d).

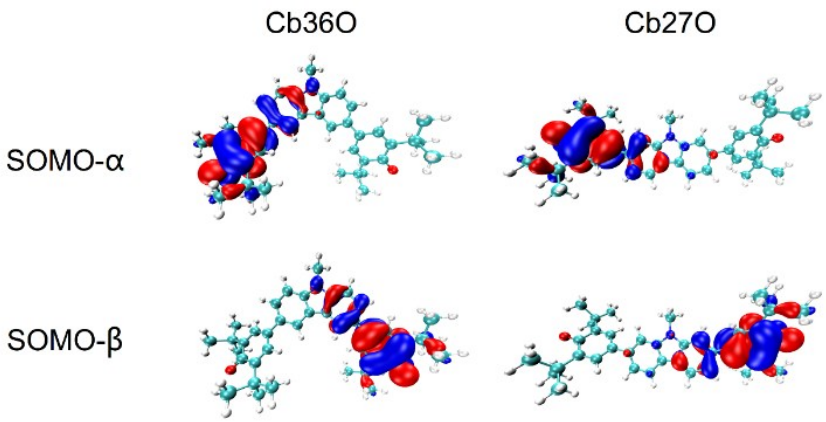


Figure S21. The frontier SOMO profiles of Cb36O and Cb27O at the open-shell singlet ground state calculated at the UB3LYP/6-311G(d) level.

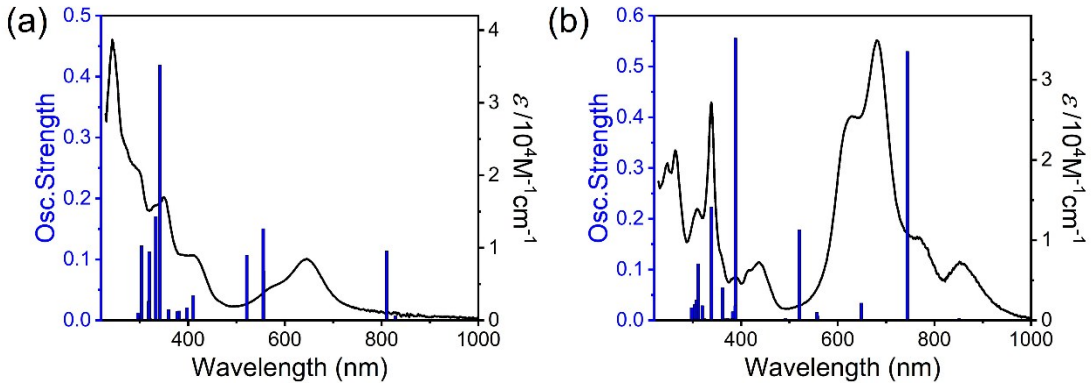


Figure S22. TD-DFT simulated spectra of **Cb36O** (a) and **Cb27O** (b) along with experimental spectra.

Table S6. Selected TD-DFT calculated energies, oscillator strength and compositions of major electronic transitions of **Cb36O**. The α and β orbitals are distinguished as A and B in the parenthesis, respectively.

Wavelength (nm)	Osc. Strength (*f*)	Major contributions
827.61	0.0072	HOMO(A)->LUMO(A) (49.9%)
		HOMO(B)->LUMO(B) (49.0%)
809.65	0.1137	HOMO(B)->LUMO(B) (49.8%)
		HOMO(A)->LUMO(A) (48.8%)
555.29	0.0091	HOMO(A)-5->LUMO(A) (53.1%)
		HOMO(B)-5->LUMO(B) (37.6%)
555.22	0.0814	HOMO(B)-5->LUMO(B) (41.0%)
		HOMO(A)-5->LUMO(A) (37.7%)
		HOMO(B)-1->LUMO(B) (6.4%)
		HOMO(A)-1->LUMO(A) (6.3%)
554.92	0.1506	HOMO(A)-1->LUMO(A) (37.8%)
		HOMO(B)-1->LUMO(B) (36.7%)
		HOMO(B)-5->LUMO(B) (14.5%)
520.87	0.1069	HOMO(B)-1->LUMO(B) (40.2%)
		HOMO(A)-1->LUMO(A) (39.8%)

Table S7. Selected TD-DFT calculated energies, oscillator strength and compositions of major electronic transitions of **Cb27O**. The α and β orbitals are distinguished as A and B in the parenthesis, respectively.

Wavelength (nm)	Osc. Strength (*f*)	Major contributions
850.86	0.0013	HOMO(A)->LUMO(A) (49.4%)
		HOMO(B)->LUMO(B) (47.7%)
743.27	0.5298	HOMO(B)->LUMO(B) (48.9%)
		HOMO(A)->LUMO(A) (47.2%)
651.60	0.0021	HOMO(A)-1->LUMO(A) (62.3%)
		HOMO(B)-1->LUMO(B) (35.4%)
648.20	0.0340	HOMO(B)-1->LUMO(B) (60.7%)
		HOMO(A)-1->LUMO(A) (33.8%)
557.15	0.0087	HOMO(A)-5->LUMO(A) (77.1%)
		HOMO(B)-5->LUMO(B) (18.2%)
556.75	0.0158	HOMO(B)-5->LUMO(B) (77.0%)
		HOMO(A)-5->LUMO(A) (18.1%)

12. References

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13. Coordinates for calculated geometries

Cb36O CS

C	-3.41653100	2.97873900	0.13130900
C	-3.06211600	1.59667200	0.11758700
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Cb36O T

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C	-6.34484900	-0.20255200	-0.37340800
C	-5.35380400	0.74948800	-0.38850100
C	3.82004900	-0.69108000	-0.83121300
C	4.74901600	-1.70111900	-0.90505900
C	6.07043200	-1.48799900	-0.27974500
C	6.33742500	-0.20065200	0.39383500
C	5.34605000	0.75112500	0.40264900
O	-6.94185400	-2.38508200	0.33269000
C	-7.71346100	0.03580400	-1.02854500
C	-7.95702200	-1.01251500	-2.14160000
C	4.45651500	-3.02574300	-1.62527800
O	6.94439600	-2.37788900	-0.32012300
C	7.69718000	0.03326000	1.06872900
C	3.03408400	-3.06143900	-2.21529900
C	-8.83168100	-0.06706400	0.03788400
C	-7.81109800	1.43151400	-1.67298500
C	-4.43705000	-3.04147900	1.60054400
C	-3.00710400	-3.08097500	2.17185200
C	-5.41902000	-3.24819400	2.77970700
C	-4.57312600	-4.21331300	0.59733600
C	5.45372900	-3.22374500	-2.79309800
C	4.58001600	-4.20474600	-0.62888200
C	7.92606400	-1.02261700	2.17775500
C	8.82950200	-0.06229600	0.01660800
C	7.78606800	1.42455300	1.72391800
H	-4.46088600	3.22617700	0.24619100
H	-1.37669500	0.22818100	0.03162900
H	-2.79973600	5.01685900	0.15848500
H	1.37645900	0.22989000	-0.06135800
H	4.45943700	3.23284900	-0.21715100
H	2.79516300	5.02118000	-0.12669800

