Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Formation of stable biradical triplet state cation versus closed shell singlet state cation by oxidation of adducts of 3,6-dimethoxycarbazole and polychlorotriphenylmethyl radicals. (Supplementary Information)

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Experimental section

General procedures. IR spectra were recorded with a FT-IR spectrophotometer, electronic spectra with a single cell spectrophotometer, emission spectra were recorded in a PTI fluorimeter, and the X-band EPR spectra at rt and at low temperature with an EMX-Plus 10/12 spectrometer. HRMS was performed in a LC/MSD-TOF apparatus by means of the electrospray (ESI-MS) technique. Cyclic voltammograms were recorded with an Autolab PGSTAT30 instrument using a conventional three-electrode cell. The cyclic graphics were recorded at scan rates ranging from 20 to 200 mV s^{-1}. All reagents were obtained from commercial sources and used as received. 3,6-dimethoxy-9*H*-carbazole was prepared from 3,6-dibromo-9*H*-carbazole.[1]

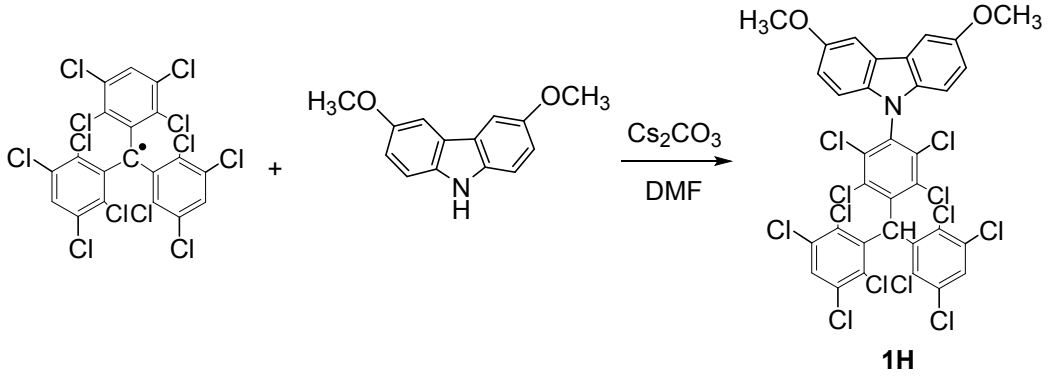
Theoretical methods.

The different stationary points have been optimized and characterized employing the density functional theory (DFT) with the B3LYP functional,[2] using the 6-31+G(2df) basis set.[3, 4] The optimized Cartesian coordinates in Å of all optimized geometries are displayed in Table S8. The Time-Dependent Density Functional theory,[5] with the B3LYP functional and employing the same basis has been used to calculate the electronic spectra. In these calculations the Polarizable Continuum Model (PCM) approach with and with a dielectric contant ε=8.93 (Dichloromethane) has been used. The ionization potential have been estimated carrying out single point energy calculations at at DLPNO-CCSD(T) level of theory[6] with the cc-pVTZ basis set.[7, 8] Regarding the DFT calculations, we have employed the unrestricted functional for the doublet and triplet electronic states and the restricted functional for the singlet electronic states. However, in these

cases, we have tried also the unrestricted approach with broken symmetry to look for possible interactions with biradical states, but the convergence procedure fall to the restricted one.

Along this work we have employed the Gaussian 09 program [9] and with the ORCA program,[10] for the ab-initio calculations, and the Molden program[11] for visualizing the electronic features.

Reaction of tris(2,3,5,6-tetrachlorophenyl)methyl radical (DTM) with 3,6-dimethoxy-9*H*-carbazole in DMF.

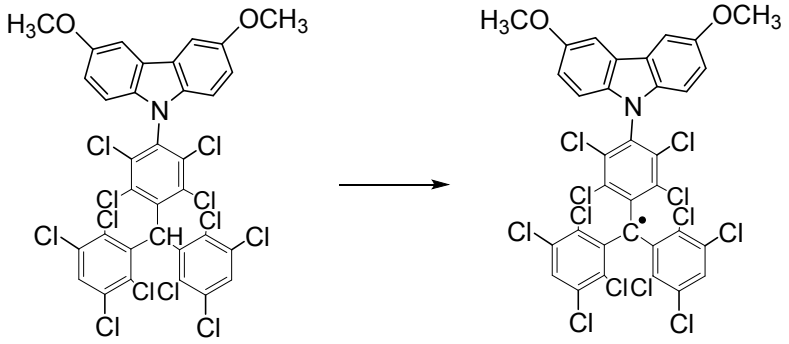


1H

A mixture of 3,6-dimethoxy-9*H*-carbazole (155 mg; 0.68 mmols), DTM (300 mg; 0.46 mmols), anhydrous Cs_2CO_3 (237 mg; 0.73 mmols), and DMF (15 mL) was stirred at reflux (2 h) in an inert atmosphere and in the dark. The resulting mixture was poured into an excess of diluted aqueous HCl acid, and the precipitate was filtered off. The solid was chromatographed in silica gel with hexane/$CHCl_3$ (2:1) to give tris(2,3,5,6-tetrachlorophenyl)methane (178 mg; 59%) and [4-(3,6-dimethoxy-9-carbazolyl)-2,3,5,6-tetrachlorophenyl]bis(2,3,5,6-tetrachlorophenyl)methane (**1H**) (153 mg; 38%). IR: $\bar{u}/cm^{-1}$, 3062(d), 3000(d), 1725(d), 1582(d), 1548(d), 1490(f), 1469(f), 1437(m), 1397(m), 1366(m), 1350(m), 1326(d), 1292(d), 1263(d), 1206(f), 1164(f), 1098(d), 1040(m), 973(d),

912(d), 867(d), 843(d), 791(m), 755(m), 721(d), 705(d), 667(d). ESI-HRMS: calculated for $C_{33}H_{14}Cl_{12}NO_2$: 875,7292, found: m/z 875,7265.

Synthesis of the [4-(3,6-dimethoxy-9-carbazolyl)-2,3,5,6-tetrachlorophenyl]bis(2,3,5,6-tetrachlorophenyl)methyl radical adduct (1).



1H **1**

Tetrabutylammonium hydroxide (TBAH) (1.0 M; 0.22 mL,) was added to a solution of [4-(3,6-dimethoxy-9-carbazolyl)-2,3,5,6-tetrachlorophenyl]bis(2,3,5,6-tetrachlorophenyl)methane (150 g; 0.17 mmol) in THF (15 mL) and the mixture was stirred (4 h). 2,3,5,6-tetrachloroquinone (59 g; 0.24 mmol) was added in solid to the reaction mixture and stirred in the dark under inert atmosphere (Ar) (30 min). The mixture was poured into an excess of acidic aqueous solution, and the precipitate, filtered, washed with water and dried, was chromatographed on silicagel with hexane/$CHCl_3$ (2:1) to give **1** (121 mg; 81 %). IR: ū/cm^{-1}, 3108(d), 3000(d), 2158(d), 2039(d), 1724(d), 1584(d), 1536(d), 1487(m), 1464(f), 1436(m), 1378(f), 1360(m), 1330(m), 1285(m), 1248(m), 1207(f), 1195(f), 1177(f), 1165(f), 1034(m), 1011(m), 984(m), 903(d), 859(m), 849(m), 786(m), 756(d), 735(m), 716(m), 704(m), 677(d), 662(m). ESI-HRMS: calculated for $C_{33}H_{14}Cl_{12}NO_2$: 875,7292, found: m/z 875,7291 $[M]^{\bullet-}$.

