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DFT study of the stabilization preconditions of the indoline spiropyrans with a cationic substituent

Vitaliy V. Koval, Anastasia S. Kozlenko and Boris S. Lukyanov

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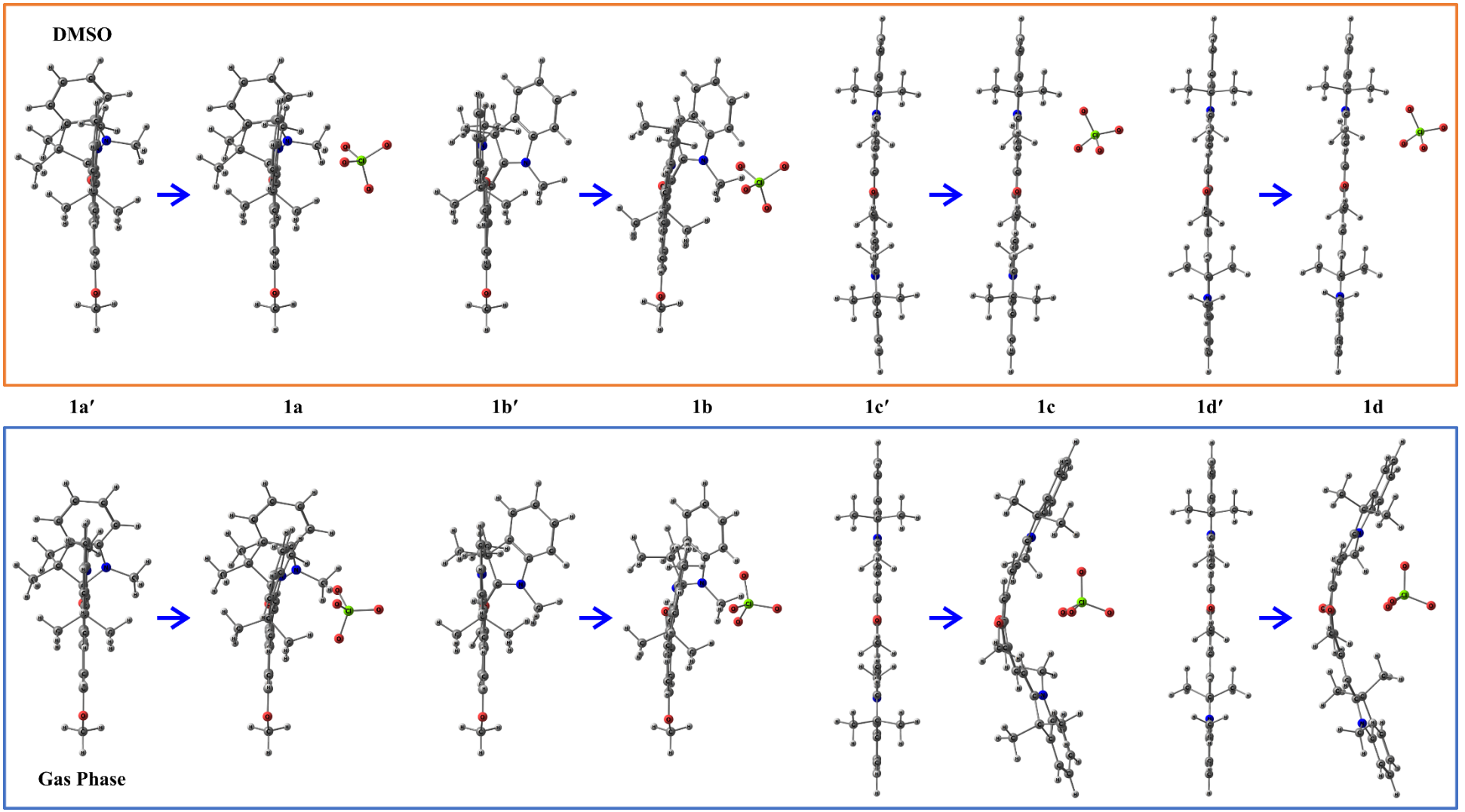


Figure S1 The quality geometry changes in the structures of the compound **1** upon going from structures without an anion to structures with an anion in DMSO and in the gas phase (updated early data [30]). For the structures **1a, 1a′, 1b, 1b′ -** profile view of molecule, for the structures **1c, 1c′, 1d, 1d′ -** bottom view of molecule.

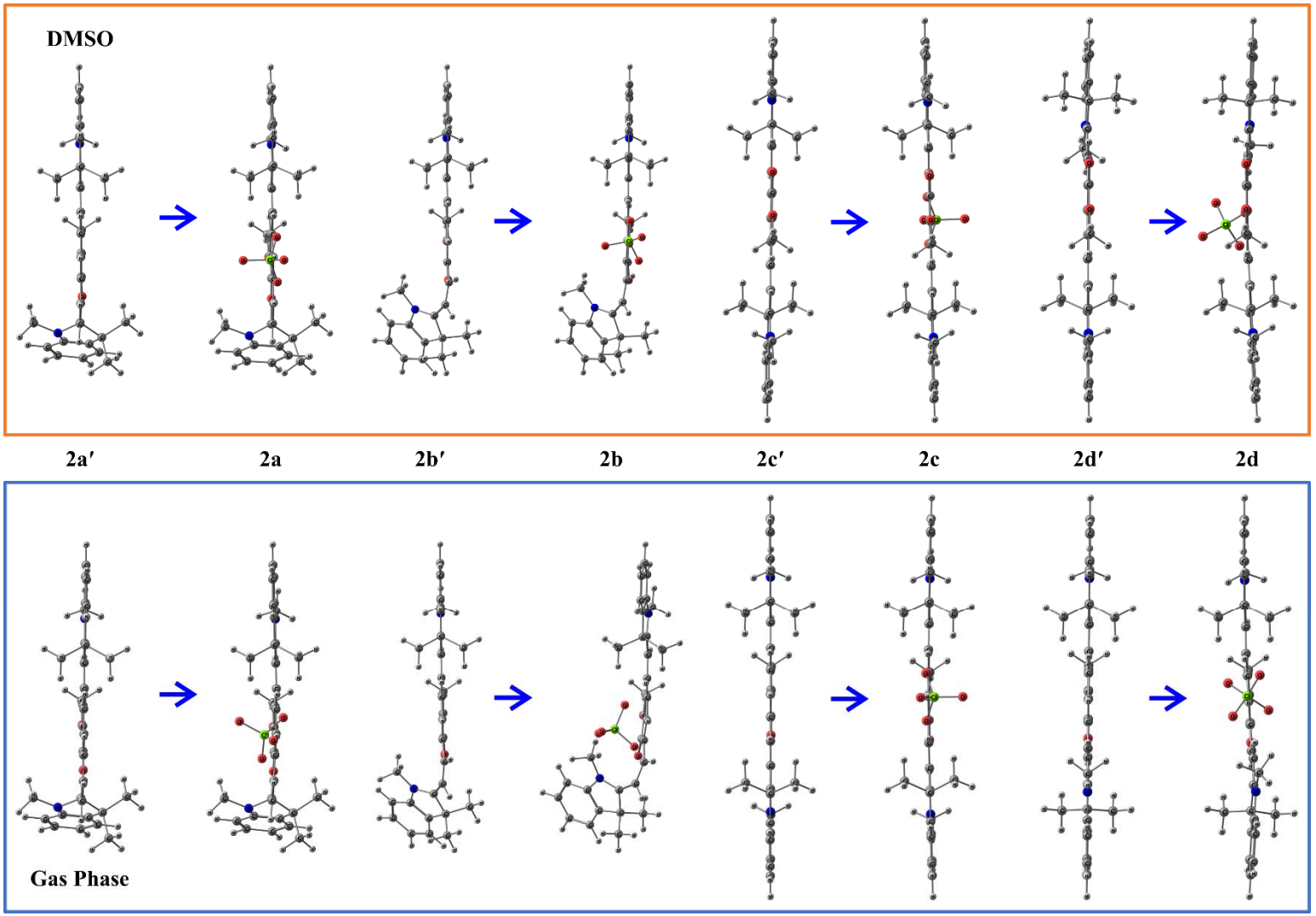
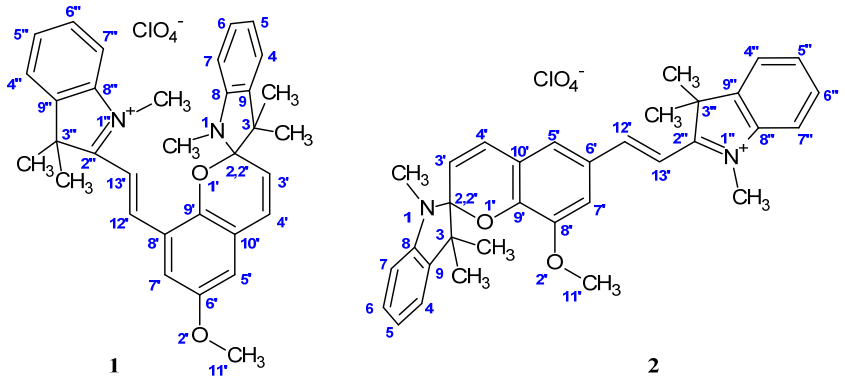


Figure S2 The quality geometry changes in the structures of the compound **2** upon going from structures without an anion to structures with an anion in DMSO and in the gas phase (updated early data [30]). For the structures **2a, 2a′, 2b, 2b′ -** profile view of molecule, for the structures **2c, 2c′, 2d, 2d′ -** bottom view of molecule).



Scheme S1 Scheme of atoms labeling in compounds **1** and **2.**

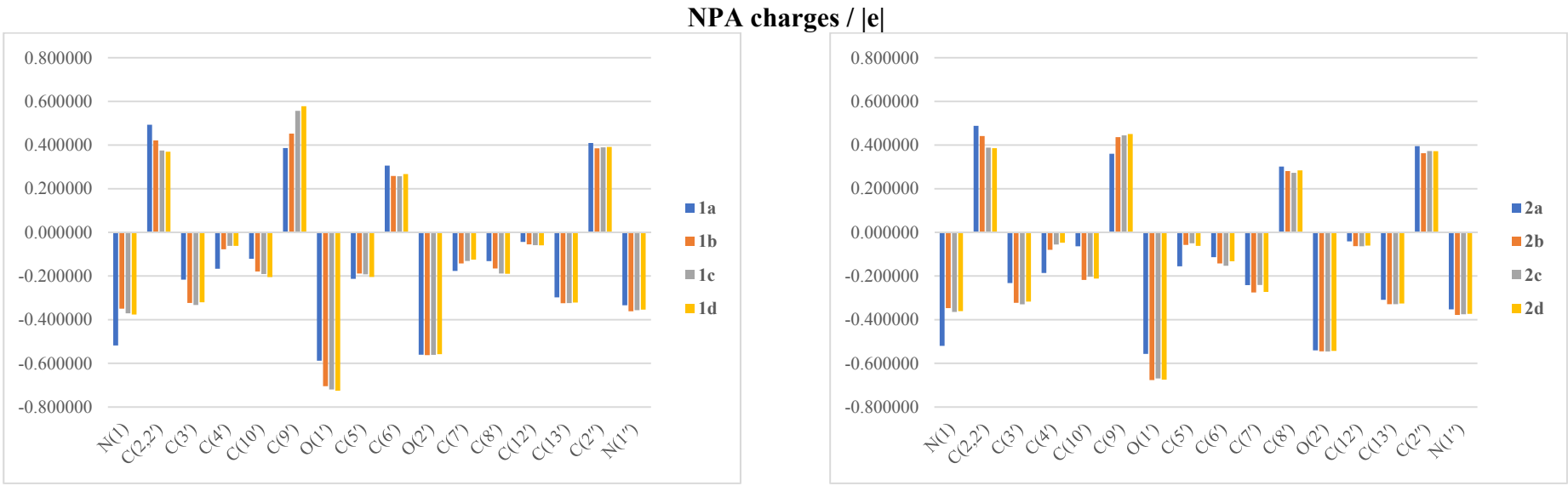


Figure S3 Histograms of the atom charges for isomeric structures **1a-1d** and **2a-2d** according to calculations of the NPA charges.