H	-0.91131400	6.27276200	-0.45606500
H	0.05931300	6.26903200	1.03265700
H	0.84622300	6.27358100	-0.56089600
H	-2.84483400	-0.82813300	1.28322300
H	-5.52638500	1.68895100	-0.89574600
H	2.85954200	-0.81495200	-1.31281500
H	5.51185500	1.68692300	0.91882200
H	-8.92032400	-0.82280000	-2.62535600
H	-7.18136400	-0.95262500	-2.91122000
H	-7.96745400	-2.02275000	-1.73846800
H	2.87405500	-4.02174900	-2.71173100
H	2.26252600	-2.96401100	-1.44580800
H	2.87365100	-2.28043600	-2.96413100
H	-9.80374800	0.13302700	-0.42372200
H	-8.68315700	0.67070700	0.83247300
H	-8.86037700	-1.05752200	0.48648700
H	-7.07579000	1.57461000	-2.47008700
H	-8.80043300	1.55268500	-2.12120000
H	-7.68741400	2.23633100	-0.94227800
H	-2.84045200	-4.04478700	2.65923500
H	-2.24556800	-2.97776900	1.39318100
H	-2.83719800	-2.30535200	2.92418200
H	-5.18377000	-4.18270900	3.29860200
H	-6.44905400	-3.29678400	2.43335700
H	-5.33372200	-2.43438000	3.50634800
H	-5.58539200	-4.28338700	0.20559800
H	-3.88247100	-4.09093900	-0.24272800
H	-4.32737000	-5.15695200	1.09437600
H	5.22546300	-4.15451900	-3.32174100
H	6.47919800	-3.27466000	-2.43377800
H	5.37764800	-2.40470700	-3.51487900
H	5.58716500	-4.27737600	-0.22462200
H	3.87851900	-4.08863300	0.20304900
H	4.34104500	-5.14483800	-1.13585200
H	8.88280100	-0.83613500	2.67559100
H	7.14021100	-0.96806500	2.93736700
H	7.94205500	-2.03007400	1.76791300
H	9.79532700	0.13458700	0.49247200
H	8.69152100	0.68091500	-0.77480400
H	8.86422700	-1.04965500	-0.43836100
H	7.04008400	1.56227700	2.51199500
H	8.76926900	1.54262100	2.18623600
H	7.67222600	2.23432200	0.99709300

Cb36O OS

C	-3.41411897	2.96300956	0.15633595
C	-3.05047398	1.59268257	0.13840944
C	-1.68378926	1.26853574	0.07598975
C	-0.72562770	2.27412815	0.02398277
C	-1.12768378	3.63495795	0.03965169
C	-2.47799423	3.98379410	0.11570947
C	1.12259924	3.63621621	-0.07173275
C	0.72236713	2.27491958	-0.05483570
C	1.68221418	1.27070912	-0.10154809
C	3.04907129	1.59687784	-0.14907402
C	3.41148273	2.96756531	-0.15211596
C	2.47364091	3.98707836	-0.11791511
N	-0.00383223	4.44263321	-0.03414514
C	-0.00155855	5.89086898	0.00657669
C	-4.07637093	0.54239022	0.18728798
C	4.07636151	0.54762611	-0.19116079
C	-3.80566047	-0.70664476	0.79900084
C	-4.73268864	-1.71766871	0.87655825
C	-6.06747680	-1.49508686	0.28338674
C	-6.34866371	-0.19684994	-0.36339611
C	-5.35817831	0.75532202	-0.37744254
C	3.81388693	-0.69718154	-0.81491665
C	4.74215538	-1.70746262	-0.88760228
C	6.06913096	-1.48869429	-0.27581716
C	6.34154310	-0.19493772	0.38359424
C	5.35072162	0.75695866	0.39146004
O	-6.94002156	-2.38578734	0.32755224
C	-7.72239885	0.04710608	-1.00570285
C	-7.97414889	-0.99067282	-2.12675446
C	4.44380126	-3.03867419	-1.59325426
O	6.94248451	-2.37885177	-0.31502746
C	7.70675134	0.04480505	1.04539782
C	3.01661510	-3.07984572	-2.17129591
C	-8.83229738	-0.06644978	0.06829471
C	-7.82565916	1.44881342	-1.63608206
C	-4.42509614	-3.05367213	1.56908438
C	-2.99066655	-3.09846455	2.12862663
C	-5.39763286	-3.27089435	2.75411607
C	-4.56930515	-4.21647610	0.55655908
C	5.43141676	-3.24741034	-2.76729904
C	4.57548921	-4.20849621	-0.58714263
C	7.94425064	-1.00079314	2.16229054
C	8.83057015	-0.06090433	-0.01482851

C	7.80134797	1.44206372	1.68692498
H	-4.46076974	3.22849911	0.24695515
H	-1.37585794	0.22990341	0.03273163
H	-2.79990820	5.01820968	0.15878022
H	1.37567176	0.23152796	-0.06125885
H	4.45942936	3.23489181	-0.21910634
H	2.79552037	5.02237060	-0.12846651
H	-0.91129833	6.27305714	-0.45641355
H	0.05970585	6.26939142	1.03210871
H	0.84637333	6.27375930	-0.56158793
H	-2.83556931	-0.83878877	1.25849295
H	-5.53540813	1.69906576	-0.87490240
H	2.84969870	-0.82619685	-1.28758719
H	5.52140991	1.69721998	0.89769751
H	-8.94132710	-0.79696951	-2.60111455
H	-7.20458367	-0.92295679	-2.90183039
H	-7.98084616	-2.00471979	-1.73322771
H	2.85257136	-4.04473544	-2.65743659
H	2.25133292	-2.97529159	-1.39646718
H	2.85003185	-2.30588117	-2.92608602
H	-9.80802450	0.13738899	-0.38386791
H	-8.67800057	0.66388906	0.86863115
H	-8.85697980	-1.06109983	0.50777119
H	-7.09660241	1.59987049	-2.43745921
H	-8.81848247	1.57370817	-2.07548003
H	-7.69674963	2.24674088	-0.89874064
H	-2.82027477	-4.06665707	2.60593497
H	-2.23530688	-2.98834413	1.34488036
H	-2.81465649	-2.32971745	2.88660513
H	-5.15860528	-4.21016624	3.26260165
H	-6.43042196	-3.31603744	2.41559339
H	-5.30626232	-2.46374383	3.48742754
H	-5.58464437	-4.28289805	0.17220194
H	-3.88529821	-4.08665235	-0.28781986
H	-4.31982569	-5.16458489	1.04314536
H	5.19914037	-4.18314430	-3.28534260
H	6.45981850	-3.29472161	-2.41595131
H	5.34918192	-2.43516175	-3.49604907
H	5.58589249	-4.27738263	-0.19041684
H	3.88078038	-4.08473956	0.24937411
H	4.33249460	-5.15322908	-1.08347608
H	8.90510598	-0.81019785	2.65055336
H	7.16463889	-0.93876478	2.92774437
H	7.95643892	-2.01203440	1.76173868

H	9.80025946	0.14000804	0.45141061
H	8.68644449	0.67500045	-0.81195632
H	8.86131238	-1.05243815	-0.46091015
H	7.06183012	1.58735043	2.47973901
H	8.78829883	1.56406418	2.14014972
H	7.68188128	2.24512670	0.95357732

Cb27O CS

C	-3.45784300	-0.66950900	-0.04665400
C	-3.01390700	-2.04045100	-0.03423200
C	-1.69079100	-2.38869200	-0.04668900
C	-0.70135800	-1.37846800	-0.05673200
C	-1.12822200	-0.00672500	-0.07538100
C	-2.45687800	0.34643600	-0.06795300
C	1.12864200	-0.00552400	-0.04202000
C	0.70298700	-1.37775900	-0.04154300
C	1.69321800	-2.38712300	-0.02741500
C	3.01609700	-2.03776200	-0.02161400
C	3.45843400	-0.66632200	-0.00679800
C	2.45650400	0.34874700	-0.01096900
N	0.00010700	0.80210600	-0.08664100
C	-0.00147500	2.24994400	-0.06424800
C	-4.85303700	-0.34668900	-0.04316000
C	4.85318500	-0.34264500	0.02299300
C	-5.31272700	0.96774300	-0.37415400
C	-6.62767200	1.32837600	-0.38815600
C	-7.64951600	0.31407900	-0.01838100
C	-7.18424000	-1.05206700	0.33241300
C	-5.84705900	-1.31933800	0.29505400
C	5.85484900	-1.31507300	-0.29251200
C	7.19247800	-1.04747800	-0.29948500
C	7.64926100	0.31867000	0.06221000
C	6.61902100	1.33262800	0.40898600
C	5.30474500	0.97196400	0.36422900
O	-8.85336700	0.60064500	-0.00554200
C	-8.21898600	-2.11437600	0.73333700
C	-8.99772300	-1.64784800	1.98752200
C	8.23629300	-2.10940500	-0.67722500
O	8.85301100	0.60555300	0.07678200
C	7.06639600	2.74484800	0.81473700
C	7.58712100	-3.46126200	-1.02800900
C	-9.20747700	-2.35239500	-0.43478400
C	-7.56177300	-3.46621000	1.06898500