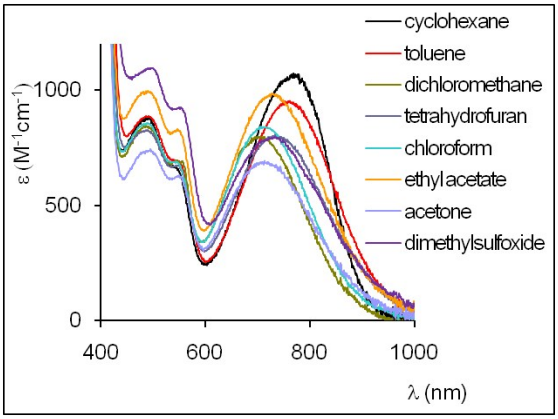


Figure S1. Details of the absorptivities of the electronic spectra of radical adduct 3,6-diMeOczDTM (**1)** (400-1000 nm) in solvents of different polarities.

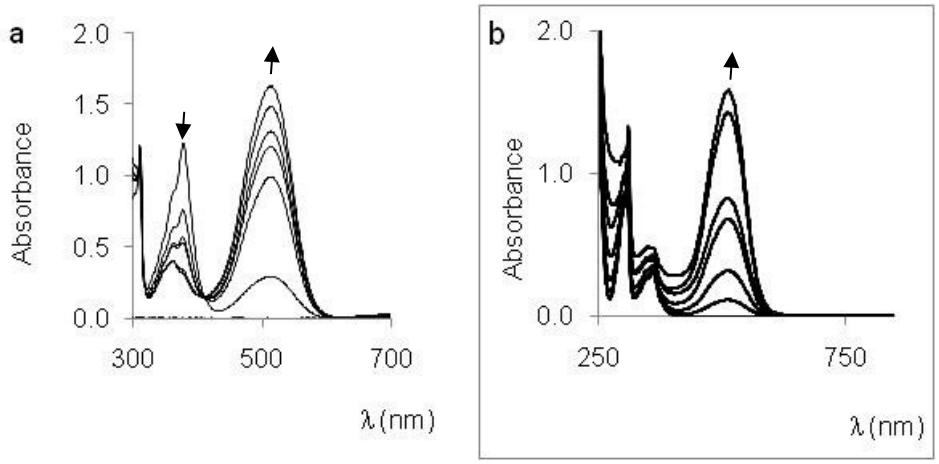


Figure S2. (Left): Evolution of the UV-vis spectra of radical adduct **1** in THF (~10^{-5} M) with additional amounts of aqueous solution of TBAH. Typical band of **1** at λ = 377 nm decreases and anion band at λ = 512 nm increases. (Right): Evolution of the UV-vis spectra of **1H** in THF (~10^{-5} M) with additional amounts of aqueous solution of TBAH (2.3x10^{-3} M) (increase in the intensity of the anion band.

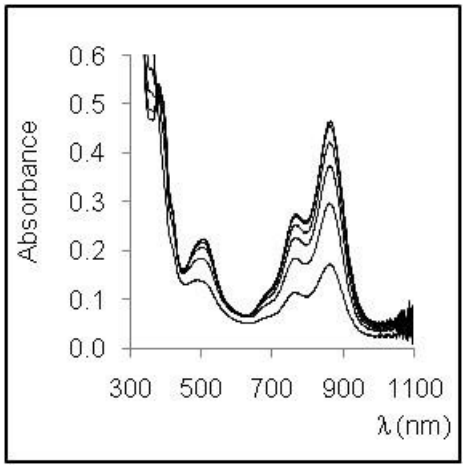


Figure S3. Oxidation details of **1H** in CH2Cl2 (0.68×10^{-4} M) with SbCl5 in CH2Cl2 (8.9×10^{-4} M). Bands at λ = 505, 766 and 862 nm.

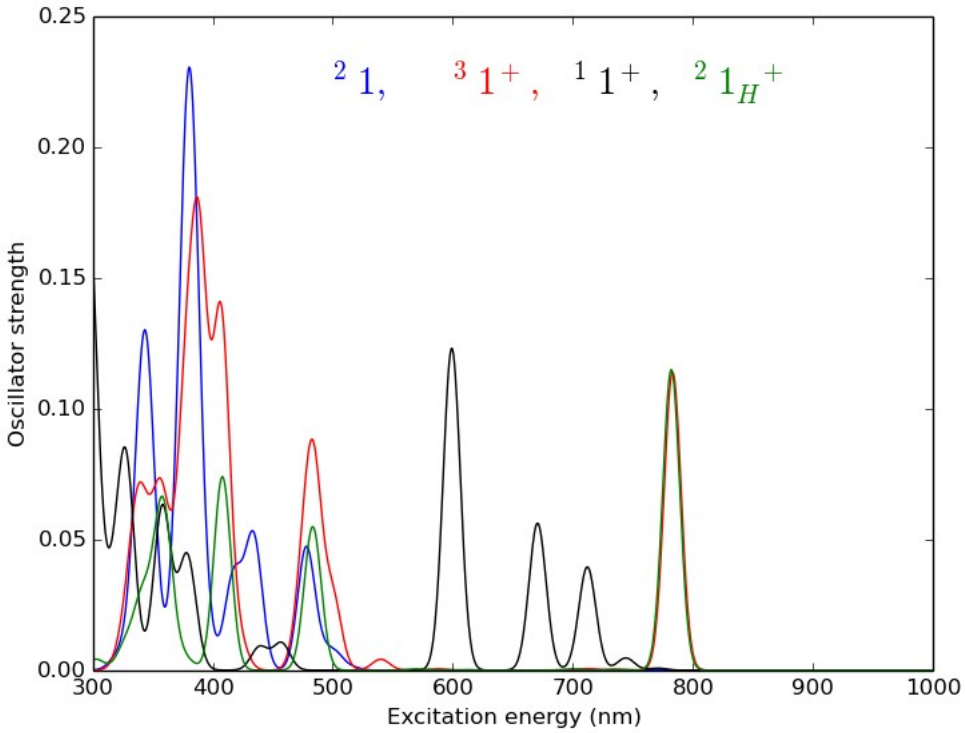


Figure S4. Calculated electronic spectra, in the 300 – 1000 nm range, of radical **^{2}1** (in blue) and the triplet (**^{3}1$^+$** in red), closed shell singlet electronic states (**^{1}1$^+$** in black), and the cation **^{2}1H$^+$** (in green). A Gaussian function with an arbitrary sigma value of 100 has been used to draw the calculated spectra.