Figure S4 Histograms of the atom charges for isomeric structures **1a-1d** and **2a-2d** according to calculations of the ESP charges.

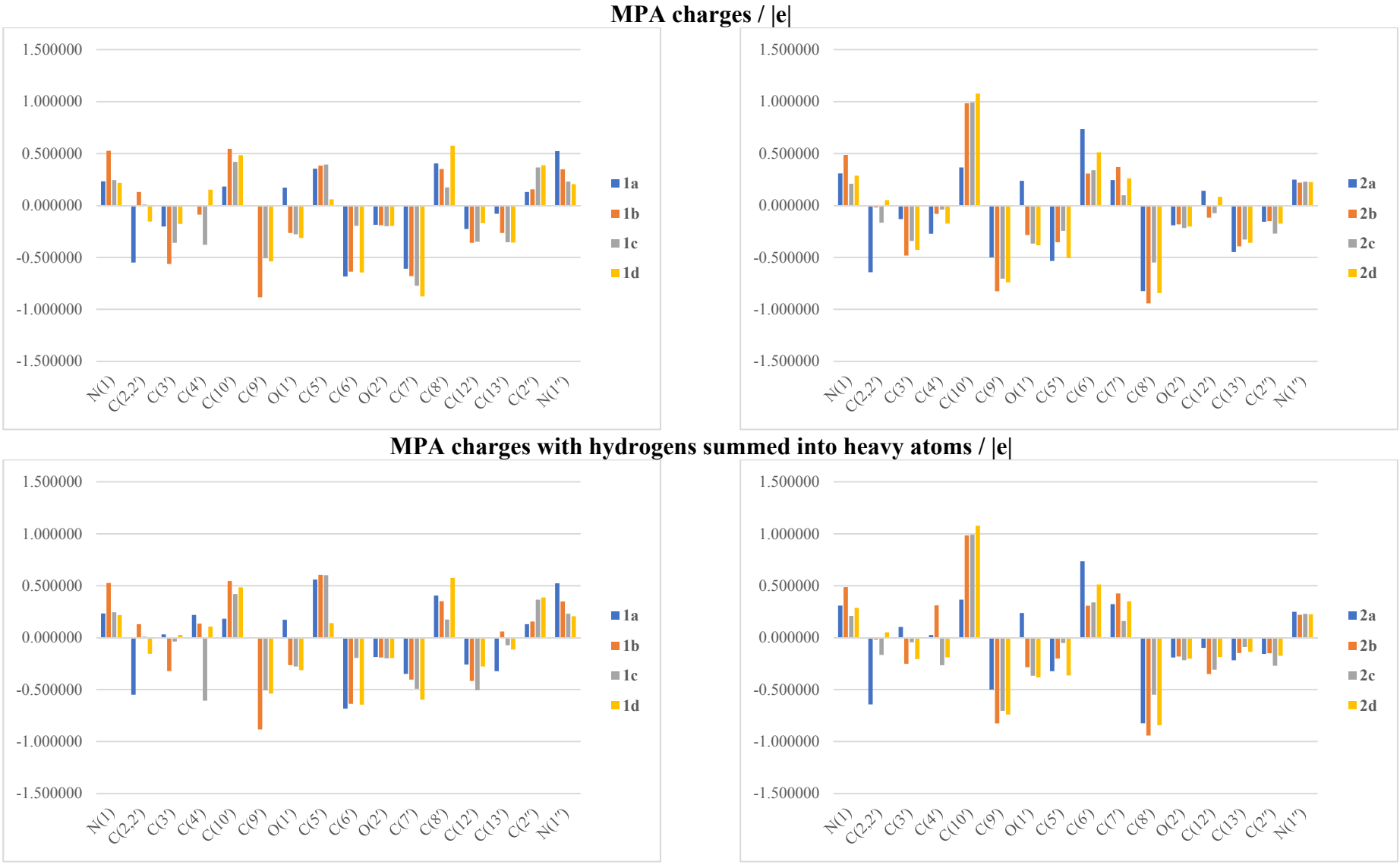


Figure S5 Histograms of the atom charges for isomeric structures **1a-1d** and **2a-2d** according to calculations of the MPA charges.

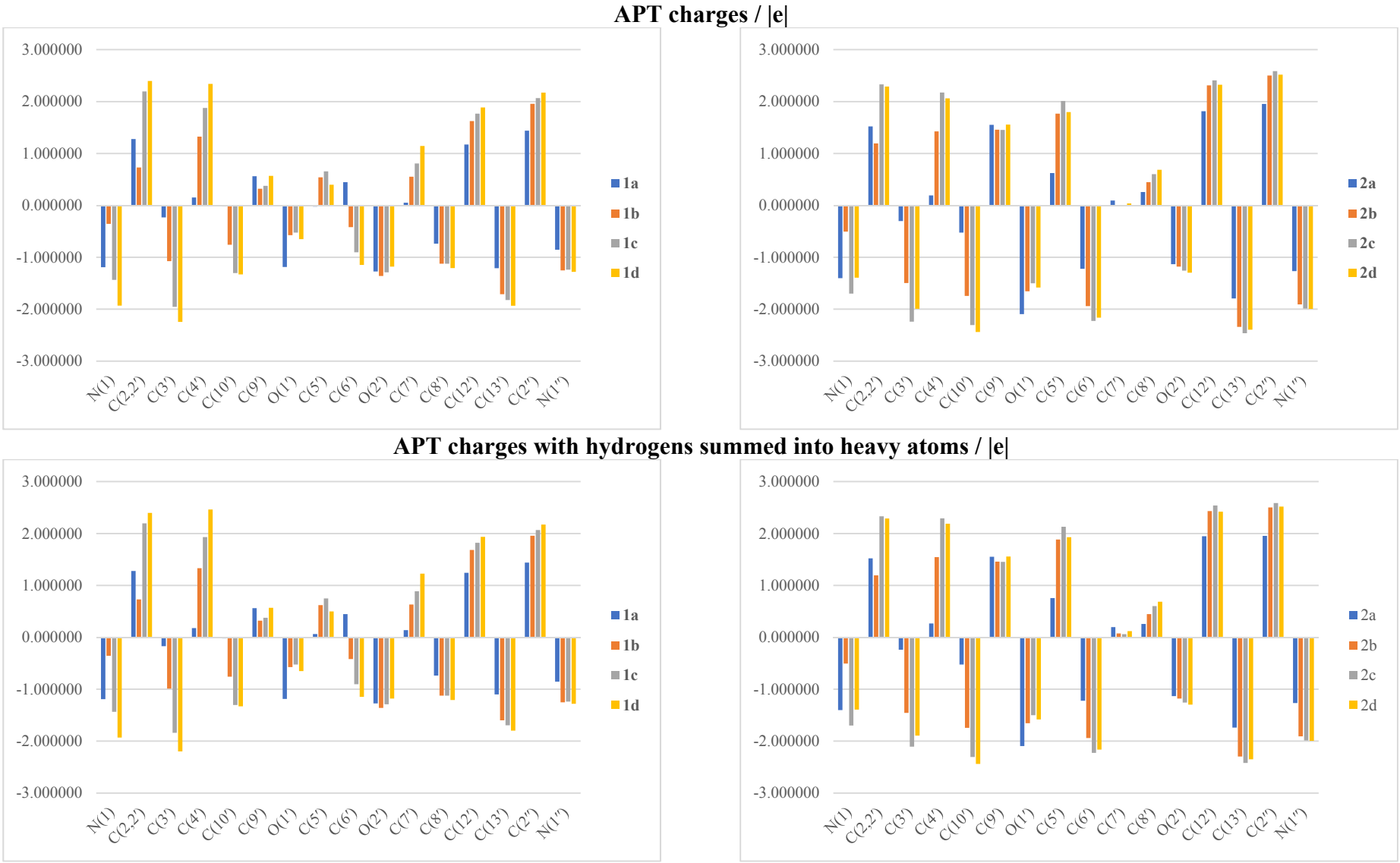
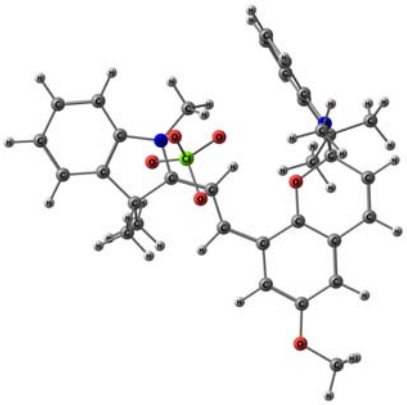
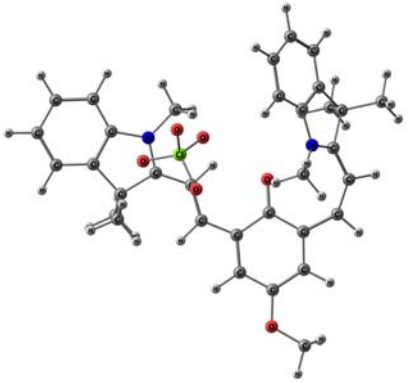
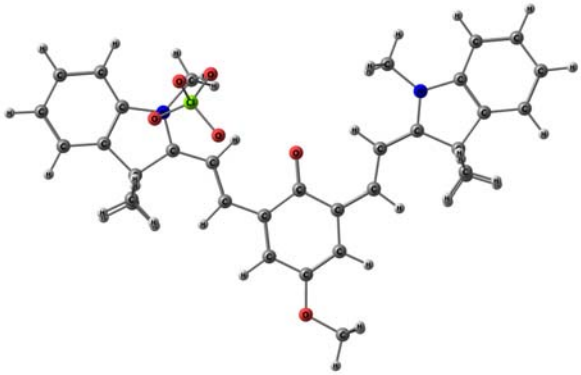
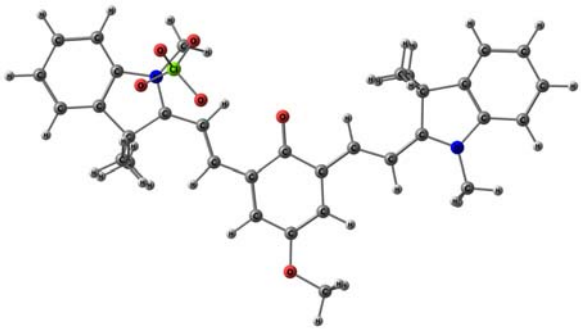
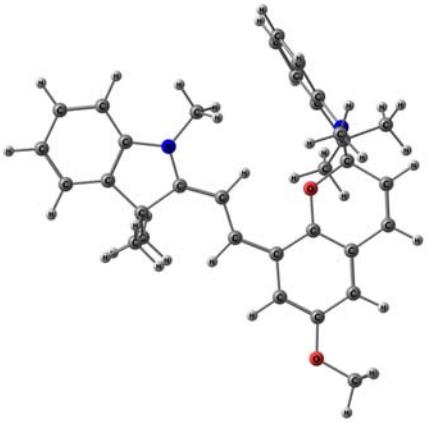
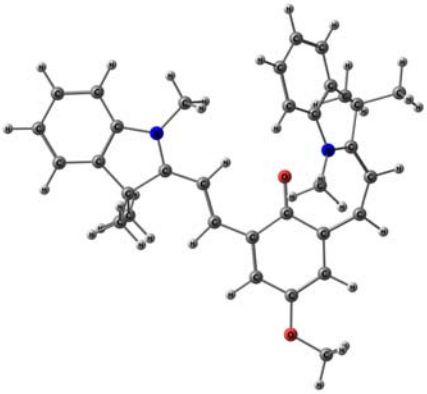
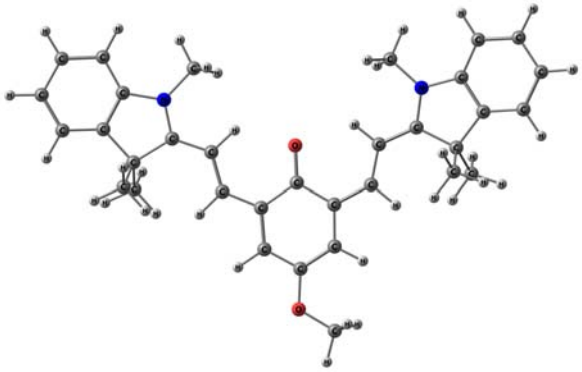
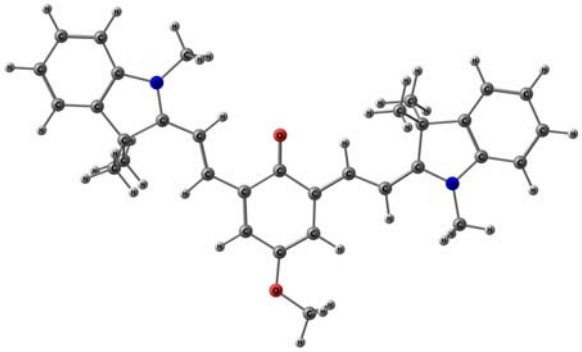
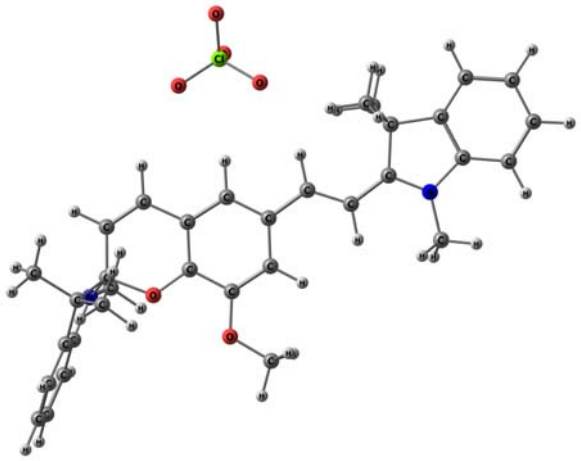
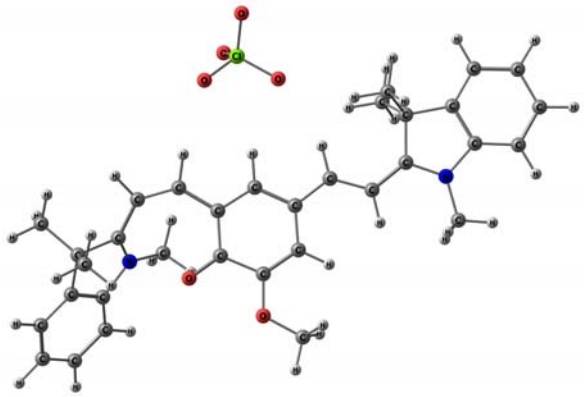
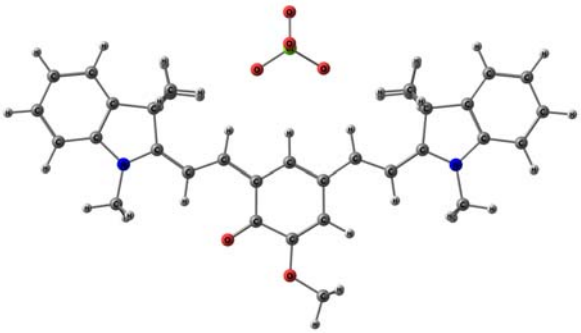
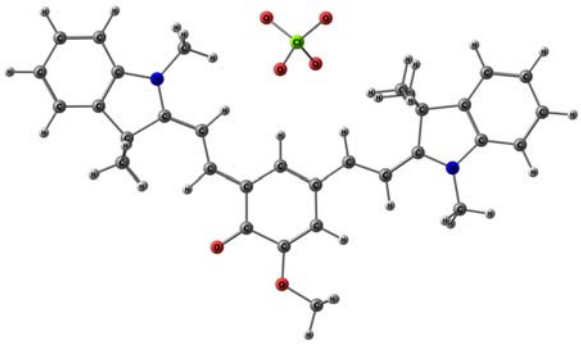