C	-7.08436000	2.74081100	-0.78261200
C	-5.89797400	3.65396200	-1.14415700
C	-8.01433200	2.67040000	-2.01852100
C	-7.83780400	3.39918000	0.39941000
C	9.04298500	-1.64231900	-1.91340800
C	9.19826700	-2.34748300	0.51281900
C	7.96815800	2.67353800	2.07133900
C	7.84633900	3.40426300	-0.34936800
C	5.87199200	3.65753400	1.15010400
H	-3.75007100	-2.83191800	-0.05812700
H	-1.40436800	-3.43517900	-0.05273100
H	-2.74103300	1.38860400	-0.02502500
H	1.40751500	-3.43372000	-0.01288900
H	3.75240800	-2.82827100	0.02195300
H	2.74049000	1.39168600	-0.02894400
H	-0.87787300	2.62435100	-0.59355500
H	-0.00973100	2.64401700	0.95729900
H	0.88130000	2.62736300	-0.58080400
H	-4.57446700	1.69684000	-0.67378700
H	-5.51097100	-2.30434400	0.58176700
H	5.52539300	-2.30001000	-0.58714600
H	4.55978100	1.70099900	0.64699200
H	-9.71802400	-2.41651800	2.28475200
H	-8.31882600	-1.48504500	2.83028400
H	-9.54015000	-0.72457100	1.79630800
H	8.36876300	-4.18046300	-1.28508300
H	7.02534300	-3.88270200	-0.18888900
H	6.91789500	-3.39091300	-1.89068900
H	-9.92891700	-3.12775700	-0.15832500
H	-8.67888000	-2.69425900	-1.32999200
H	-9.75483000	-1.44535800	-0.68120800
H	-6.87338100	-3.39610800	1.91647700
H	-8.33730200	-4.18568800	1.34322600
H	-7.01888500	-3.88720400	0.21730200
H	-6.27420800	4.64373600	-1.41445500
H	-5.20817100	3.78976400	-0.30546600
H	-5.33057600	3.27961800	-2.00155400
H	-8.31944100	3.67979500	-2.31189300
H	-8.90901800	2.08877800	-1.80794000
H	-7.49754000	2.21841900	-2.87073700
H	-7.19469600	3.46860100	1.28222700
H	-8.13984900	4.41542900	0.12717200
H	-8.72884100	2.83443100	0.66402900
H	9.77009000	-2.41066800	-2.19446100

H	9.58064700	-0.71889700	-1.70980400
H	8.38323000	-1.47959200	-2.77125700
H	8.64965800	-2.68927700	1.39592800
H	9.92563000	-3.12293900	0.25264200
H	9.74004200	-1.44050000	0.77146900
H	8.26621700	3.68275800	2.37243900
H	7.43231300	2.22065700	2.91121500
H	8.86754000	2.09233500	1.88053900
H	8.14202800	4.42031400	-0.06952200
H	7.22336200	3.47439500	-1.24645700
H	8.74320200	2.83982200	-0.59423800
H	5.28505500	3.28240000	1.99385200
H	6.24190200	4.64706700	1.42985500
H	5.20144700	3.79417800	0.29606900

Cb27O T

C	-3.44623000	-0.69519000	-0.06531500
C	-3.03399500	-2.05166900	-0.05025800
C	-1.69571700	-2.40572400	-0.04757300
C	-0.71883900	-1.40488500	-0.04977200
C	-1.12675100	-0.04427100	-0.07097300
C	-2.47077800	0.31576200	-0.07664400
C	1.12762600	-0.04285200	-0.02802000
C	0.72107200	-1.40401900	-0.02687600
C	1.69884400	-2.40378900	-0.00686900
C	3.03664200	-2.04819700	0.00817600
C	3.44703600	-0.69112900	0.01968600
C	2.47067300	0.31873900	0.00685900
N	0.00037800	0.76645200	-0.07603000
C	-0.00122700	2.21374900	-0.04452400
C	-4.87692200	-0.34896800	-0.06602700
C	4.87724100	-0.34372400	0.04881600
C	-5.33970800	0.80919300	-0.73656500
C	-6.66452300	1.17367000	-0.76891900
C	-7.64385300	0.32358500	-0.06057500
C	-7.16109600	-0.88184200	0.64434100
C	-5.81686400	-1.16711200	0.60596400
C	5.83033900	-1.16262300	-0.60331400
C	7.17489800	-0.87646000	-0.61647800
C	7.64315400	0.33065200	0.09520800
C	6.64994500	1.18102300	0.78359500
C	5.32612900	0.81583600	0.72625500
O	-8.85630000	0.61825500	-0.05896400

C	-8.16051800	-1.76870300	1.40108800
C	-8.86325100	-0.94673500	2.50930000
C	8.18926500	-1.76410300	-1.35214100
O	8.85516900	0.62649800	0.11578300
C	7.11938100	2.42819600	1.54671300
C	7.51391200	-2.96686100	-2.03779700
C	-9.21750100	-2.32800800	0.41700800
C	-7.47119400	-2.96926400	2.07663100
C	-7.14919900	2.41960500	-1.52448700
C	-5.98856700	3.17257000	-2.20191400
C	-8.15152900	2.00953400	-2.63118800
C	-7.83222200	3.40030800	-0.53964600
C	8.91213600	-0.94407900	-2.44878800
C	9.22793600	-2.32013300	-0.34693000
C	8.10087900	2.02018400	2.67269100
C	7.82033300	3.40813100	0.57377000
C	5.94569300	3.18116300	2.20122200
H	-3.78505700	-2.83189600	-0.07913400
H	-1.41209400	-3.45327000	-0.04685700
H	-2.76898000	1.35642400	-0.04050800
H	1.41619500	-3.45153000	0.00489600
H	3.78809900	-2.82711200	0.05654900
H	2.76816900	1.36009700	-0.01081000
H	-0.87534900	2.59256200	-0.57461800
H	-0.01396800	2.60245400	0.97935700
H	0.88379700	2.59511700	-0.55450200
H	-4.61084300	1.39808400	-1.27674600
H	-5.43810500	-2.02756700	1.14022800
H	5.46228000	-2.02442200	-1.14292500
H	4.58669300	1.40514200	1.25145800
H	-9.55255000	-1.58916500	3.06600100
H	-8.13434300	-0.54682100	3.22083600
H	-9.42872100	-0.11758300	2.08979600
H	8.27482100	-3.56692600	-2.54294600
H	7.00807600	-3.62270500	-1.32317500
H	6.78813300	-2.66050700	-2.79658800
H	-9.91018700	-2.98505100	0.95208900
H	-8.74276600	-2.91855500	-0.37259800
H	-9.79018400	-1.52770300	-0.04628500
H	-6.73133800	-2.66052900	2.82072200
H	-8.22183300	-3.56871000	2.59762600
H	-6.97854700	-3.62642300	1.35404300
H	-6.38275600	4.04933200	-2.72164800
H	-5.24906700	3.53136100	-1.47971400

H	-5.47310000	2.56005300	-2.94725800
H	-8.47343000	2.89583600	-3.18676800
H	-9.03190300	1.52924400	-2.20987100
H	-7.68683300	1.32139100	-3.34389700
H	-7.13897400	3.70877700	0.24904300
H	-8.14926500	4.30119300	-1.07419600
H	-8.70631200	2.94988700	-0.07482700
H	9.61220600	-1.58724700	-2.99101200
H	9.46907300	-0.11359000	-2.02060600
H	8.19645400	-0.54627800	-3.17479000
H	8.73891800	-2.90954100	0.43476700
H	9.93139800	-2.97753700	-0.86731100
H	9.79085700	-1.51821400	0.12546100
H	8.41151500	2.90739900	3.23320500
H	7.62325800	1.33256700	3.37731800
H	8.98945000	1.54006900	2.26875300
H	8.12673500	4.30981500	1.11315200
H	7.14189400	3.71529400	-0.22820000
H	8.70328100	2.95767000	0.12604000
H	5.41651900	2.56911300	2.93727700
H	6.32953000	4.05863700	2.72747400
H	5.21966300	3.53881900	1.46495700