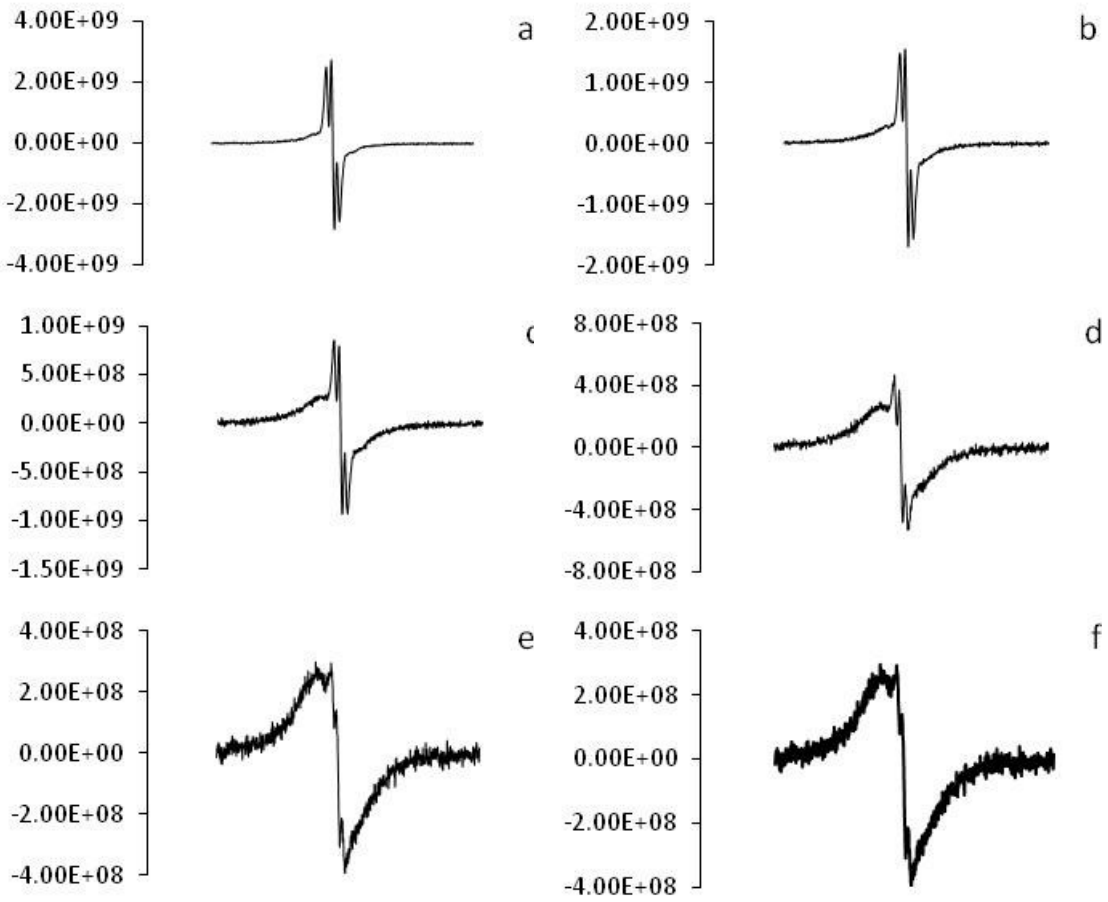


Figure S5. Evolution (every 5 min) of the epr spectra of a solution of **1** ($3.0 \cdot 10^{-5}$ M) in CH_2Cl_2 in the presence of an excess of $SbCl_5$ (7.1×10^{-3}). (a) spectrum before oxidation.

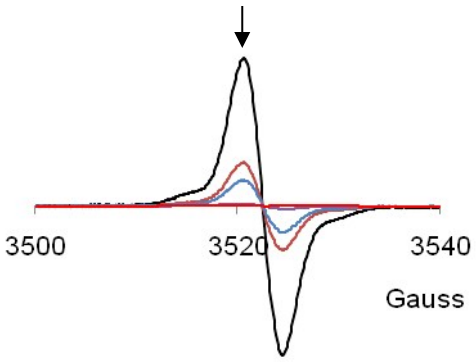


Figure S6. Sequential decrease of the epr band of **3** in CH_2Cl_2 (1.97×10^{-4} M) in the presence of an excess of $SbCl_5$.

Table S1. The UV-vis absorption data of the spectra of radical adduct **1**$^{\bullet}$ in solvents of different polarity

Solvent	λ_{max}nm(ε)[a]
cyclohexane	297(15 880), 302(16 570), 309(20 770), 361(17 210), 376(23 700), 485(880), 543(sh)(665), 769(1070)
Toluene	299(sh)(12 560), 304(sh)(14 160), 310(18 650), 363(16 980), 376(20 950), 487(890), 550(690), 761(950)
CH_2Cl_2	298(sh)(15 640), 303(16 590), 309(20 600), 362(18 790), 378(26 695), 487(845), 550(sh)(690), 706(800)
THF	297(18 240), 302(18 000), 308(20 610), 363(16 520), 377(22 670), 487(830), 547(670), 734(810)
$CHCl_3$	298(sh)(14890), 303(sh)(15 890), 309(19 060), 362(17 860), 377(24945), 489(860), 544(690), 707(840)
Ethyl acetate	296(sh)(17 550), 301(sh)(18620), 308(23 055), 361(21 000), 375(28 910), 489(1000), 547(830), 729(990)
Acetone	376(22 815), 495(740), 550(630), 713(690)

[a]Units: $dm^3\ mol^{-1}\ cm^{-1}$.

Table S2. Calculated electronic spectra λ (nm), the corresponding oscillator strengths, f_{osc}, and the electronic nature of the transitions for the radical adduct **^{2}1**.

band	λ (nm)	f_{osc}	Transition nature
1	1031	0.02	$\pi_{carbazol} \rightarrow n_{SOMO}$
2	502	0.06	$\pi_{phenyl\text{-}bridge} \rightarrow n_{SOMO}$
	490	0.05	$\pi_{carbazol} \rightarrow n_{SOMO}$
	479	0.03	$\pi_{diphenyl} \rightarrow n_{SOMO}$
	477	0.02	$\sigma_{phenyl\text{-}bridge} \rightarrow n_{SOMO}$
3	434	0.05	$\pi_{carbazol} \rightarrow \pi^*_{phenyl}$
	431	0.05	$\pi_{carbazol} \rightarrow \pi^*_{carbazol}$
	419	0.02	$\pi_{triphenyl} \rightarrow n_{SOMO}$
	416	0.02	$\pi_{carbazol} \rightarrow \pi^*_{phenyl\text{-}bridge}$
4	394	0.011	$\pi_{carbazol} \rightarrow \pi^*_{biphenyl}$
	386	0.03	$\pi_{carbazol} \rightarrow \pi^*_{biphenyl}$
	382	0.16	$n_{SOMO} \rightarrow \pi^*_{phenyl\text{-}bridge}$