Figure S6 Histograms of the atom charges for isomeric structures **1a-1d** and **2a-2d** according to calculations of the APT charges.

Table S1 Graphical summary of the compounds **1** and **2** and the links to sections with calculation experiment details.

Structure	**Calculation visualization (front view of molecule)**	**Geo-metry**	**Over-view**
SP form **1a**		g.1a	o.1a
Cis-isomer of *MC* form **1b**		g.1b	o.1b
TTC-TTC isomer of *MC* form **1c**		g.1c	o.1c
TTT-TTC isomer of *MC* form **1d**		g.1d	o.1d

SP form without perchlorate anion **1a′**		g.1a′	o.1a′
Cis-isomer of *MC* form without perchlorate anion **1b′**		g.1b′	o.1b′
TTC-TTC isomer of *MC* form without perchlorate anion **1c′**		g.1c′	o.1c′
TTT-TTC isomer of *MC* form without perchlorate anion **1d′**		g.1d′	o.1d′

Structure	Calculation visualization (front view of molecule)	Geo-metry	Over-view
SP form **2a**		g.2a	o.2a
Cis-isomer of *MC* form **2b**		g.2b	o.2b
TTC-TTC isomer of *MC* form **2c**		g.2c	o.2c
TTT-TTC isomer of *MC* form **2d**		g.2d	o.2d

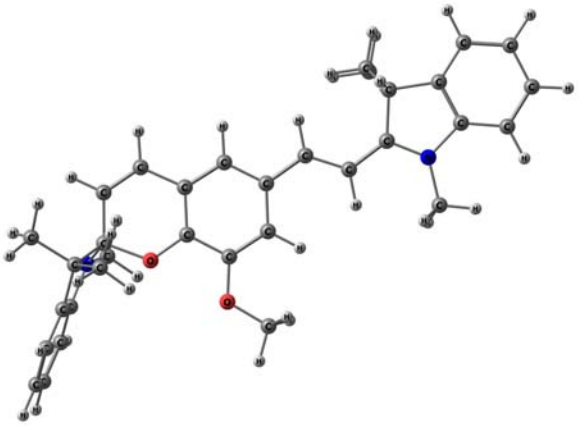
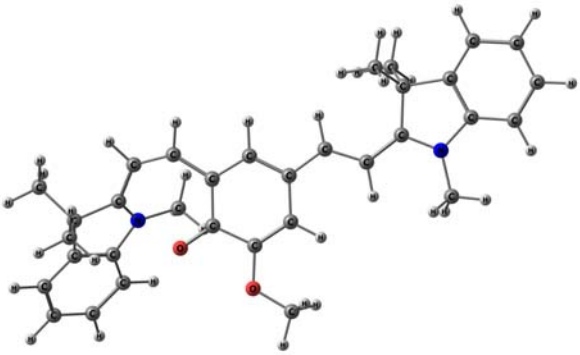
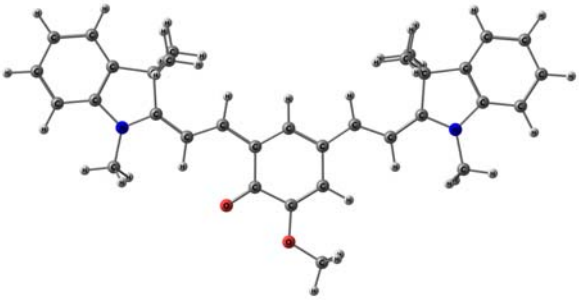
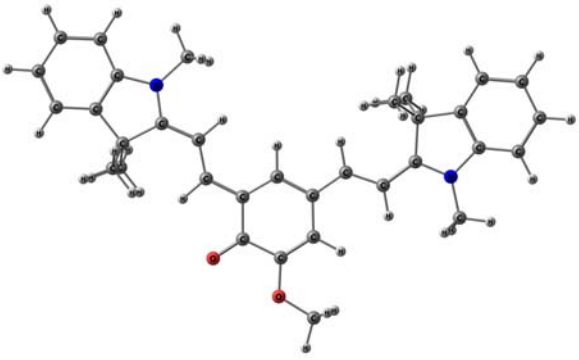
SP form without perchlorate anion **2a′**		g.2a′	o.2a′
Cis-isomer of *MC* form without perchlorate anion **2b′**		g.2b′	o.2b′
TTC-TTC isomer of *MC* form without perchlorate anion **2c′**		g.2c′	o.2c′
TTT-TTC isomer of *MC* form without perchlorate anion **2d′**		g.2d′	o.2d′

Table S2 The lengths of some bonds, distances (Å) and angles (°) for the structures **1a** and **2d** calculated by B3LYP/6-311++G(d,p) method in DMSO and obtained from updated early calculations in the gas phase [30], and from XRD data [20].