Cb27O OS

C	-3.44801726	-0.69241851	-0.06309511
C	-3.03100064	-2.05084492	-0.04764361
C	-1.69489016	-2.40417626	-0.04755027
C	-0.71626123	-1.40211093	-0.05109576
C	-1.12686383	-0.04005521	-0.07252524
C	-2.46873725	0.31887157	-0.07653480
C	1.12773188	-0.03865566	-0.02824244
C	0.71845098	-1.40126524	-0.02814663
C	1.69793722	-2.40232653	-0.00956271
C	3.03361428	-2.04756994	0.00369782
C	3.44881814	-0.68856897	0.01679714
C	2.46865619	0.32169906	0.00624711
N	0.00038772	0.77040283	-0.07696179
C	-0.00137663	2.21778497	-0.04609140
C	-4.87354981	-0.34984731	-0.06435973
C	4.87385266	-0.34486212	0.04706871
C	-5.33239150	0.84548925	-0.67447690
C	-6.65545649	1.21032702	-0.70374964
C	-7.64437367	0.32354545	-0.05384547

C	-7.16830227	-0.92063654	0.58730752
C	-5.82540684	-1.20442636	0.54761414
C	5.83781684	-1.19976622	-0.54505309
C	7.18106074	-0.91508819	-0.55922089
C	7.64373348	0.33029478	0.08928295
C	6.64194639	1.21689636	0.71944807
C	5.31982169	0.85142381	0.66472024
O	-8.85509111	0.61911990	-0.04813789
C	-8.17671868	-1.84708539	1.28271672
C	-8.88964882	-1.08765242	2.42825532
C	8.20337673	-1.84175965	-1.23374212
O	8.85408149	0.62707711	0.10592828
C	7.10450810	2.50248986	1.42097368
C	7.53596118	-3.08167909	-1.85815977
C	-9.22426257	-2.34773088	0.25786924
C	-7.49639058	-3.08545713	1.89617844
C	-7.13216312	2.49523464	-1.39701580
C	-5.96474244	3.28250970	-2.02153694
C	-8.12321193	2.14607144	-2.53420570
C	-7.82482174	3.42238929	-0.36802334
C	8.93750184	-1.08353367	-2.36661540
C	9.23145028	-2.33988186	-0.18814822
C	8.07425685	2.15462793	2.57679425
C	7.81571143	3.42968045	0.40475910
C	5.92495185	3.28911308	2.02311444
H	-3.77949713	-2.83302879	-0.07745580
H	-1.41102929	-3.45161228	-0.04822978
H	-2.76441584	1.35981446	-0.03760305
H	1.41497888	-3.44993046	0.00277502
H	3.78244068	-2.82850054	0.05274698
H	2.76383000	1.36334501	-0.01320208
H	-0.87513939	2.59611814	-0.57709999
H	-0.01489182	2.60675358	0.97762584
H	0.88394075	2.59894699	-0.55567460
H	-4.60007191	1.46439456	-1.17445878
H	-5.45610944	-2.09342445	1.03953109
H	5.47846575	-2.08971475	-1.04264297
H	4.57759980	1.47038932	1.14987549
H	-9.58653281	-1.75854037	2.94020149
H	-8.16758757	-0.73083111	3.16910659
H	-9.44862721	-0.23439425	2.05044033
H	8.30255222	-3.70869920	-2.32018842
H	7.02237540	-3.69669647	-1.11330925
H	6.81871836	-2.81927653	-2.64122778

H	-9.92411139	-3.03179436	0.74790330
H	-8.74232968	-2.89448715	-0.55847948
H	-9.79031315	-1.52125758	-0.16594899
H	-6.76446351	-2.82121640	2.66490957
H	-8.25343452	-3.71236263	2.37382871
H	-6.99670200	-3.70125828	1.14257034
H	-6.35371994	4.18543332	-2.49867816
H	-5.23302820	3.60288171	-1.27372651
H	-5.44133222	2.70977947	-2.79262240
H	-8.43956457	3.06121288	-3.04440405
H	-9.00785357	1.64432158	-2.14839202
H	-7.65134151	1.49708957	-3.27828322
H	-7.13936326	3.68760990	0.44289580
H	-8.13644644	4.35090381	-0.85657047
H	-8.70356591	2.94830780	0.06329479
H	9.64464029	-1.75461786	-2.86404179
H	9.48839769	-0.22916454	-1.97955872
H	8.22946353	-0.72856174	-3.12175183
H	8.73437684	-2.88573530	0.61968275
H	9.94114396	-3.02415506	-0.66350481
H	9.78859798	-1.51227456	0.24515750
H	8.37988322	3.07024523	3.09264823
H	7.58907232	1.50534193	3.31198877
H	8.96656785	1.65372261	2.20793425
H	8.11755889	4.35858573	0.89866886
H	7.14533503	3.69415027	-0.41891964
H	8.70264758	2.95597770	-0.00989119
H	5.38744837	2.71632408	2.78438829
H	6.30427108	4.19246148	2.50718237
H	5.20710125	3.60872981	1.26169547

CDR1 CS

C	-3.43672200	-1.48935000	0.21268600
C	-3.01172800	-0.09242500	0.11631900
C	-1.67753400	0.24834800	0.08147200
C	-0.69983900	-0.76777000	0.20636500
C	-1.12523900	-2.13811900	0.36750400
C	-2.44560300	-2.50100400	0.36649200
C	0.69982800	-0.76775800	0.20636400
C	1.12523800	-2.13809700	0.36750700
N	0.00001200	-2.93886800	0.49150000
C	1.67752400	0.24835800	0.08147000
C	3.01172000	-0.09242100	0.11632000

C	3.43671900	-1.48934600	0.21269200
C	2.44559600	-2.50099900	0.36650300
N	4.07001400	0.81678800	0.04732600
N	5.36304100	0.43272300	-0.10982800
C	5.62636800	-0.85053500	-0.06478500
N	4.70964300	-1.84206100	0.13369000
N	-4.70964600	-1.84206800	0.13368300
C	-5.62637400	-0.85054400	-0.06478500
N	-5.36305000	0.43271500	-0.10982700
N	-4.07002400	0.81678300	0.04732400
C	3.88308400	2.23461000	0.05273200
C	7.04549800	-1.25424300	-0.22837400
C	-3.88309500	2.23460500	0.05272500
C	-7.04550500	-1.25425300	-0.22837000
C	7.38927200	-2.61190500	-0.23683600
C	8.71628900	-3.00291600	-0.39309500
C	9.71805200	-2.04675200	-0.54104900
C	9.38336500	-0.69197700	-0.53082200
C	8.06020900	-0.29710200	-0.37611600
C	4.49037800	3.00842700	-0.93821600
C	4.34452700	4.39181300	-0.91941900
C	3.59636100	5.00862700	0.08173100
C	3.00018600	4.23229400	1.07426500
C	3.14218800	2.84805500	1.06580400
C	-3.14219600	2.84805300	1.06579300
C	-3.00019300	4.23229200	1.07424900
C	-3.59637200	5.00862200	0.08171600
C	-4.34454200	4.39180400	-0.91943000
C	-4.49039300	3.00841900	-0.93822300
C	-8.06021700	-0.29711300	-0.37610400
C	-9.38337300	-0.69198900	-0.53080500
C	-9.71805800	-2.04676400	-0.54103700
C	-8.71629300	-3.00292800	-0.39309100
C	-7.38927600	-2.61191600	-0.23683600
C	0.00012000	-4.38264000	0.60206400
H	-1.37165900	1.27883600	-0.03949300
H	-2.78958000	-3.52467200	0.44001200
H	1.37165600	1.27884700	-0.03950000
H	2.78954500	-3.52467700	0.44003600
H	6.60517800	-3.34867100	-0.11865800
H	8.96743100	-4.05902300	-0.39857800
H	10.75258600	-2.35253200	-0.66178700
H	10.15854600	0.05979200	-0.64220500
H	7.79968100	0.75405500	-0.36305100