	376	0.04	$n_{SOMO} \rightarrow \pi^*_{biphenyl}$
	373	0.03	$\pi_{carbazol} \rightarrow \pi^*_{diphenyl}$
5	346	0.08	$\pi_{carbazol} \rightarrow \pi^*_{carbazol}$
	343	0.02	$n_{SOMO} \rightarrow \pi^*_{phenyl}$
	338	0.03	$n_{SOMO} \rightarrow \pi^*_{biphenyl}$

Table S3. Calculated electronic spectra λ (nm), the corresponding oscillator strengths, f_{osc}, and the electronic nature of the transitions for the radical adduct $^3\mathbf{1}^+$.

band	**λ (nm)**	f_{osc}	**Transition nature**[a]
1	1511	0.05	$\pi_{carbazol} \rightarrow p_{N+}\pi_{carbazol}$
2	783	0.11	$\pi_{carbazol} \rightarrow p_{N+}\pi_{carbazol}$
3	539	00038	$\pi_{diphenyl} \rightarrow p_{C\text{-}tris}$
4	503	0.0029	$\pi_{bridge} \rightarrow p_{N+}\pi_{carbazol}$
	500	0.03	$\pi_{diphenyl} \rightarrow p_{C\text{-}tris}$
			$\pi_{bridge} \rightarrow p_{C\text{-}tris}$
	484	0.07	$\pi_{carbazol} \rightarrow p_{N+}\pi_{carbazol}$
	475	0.01	$\pi_{triphenyl} \rightarrow p_{C\text{-}tris}$
	475	0.02	$\pi_{diphenyl} \rightarrow p_{C\text{-}tris}$
4	422	0.01	$\pi_{bridge} \rightarrow p_{C\text{-}tris}$
	407	0.13	$\pi_{carbazol} + p_{Cl} \rightarrow p_{N+}\pi_{carbazol}$
5	389	0.15	$p_{C\text{-}tris} \rightarrow \pi^*_{phenyl\text{-}bridge}$
	377	0.09	$p_{C\text{-}tris} \rightarrow \pi^*_{biphenyl}$
6	362	0.015	$\pi_{carbazol} \rightarrow \pi^*_{carbazol}$
	357	0.05	$p_{Cl} \rightarrow p_{N+}\pi_{carbazol}$
			$p_{Cl} \rightarrow p_{N+}\pi_{carbazol}$
			$\pi_{carbazol} \rightarrow \pi^*_{carbazol}$
7	348	0.012	$p_{C\text{-}tris} \rightarrow \pi^*_{phenyl\text{-}bridge}$
			$p_{Cl} \rightarrow \pi^*_{bridge}$
	341	0.022	$\pi_{carbazol} \rightarrow p_{N+}\pi_{carbazol}$

a) $p_{C\text{-}tris}$ corresponds to the p orbital of the trisaryl-substituted carbon atom.

Table S4. Calculated electronic spectra λ (nm), the corresponding oscillator strengths, f_{osc}, and the electronic nature of the transitions for the radical adduct $^1\mathbf{1}^+$.

band	λ (nm)	f_{osc}	Transition nature[a]
1	1295	0.08	$\pi_{carbazol} \rightarrow p^*_{C\text{-}tris}$
2	1226	0.57	$\pi_{carbazol} \rightarrow p^*_{C\text{-}tris}$
3	744	0.047	$\pi_{diphenyl} \rightarrow p^*_{C\text{-}tris}$
	712	0.04	$\pi_{carbazol} \rightarrow p^*_{C\text{-}tris}$
4	670	0.05	$\pi_{bridge} \rightarrow p^*_{C\text{-}tris}$
5	600	0.07	$\pi_{triphenyl} \rightarrow p^*_{C\text{-}tris}$
6	457	0.01	$\pi_{carbazol} \rightarrow p^*_{C\text{-}tris}$
	439	0.009	$\pi_{c\text{-}bridge} \rightarrow p^*_{C\text{-}tris}$
7	379	0.01	$p_{Cl} \rightarrow p^*_{C\text{-}tris}$
	379	0.015	$p_{Cl} \rightarrow p^*_{C\text{-}tris}$
	376	0.01	$n_{SOMO} \rightarrow \pi^*_{triphenyl}$
8	358	0.036	$n_{SOMO} \rightarrow \pi^*_{bridgel}$
	358	0.0248	$p_{Cl} \rightarrow p^*_{C\text{-}tris}$
9	328	0.065	$\pi_{carbazol} \rightarrow \pi^*_{carbazol}$
	321	0.0034	$\sigma_{carbazol} \rightarrow p^*_{C\text{-}tris}$
10	309	0.0140	$p_{Cl} \rightarrow p^*_{C\text{-}tris}$
	296	0.160	$\pi_{carbazol} \rightarrow \pi^*_{carbazol}$
	290	0.017	$\pi_{diphenyl} \rightarrow \pi^*_{bridge}$

a) $p_{C\text{-}tris}$ corresponds to the p orbital of the trisaryl-substituted carbon atom.

Table S5. Calculated electronic spectra λ (nm), the corresponding oscillator strengths, f_{osc}, and the electronic nature of the transitions for the radical adduct ^{2}**2**.

band	λ (nm)	f_{osc}	Transition nature
1	820	0.1391	$\pi_{carbazol} \rightarrow n_{SOMO}$
2	583	0.0012	$\pi_{carbazol} \rightarrow n_{SOMO}$
3	473	0.0188	$\pi_{phenyl} \rightarrow n_{SOMO}$
4	439	0.0026	$\pi_{triphenyl} \rightarrow n_{SOMO}$
	429	0.0287	$\pi_{biphenyl} \rightarrow n_{SOMO}$
			$\pi_{carbazol} \rightarrow \pi^*_{phenyl}$
			$\pi_{triphenyl} \rightarrow n_{SOMO}$
	426	0.0043	$\pi_{diphenyl} \rightarrow n_{SOMO}$