Structure 1a				**Structure 2d**			
Bond	**Gas**	**DMSO**	**XRD**	**Bond**	**Gas**	**DMSO**	**XRD**
N(1)–C(2,2′)	1.439	1.441	1.448(4)	N(1)–C(2,2′)	1.349	1.343	1.341(2)
C(2,2′)–C(3′)	1.498	1.499	1.497(5)	C(2,2′)–C(3′)	1.404	1.411	1.402(2)
C(3′)–C(4′)	1.336	1.336	1.317(5)	C(3′)–C(4′)	1.381	1.376	1.374(2)
C(4′)–C(10′)	1.451	1.454	1.451(5)	C(4′)–C(10′)	1.419	1.425	1.419(2)
C(10′)–C(9′)	1.403	1.403	1.398(5)	C(10′)–C(9′)	1.482	1.473	1.454(2)
C(9′)–O(1′)	1.348	1.351	1.367(4)	C(9′)–O(1′)	1.223	1.242	1.245(2)
O(1′)–C(2,2′)	1.500	1.500	1.478(4)	O(1′)–C(2,2′)	-	-	-
C(10′)–C(5′)	1.401	1.399	1.402(4)	C(10′)–C(5′)	1.394	1.399	1.399(2)
C(5′)–C(6′)	1.394	1.397	1.389(5)	C(5′)–C(6′)	1.407	1.402	1.391(2)
C(6′)–O(2′)	1.367	1.366	1.368(4)	C(6′)–C(7′)	1.448	1.442	1.437(2)
C(6′)–C(7′)	1.389	1.388	1.388(5)	C(7′)–C(8′)	1.359	1.361	1.359(2)
C(7′)–C(8′)	1.409	1.412	1.403(4)	C(8′)–O(2′)	1.352	1.356	1.359(2)
C(8′)–C(9′)	1.422	1.421	1.411(5)	C(8′)–C(9′)	1.486	1.476	1.475(2)
C(8′)–C(12′)	1.444	1.444	1.459(4)	C(6′)–C(12′)	1.409	1.419	1.426(2)
C(12′)–C(13′)	1.362	1.364	1.357(4)	C(12′)–C(13′)	1.397	1.385	1.368(2)
C(13′)–C(2″)	1.423	1.424	1.431(4)	C(13′)–C(2″)	1.391	1.402	1.404(2)
C(2″)–N(1″)	1.331	1.330	1.325(4)	C(2″)–N(1″)	1.362	1.348	1.334(2)
Distance	**Gas**	**DMSO**	**XRD**	**Distance**	**Gas**	**DMSO**	**XRD**
Cl(1)–N(1)	5.277	5.859	5.905(4)	Cl(1)–N(1)	4.956	5.238	5.0458(15)
Cl(1)–N(1″)	3.992	4.284	3.921(3)	Cl(1)–N(1″)	6.954	7.277	7.0981(15)
Cl(1)–C(2,2′)	5.854	6.467	6.470(4)	Cl(1)–C(2,2′)	5.154	5.482	5.3635(18)
Cl(1)–O(1′)	4.995	5.576	5.537(3)	Cl(1)–O(1′)	7.484	7.868	7.8497(15)
Cl(1)–C(8′)	4.694	5.681	5.688(3)	Cl(1)–C(3′)	4.356	4.738	4.6647(18)
Cl(1)–C(13′)	3.673	4.384	4.289(4)	Cl(1)–C(10′)	5.109	5.527	5.5011(18)
Cl(1)–C(2″)	3.812	4.350	4.151(3)	Cl(1)–C(2″)	5.635	5.992	5.8180(17)
C(2,2′)–C(2″)	5.501	5.500	5.449(5)	C(2,2′)–C(2″)	9.027	9.073	9.010(3)
C(2,2′)–C(6′)	5.177	5.165	5.126(6)	C(2,2′)–C(8′)	6.243	6.241	6.204(3)
C(2″)–C(6′)	6.172	6.183	6.164(5)	C(2″)–C(8′)	5.790	5.789	5.763(3)
Angle	**Gas**	**DMSO**	**XRD**	**Angle**	**Gas**	**DMSO**	**XRD**
A(C(2,2′), C(6′),C(2″))	57.18	57.14	56.82(7)	A(C(2,2′), C(8′),C(2″))	97.14	97.84	96.84(4)
A(N(1), C(6′),N(1″))	49.25	48.54	47.83(5)	A(N(1), C(8′),N(1″))	101.82	102.52	101.04(3)
A(C(2,2′), C(3′),C(4′))	123.56	123.29	123.0(4)	A(C(2,2′), C(3′),C(4′))	123.73	123.84	123.70(16)
A(C(3′), C(4′),C(10′))	121.84	121.56	121.7(4)	A(C(3′), C(4′),C(10′))	127.87	128.21	126.69(16)
A(C(4′), C(10′),C(9′))	117.66	117.69	117.6(4)	A(C(4′), C(10′),C(9′))	115.62	115.83	116.59(15)
A(C(9′), C(8′),C(12′))	125.98	125.98	125.5(3)	A(C(7′), C(6′),C(12′))	123.84	122.92	122.80(15)

A(C(8′), C(12′),C(13′))	129.70	129.53	128.5(3)	A(C(6′), C(12′),C(13′))	126.25	126.44	125.51(16)
A(C(12′), C(13′),C(2″))	123.41	123.72	122.8(4)	A(C(12′), C(13′),C(2″))	126.10	126.04	125.37(16)
A(N(1), C(6′),Cl(1))	50.04	49.40	50.03(4)	A(N(1), C(8′),Cl(1))	40.18	35.48	40.388(15)
A(N(1″), C(6′),Cl(1))	32.90	33.51	30.75(3)	A(N(1″), C(8′),Cl(1))	61.69	53.32	61.66(2)
Dihedral Angle	**Gas**	**DMSO**	**XRD**	**Dihedral Angle**	**Gas**	**DMSO**	**XRD**
D(C(2,2′), C(6′), C(8′), C(2″))	-171.30	-179.48	-168.6(5)	D(C(2,2′), C(8′), C(6′), C(2″))	178.03	176.62	177.03(11)

Table S3 The overview of the compounds **1** and **2** calculated by B3LYP/6-311++G(d,p) method in DMSO. E_{tot} - total electronic energy, E_0 - total electronic energy with zero point vibrational energy, $E_{298K,1atm}$ − sum E_0 and thermal correction to the internal energy under standard conditions (T = 298.15 K, P = 1.0 atm.), $H_{298K,1atm}$ - enthalpy, $G_{298K,1atm}$ − Gibbs free energy, μ - dipole moment (Debye), λ - number of negative eigenvalues of the Hessian. Energy values are given in Hartree.

Compound 1										
Key	**Structure**	**Charge**	**E_{tot}**	**E_0**	**$E_{298K,1atm}$**	**$H_{298K,1atm}$**	**$G_{298K,1atm}$**	**μ**	**λ**	**Point group**
o.1a	**1a**	0	-2299.7903	-2299.1731	-2299.1323	-2299.1314	-2299.7908	19.762	0	C_1
o.1b	**1b**	0	-2299.7878	-2299.1718	-2299.1301	-2299.1292	-2299.2522	19.386	0	C_1
o.1c	**1c**	0	-2299.8004	-2299.1845	-2299.1425	-2299.1415	-2299.1669	26.112	0	C_1
o.1d	**1d**	0	-2299.8001	-2299.1842	-2299.1422	-2299.1413	-2299.2666	28.909	0	C_1
o.1a′	**1a′**	1	-1538.7656	-1538.1630	-1538.1287	-1538.1278	-1538.2284	4.968	0	C_1
o.1b′	**1b′**	1	-1538.7640	-1538.1625	-1538.1275	-1538.1265	-1538.2298	3.423	0	C_1
o.1c′	**1c′**	1	-1538.7770	-1538.1753	-1538.1400	-1538.1391	-1538.2433	3.544	0	C_1
o.1d′	**1d′**	1	-1538.7768	-1538.1754	-1538.1399	-1538.1390	-1538.2445	1.577	0	C_1
Compound 2										
Key	**Structure**	**Charge**	**E_{tot}**	**E_0**	**$E_{298K,1atm}$**	**$H_{298K,1atm}$**	**$G_{298K,1atm}$**	**μ**	**λ**	**Point group**
o.2a	**2a**	0	-2299.7939	-2299.1766	-2299.1357	-2299.1348	-2299.2564	26.635	0	C_1
o.2b	**2b**	0	-2299.7941	-2299.1775	-2299.1359	-2299.1349	-2299.2576	21.848	0	C_1
o.2c	**2c**	0	-2299.8071	-2299.1900	-2299.1483	-2299.1474	-2299.2696	13.356	0	C_1
o.2d	**2d**	0	-2299.8063	-2299.1892	-2299.1475	-2299.1465	-2299.2692	11.069	0	C_1
o.2a′	**2a′**	1	-1538.7691	-1538.1666	-1538.1322	-1538.1313	-1538.2336	18.540	0	C_1
o.2b′	**2b′**	1	-1538.7695	-1538.1677	-1538.1326	-1538.1317	-1538.2356	6.843	0	C_1
o.2c′	**2c′**	1	-1538.7820	-1538.1799	-1538.1446	-1538.1437	-1538.2485	6.978	0	C_1
o.2d′	**2d′**	1	-1538.7811	-1538.1793	-1538.1438	-1538.1429	-1538.2486	12.325	0	C_1

Table S4 The overview of the compounds **1** and **2** calculated by B3LYP/6-311++G(d,p) method in the gas phase, that updates early data [30]. E_{tot} - total electronic energy, E_0 - total electronic energy with zero point vibrational energy, $E_{298K,1atm}$ − sum E_0 and thermal correction to the internal energy under standard conditions (T = 298.15 K, P = 1.0 atm.), $H_{298K,1atm}$ - enthalpy, $G_{298K,1atm}$ − Gibbs free energy, μ - dipole moment (Debye), λ - number of negative eigenvalues of the Hessian. Energy values are given in Hartree.

Compound 1									
Structure	**Charge**	**E_{tot}**	**E_0**	**$E_{298K,1atm}$**	**$H_{298K,1atm}$**	**$G_{298K,1atm}$**	**μ**	**λ**	**Point group**
1a	0	-2299.7504	-2299.1321	-2299.0919	-2299.0909	-2299.2071	11.276	0	C_1
1b	0	-2299.7486	-2299.1313	-2299.0903	-2299.0893	-2299.2072	10.622	0	C_1
1c	0	-2299.7520	-2299.1352	-2299.0937	-2299.0928	-2299.2129	6.279	0	C_1
1d	0	-2299.7453	-2299.1289	-2299.0872	-2299.0863	-2299.2080	7.075	0	C_1
1a′	1	-1538.7105	-1538.1073	-1538.0731	-1538.0721	-1538.1731	3.793	0	C_1
1b′	1	-1538.7086	-1538.1067	-1538.0716	-1538.0707	-1538.1742	1.870	0	C_1
1c′	1	-1538.7210	-1538.1191	-1538.0836	-1538.0826	-1538.1887	2.508	0	C_S
1d′	1	-1538.7200	-1538.1183	-1538.0827	-1538.0817	-1538.1882	0.548	0	C_S
Compound 2									
Structure	**Charge**	**E_{tot}**	**E_0**	**$E_{298K,1atm}$**	**$H_{298K,1atm}$**	**$G_{298K,1atm}$**	**μ**	**λ**	**Point group**
2a	0	-2299.7461	-2299.1280	-2299.0874	-2299.0864	-2299.2060	17.065	0	C_1
2b	0	-2299.7436	-2299.1264	-2299.0852	-2299.0842	-2299.2043	11.947	0	C_1
2c	0	-2299.7600	-2299.1422	-2299.1006	-2299.0996	-2299.2215	9.042	0	C_1
2d	0	-2299.7626	-2299.1450	-2299.1034	-2299.1024	-2299.2237	5.598	0	C_1
2a′	1	-1538.7084	-1538.1057	-1538.0713	-1538.0703	-1538.1729	12.613	0	C_1
2b′	1	-1538.7107	-1538.1082	-1538.0731	-1538.0722	-1538.1761	3.219	0	C_1
2c′	1	-1538.7193	-1538.1173	-1538.0818	-1538.0808	-1538.1870	3.387	0	C_S
2d′	1	-1538.7148	-1538.1129	-1538.0773	-1538.0764	-1538.1829	7.119	0	C_S

Table S5 The summary of NBO deletion analysis for the compounds **1** and **2** calculated by B3LYP/6-311++G(d,p) method in DMSO. Energy values are given in Hartree.