H	5.07726600	2.51885100	-1.70529900
H	4.81589200	4.98898500	-1.69304700
H	3.48430400	6.08762300	0.09282800
H	2.43219200	4.70548400	1.86855500
H	2.69832300	2.24609300	1.84992400
H	-2.69832800	2.24609300	1.84991300
H	-2.43219700	4.70548400	1.86853600
H	-3.48431600	6.08761800	0.09280800
H	-4.81591000	4.98897400	-1.69305800
H	-5.07728400	2.51884000	-1.70530200
H	-7.79969100	0.75404400	-0.36303500
H	-10.15855500	0.05977900	-0.64218200
H	-10.75259200	-2.35254500	-0.66177100
H	-8.96743500	-4.05903500	-0.39857700
H	-6.60518200	-3.34868200	-0.11866500
H	0.88070200	-4.70700100	1.15669200
H	-0.88136800	-4.70721500	1.15509700
H	0.00106300	-4.86820500	-0.37954000

CDR1 T

C	-3.43982900	-1.50068700	0.21163300
C	-3.02996300	-0.12858400	0.11916400
C	-1.67686300	0.21751500	0.07979400
C	-0.72161600	-0.78956200	0.19168500
C	-1.12955000	-2.14815700	0.33935400
C	-2.46730700	-2.50671500	0.33572100
C	0.72156400	-0.78953100	0.19175600
C	1.12951000	-2.14814000	0.33944900
N	-0.00000900	-2.94587200	0.45135600
C	1.67682700	0.21752400	0.07996300
C	3.02992400	-0.12859900	0.11947900
C	3.43978500	-1.50069300	0.21192900
C	2.46723100	-2.50672100	0.33595700
N	4.06801100	0.80236000	0.03666000
N	5.36697800	0.43615000	-0.12542900
C	5.63382400	-0.87046200	-0.05794200
N	4.75667800	-1.85363700	0.14742400
N	-4.75673500	-1.85360600	0.14714000
C	-5.63390100	-0.87041900	-0.05796400
N	-5.36705900	0.43619600	-0.12555100
N	-4.06802600	0.80236700	0.03615300
C	3.86019600	2.21724300	0.05039600
C	7.06687900	-1.23952500	-0.21627600

C	-3.86011200	2.21724200	0.04931100
C	-7.06701600	-1.23942800	-0.21588900
C	7.44021700	-2.58935000	-0.22680700
C	8.77535800	-2.95040200	-0.37622200
C	9.75651500	-1.97035700	-0.51640900
C	9.39274900	-0.62427700	-0.50470800
C	8.05906000	-0.25933900	-0.35557400
C	4.44689200	3.00217100	-0.94423400
C	4.27794400	4.38248800	-0.92099400
C	3.52981200	4.98490600	0.08957600
C	2.95755100	4.19793100	1.08714200
C	3.12281700	2.81577300	1.07458200
C	-3.12324400	2.81622100	1.07359300
C	-2.95782500	4.19836700	1.08552600
C	-3.52943200	4.98488600	0.08722300
C	-4.27707400	4.38202400	-0.92344300
C	-4.44615900	3.00171100	-0.94605600
C	-8.05937000	-0.25917200	-0.35344700
C	-9.39311700	-0.62406400	-0.50218400
C	-9.75676000	-1.97016500	-0.51525400
C	-8.77542500	-2.95028100	-0.37682300
C	-7.44023100	-2.58927500	-0.22777100
C	0.00018400	-4.38977000	0.55503200
H	-1.37526200	1.24884200	-0.04768100
H	-2.81106200	-3.53171700	0.39655500
H	1.37526600	1.24886700	-0.04748100
H	2.81093400	-3.53174400	0.39678600
H	6.66962200	-3.34150900	-0.11554500
H	9.05082000	-4.00039300	-0.38346300
H	10.79821000	-2.25303700	-0.63247000
H	10.15174500	0.14467600	-0.60986300
H	7.77428900	0.78513500	-0.33999600
H	5.03465300	2.52246100	-1.71672500
H	4.73170100	4.98923500	-1.69761800
H	3.40123100	6.06200400	0.10449400
H	2.39191100	4.66050300	1.88924900
H	2.70303800	2.20539900	1.86559200
H	-2.70396900	2.20621200	1.86515300
H	-2.39255200	4.66128100	1.88769400
H	-3.40072900	6.06197500	0.10164400
H	-4.73035200	4.98840400	-1.70063300
H	-5.03354000	2.52168200	-1.71864100
H	-7.77467400	0.78530700	-0.33686600
H	-10.15225300	0.14493900	-0.60595100

H	-10.79849900	-2.25280700	-0.63101000
H	-9.05078900	-4.00029000	-0.38515100
H	-6.66950600	-3.34149300	-0.11780300
H	0.88081600	-4.71739300	1.10801200
H	-0.88216300	-4.71777700	1.10498700
H	0.00197100	-4.87042200	-0.42914800

CDR1 OS

C	-3.43811300	-1.49410600	0.21119100
C	-3.02351800	-0.11444800	0.11823100
C	-1.67795900	0.23023500	0.08110600
C	-0.71407700	-0.77926300	0.19671300
C	-1.12735900	-2.14151700	0.34675700
C	-2.45887000	-2.50208300	0.34378400
C	0.71405700	-0.77924600	0.19671800
C	1.12735000	-2.14148800	0.34677000
N	0.00001200	-2.94208800	0.46184000
C	1.67794200	0.23024700	0.08111500
C	3.02350200	-0.11444500	0.11825600
C	3.43810100	-1.49410400	0.21121500
C	2.45885300	-2.50207900	0.34381100
N	4.07160100	0.80949800	0.04131100
N	5.36708800	0.43386500	-0.11762500
C	5.63126700	-0.86373900	-0.05877700
N	4.73821500	-1.84945300	0.14224100
N	-4.73822800	-1.84945600	0.14222300
C	-5.63128400	-0.86374200	-0.05877300
N	-5.36710500	0.43386300	-0.11763100
N	-4.07161600	0.80949400	0.04127200
C	3.87267900	2.22556400	0.05046600
C	7.05905200	-1.24744100	-0.21807300
C	-3.87268300	2.22556000	0.05037100
C	-7.05907300	-1.24744100	-0.21803400
C	7.41978800	-2.60066600	-0.22900800
C	8.75171500	-2.97435400	-0.37989700
C	9.74197200	-2.00422900	-0.52071300
C	9.39062100	-0.65443300	-0.50837300
C	8.06106000	-0.27688100	-0.35822400
C	4.46635200	3.00506000	-0.94421200
C	4.30701300	4.38675800	-0.92379100
C	3.55996600	4.99591500	0.08323100
C	2.97902400	4.21414300	1.08011300
C	3.13499500	2.83106400	1.07039700

C	-3.13503500	2.83109600	1.07030600
C	-2.97904800	4.21417400	1.07996600
C	-3.55993900	4.99590600	0.08302300
C	-4.30694900	4.38671300	-0.92400500
C	-4.46630200	3.00501500	-0.94436900
C	-8.06108200	-0.27687900	-0.35816700
C	-9.39064800	-0.65442800	-0.50828200
C	-9.74200300	-2.00422300	-0.52060500
C	-8.75174600	-2.97435000	-0.37980700
C	-7.41981400	-2.60066500	-0.22895200
C	0.00016400	-4.38613400	0.56296500
H	-1.37528300	1.26159900	-0.04275800
H	-2.80245500	-3.52680600	0.40779200
H	1.37527800	1.26161300	-0.04275600
H	2.80239700	-3.52681500	0.40783200
H	6.64318500	-3.34640200	-0.11688900
H	9.01682100	-4.02701300	-0.38741800
H	10.78083900	-2.29666000	-0.63765700
H	10.15672300	0.10737800	-0.61404000
H	7.78662400	0.77049200	-0.34272300
H	5.05270400	2.52064600	-1.71491900
H	4.76712800	4.98894600	-1.70025400
H	3.43806600	6.07382700	0.09571000
H	2.41311600	4.68174800	1.87914000
H	2.70625800	2.22472900	1.85966100
H	-2.70633900	2.22478900	1.85961400
H	-2.41316900	4.68181000	1.87899500
H	-3.43802700	6.07381800	0.09545700
H	-4.76702300	4.98887200	-1.70051400
H	-5.05262600	2.52057200	-1.71508000
H	-7.78664200	0.77049300	-0.34268000
H	-10.15675000	0.10738500	-0.61393600
H	-10.78087500	-2.29665100	-0.63752200
H	-9.01685500	-4.02700900	-0.38731400
H	-6.64321200	-3.34640400	-0.11684800
H	0.88068400	-4.71465500	1.11552500
H	-0.88164000	-4.71494300	1.11326000
H	0.00150200	-4.86581400	-0.42172100