	425	0.0088	$\pi_{carbazol} \rightarrow n_{SOMO}$
5	413	0.2165	$\pi_{carbazol} \rightarrow \pi^*_{phenyl}$
			$\pi_{diphenyl} \rightarrow n_{SOMO}$
6	397	0.0117	$\pi_{carbazol} \rightarrow \pi^*_{carbazol}$
			$\pi_{carbazol} \rightarrow \pi^*_{carbazol}$
	396	0.1796	$\pi_{carbazol} \rightarrow \pi^*_{diohenyl}$
			$n_{SOMO} \rightarrow \pi^*_{diohenyl}$
			$\pi_{diphenyl} \rightarrow n_{SOMO}$
	393	0.0977	$\pi_{triphenyl} \rightarrow n_{SOMO}$
			$\pi_{carbazol} \rightarrow \pi^*_{phenyl}$
	388	0.0162	$\pi_{carbazol} \rightarrow \pi^*_{phenyl}$
			$\pi_{carbazol} \rightarrow \pi^*_{phenyl}$
	373	0.1558	$\pi_{carbazol} \rightarrow \pi^*_{phenyl}$
7	355	0.0393	$\pi_{carbazol} \rightarrow \pi^*_{carbazol}$
			$\pi_{carbazol} \rightarrow \pi^*_{carbazol}$
	348	0.0136	$n_{SOMO} \rightarrow \pi^*_{phenyl}$
			$\pi_{carbazol} \rightarrow \pi^*_{phenyl}$
	341	0.022	$\pi_{carbazol} \rightarrow \pi^*_{diphenyl}$
			$\pi_{carbazol} \rightarrow \pi^*_{triphenyl}$
	324	0.0152	$n_{SOMO} \rightarrow \pi^*_{diohenyl}$
			$\pi_{carbazol} \rightarrow \pi^*_{phenyl}$
	298	0.2330	$\pi_{carbazol} \rightarrow \pi^*_{carbazol}$
			$\pi_{carbazol} \rightarrow \pi^*_{carbazol}$

Table S6. Calculated electronic spectra λ (nm), the corresponding oscillator strengths, f_{osc}, and the electronic nature of the transitions for the radical adduct $^3\mathbf{2}^+$.

band	**λ (nm)**	f_{osc}	**Transition nature**[a]
1	1435	0.0495	$\pi_{carbazol} \rightarrow p_{N+}\pi_{carbazol}$
2	766	0.1063	$\pi_{phenyl} \rightarrow p_{N+}\pi_{carbazol}$
			$\pi_{phenyl} \rightarrow p_{N+}\pi_{carbazol}$
3	696	0.012	$\pi_{diphenyl} \rightarrow p_{N+}\pi_{carbazol}$
			$\pi_{phenyl+carbazol} \rightarrow p_{N+}\pi_{carbazol}$
	668	0.041	$\pi_{diphenyl} \rightarrow p_{N+}\pi_{carbazol}$
4	614	0.0551	$\pi_{diphenyl} \rightarrow p_{N+}\pi_{carbazol}$

5	527	0.047	$\pi_{triphenyl} \rightarrow p_{N+}\pi_{carbazol}$
6	488	0.038	$\pi_{diphenyl} \rightarrow p_{C\text{-}tris}$
	475	0.0298	$\pi_{carbazol} \rightarrow p_{N+}\pi_{carbazol}$
7	418	0.0029	$\pi_{phenyl+carbazol} \rightarrow p_{C\text{-}tris}$
	408	0.1913	$p_{C\text{-}tris} \rightarrow \pi^*_{phenyl}$
			$\pi_{triphenyl} \rightarrow p_{C\text{-}tris}$
			$\pi_{diphenyl} \rightarrow p_{C\text{-}tris}$
8	395	0.0444	$lp_{Cl} \rightarrow p_{N+}\pi_{carbazol}$
	385	0.1388	$p_{C\text{-}tris} \rightarrow \pi^*_{phenyl}$
	381	0.0227	$p_{C\text{-}tris} \rightarrow \pi^*_{carbazol}$
			$\pi_{carbazol} \rightarrow \pi^*_{carbazol}$
	381	0.1864	$p_{C\text{-}tris} \rightarrow \pi^*_{phenyl}$
			$p_{C\text{-}tris} \rightarrow \pi^*_{diphenyl}$
	376	0.0185	$lp_{Cl} \rightarrow p_{N+}\pi_{carbazol}$
9	367	0.0169	$p_{C\text{-}tris} \rightarrow \pi^*_{phenyl}$
			$p_{C\text{-}tris} \rightarrow \pi^*_{diphenyl}$
10	354	0.129	$\pi_{carbazol} \rightarrow \pi^*_{carbazol}$
			$p_{C\text{-}tris} \rightarrow \pi^*_{carbazol}$
11	337	0.0202	$\pi_{carbazol} \rightarrow p_{N+}\pi_{carbazol}$
			$\pi_{carbazol} \rightarrow \pi^*_{carbazol}$
12	324	0.0173	$\pi_{diphenyl} \rightarrow \pi^*_{diphenyl}$
			$p_{C\text{-}tris} \rightarrow \pi^*_{diphenyl}$
			$\pi_{diphenyl} \rightarrow \pi^*_{diphenyl}$

a) $p_{C\text{-}tris}$ corresponds to the p orbital of the trisaryl-substituted carbon atom.

Table S7. Calculated electronic spectra λ (nm), the corresponding oscillator strengths, f_{osc}, and the electronic nature of the transitions for the radical adduct $^{1}\mathbf{2}^{+}$.

band	λ (nm)	f_{osc}	Transition nature[a]
1	903	0.2562	$\pi_{carbazol} \rightarrow p^*_{C\text{-}tris}$
			$\pi_{carbazol} \rightarrow p^*_{C\text{-}tris}$
2	869	0.771	$\pi_{carbazol} \rightarrow p^*_{C\text{-}tris}$
			$\pi_{carbazol} \rightarrow p^*_{C\text{-}tris}$
3	572	0.0895	$\pi_{carbazol} \rightarrow p^*_{C\text{-}tris}$
			$\pi_{carbazol} \rightarrow p^*_{C\text{-}tris}$

4	566	0.072	$\pi_{diphenyl} \rightarrow p^*_{C\text{-}tris}$
			$\pi_{phenyl} \rightarrow p^*_{C\text{-}tris}$
	561	0.001	$\pi_{triphenyl} \rightarrow p^*_{C\text{-}tris}$
5	538	0.013	$\pi_{diphenyl} \rightarrow p^*_{C\text{-}tris}$
6	512	0.048	$\pi_{diphenyl} \rightarrow p^*_{C\text{-}tris}$
			$\pi_{triphenyl} \rightarrow p^*_{C\text{-}tris}$
7	491	0.078	$\pi_{phenyl} \rightarrow p^*_{C\text{-}tris}$
	370	0.016	$\pi_{C\text{-}tris\text{-}Cpheny} \rightarrow p^*_{C\text{-}tris}$
	347	0.064	$\pi_{carbazol} \rightarrow lp_N$
8	342	0.004	$\pi_{carbazol} \rightarrow \pi^*_{diphenyl}$
			$\pi_{carbazol} \rightarrow \pi^*_{triphenyl}$
9	332	0.029	$\pi_{carbazol} \rightarrow p^*_{C\text{-}tris}$
	330	0.078	$\pi_{carbazol} \rightarrow \pi^*_{diphenyl}$
			$\pi_{carbazol} \rightarrow \pi^*_{triphenyl}$
	325	0.020	$lp_{Cl} \rightarrow p^*_{C\text{-}tris}$
	324	0.033	$\pi_{carbazol} \rightarrow \pi^*_{carbazol}$
	295	0.208	$\pi_{carbazol} \rightarrow \pi^*_{carbazol}$
			$\pi_{carbazol} \rightarrow p^*_{C\text{-}tris}$

a) $p_{C\text{-}tris}$ corresponds to the p orbital of the trisaryl-substituted carbon atom.