Compound 1			
Structure	**E(L)**	**E(NL)**	**E_{tot}**
1a	-2295.8379	-3.9524	-2299.7903
1b	-2295.6297	-4.1581	-2299.7878
1c	-2295.6020	-4.1984	-2299.8004
1d	-2295.6008	-4.1993	-2299.8001
1a′	-1535.6868	-3.0788	-1538.7656
1b′	-1535.3981	-3.3659	-1538.7640
1c′	-1535.4354	-3.3416	-1538.7770
1d′	-1535.4336	-3.3432	-1538.7768
Compound 2			
Structure	**E(L)**	**E(NL)**	**E_{tot}**
2a	-2295.8350	-3.9589	-2299.7939
2b	-2295.7863	-4.0078	-2299.7941
2c	-2295.7781	-4.0290	-2299.8071
2d	-2295.7888	-4.0174	-2299.8063
2a′	-1535.6816	-3.0875	-1538.7691
2b′	-1535.6245	-3.1450	-1538.7695
2c′	-1535.5235	-3.2586	-1538.7820
2d′	-1535.4331	-3.3480	-1538.7811

Table S6 The summary of NBO deletion analysis for the compounds **1** and **2** calculated by B3LYP/6-311++G(d,p) method in the gas phase, that updates early data [30].

Compound 1			
Structure	**E(L)**	**E(NL)**	**E_{tot}**
1a	-2 295.7544	-3.9960	-2299.7504
1b	-2 295.5193	-4.2294	-2299.7486
1c	-2 295.7319	-4.0201	-2299.7520
1d	-2 295.7627	-3.9826	-2299.7453
1a′	-1 535.5869	-3.1235	-1538.7105
1b′	-1 535.5218	-3.1869	-1538.7086
1c′	-1 535.5160	-3.2050	-1538.7210
1d′	-1 535.5244	-3.1956	-1538.7200
Compound 2			
Structure	**E(L)**	**E(NL)**	**E_{tot}**
2a	-2295.7084	-4.0377	-2299.7461
2b	-2295.7248	-4.0189	-2299.7436
2c	-2295.6899	-4.0701	-2299.7600
2d	-2295.7215	-4.0411	-2299.7626
2a′	-1535.5421	-3.1663	-1538.7084
2b′	-1535.5562	-3.1542	-1538.7104
2c′	-1535.5194	-3.2000	-1538.7193
2d′	-1535.5465	-3.1683	-1538.7148

Table S7 ESP, Mulliken, APT and NPA charges for structures of compounds **1** and **2** calculated by B3LYP/6-311++G(d,p) method in DMSO. Charges marked with asterisk is summed with hydrogen atom.

Compound 1					
Atom	**Charge**	**Structure**			
		1a	**1b**	**1c**	**1d**
N(1)	ESP	-0.438	0.072	0.075	0.126
	ESP*	-0.438	0.072	0.075	0.126
	Mulliken	0.232	0.527	0.245	0.218
	Mulliken*	0.232	0.527	0.245	0.218
	APT	-1.192	-0.356	-1.435	-1.932
	APT*	-1.192	-0.356	-1.435	-1.932
	NPA	-0.518	-0.349	-0.371	-0.377
C(3)	ESP	0.235	0.355	0.313	0.417
	ESP*	0.235	0.355	0.313	0.417
	Mulliken	0.640	0.265	0.666	0.537
	Mulliken*	0.640	0.265	0.666	0.537
	APT	0.116	-0.012	0.150	0.202
	APT*	0.116	-0.012	0.150	0.202
	NPA	-0.080	-0.109	-0.107	-0.105
C(4)	ESP	-0.174	-0.220	-0.203	-0.204
	ESP*	-0.014	-0.046	-0.030	-0.033
	Mulliken	-0.149	-0.379	-0.509	-0.177
	Mulliken*	0.040	-0.182	-0.331	0.005
	APT	0.096	0.016	0.087	0.074
	APT*	0.145	0.069	0.147	0.143
	NPA	-0.193	-0.186	-0.185	-0.185
C(5)	ESP	-0.222	-0.117	-0.139	-0.150
	ESP*	-0.071	0.027	0.006	-0.001
	Mulliken	-0.524	-0.451	-0.505	-0.581
	Mulliken*	-0.331	-0.245	-0.308	-0.385
	APT	-0.255	-0.100	-0.243	-0.275
	APT*	-0.220	-0.052	-0.206	-0.238
	NPA	-0.253	-0.205	-0.210	-0.212
C(6)	ESP	-0.168	-0.162	-0.133	-0.135
	ESP*	-0.009	-0.014	0.019	0.015
	Mulliken	-0.247	-0.270	-0.280	-0.244
	Mulliken*	-0.048	-0.056	-0.071	-0.035
	APT	0.053	-0.096	-0.082	-0.037
	APT*	0.090	-0.051	-0.050	-0.008
	NPA	-0.202	-0.197	-0.197	-0.197
C(7)	ESP	-0.307	-0.169	-0.249	-0.207
	ESP*	-0.127	0.002	-0.057	-0.034
	Mulliken	-0.231	-0.279	-0.606	-0.300
	Mulliken*	-0.051	-0.011	-0.429	-0.122
	APT	-0.221	-0.089	-0.087	-0.075
	APT*	-0.157	0.047	0.000	0.007
	NPA	-0.261	-0.219	-0.218	-0.220
C(8)	ESP	0.361	0.065	0.103	0.055
	ESP*	0.361	0.065	0.103	0.055
	Mulliken	0.009	0.262	0.773	0.475
	Mulliken*	0.009	0.262	0.773	0.475
	APT	0.616	0.433	0.680	0.640
	APT*	0.616	0.433	0.680	0.640
	NPA	0.197	0.159	0.162	0.163

C(9)	ESP	-0.122	-0.015	0.011	-0.009
	ESP*	-0.122	-0.015	0.011	-0.009
	Mulliken	-0.178	0.393	0.735	0.524
	Mulliken*	-0.178	0.393	0.735	0.524
	APT	-0.169	-0.126	-0.234	-0.222
	APT*	-0.169	-0.126	-0.234	-0.222
	NPA	-0.061	-0.021	-0.021	-0.022
$C(CH_3\text{-}N(1))$**	ESP	-0.155	-0.337	-0.264	-0.318
	ESP*	0.132	0.139	0.147	0.130
	Mulliken	-0.308	-0.453	-0.368	-0.334
	Mulliken*	0.287	0.108	0.234	0.252
	APT	0.424	0.179	0.221	0.368
	APT*	0.389	0.306	0.373	0.471
	NPA	-0.375	-0.372	-0.373	-0.374
$C(CH_3\text{-}C(3))$	ESP	-0.370	-0.368	-0.503	-0.453
	ESP*	-0.096	-0.053	-0.068	-0.074
	Mulliken	-0.621	-0.663	-0.708	-0.758
	Mulliken*	-0.146	-0.114	-0.157	-0.209
	APT	0.014	0.034	0.024	0.036
	APT*	-0.010	0.026	0.011	0.031
	NPA	-0.584	-0.565	-0.563	-0.564
$C(C'H_3\text{-}C(3))$***	ESP	-0.293	-0.525	-0.471	-0.443
	ESP*	-0.066	-0.088	-0.058	-0.074
	Mulliken	-0.554	-0.624	-0.712	-0.754
	Mulliken*	-0.009	-0.066	-0.161	-0.204
	APT	0.031	0.078	0.025	0.035
	APT*	-0.014	0.035	0.017	0.028
	NPA	-0.577	-0.563	-0.563	-0.563
C(2,2′)	ESP	0.522	0.326	0.127	0.045
	ESP*	0.522	0.326	0.127	0.045
	Mulliken	-0.549	0.130	0.010	-0.155
	Mulliken*	-0.549	0.130	0.010	-0.155
	APT	1.277	0.731	2.196	2.396
	APT*	1.277	0.731	2.196	2.396
	NPA	0.493	0.421	0.375	0.369
O(1′)	ESP	-0.004	-0.613	-0.632	-0.653
	ESP*	-0.004	-0.613	-0.632	-0.653
	Mulliken	0.172	-0.265	-0.278	-0.312
	Mulliken*	0.172	-0.265	-0.278	-0.312
	APT	-1.187	-0.574	-0.525	-0.650
	APT*	-1.187	-0.574	-0.525	-0.650
	NPA	-0.588	-0.705	-0.720	-0.726
O(2′)	ESP	-0.394	-0.414	-0.404	-0.390
	ESP*	-0.394	-0.414	-0.404	-0.390
	Mulliken	-0.186	-0.191	-0.199	-0.197
	Mulliken*	-0.186	-0.191	-0.199	-0.197
	APT	-1.273	-1.359	-1.290	-1.180
	APT*	-1.273	-1.359	-1.290	-1.180
	NPA	-0.561	-0.563	-0.561	-0.558
C(3′)	ESP	-0.299	-0.520	-0.311	-0.320
	ESP*	-0.125	-0.314	-0.123	-0.137
	Mulliken	-0.202	-0.563	-0.360	-0.177
	Mulliken*	0.031	-0.322	-0.037	0.027
	APT	-0.232	-1.074	-1.955	-2.244
	APT*	-0.171	-0.989	-1.841	-2.198
	NPA	-0.216	-0.323	-0.333	-0.321