CDR2 CS

C	-1.12359000	-1.12964400	-0.00046400
C	-0.70581900	0.23854300	-0.11416400
C	-2.44871200	-1.50894900	0.04921800

C	-3.41976200	-0.48638400	-0.03473000
C	-3.03402200	0.91336300	-0.11762700
C	-1.68892000	1.24410700	-0.16645900
N	-4.75572800	-0.73374800	-0.01755900
N	-5.71825700	0.23310900	0.01642000
C	-5.26503600	1.49451100	-0.03871500
N	-4.00236000	1.88272000	-0.12771400
C	-5.30194900	-2.06497600	0.00899800
C	-6.31913800	2.54630800	-0.00634900
C	-5.95175200	3.89747500	-0.00741000
C	-6.92399900	4.89178400	0.02481600
C	-8.27567600	4.55177800	0.05752300
C	-8.64880400	3.20852900	0.05692300
C	-7.67924900	2.21122700	0.02526400
C	-6.12672800	-2.43561700	1.06949100
C	-6.68269900	-3.71084700	1.08968200
C	-6.42470400	-4.60725900	0.05313100
C	-5.61256300	-4.22210600	-1.01167700
C	-5.05021900	-2.94809600	-1.03974400
C	0.70579100	0.23857300	-0.11416700
C	1.12358400	-1.12959300	-0.00048300
N	0.00002700	-1.94426700	0.04802500
C	1.68889400	1.24413200	-0.16645500
C	3.03399900	0.91337000	-0.11762400
C	3.41974900	-0.48637600	-0.03474300
C	2.44869300	-1.50894200	0.04918700
N	4.00233400	1.88273000	-0.12770200
C	5.26501300	1.49452600	-0.03870300
N	5.71824100	0.23312800	0.01642200
N	4.75571400	-0.73373400	-0.01757200
C	0.00029900	-3.37915400	0.23279300
C	6.31910800	2.54632900	-0.00632600
C	5.30193900	-2.06496000	0.00897300
C	5.05021600	-2.94806800	-1.03978100
C	5.61256600	-4.22207600	-1.01172900
C	6.42470500	-4.60723800	0.05307700
C	6.68269300	-3.71083900	1.08964000
C	6.12671500	-2.43561100	1.06946400
C	7.67922100	2.21125600	0.02528200
C	8.64877000	3.20856400	0.05695100
C	8.27563400	4.55181100	0.05756500
C	6.92395400	4.89180900	0.02486300
C	5.95171400	3.89749400	-0.00737300
H	-2.74485900	-2.54108200	0.16870900

H	-1.42691600	2.29349000	-0.22827900
H	-4.89872800	4.14753100	-0.03464300
H	-6.62578200	5.93557700	0.02425700
H	-9.03368500	5.32862700	0.08199400
H	-9.69950500	2.93627700	0.07953600
H	-7.96541500	1.16702000	0.02034900
H	-6.33135600	-1.72045900	1.85674700
H	-7.32168400	-4.00329500	1.91612600
H	-6.86421100	-5.59897200	0.07014400
H	-5.42627300	-4.90777300	-1.83156800
H	-4.43707100	-2.63198300	-1.87593500
H	1.42691000	2.29352000	-0.22826700
H	2.74477400	-2.54110100	0.16864100
H	0.87920300	-3.81207000	-0.24583400
H	0.00255100	-3.65838800	1.29208800
H	-0.88076700	-3.81181200	-0.24199200
H	4.43707000	-2.63194700	-1.87597000
H	5.42628200	-4.90773400	-1.83162900
H	6.86421700	-5.59895000	0.07007800
H	7.32167600	-4.00329500	1.91608200
H	6.33133700	-1.72046200	1.85673000
H	7.96539400	1.16705200	0.02035700
H	9.69947300	2.93631900	0.07955900
H	9.03363800	5.32866400	0.08204300
H	6.62573100	5.93560000	0.02431400
H	4.89868800	4.14754300	-0.03460200

CDR2 T

C	-1.12953100	-1.15633000	0.02215700
C	-0.72291000	0.19998700	-0.13639600
C	-2.46833400	-1.52676000	0.08002400
C	-3.42754200	-0.51538200	-0.04414400
C	-3.04893100	0.86273900	-0.16880800
C	-1.68517800	1.19461800	-0.22605400
N	-4.79909600	-0.75715300	-0.02453000
N	-5.72149600	0.24494300	0.04022900
C	-5.25890900	1.49182900	-0.05527200
N	-3.98302200	1.85742200	-0.19904400
C	-5.36718300	-2.06989800	0.00532000
C	-6.28856200	2.56578700	-0.00608500
C	-5.89326100	3.90906700	-0.02667600
C	-6.84347000	4.92423400	0.02091500
C	-8.20047300	4.61370500	0.08869700

C	-8.60162000	3.27833600	0.10728600
C	-7.65484700	2.26068700	0.06010200
C	-6.29869200	-2.38871700	0.99488700
C	-6.87962500	-3.65263900	1.01255100
C	-6.53785100	-4.59957800	0.04807700
C	-5.61712100	-4.27176300	-0.94547100
C	-5.03337200	-3.00808500	-0.97385400
C	0.72288000	0.20003500	-0.13645200
C	1.12954400	-1.15625500	0.02206900
N	0.00006000	-1.95957200	0.09840500
C	1.68514300	1.19467300	-0.22603300
C	3.04889800	0.86277100	-0.16879100
C	3.42753000	-0.51535600	-0.04419200
C	2.46833100	-1.52674500	0.07994000
N	3.98299300	1.85745800	-0.19895100
C	5.25886400	1.49187600	-0.05504500
N	5.72146300	0.24498400	0.04039100
N	4.79908500	-0.75711000	-0.02460200
C	0.00050200	-3.38952500	0.32057800
C	6.28849700	2.56584900	-0.00566700
C	5.36717800	-2.06987100	0.00487800
C	5.03331400	-3.00779700	-0.97452700
C	5.61708200	-4.27147400	-0.94652000
C	6.53786500	-4.59955500	0.04689200
C	6.87967600	-3.65287700	1.01160800
C	6.29873800	-2.38895100	0.99431100
C	7.65477000	2.26077000	0.06085000
C	8.60151900	3.27843300	0.10821300
C	8.20036000	4.61379600	0.08947200
C	6.84336900	4.92430500	0.02135900
C	5.89318400	3.90912300	-0.02640700
H	-2.76734900	-2.55420800	0.23233900
H	-1.42745400	2.24297800	-0.32172300
H	-4.83672100	4.13866300	-0.08142700
H	-6.52304700	5.96127600	0.00505000
H	-8.94113900	5.40655500	0.12509700
H	-9.65694300	3.02855900	0.15637700
H	-7.96388700	1.22296400	0.06876500
H	-6.56439800	-1.63979700	1.73054000
H	-7.60167800	-3.89808100	1.78430900
H	-6.99422700	-5.58364700	0.06447500
H	-5.36326100	-4.99504800	-1.71349900
H	-4.34012900	-2.74035200	-1.76286100
H	1.42744200	2.24304300	-0.32164800