Table S8. Cartesian coordinates of the optimized structures.

Adduct ^{2}**1**.

6	6.390357	-3.037298	-0.714032
6	5.034226	-3.409447	-0.811754
6	4.016401	-2.491849	-0.597786
6	4.371998	-1.181946	-0.277639
6	5.723327	-0.791821	-0.180443
6	6.744007	-1.727280	-0.400692
7	3.555760	-0.071022	-0.027786
6	4.380452	1.030904	0.232144
6	5.733421	0.618730	0.147653
6	6.752122	1.540844	0.378518
6	6.419261	2.860022	0.690287
6	5.072597	3.254732	0.775078
6	4.042838	2.339410	0.547592
6	1.432316	0.485586	-1.100234
6	0.033928	0.501132	-1.093673

6	-0.710898	-0.034618	-0.015133
6	0.030649	-0.588692	1.056343
6	1.429156	-0.600586	1.052929
6	2.151536	-0.063328	-0.025554
6	-2.188306	-0.013210	-0.006926
6	-4.648915	2.478517	-1.509492
6	-4.287714	3.656140	-0.868627
6	-3.249258	3.645952	0.052938
6	-2.570642	2.459386	0.345900
6	-2.909172	1.243275	-0.300883
6	-3.968988	1.286419	-1.242576
6	-2.943268	-1.247059	0.296904
6	-3.990184	-1.258376	1.253691
6	-4.701792	-2.429503	1.530383
6	-4.385531	-3.617093	0.884099
6	-3.360722	-3.637971	-0.052524
6	-2.650824	-2.472188	-0.354978
17	-4.392252	-0.118905	-2.167251
17	-1.369391	2.494515	1.597952
17	-4.356742	0.158865	2.184578
17	-1.469289	-2.541945	-1.623869
17	-0.783028	-1.165356	2.476771
17	-0.779057	1.092179	-2.508640
17	-3.017592	-5.145629	-0.843350
17	-5.983080	-2.462737	2.702397
17	-2.849268	5.143040	0.837771
17	-5.945529	2.550360	-2.662721
17	2.316329	1.096200	-2.456523
17	2.310460	-1.228960	2.402803
8	7.285034	-4.044862	-0.948793
1	4.804664	-4.440857	-1.061046
1	2.977261	-2.796029	-0.678386
1	7.781023	-1.420938	-0.327797
1	7.800144	1.261136	0.325719
8	7.476099	3.704566	0.900949
1	4.812326	4.277515	1.019799
1	3.007467	2.658723	0.617758
1	-4.813766	4.577809	-1.086087
1	-4.935884	-4.522625	1.109093
6	8.666027	-3.750079	-0.857607
1	9.187809	-4.686358	-1.069714
1	8.962854	-2.991134	-1.595875
1	8.934397	-3.401871	0.150293
6	7.211789	5.058544	1.215869
1	8.188575	5.533898	1.334681
1	6.659793	5.558872	0.407189
1	6.646281	5.150209	2.15436

Cation $^{3}\mathbf{1}^{+}$.

6	6.322279	-2.936895	-1.096315
6	4.950363	-3.281947	-1.220825
6	3.958652	-2.388795	-0.883414
6	4.352091	-1.126698	-0.412909
6	5.720291	-0.763774	-0.279108
6	6.712900	-1.663357	-0.619313
7	3.567270	-0.065813	-0.017064
6	4.372338	0.991013	0.377013
6	5.732245	0.604957	0.233319
6	6.728904	1.492526	0.567610
6	6.366323	2.779829	1.050396
6	5.012534	3.146502	1.185327
6	4.004789	2.250445	0.847507
6	1.441922	0.368254	-1.150862
6	0.042807	0.368554	-1.151751
6	-0.698691	-0.028216	-0.009841
6	0.039323	-0.440490	1.128790
6	1.438227	-0.466003	1.122844
6	2.140297	-0.054921	-0.015075
6	-2.177139	-0.011464	-0.006134
6	-4.643145	2.259580	-1.814516
6	-4.284900	3.509446	-1.325074
6	-3.243970	3.623040	-0.412198
6	-2.560791	2.484434	0.023615
6	-2.897661	1.195314	-0.460425
6	-3.957311	1.112626	-1.399987
6	-2.923611	-1.200762	0.451675
6	-3.976952	-1.093104	1.395785
6	-4.688479	-2.223359	1.812554
6	-4.362373	-3.481181	1.320961
6	-3.327921	-3.619528	0.404053
6	-2.619213	-2.497375	-0.033943
17	-4.370942	-0.398828	-2.140415
17	-1.355961	2.680115	1.261938
17	-4.350256	0.427581	2.139188
17	-1.423743	-2.721203	-1.276110
17	-0.764228	-0.836089	2.606897
17	-0.758666	0.777016	-2.627478
17	-2.972073	-5.210590	-0.186281
17	-5.975244	-2.112154	2.966935
17	-2.847910	5.205655	0.176208
17	-5.937009	2.178923	-2.963406
17	2.341101	0.851800	-2.548500
17	2.333458	-0.967762	2.516621
8	7.178006	-3.892895	-1.458767
1	4.710929	-4.273247	-1.591026
1	2.911009	-2.654601	-0.978897

1	7.759454	-1.399718	-0.523797
1	7.784385	1.254269	0.480292
8	7.398770	3.572442	1.350084
1	4.743649	4.128848	1.552873
1	2.961525	2.531561	0.950113
1	-4.816892	4.394022	-1.654656
1	-4.914140	-4.352927	1.652263
6	8.591884	-3.674201	-1.383865
1	9.045108	-4.601277	-1.735904
1	8.887139	-2.843810	-2.035512
1	8.896430	-3.479817	-0.349035
6	7.170984	4.896012	1.848930
1	8.163407	5.318324	2.009014
1	6.623640	5.494893	1.111942
1	6.622349	4.859119	2.797113

Cation $^{1}\mathbf{1}^{+}$.