C(4′)	ESP	-0.179	0.121	0.034	0.117
	ESP*	-0.020	0.234	0.193	0.232
	Mulliken	-0.007	-0.088	-0.378	0.152
	Mulliken*	0.219	0.134	-0.606	0.106
	APT	0.151	1.325	1.878	2.341
	APT*	0.178	1.331	1.931	2.463
	NPA	-0.167	-0.078	-0.062	-0.062
C(5′)	ESP	-0.449	-0.283	-0.261	-0.177
	ESP*	-0.233	-0.105	-0.093	-0.012
	Mulliken	0.355	0.384	0.394	0.059
	Mulliken*	0.559	0.605	0.602	0.141
	APT	-0.023	0.540	0.656	0.397
	APT*	0.064	0.619	0.750	0.497
	NPA	-0.213	-0.189	-0.192	-0.204
C(6′)	ESP	0.569	0.484	0.480	0.402
	ESP*	0.569	0.484	0.480	0.402
	Mulliken	-0.684	-0.637	-0.195	-0.645
	Mulliken*	-0.684	-0.637	-0.195	-0.645
	APT	0.448	-0.418	-0.903	-1.146
	APT*	0.448	-0.418	-0.903	-1.146
	NPA	0.306	0.258	0.257	0.267
C(7′)	ESP	-0.522	-0.410	-0.416	-0.345
	ESP*	-0.329	-0.227	-0.231	-0.166
	Mulliken	-0.609	-0.681	-0.773	-0.875
	Mulliken*	-0.348	-0.404	-0.492	-0.597
	APT	0.052	0.553	0.808	1.144
	APT*	0.138	0.631	0.886	1.226
	NPA	-0.177	-0.143	-0.131	-0.125
C(8′)	ESP	0.236	-0.056	-0.002	-0.042
	ESP*	0.236	-0.056	-0.002	-0.042
	Mulliken	0.405	0.351	0.174	0.576
	Mulliken*	0.405	0.351	0.174	0.576
	APT	-0.738	-1.123	-1.124	-1.209
	APT*	-0.738	-1.123	-1.124	-1.209
	NPA	-0.132	-0.165	-0.189	-0.190
C(9′)	ESP	-0.142	0.532	0.578	0.587
	ESP*	-0.142	0.532	0.578	0.587
	Mulliken	0.001	-0.883	-0.508	-0.538
	Mulliken*	0.001	-0.883	-0.508	-0.538
	APT	0.563	0.320	0.376	0.570
	APT*	0.563	0.320	0.376	0.570
	NPA	0.386	0.452	0.557	0.578
C(10′)	ESP	0.210	-0.214	-0.245	-0.313
	ESP*	0.210	-0.214	-0.245	-0.313
	Mulliken	0.183	0.545	0.420	0.485
	Mulliken*	0.183	0.545	0.420	0.485
	APT	-0.022	-0.758	-1.304	-1.329
	APT*	-0.022	-0.758	-1.304	-1.329
	NPA	-0.121	-0.179	-0.191	-0.205
C(11′)	ESP	-0.056	0.008	-0.019	0.001
	ESP*	0.222	0.230	0.227	0.230
	Mulliken	-0.365	-0.366	-0.346	-0.359
	Mulliken*	0.171	0.166	0.194	0.186
	APT	0.700	0.743	0.687	0.641
	APT*	0.609	0.640	0.619	0.600
	NPA	-0.215	-0.215	-0.215	-0.216

C(12′)	ESP	-0.203	-0.035	-0.114	-0.087
	ESP*	0.050	0.169	0.113	0.120
	Mulliken	-0.226	-0.359	-0.349	-0.169
	Mulliken*	-0.258	-0.417	-0.506	-0.278
	APT	1.173	1.624	1.768	1.886
	APT*	1.244	1.683	1.820	1.937
	NPA	-0.044	-0.055	-0.059	-0.059
C(13′)	ESP	-0.076	-0.366	-0.282	-0.251
	ESP*	-0.036	-0.167	-0.116	-0.081
	Mulliken	-0.080	-0.264	-0.354	-0.357
	Mulliken*	-0.324	0.060	-0.073	-0.115
	APT	-1.210	-1.710	-1.824	-1.934
	APT*	-1.100	-1.598	-1.694	-1.799
	NPA	-0.298	-0.325	-0.324	-0.322
N(1″)	ESP	0.073	-0.024	0.082	0.111
	ESP*	0.073	-0.024	0.082	0.111
	Mulliken	0.523	0.349	0.230	0.206
	Mulliken*	0.523	0.349	0.230	0.206
	APT	-0.855	-1.253	-1.239	-1.280
	APT*	-0.855	-1.253	-1.239	-1.280
	NPA	-0.334	-0.361	-0.357	-0.354
C(2″)	ESP	0.148	0.245	0.219	0.165
	ESP*	0.148	0.245	0.219	0.165
	Mulliken	0.130	0.155	0.366	0.387
	Mulliken*	0.130	0.155	0.366	0.387
	APT	1.441	1.958	2.066	2.172
	APT*	1.441	1.958	2.066	2.172
	NPA	0.409	0.385	0.389	0.391
C(3″)	ESP	0.186	0.309	0.240	0.248
	ESP*	0.186	0.309	0.240	0.248
	Mulliken	0.385	0.395	0.516	0.475
	Mulliken*	0.385	0.395	0.516	0.475
	APT	0.077	0.127	0.122	0.126
	APT*	0.077	0.127	0.122	0.126
	NPA	-0.110	-0.108	-0.109	-0.109
C(4″)	ESP	-0.263	-0.194	-0.224	-0.250
	ESP*	-0.069	-0.025	-0.050	-0.070
	Mulliken	-0.191	-0.103	-0.166	-0.143
	Mulliken*	-0.003	0.085	0.021	0.044
	APT	0.008	0.069	0.069	0.067
	APT*	0.071	0.129	0.130	0.130
	NPA	-0.184	-0.185	-0.185	-0.185
C(5″)	ESP	-0.134	-0.144	-0.129	-0.106
	ESP*	0.018	0.002	0.018	0.036
	Mulliken	-0.480	-0.567	-0.580	-0.586
	Mulliken*	-0.278	-0.370	-0.383	-0.388
	APT	-0.146	-0.212	-0.215	-0.222
	APT*	-0.099	-0.174	-0.177	-0.184
	NPA	-0.196	-0.207	-0.205	-0.204
C(6″)	ESP	-0.106	-0.134	-0.167	-0.170
	ESP*	0.042	0.018	-0.006	-0.011
	Mulliken	-0.422	-0.405	-0.278	-0.241
	Mulliken*	-0.205	-0.193	-0.066	-0.028
	APT	-0.096	-0.085	-0.104	-0.110
	APT*	-0.054	-0.051	-0.071	-0.078
	NPA	-0.195	-0.196	-0.196	-0.196

C(7″)	ESP	-0.272	-0.257	-0.196	-0.186
	ESP*	-0.075	-0.058	-0.017	-0.010
	Mulliken	-0.264	-0.242	-0.321	-0.279
	Mulliken*	-0.090	-0.062	-0.142	-0.099
	APT	0.016	-0.059	-0.043	-0.026
	APT*	0.105	0.026	0.046	0.064
	NPA	-0.207	-0.215	-0.214	-0.213
C(8″)	ESP	0.152	0.142	0.049	0.025
	ESP*	0.152	0.142	0.049	0.025
	Mulliken	0.796	0.801	0.591	0.478
	Mulliken*	0.796	0.801	0.591	0.478
	APT	0.313	0.571	0.567	0.547
	APT*	0.313	0.571	0.567	0.547
	NPA	0.158	0.161	0.161	0.160
C(9″)	ESP	0.098	0.004	0.087	0.109
	ESP*	0.098	0.004	0.087	0.109
	Mulliken	0.114	0.335	0.373	0.373
	Mulliken*	0.114	0.335	0.373	0.373
	APT	-0.158	-0.210	-0.219	-0.225
	APT*	-0.158	-0.210	-0.219	-0.225
	NPA	-0.012	-0.018	-0.017	-0.016
$C(CH_3\text{-}N(1''))$	ESP	-0.327	-0.235	-0.375	-0.348
	ESP*	0.168	0.172	0.151	0.154
	Mulliken	-0.571	-0.439	-0.440	-0.405
	Mulliken*	0.188	0.165	0.247	0.279
	APT	0.267	0.231	0.197	0.198
	APT*	0.461	0.407	0.399	0.407
	NPA	-0.388	-0.379	-0.381	-0.382
$C(CH_3\text{-}C(3''))$	ESP	-0.364	-0.416	-0.331	-0.350
	ESP*	-0.021	-0.052	-0.032	-0.030
	Mulliken	-0.825	-0.845	-0.885	-0.891
	Mulliken*	-0.236	-0.238	-0.299	-0.304
	APT	0.041	0.011	0.018	0.016
	APT*	0.076	0.043	0.045	0.043
	NPA	-0.566	-0.569	-0.569	-0.569
$C(C'H_3\text{-}C(3''))$	ESP	-0.439	-0.494	-0.529	-0.524
	ESP*	-0.046	-0.083	-0.084	-0.078
	Mulliken	-0.750	-0.742	-0.734	-0.745
	Mulliken*	-0.180	-0.179	-0.169	-0.180
	APT	0.056	0.042	0.033	0.033
	APT*	0.056	0.029	0.021	0.021
	NPA	-0.562	-0.563	-0.562	-0.562
Cl(1′)	ESP	1.073	1.045	1.132	1.131
	ESP*	1.073	1.045	1.132	1.131
	Mulliken	-0.310	-0.327	-0.073	-0.060
	Mulliken*	-0.310	-0.327	-0.073	-0.060
	APT	3.196	3.227	3.191	3.190
	APT*	3.196	3.227	3.191	3.190
	NPA	2.363	2.364	2.363	2.364
O(3′)	ESP	-0.521	-0.519	-0.537	-0.536
	ESP*	-0.521	-0.519	-0.537	-0.536
	Mulliken	-0.231	-0.242	-0.281	-0.282
	Mulliken*	-0.231	-0.242	-0.281	-0.282
	APT	-1.071	-1.069	-1.067	-1.068
	APT*	-1.071	-1.069	-1.067	-1.068
	NPA	-0.836	-0.838	-0.838	-0.838

O(4′)	ESP	-0.514	-0.467	-0.542	-0.542
	ESP*	-0.514	-0.467	-0.542	-0.542
	Mulliken	-0.110	-0.092	-0.197	-0.203
	Mulliken*	-0.110	-0.092	-0.197	-0.203
	APT	-1.080	-1.100	-1.069	-1.068
	APT*	-1.080	-1.100	-1.069	-1.068
	NPA	-0.838	-0.838	-0.841	-0.840
O(5′)	ESP	-0.508	-0.508	-0.517	-0.518
	ESP*	-0.508	-0.508	-0.517	-0.518
	Mulliken	-0.123	-0.138	-0.190	-0.195
	Mulliken*	-0.123	-0.138	-0.190	-0.195
	APT	-1.066	-1.071	-1.059	-1.060
	APT*	-1.066	-1.071	-1.059	-1.060
	NPA	-0.836	-0.836	-0.836	-0.836
O(6′)	ESP	-0.514	-0.514	-0.529	-0.528
	ESP*	-0.514	-0.514	-0.529	-0.528
	Mulliken	-0.209	-0.200	-0.245	-0.245
	Mulliken*	-0.209	-0.200	-0.245	-0.245
	APT	-1.036	-1.044	-1.037	-1.037
	APT*	-1.036	-1.044	-1.037	-1.037
	NPA	-0.835	-0.837	-0.836	-0.836