H	2.76724600	-2.55423700	0.23219800
H	0.87949100	-3.83480600	-0.14643000
H	0.00414500	-3.63840000	1.38721200
H	-0.88193800	-3.83426200	-0.14025400
H	4.34002200	-2.73986500	-1.76342200
H	5.36318300	-4.99455300	-1.71472900
H	6.99424900	-5.58362500	0.06299500
H	7.60176700	-3.89852000	1.78326600
H	6.56446900	-1.64023400	1.73016100
H	7.96382400	1.22305200	0.06962200
H	9.65683300	3.02867100	0.15756800
H	8.94100800	5.40665700	0.12601000
H	6.52293600	5.96134200	0.00537200
H	4.83665300	4.13870400	-0.08140400

CDR2 OS

C	-1.12857400	-1.15081800	0.01491700
C	-0.72109500	0.20680000	-0.13223300
C	-2.46541500	-1.52262100	0.07048500
C	-3.42596900	-0.50873500	-0.04374500
C	-3.04662400	0.87048000	-0.15903700
C	-1.68657700	1.20282800	-0.21313600
N	-4.79293900	-0.75278600	-0.02243400
N	-5.72164300	0.24294800	0.03747500
C	-5.25945700	1.49475300	-0.05149500
N	-3.98800100	1.86389100	-0.18533700
C	-5.35644800	-2.06916600	0.00697300
C	-6.29507800	2.56332800	-0.00573700
C	-5.90639200	3.90865500	-0.02170900
C	-6.86179200	4.91885500	0.02264500
C	-8.21772100	4.60130000	0.08263400
C	-8.61224900	3.26407100	0.09675100
C	-7.66001000	2.25114100	0.05277400
C	-6.26707100	-2.39855400	1.01177100
C	-6.84308800	-3.66476900	1.03022900
C	-6.51706000	-4.60184800	0.05073100
C	-5.61730800	-4.26268400	-0.95802600
C	-5.03830300	-2.99667800	-0.98677700
C	0.72106400	0.20683200	-0.13223800
C	1.12856700	-1.15076600	0.01489500
N	0.00002900	-1.95738300	0.08428300
C	1.68654700	1.20285500	-0.21313400
C	3.04659700	0.87048900	-0.15903300

C	3.42595300	-0.50872700	-0.04375500
C	2.46539400	-1.52261600	0.07045800
N	3.98797200	1.86390300	-0.18532700
C	5.25943000	1.49477000	-0.05148800
N	5.72162300	0.24296700	0.03747700
N	4.79292200	-0.75277000	-0.02243900
C	0.00031500	-3.38832900	0.29739900
C	6.29504500	2.56335000	-0.00572500
C	5.35643700	-2.06914800	0.00696200
C	5.03831500	-2.99664800	-0.98680500
C	5.61732900	-4.26265000	-0.95806200
C	6.51706700	-4.60182000	0.05070500
C	6.84307200	-3.66475200	1.03022100
C	6.26704500	-2.39854200	1.01177200
C	7.65997900	2.25116900	0.05278000
C	8.61221300	3.26410400	0.09676000
C	8.21767800	4.60133100	0.08265200
C	6.86174800	4.91887900	0.02266900
C	5.90635200	3.90867600	-0.02168800
H	-2.76405300	-2.55126000	0.21483900
H	-1.42834300	2.25175300	-0.30077800
H	-4.85061400	4.14324800	-0.07027900
H	-6.54659000	5.95754800	0.01040900
H	-8.96251600	5.39039700	0.11657400
H	-9.66654700	3.00891000	0.13994300
H	-7.96378000	1.21188000	0.05822500
H	-6.52094000	-1.65636000	1.75841700
H	-7.54908200	-3.91953800	1.81368800
H	-6.96986200	-5.58756800	0.06751000
H	-5.37619800	-4.97865600	-1.73689200
H	-4.36078000	-2.71930600	-1.78609000
H	1.42833400	2.25178600	-0.30076800
H	2.76396300	-2.55128100	0.21478200
H	0.87967200	-3.83080600	-0.17172900
H	0.00269100	-3.64525200	1.36229200
H	-0.88130600	-3.83046700	-0.16769100
H	4.36080300	-2.71926900	-1.78612500
H	5.37623600	-4.97861300	-1.73694100
H	6.96987600	-5.58753700	0.06747800
H	7.54905500	-3.91952800	1.81368800
H	6.52089700	-1.65635600	1.75843200
H	7.96375400	1.21191000	0.05822400
H	9.66651300	3.00894800	0.13994700
H	8.96246900	5.39043100	0.11659400

H	6.54654000	5.95757100	0.01044000
H	4.85057300	4.14326400	-0.07025300

***m*-Cz-ph CS**

C	3.42856700	0.18184700	0.04629300
C	3.06787700	-1.20496700	0.03195100
C	1.67821300	-1.55412300	0.01545600
C	0.73220300	-0.56312400	0.00186000
C	1.13042300	0.80807800	0.00378900
C	2.48410100	1.17893700	0.03555300
C	-0.73220300	-0.56312400	-0.00180900
C	-1.13042400	0.80807800	-0.00376100
N	-0.00000100	1.59417000	0.00000800
C	-1.67821300	-1.55412400	-0.01539000
C	-3.06787600	-1.20496900	-0.03188900
C	-3.42856700	0.18184500	-0.04625600
C	-2.48410200	1.17893600	-0.03553100
C	-0.00000100	3.03075900	-0.00000300
C	4.05639100	-2.21635400	0.03996700
C	-4.05639000	-2.21635600	-0.03989100
C	-0.49938200	3.71754100	1.10609700
C	-0.49883500	5.10988200	1.09974700
C	-0.00000100	5.80573900	-0.00002500
C	0.49883300	5.10986500	-1.09978600
C	0.49938000	3.71752400	-1.10611400
C	5.43521300	-1.89717800	0.05656300
N	6.55835900	-1.61174400	0.06973800
C	3.71393600	-3.58921700	0.03131700
N	3.41327100	-4.70854100	0.02385700
C	-5.43521200	-1.89718200	-0.05658400
N	-6.55835700	-1.61174900	-0.06986600
C	-3.71393500	-3.58921900	-0.03130600
N	-3.41326600	-4.70854300	-0.02395400
H	4.47933100	0.44444300	0.07043100
H	1.39289500	-2.60027200	0.01731100
H	2.78017200	2.22088300	0.05515800
H	-1.39289400	-2.60027300	-0.01722900
H	-4.47933100	0.44444000	-0.07039800
H	-2.78017400	2.22088000	-0.05515200
H	-0.86950500	3.16562600	1.96275300
H	-0.88265700	5.64939200	1.95848700
H	-0.00000200	6.89022000	-0.00003300
H	0.88265400	5.64936100	-1.95853500

H	0.86950400	3.16559500	-1.96276100

***m*-Cz-ph T**

C	-3.42103600	0.16486200	-0.04277300
C	-3.05139900	-1.21137500	-0.03108900
C	-1.68116500	-1.55710800	-0.01455900
C	-0.72589400	-0.55411200	-0.00303600
C	-1.12873500	0.80750900	-0.00572900
C	-2.47919900	1.17282900	-0.03181100
C	0.72589500	-0.55411000	0.00304700
C	1.12873400	0.80751100	0.00573600
N	-0.00000100	1.61830900	0.00000200
C	1.68116800	-1.55710500	0.01457000
C	3.05140100	-1.21137000	0.03109300
C	3.42103600	0.16486800	0.04277700
C	2.47919700	1.17283300	0.03181600
C	-0.00000300	3.04968300	-0.00000200
C	-4.06638700	-2.23238500	-0.04001900
C	4.06639100	-2.23237800	0.04002400
C	0.48733900	3.74212600	-1.10936800
C	0.49114900	5.13462200	-1.10257300
C	-0.00000600	5.83141400	-0.00001100
C	-0.49116000	5.13462700	1.10255600
C	-0.48734600	3.74213200	1.10935900
C	-5.43984200	-1.90727900	-0.05610400
N	-6.56338600	-1.61919300	-0.06881900
C	-3.73078500	-3.60336900	-0.03247100
N	-3.43370200	-4.72448200	-0.02601300
C	5.43984600	-1.90727000	0.05610700
N	6.56338900	-1.61918400	0.06885300
C	3.73078900	-3.60336300	0.03255400
N	3.43371300	-4.72447500	0.02590200
H	-4.47294900	0.42511700	-0.06347200
H	-1.38786800	-2.60107200	-0.01325600
H	-2.78096800	2.21300300	-0.04716600
H	1.38787200	-2.60106900	0.01327400
H	4.47294900	0.42512500	0.06347000
H	2.78096500	2.21300800	0.04716600
H	0.84939000	3.19112900	-1.97038600
H	0.86979300	5.67401200	-1.96394100
H	-0.00000700	6.91601100	-0.00001500
H	-0.86980500	5.67402300	1.96391900
H	-0.84939600	3.19113900	1.97038100