6	6.357092	-3.089980	-0.499298
6	4.994412	-3.459277	-0.569614
6	3.988309	-2.525111	-0.408491
6	4.357360	-1.201611	-0.153544
6	5.711577	-0.812045	-0.108912
6	6.721967	-1.751312	-0.282050
7	3.547821	-0.059344	-0.015611
6	4.387279	1.063995	0.125713
6	5.733713	0.631989	0.081816
6	6.757999	1.543314	0.256658
6	6.437190	2.898283	0.474175
6	5.093455	3.310163	0.542831
6	4.059735	2.390333	0.379526
6	1.438833	0.716565	-0.966384
6	0.051442	0.737912	-0.958925
6	-0.714712	-0.017122	-0.002983
6	0.042314	-0.783748	0.951109
6	1.429717	-0.788599	0.951306
6	2.162468	-0.043742	-0.010238
6	-2.146868	-0.007831	-0.001826
6	-4.690845	2.498565	-1.313475
6	-4.364664	3.626557	-0.568955
6	-3.312063	3.589564	0.339276
6	-2.572080	2.417106	0.513777
6	-2.888071	1.243446	-0.226957
6	-3.964994	1.314810	-1.151872
6	-2.902402	-1.250230	0.224402
6	-3.978796	-1.309101	1.150893
6	-4.717334	-2.484617	1.314399
6	-4.404705	-3.616626	0.570077
6	-3.353458	-3.591883	-0.340140
6	-2.600800	-2.427686	-0.516553

17	-4.323402	-0.008636	-2.207114
17	-1.351244	2.408719	1.745893
17	-4.320983	0.018858	2.206028
17	-1.383039	-2.433478	-1.751518
17	-0.751419	-1.539516	2.287295
17	-0.734459	1.512051	-2.289268
17	-3.032435	-5.031466	-1.244560
17	-6.019265	-2.591428	2.446906
17	-2.973440	5.025255	1.243967
17	-5.993287	2.620314	-2.443863
17	2.311655	1.457052	-2.261675
17	2.295476	-1.544681	2.242031
8	7.232124	-4.096406	-0.672246
1	4.759249	-4.500768	-0.762807
1	2.949302	-2.826972	-0.483587
1	7.761288	-1.446039	-0.265642
1	7.803031	1.250021	0.249938
8	7.492043	3.721059	0.623056
1	4.844979	4.346932	0.732293
1	3.029656	2.722028	0.453698
1	-4.932789	4.540724	-0.698535
1	-4.982532	-4.524464	0.701294
6	8.632603	-3.829761	-0.621766
1	9.119411	-4.794161	-0.773628
1	8.926690	-3.137341	-1.420552
1	8.916419	-3.421294	0.356242
6	7.276518	5.113035	0.848721
1	8.271660	5.553985	0.923257
1	6.733180	5.564928	0.009452
1	6.728519	5.276721	1.785131

Cation ^{2}**1H**$^{+}$.

6	6.277938	-3.013046	-1.061202
6	4.898784	-3.343925	-1.134493
6	3.928396	-2.429065	-0.793400
6	4.350895	-1.158971	-0.371725
6	5.726861	-0.809548	-0.290959
6	6.697898	-1.731152	-0.634114
7	3.591782	-0.077392	0.018062
6	4.421194	0.980226	0.355760
6	5.771118	0.573206	0.180102
6	6.788249	1.457814	0.455346
6	6.456610	2.763527	0.910039
6	5.112211	3.150611	1.078075
6	4.083811	2.257324	0.800428
6	1.430977	0.364224	-1.043391
6	0.028068	0.388418	-0.995296
6	-0.670962	0.026172	0.173211

6	0.102398	-0.387085	1.281744
6	1.500702	-0.435976	1.235642
6	2.165801	-0.049139	0.069927
6	-2.194789	0.137491	0.387162
6	-4.531723	2.256904	-1.906146
6	-4.265554	3.532036	-1.429575
6	-3.322860	3.706086	-0.426809
6	-2.661426	2.596899	0.109566
6	-2.909527	1.285771	-0.354796
6	-3.855963	1.141063	-1.387801
6	-2.961526	-1.191921	0.532005
6	-4.048873	-1.204350	1.434957
6	-4.768415	-2.375478	1.698990
6	-4.407107	-3.566928	1.086494
6	-3.339888	-3.586005	0.201096
6	-2.627906	-2.412327	-0.084798
17	-4.184817	-0.395799	-2.119668
17	-1.516387	2.878579	1.397214
17	-4.524562	0.249370	2.264502
17	-1.374936	-2.518427	-1.286241
17	-0.662049	-0.840947	2.770628
17	-0.792837	0.813325	-2.454155
17	-2.934684	-5.100276	-0.543113
17	-6.108502	-2.394630	2.796157
17	-3.013871	5.317140	0.135366
17	-5.708611	2.098409	-3.168789
17	2.287768	0.820539	-2.476472
17	2.432370	-0.947131	2.600792
8	7.110739	-3.990148	-1.420220
1	4.636419	-4.342299	-1.468375
1	2.875385	-2.684745	-0.849450
1	7.749903	-1.478195	-0.577638
1	7.837520	1.203937	0.341222
8	7.507387	3.551985	1.150861
1	4.866674	4.146700	1.424372
1	3.047851	2.554556	0.928492
1	-4.788741	4.387192	-1.840522
1	-4.957794	-4.476229	1.295822
6	8.528958	-3.788287	-1.393324
1	8.959763	-4.731474	-1.730346
1	8.815190	-2.981732	-2.078072
1	8.866432	-3.567360	-0.374160
6	7.311590	4.893574	1.614183
1	8.313591	5.308048	1.728391
1	6.747410	5.475637	0.876441
1	6.793840	4.893770	2.580270
1	-2.227533	0.507772	1.414833

Adduct ^{2}**2**.

6	6.278789	-3.131832	-0.043049
6	4.922801	-3.515415	-0.061150
6	3.903435	-2.575369	-0.042912
6	4.251494	-1.222814	0.001968
6	5.604958	-0.826902	-0.000480
6	6.628060	-1.784180	-0.019560
7	3.435076	-0.079182	-0.009868
6	4.272169	1.049167	-0.016630
6	5.622852	0.620188	-0.007166
6	6.653998	1.555920	0.017463
6	6.339725	2.915470	0.040130
6	4.997511	3.332401	0.051286
6	3.956325	2.402517	0.026795
6	1.326513	0.747625	-0.901088
6	-0.058823	0.758759	-0.887195
6	-0.840207	-0.031330	-0.004205
6	-0.074922	-0.840604	0.875489
6	1.310494	-0.862056	0.885106
6	2.032311	-0.065154	-0.008741
6	-2.305735	-0.012537	-0.000836
6	-4.784494	2.744366	-0.938488
6	-4.425124	3.744308	-0.043928
6	-3.391112	3.549622	0.862927
6	-2.718801	2.333926	0.865612
6	-3.027680	1.270154	-0.018639
6	-4.090410	1.541149	-0.916292
6	-3.060819	-1.275996	0.019971
6	-4.125562	-1.519690	0.922896
6	-4.850950	-2.704167	0.947679
6	-4.522579	-3.712438	0.050466
6	-3.488177	-3.544362	-0.861313
6	-2.784237	-2.346731	-0.866501
17	-4.548068	0.386424	-2.144829
17	-1.503604	2.150850	2.108030
17	-4.546143	-0.354038	2.154486
17	-1.570685	-2.194023	-2.114388
17	-0.849037	-1.794427	2.121115
17	-0.814101	1.730064	-2.131246
1	-3.243131	-4.322184	-1.574143
1	-5.644923	-2.840752	1.671606
1	-3.122636	4.321044	1.574263
1	-5.578291	2.901200	-1.658491
1	1.856138	1.336137	-1.640300
1	1.828235	-1.463453	1.622402
8	7.174003	-4.163584	-0.058832
1	4.692479	-4.575871	-0.093949
1	2.868785	-2.898942	-0.074520
1	7.663851	-1.465217	-0.023444
1	7.697737	1.256180	0.028031