Compound 2

Atom	Charge	Structure			
		2a	2b	2c	2d
N(1)	ESP	-0.348	-0.058	-0.051	-0.067
	ESP*	-0.348	-0.058	-0.051	-0.067
	Mulliken	0.309	0.487	0.209	0.287
	Mulliken*	0.309	0.487	0.209	0.287
	APT	-1.403	-0.506	-1.700	-1.392
	APT*	-1.403	-0.506	-1.700	-1.392
	NPA	-0.520	-0.347	-0.365	-0.361
C(3)	ESP	0.238	0.273	0.206	0.099
	ESP*	0.238	0.273	0.206	0.099
	Mulliken	0.585	0.462	0.602	0.529
	Mulliken*	0.585	0.462	0.602	0.529
	APT	0.151	0.014	0.160	0.156
	APT*	0.151	0.014	0.160	0.156
	NPA	-0.077	-0.111	-0.108	-0.104
C(4)	ESP	-0.140	-0.203	-0.204	-0.228
	ESP*	0.012	-0.028	-0.030	-0.044
	Mulliken	-0.177	-0.491	-0.232	-0.172
	Mulliken*	0.008	-0.296	-0.049	0.008
	APT	0.109	0.030	0.054	0.089
	APT*	0.157	0.085	0.122	0.148
	NPA	-0.192	-0.181	-0.183	-0.184
C(5)	ESP	-0.244	-0.128	-0.163	-0.135
	ESP*	-0.091	0.014	-0.014	0.010
	Mulliken	-0.587	-0.504	-0.580	-0.520
	Mulliken*	-0.407	-0.306	-0.382	-0.321
	APT	-0.261	-0.119	-0.243	-0.234
	APT*	-0.230	-0.072	-0.205	-0.197
	NPA	-0.249	-0.202	-0.207	-0.206

C(6)	ESP	-0.144	-0.135	-0.110	-0.144
	ESP*	0.007	0.019	0.038	0.011
	Mulliken	-0.230	-0.232	-0.259	-0.417
	Mulliken*	-0.032	-0.018	-0.049	-0.206
	APT	0.040	-0.121	-0.060	-0.110
	APT*	0.071	-0.079	-0.028	-0.079
	NPA	-0.199	-0.196	-0.197	-0.197
C(7)	ESP	-0.299	-0.264	-0.300	-0.250
	ESP*	-0.124	-0.070	-0.102	-0.074
	Mulliken	-0.382	-0.554	-0.329	-0.243
	Mulliken*	-0.217	-0.372	-0.147	-0.059
	APT	-0.230	-0.066	-0.034	-0.043
	APT*	-0.167	0.029	0.052	0.051
	NPA	-0.268	-0.213	-0.217	-0.218
C(8)	ESP	0.311	0.226	0.229	0.219
	ESP*	0.311	0.226	0.229	0.219
	Mulliken	0.166	0.462	0.528	0.499
	Mulliken*	0.166	0.462	0.528	0.499
	APT	0.737	0.480	0.545	0.609
	APT*	0.737	0.480	0.545	0.609
	NPA	0.198	0.166	0.169	0.167
C(9)	ESP	-0.107	-0.026	0.044	0.046
	ESP*	-0.107	-0.026	0.044	0.046
	Mulliken	0.065	0.518	0.601	0.471
	Mulliken*	0.065	0.518	0.601	0.471
	APT	-0.171	-0.157	-0.211	-0.233
	APT*	-0.171	-0.157	-0.211	-0.233
	NPA	-0.052	-0.028	-0.029	-0.029
$C(CH_3\text{-}N(1))$	ESP	-0.236	-0.294	-0.254	-0.336
	ESP*	0.129	0.168	0.160	0.174
	Mulliken	-0.374	-0.451	-0.353	-0.545
	Mulliken*	0.164	0.210	0.241	0.324
	APT	0.386	0.146	0.344	0.187
	APT*	0.348	0.302	0.465	0.337
	NPA	-0.372	-0.373	-0.373	-0.381
$C(CH_3\text{-}C(3))$	ESP	-0.443	-0.408	-0.440	-0.382
	ESP*	-0.077	-0.031	-0.034	-0.024
	Mulliken	-0.473	-0.664	-0.783	-0.758
	Mulliken*	0.039	-0.111	-0.209	-0.191
	APT	0.002	0.018	0.030	0.028
	APT*	-0.019	0.031	0.045	0.023
	NPA	-0.584	-0.564	-0.565	-0.563
$C(C'H_3\text{-}C(3))$	ESP	-0.327	-0.554	-0.414	-0.364
	ESP*	-0.066	-0.073	-0.032	-0.019
	Mulliken	-0.600	-0.630	-0.823	-0.740
	Mulliken*	-0.063	-0.071	-0.234	-0.179
	APT	-0.001	0.044	0.035	0.024
	APT*	-0.046	0.014	0.045	0.021
	NPA	-0.579	-0.562	-0.563	-0.563
O(1′)	ESP	-0.519	-0.672	-0.716	-0.683
	ESP*	-0.519	-0.672	-0.716	-0.683
	Mulliken	0.238	-0.285	-0.366	-0.383
	Mulliken*	0.238	-0.285	-0.366	-0.383
	APT	-2.095	-1.654	-1.500	-1.581
	APT*	-2.095	-1.654	-1.500	-1.581
	NPA	-0.557	-0.676	-0.669	-0.675

O(2′)	ESP	-0.292	-0.361	-0.361	-0.366
	ESP*	-0.292	-0.361	-0.361	-0.366
	Mulliken	-0.190	-0.181	-0.217	-0.203
	Mulliken*	-0.190	-0.181	-0.217	-0.203
	APT	-1.132	-1.179	-1.258	-1.297
	APT*	-1.132	-1.179	-1.258	-1.297
	NPA	-0.541	-0.545	-0.545	-0.543
N(1″)	ESP	0.212	0.118	-0.038	-0.050
	ESP*	0.212	0.118	-0.038	-0.050
	Mulliken	0.249	0.220	0.229	0.226
	Mulliken*	0.249	0.220	0.229	0.226
	APT	-1.267	-1.907	-1.988	-1.994
	APT*	-1.267	-1.907	-1.988	-1.994
	NPA	-0.353	-0.378	-0.375	-0.373
C(2,2′)	ESP	0.607	0.428	0.235	0.332
	ESP*	0.607	0.428	0.235	0.332
	Mulliken	-0.643	-0.019	-0.166	0.052
	Mulliken*	-0.643	-0.019	-0.166	0.052
	APT	1.521	1.194	2.331	2.290
	APT*	1.521	1.194	2.331	2.290
	NPA	0.488	0.441	0.388	0.386
C(3′)	ESP	-0.380	-0.510	-0.404	-0.407
	ESP*	-0.192	-0.304	-0.121	-0.168
	Mulliken	-0.131	-0.482	-0.341	-0.428
	Mulliken*	0.103	-0.251	-0.044	-0.206
	APT	-0.303	-1.495	-2.240	-1.992
	APT*	-0.239	-1.456	-2.107	-1.894
	NPA	-0.232	-0.323	-0.330	-0.317
C(4′)	ESP	-0.090	0.090	0.073	-0.007
	ESP*	0.081	0.228	0.201	0.219
	Mulliken	-0.271	-0.081	-0.039	-0.175
	Mulliken*	0.026	0.311	-0.265	-0.189
	APT	0.192	1.426	2.175	2.061
	APT*	0.267	1.544	2.292	2.189
	NPA	-0.186	-0.080	-0.056	-0.048
C(7′)	ESP	-0.394	-0.334	-0.179	-0.286
	ESP*	-0.181	-0.143	-0.018	-0.109
	Mulliken	0.245	0.370	0.098	0.260
	Mulliken*	0.323	0.425	0.161	0.350
	APT	0.094	-0.008	-0.020	0.038
	APT*	0.197	0.076	0.061	0.120
	NPA	-0.242	-0.276	-0.241	-0.273
C(6′)	ESP	0.069	0.086	-0.181	0.036
	ESP*	0.069	0.086	-0.181	0.036
	Mulliken	0.735	0.308	0.339	0.512
	Mulliken*	0.735	0.308	0.339	0.512
	APT	-1.223	-1.940	-2.226	-2.163
	APT*	-1.223	-1.940	-2.226	-2.163
	NPA	-0.114	-0.142	-0.153	-0.132
C(5′)	ESP	-0.373	-0.333	-0.135	-0.298
	ESP*	-0.140	-0.123	0.051	-0.026
	Mulliken	-0.533	-0.354	-0.244	-0.506
	Mulliken*	-0.323	-0.201	-0.051	-0.364
	APT	0.623	1.768	2.012	1.797
	APT*	0.757	1.884	2.131	1.928
	NPA	-0.156	-0.057	-0.050	-0.062

C(10′)	ESP	0.060	-0.089	-0.227	-0.121
	ESP*	0.060	-0.089	-0.227	-0.121
	Mulliken	0.366	0.985	0.992	1.078
	Mulliken*	0.366	0.985	0.992	1.078
	APT	-0.525	-1.744	-2.307	-2.438
	APT*	-0.525	-1.744	-2.307	-2.438
	NPA	-0.064	-0.218	-0.203	-0.212
C(9′)	ESP	0.306	0.511	0.620	0.491
	ESP*	0.306	0.511	0.620	0.491
	Mulliken	-0.500	-0.825	-0.705	-0.740
	Mulliken*	-0.500	-0.825	-0.705	-0.740
	APT	1.551	1.459	1.452	1.556
	APT*	1.551	1.459	1.452	1.556
	NPA	0.360	0.436	0.444	0.451
C(CH_3-N(1″))	ESP	-0.297	-0.320	-0.304	-0.307
	ESP*	0.136	0.127	0.148	0.154
	Mulliken	-0.343	-0.333	-0.363	-0.350
	Mulliken*	0.271	0.252	0.225	0.240
	APT	0.294	0.309	0.340	0.366
	APT*	0.428	0.432	0.458	0.476
	NPA	-0.376	-0.374	-0.374	-0.374
C(11′)	ESP	-0.109	0.020	0.039	0.001
	ESP*	0.207	0.244	0.244	0.240
	Mulliken	-0.306	-0.293	-0.317	-0.343
	Mulliken*	0.235	0.247	0.226	0.205
	APT	0.582	0.574	0.605	0.608
	APT*	0.545	0.525	0.542	0.546
	NPA	-0.216	-0.217	-0.217	-0.217
C(2″)	ESP	0.076	0.061	0.356	0.200
	ESP*	0.076	0.061	0.356	0.200
	Mulliken	-0.157	-0.150	-0.270	-0.174
	Mulliken*	-0.157	-0.150	-0.270	-0.174
	APT	1.955	2.502	2.587	2.518
	APT*	1.955	2.502	2.587	2.518
	NPA	0.395	0.362	0.373	0.372
C(3″)	ESP	0.344	0.362	-0.030	0.209
	ESP*	0.344	0.362	-0.030	0.209
	Mulliken	0.639	0.561	0.651	0.684
	Mulliken*	0.639	0.561	0.651	0.684
	APT	0.121	0.200	0.205	0.205
	APT*	0.121	0.200	0.205	0.205
	NPA	-0.107	-0.105	-0.106	-0.107
C(4″)	ESP	-0.212	-0.198	-0.279	-0.216
	ESP*	-0.028	-0.024	-0.088	-0.040
	Mulliken	-0.253	-0.175	-0.232	-0.184
	Mulliken*	-0.067	0.006	-0.051	0.001
	APT	0.033	0.096	0.084	0.073
	APT*	0.099	0.161	0.152	0.143
	NPA	-0.183	-0.185	-0.185	-0.185
C(5″)	ESP	-0.153	-0.181	-0.145	-0.170
	ESP*	0.006	-0.023	0.001	-0.020
	Mulliken	-0.557	-0.599	-0.578	-0.560
	Mulliken*	-0.356	-0.403	-0.381	-0.364
	APT	-0.191	-0.281	-0.283	-0.279
	APT*	-0.149	-0.246	-0.249	-0.242
	NPA	-0.201	-0.213	-0.211	-0.210