***m*-Cz-ph OS**

C	3.42345230	0.16923625	0.04284267
C	3.05517930	-1.20817645	0.03091192
C	1.68066982	-1.55452762	0.01452075
C	0.72731243	-0.55385478	0.00266187
C	1.12953818	0.80951896	0.00508574
C	2.48077627	1.17508797	0.03204580
C	-0.72731110	-0.55385614	-0.00270637
C	-1.12953938	0.80951689	-0.00511386
N	-0.00000137	1.61390597	-0.00001008
C	-1.68066660	-1.55453061	-0.01457694
C	-3.05517668	-1.20818187	-0.03096996
C	-3.42345230	0.16923035	-0.04287809
C	-2.48077821	1.17508372	-0.03206809
C	-0.00000280	3.04644438	-0.00000206
C	4.06230938	-2.23000819	0.03967612
C	-4.06230499	-2.23001530	-0.03974086
C	-0.48847670	3.73776269	1.10923014
C	-0.49137018	5.13022521	1.10258847
C	-0.00000545	5.82685948	0.00001351
C	0.49136055	5.13023853	-1.10256928
C	0.48846976	3.73777607	-1.10922661
C	5.43762284	-1.90880071	0.05548686
N	6.56176831	-1.62422792	0.06807179
C	3.72274118	-3.60104475	0.03230181
N	3.42377721	-4.72138802	0.02581125
C	-5.43762041	-1.90881010	-0.05542411
N	-6.56176561	-1.62423264	-0.06792935
C	-3.72273595	-3.60105096	-0.03224741
N	-3.42376785	-4.72139342	-0.02579857
H	4.47515149	0.42978902	0.06392765
H	1.38880270	-2.59892364	0.01388573
H	2.78168624	2.21556506	0.04802967
H	-1.38879753	-2.59892611	-0.01395229
H	-4.47515198	0.42978141	-0.06396025
H	-2.78169004	2.21556044	-0.04804014
H	-0.85128651	3.18652081	1.96970270
H	-0.87004363	5.66962029	1.96389413
H	-0.00000646	6.91143853	0.00001955
H	0.87003296	5.66964394	-1.96386894
H	0.85128059	3.18654452	-1.96970532

***p*-Cz-alkyl CS**

C	-3.43206500	-0.25058600	-0.00000400
C	-3.00040800	-1.63500400	-0.00002200
C	-1.68360500	-1.96855300	-0.00009600
C	-0.69782100	-0.93876400	-0.00017700
C	-1.12791000	0.44721700	-0.00023000
C	-2.45003800	0.79180000	-0.00008000
C	0.68957600	-0.94336300	-0.00017500
C	1.12392300	0.43877400	-0.00023700
N	0.00268500	1.24902100	-0.00042000
C	1.67519800	-1.97318600	-0.00008900
C	2.99215800	-1.63771800	-0.00001800
C	3.42650600	-0.25359200	-0.00001200
C	2.44443400	0.78919100	-0.00010000
C	0.04386900	2.70114600	-0.00027300
C	-4.79822000	0.05382100	0.00011100
C	4.79294200	0.04868000	0.00009600
C	-5.79533100	-0.95644900	0.00024800
N	-6.60286200	-1.78588900	0.00035800
C	-5.25292600	1.39885300	0.00018600
N	-5.59581000	2.50454800	0.00024200
C	5.24933300	1.39315500	0.00012100
N	5.59435900	2.49816600	0.00013600
C	5.78869300	-0.96298100	0.00020700
N	6.59488600	-1.79371800	0.00029600
H	-3.75798500	-2.40929600	0.00004400
H	-1.38238400	-3.01024100	-0.00008100
H	-2.77699800	1.82388200	0.00002700
H	1.37598400	-3.01543600	-0.00006500
H	3.74948200	-2.41234600	0.00005300
H	2.76273600	1.82432100	-0.00001700
H	-0.96944900	3.09515400	-0.00285200
H	0.55583900	3.07230800	0.89093000
H	0.56011600	3.07211600	-0.88906200

***p*-Cz-alkyl T**

C	3.43555700	-0.26495700	0.00004300
C	3.03198100	-1.63049800	0.00007300
C	1.69714700	-1.97453000	0.00013300
C	0.72221900	-0.96566500	0.00018000
C	1.12542900	0.40104600	0.00017600
C	2.46670400	0.76006800	0.00006100

C	-0.71420100	-0.97045400	0.00014100
C	-1.12164100	0.39305300	0.00011500
N	-0.00271900	1.20757900	0.00018700
C	-1.68899300	-1.97917700	0.00015300
C	-3.02411800	-1.63300300	0.00012200
C	-3.43006000	-0.26784100	0.00003200
C	-2.46102200	0.75756700	0.00003000
C	-0.04271200	2.65914500	0.00044400
C	4.83918100	0.07684300	-0.00001300
C	-4.83396000	0.07196700	-0.00006300
C	5.84250100	-0.91425800	-0.00036900
N	6.65817700	-1.73919900	-0.00066100
C	5.26564100	1.42194000	0.00003600
N	5.58712000	2.53654600	0.00008400
C	-5.26207700	1.41653500	-0.00042700
N	-5.58593400	2.53044100	-0.00073100
C	-5.83605400	-0.92044000	0.00001200
N	-6.65046400	-1.74661700	0.00007400
H	3.78929700	-2.40514200	0.00003500
H	1.40756900	-3.01974000	0.00011300
H	2.77997500	1.79679100	-0.00006100
H	-1.40155100	-3.02495500	0.00019400
H	-3.78125200	-2.40791200	0.00013300
H	-2.76568100	1.79724800	-0.00009800
H	0.97067300	3.05321000	0.00259600
H	-0.55400300	3.03291500	-0.89028300
H	-0.55742100	3.03230600	0.88943900

_p_-Cz-alkyl OS

C	-3.43297548	-0.25557153	0.00000794
C	-3.01212473	-1.63210597	-0.00000235
C	-1.68787487	-1.96940884	-0.00005707
C	-0.70734332	-0.94768869	-0.00012488
C	-1.12688778	0.43013135	-0.00017497
C	-2.45686609	0.77979394	-0.00005672
C	0.69918801	-0.95234799	-0.00012369
C	1.12298597	0.42188375	-0.00018125
N	0.00270584	1.23369387	-0.00033010
C	1.67958130	-1.97403125	-0.00005146
C	3.00402913	-1.63472513	-0.00000074
C	3.42745445	-0.25851605	-0.00000307
C	2.45124950	0.77724164	-0.00007536
C	0.04336465	2.68560818	-0.00022166

C	-4.81373688	0.06179256	0.00010057
C	4.80849159	0.05675512	0.00008292
C	-5.81286391	-0.94176831	0.00018710
N	-6.62360574	-1.76930905	0.00025820
C	-5.25866626	1.40673560	0.00012130
N	-5.59479780	2.51538769	0.00013335
C	5.25508883	1.40115494	0.00008578
N	5.59342665	2.50911981	0.00008405
C	5.80631084	-0.94816020	0.00016782
N	6.61575222	-1.77696643	0.00023634
H	-3.76922920	-2.40687855	0.00005294
H	-1.39088371	-3.01239391	-0.00003630
H	-2.77875652	1.81362924	0.00003288
H	1.38464836	-3.01758373	-0.00002359
H	3.76090663	-2.40980834	0.00005946
H	2.76450926	1.81408818	-0.00000806
H	-0.97000945	3.07955965	-0.00252609
H	0.55510299	3.05773219	0.89078733
H	0.55891372	3.05753527	-0.88909279