8	7.405341	3.772253	0.058025
1	4.748316	4.386245	0.082534
1	2.929003	2.749084	0.053201
17	-5.281980	5.261753	-0.059387
17	-5.419276	-5.206461	0.068921
6	8.555510	-3.854397	-0.049909
1	9.077790	-4.813931	-0.062908
1	8.839946	-3.271306	-0.937593
1	8.834343	-3.298298	0.856650
6	7.157204	5.165531	0.099519
1	8.139750	5.643503	0.108826
1	6.598067	5.500158	-0.785930
1	6.606324	5.448146	1.008016

Cation $^{3}\mathbf{2}^{+}$.

6	-6.214622	-3.125406	0.350115
6	-4.843825	-3.488968	0.400041
6	-3.849591	-2.541582	0.292805
6	-4.237628	-1.202497	0.123409
6	-5.606120	-0.820329	0.084453
6	-6.600962	-1.774199	0.196468
7	-3.450219	-0.072263	0.009632
6	-4.263594	1.047773	-0.103961
6	-5.622682	0.632514	-0.063171
6	-6.626416	1.566996	-0.175949
6	-6.275341	2.934452	-0.332235
6	-4.923970	3.330107	-0.382753
6	-3.908583	2.386556	-0.273593
6	-1.337851	0.640957	0.997989
6	0.051886	0.644874	0.989588
6	0.819256	-0.026108	0.003190
6	0.063756	-0.712665	-0.981817
6	-1.325786	-0.739075	-0.986137
6	-2.021762	-0.056969	0.007185
6	2.293385	-0.012110	0.002119
6	4.778269	2.642893	1.166536
6	4.411669	3.723955	0.372961
6	3.364435	3.615171	-0.535915
6	2.690572	2.406867	-0.641538
6	3.011287	1.263192	0.131701
6	4.085363	1.446031	1.041133
6	3.034101	-1.274291	-0.128230
6	4.109390	-1.438287	-1.039637
6	4.822701	-2.622857	-1.166662
6	4.476456	-3.710257	-0.372480
6	3.429462	-3.619674	0.538711
6	2.735022	-2.423235	0.645996
17	4.552821	0.183661	2.150347
17	1.457842	2.337617	-1.882201

17	4.552717	-0.167553	-2.149514
17	1.504632	-2.374937	1.889624
17	0.836013	-1.501270	-2.325718
17	0.810645	1.451312	2.330883
1	3.172515	-4.459112	1.173276
1	5.625374	-2.698524	-1.890250
1	3.091919	4.449855	-1.170241
1	5.581085	2.732528	1.888373
1	-1.872040	1.141002	1.797836
1	-1.851250	-1.251304	-1.784085
8	-7.073125	-4.140018	0.465543
1	-4.604074	-4.538886	0.531734
1	-2.804060	-2.825344	0.343935
1	-7.646558	-1.491229	0.172300
1	-7.679612	1.304625	-0.156445
8	-7.313405	3.769711	-0.430227
1	-4.661779	4.372498	-0.513087
1	-2.869075	2.692575	-0.325330
17	5.268858	5.226537	0.517292
17	5.359140	-5.197598	-0.518936
6	-8.485630	-3.904508	0.436156
1	-8.943734	-4.887875	0.545608
1	-8.785150	-3.258952	1.269925
1	-8.781431	-3.459738	-0.521051
6	-7.094057	5.175766	-0.596427
1	-8.089205	5.618742	-0.645116
1	-6.544813	5.582680	0.260402
1	-6.551220	5.372177	-1.528243

Cation $^{1}\mathbf{2}^{+}$.

6	-6.274873	-3.129145	-0.026739
6	-4.919262	-3.518813	-0.005677
6	-3.897689	-2.583996	-0.007606
6	-4.240537	-1.228838	-0.055227
6	-5.589908	-0.829595	-0.030055
6	-6.615836	-1.769696	-0.021126
7	-3.416790	-0.074289	0.001820
6	-4.267147	1.062183	0.058821
6	-5.610886	0.624042	0.033969
6	-6.648114	1.538541	0.025286
6	-6.347871	2.912091	0.030941
6	-5.009578	3.340761	0.010432
6	-3.962597	2.418625	0.011575
6	-1.330757	0.907939	0.742197
6	0.039480	0.920580	0.742025
6	0.843181	-0.025418	-0.002365
6	0.060023	-0.988621	-0.746790
6	-1.310147	-1.007582	-0.744435

6	-2.048392	-0.058551	0.000021
6	2.259581	-0.011147	-0.001483
6	4.814183	2.667941	0.920729
6	4.507364	3.654514	-0.012296
6	3.465366	3.481061	-0.920225
6	2.726282	2.309073	-0.884154
6	3.002762	1.255318	0.029085
6	4.076861	1.493575	0.927287
6	3.027821	-1.262479	-0.030228
6	4.108900	-1.479175	-0.925576
6	4.869406	-2.638531	-0.917213
6	4.579804	-3.631278	0.014892
6	3.532094	-3.478788	0.920052
6	2.769894	-2.321791	0.882258
17	4.459420	0.368664	2.199513
17	1.497934	2.159874	-2.113724
17	4.472348	-0.346596	-2.196702
17	1.535953	-2.197277	2.108793
17	0.801627	-2.075344	-1.885368
17	0.757568	2.025554	1.878525
1	3.322126	-4.245933	1.655523
1	5.666669	-2.772421	-1.638398
1	3.242402	4.243576	-1.656672
1	5.606823	2.817669	1.643890
1	-1.860863	1.577696	1.406287
1	-1.825817	-1.689364	-1.407663
8	-7.165084	-4.139245	-0.028607
1	-4.694306	-4.579933	0.025140
1	-2.871008	-2.923502	0.051194
1	-7.649506	-1.446631	0.007251
1	-7.688557	1.230690	-0.003692
8	-7.411911	3.738603	0.033803
1	-4.770317	4.396461	-0.019060
1	-2.944826	2.784244	-0.047864
17	5.428615	5.116825	-0.042025
17	5.529824	-5.074765	0.046793
6	-8.559781	-3.843218	-0.031689
1	-9.064525	-4.810425	-0.042409
1	-8.843709	-3.288882	0.871980
1	-8.836099	-3.272022	-0.927103
6	-7.206336	5.149429	0.020858
1	-8.204311	5.590354	0.033048
1	-6.649144	5.472120	0.909468
1	-6.677217	5.459525	-0.889212

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