C(6″)	ESP	-0.127	-0.120	-0.127	-0.101
	ESP*	0.029	0.027	0.022	0.044
	Mulliken	-0.257	-0.264	-0.266	-0.252
	Mulliken*	-0.045	-0.056	-0.057	-0.043
	APT	-0.087	-0.047	-0.046	-0.039
	APT*	-0.050	-0.019	-0.019	-0.011
	NPA	-0.195	-0.197	-0.197	-0.197
C(7″)	ESP	-0.204	-0.221	-0.274	-0.321
	ESP*	-0.017	-0.044	-0.084	-0.118
	Mulliken	-0.387	-0.260	-0.362	-0.285
	Mulliken*	-0.209	-0.082	-0.183	-0.104
	APT	-0.008	-0.106	-0.074	-0.067
	APT*	0.081	-0.024	0.009	0.015
	NPA	-0.211	-0.221	-0.220	-0.219
C(8″)	ESP	-0.012	0.066	0.151	0.236
	ESP*	-0.012	0.066	0.151	0.236
	Mulliken	0.616	0.485	0.558	0.510
	Mulliken*	0.616	0.485	0.558	0.510
	APT	0.435	0.737	0.682	0.646
	APT*	0.435	0.737	0.682	0.646
	NPA	0.158	0.164	0.162	0.162
C(9″)	ESP	0.027	-0.001	0.218	0.071
	ESP*	0.027	-0.001	0.218	0.071
	Mulliken	0.611	0.546	0.621	0.523
	Mulliken*	0.611	0.546	0.621	0.523
	APT	-0.192	-0.235	-0.233	-0.228
	APT*	-0.192	-0.235	-0.233	-0.228
	NPA	-0.015	-0.022	-0.020	-0.020
C(8′)	ESP	0.344	0.219	0.168	0.252
	ESP*	0.344	0.219	0.168	0.252
	Mulliken	-0.824	-0.942	-0.549	-0.842
	Mulliken*	-0.824	-0.942	-0.549	-0.842
	APT	0.257	0.446	0.602	0.685
	APT*	0.257	0.446	0.602	0.685
	NPA	0.301	0.281	0.273	0.284
C(CH_3-C(3″))	ESP	-0.448	-0.405	-0.473	-0.477
	ESP*	-0.050	-0.061	-0.010	-0.024
	Mulliken	-0.802	-0.780	-0.833	-0.944
	Mulliken*	-0.222	-0.216	-0.247	-0.311
	APT	0.037	0.019	0.026	0.029
	APT*	0.059	0.023	0.033	0.047
	NPA	-0.566	-0.565	-0.565	-0.568
C(C′H_3-C(3″))	ESP	-0.450	-0.393	-0.500	-0.497
	ESP*	-0.054	-0.057	-0.013	-0.048
	Mulliken	-0.831	-0.839	-0.798	-0.855
	Mulliken*	-0.236	-0.256	-0.228	-0.277
	APT	0.039	0.026	0.022	0.026
	APT*	0.056	0.028	0.034	0.023
	NPA	-0.564	-0.565	-0.567	-0.563
C(12′)	ESP	0.083	-0.039	0.145	-0.045
	ESP*	0.205	0.105	0.243	0.067
	Mulliken	0.142	-0.117	-0.073	0.084
	Mulliken*	-0.098	-0.350	-0.308	-0.186
	APT	1.814	2.312	2.409	2.324
	APT*	1.947	2.431	2.540	2.421
	NPA	-0.042	-0.063	-0.064	-0.060

C(13′)	ESP	-0.309	-0.289	-0.407	-0.260
	ESP*	-0.134	-0.124	-0.221	-0.102
	Mulliken	-0.448	-0.393	-0.328	-0.359
	Mulliken*	-0.218	-0.147	-0.091	-0.137
	APT	-1.794	-2.341	-2.462	-2.396
	APT*	-1.740	-2.298	-2.422	-2.350
	NPA	-0.309	-0.329	-0.329	-0.326
Cl(1′)	ESP	1.128	1.074	1.115	1.108
	ESP*	1.128	1.074	1.115	1.108
	Mulliken	-0.129	-0.116	-0.269	-0.446
	Mulliken*	-0.129	-0.116	-0.269	-0.446
	APT	3.268	3.246	3.241	3.193
	APT*	3.268	3.246	3.241	3.193
	NPA	2.366	2.366	2.369	2.366
O(3′)	ESP	-0.537	-0.517	-0.520	-0.561
	ESP*	-0.537	-0.517	-0.520	-0.561
	Mulliken	-0.179	-0.213	-0.116	-0.125
	Mulliken*	-0.179	-0.213	-0.116	-0.125
	APT	-1.091	-1.087	-1.112	-1.117
	APT*	-1.091	-1.087	-1.112	-1.117
	NPA	-0.837	-0.838	-0.840	-0.847
O(4′)	ESP	-0.512	-0.494	-0.514	-0.525
	ESP*	-0.512	-0.494	-0.514	-0.525
	Mulliken	-0.141	-0.107	-0.122	-0.140
	Mulliken*	-0.141	-0.107	-0.122	-0.140
	APT	-1.139	-1.116	-1.108	-1.040
	APT*	-1.139	-1.116	-1.108	-1.040
	NPA	-0.843	-0.841	-0.840	-0.830
O(5′)	ESP	-0.528	-0.516	-0.520	-0.510
	ESP*	-0.528	-0.516	-0.520	-0.510
	Mulliken	-0.267	-0.274	-0.183	-0.164
	Mulliken*	-0.267	-0.274	-0.183	-0.164
	APT	-1.078	-1.075	-1.044	-1.043
	APT*	-1.078	-1.075	-1.044	-1.043
	NPA	-0.833	-0.833	-0.832	-0.830
O(6′)	ESP	-0.525	-0.516	-0.523	-0.518
	ESP*	-0.525	-0.516	-0.523	-0.518
	Mulliken	-0.227	-0.236	-0.243	-0.144
	Mulliken*	-0.227	-0.236	-0.243	-0.144
	APT	-1.050	-1.048	-1.070	-1.048
	APT*	-1.050	-1.048	-1.070	-1.048
	NPA	-0.833	-0.834	-0.832	-0.833

* Charges with hydrogens, summed into heavy atoms.

** Notation, such as C(CH_3-N(1)), means the carbon of fragment CH_3-N(1).

*** Apostrophe in a notation, such as C(C′H_3-C(3)), indicates the second group CH_3-C(3) at the atom C(3).

Table S8 The absolute values of the percentage changes of the atomic charge during the transitions from **1a** to **1b** in compound **1** and from **2a** to **2b** in compound **2** according to ESP, MPA, APT and NPA calculation schemas.

Compound 1, 1a→1b							
Atom	$\|\Delta q_{ESP}\|$	$\|\Delta q_{ESP*}\|$	$\|\Delta q_{MPA}\|$	$\|\Delta q_{MPA*}\|$	$\|\Delta q_{APT}\|$	$\|\Delta q_{APT*}\|$	$\|\Delta q_{NPA}\|$
N(1)	116%	116%	127%	127%	70%	70%	33%
C(2,2′)	37%	37%	124%	124%	43%	43%	15%
C(3′)	74%	151%	178%	1140%	363%	479%	49%
C(4′)	168%	1251%	1212%	39%	775%	649%	53%
C(10′)	202%	202%	198%	198%	3336%	3336%	48%
C(9′)	476%	476%	61734%	61734%	43%	43%	17%
O(1′)	16256%	16256%	254%	254%	52%	52%	20%
C(5′)	37%	55%	8%	8%	2406%	869%	11%
C(6′)	15%	15%	7%	7%	193%	193%	16%
O(2′)	5%	5%	2%	2%	7%	7%	0%
C(7′)	21%	31%	12%	16%	955%	357%	19%
C(8′)	124%	124%	13%	13%	52%	52%	25%
C(12′)	83%	239%	59%	61%	38%	35%	26%
C(13′)	379%	361%	230%	119%	41%	45%	9%
C(2″)	66%	66%	19%	19%	36%	36%	6%
N(1″)	133%	133%	33%	33%	47%	47%	8%
Compound 2, 2a→2b							
Atom	$\|\Delta q_{ESP}\|$	$\|\Delta q_{ESP*}\|$	$\|\Delta q_{MPA}\|$	$\|\Delta q_{MPA*}\|$	$\|\Delta q_{APT}\|$	$\|\Delta q_{APT*}\|$	$\|\Delta q_{NPA}\|$
N(1)	83%	83%	58%	58%	64%	64%	33%
C(2,2′)	30%	30%	97%	97%	22%	22%	10%
C(3′)	34%	59%	268%	343%	393%	508%	39%
C(4′)	201%	182%	70%	1092%	641%	479%	57%
C(10′)	248%	248%	169%	169%	233%	233%	241%
C(9′)	67%	67%	65%	65%	6%	6%	21%
O(1′)	30%	30%	220%	220%	21%	21%	22%
C(5′)	11%	12%	34%	38%	184%	149%	63%
C(6′)	25%	25%	58%	58%	59%	59%	25%
C(7′)	15%	21%	51%	32%	109%	62%	14%
C(8′)	36%	36%	14%	14%	74%	74%	7%
O(2′)	24%	24%	5%	5%	4%	4%	1%
C(12′)	146%	49%	182%	257%	27%	25%	53%
C(13′)	7%	8%	12%	32%	30%	32%	7%
C(2″)	21%	21%	4%	4%	28%	28%	8%
N(1″)	44%	44%	12%	12%	51%	51%	7%

* Charges with hydrogens, summed into heavy atoms.

Table S9 The absolute values of the percentage changes of the atomic charge during the transitions from **1b** to **1c** in compound **1** and from **2b** to **2c** in compound **2** according to ESP, MPA, APT and NPA calculation schemas.

Compound 1, 1b→1c							
Atom	$\|\Delta q_{ESP}\|$	$\|\Delta q_{ESP*}\|$	$\|\Delta q_{MPA}\|$	$\|\Delta q_{MPA*}\|$	$\|\Delta q_{APT}\|$	$\|\Delta q_{APT*}\|$	$\|\Delta q_{NPA}\|$
N(1)	4%	4%	54%	54%	303%	303%	6%
C(2,2′)	61%	61%	92%	92%	200%	200%	11%
C(3′)	40%	61%	36%	88%	82%	86%	3%
C(4′)	72%	18%	331%	552%	42%	45%	20%
C(10′)	15%	15%	23%	23%	72%	72%	7%
C(9′)	9%	9%	43%	43%	17%	17%	23%
O(1′)	3%	3%	5%	5%	9%	9%	2%
C(5′)	8%	11%	3%	1%	21%	21%	2%
C(6′)	1%	1%	69%	69%	116%	116%	0%
O(2′)	2%	2%	4%	4%	5%	5%	0%
C(7′)	1%	2%	14%	22%	46%	41%	8%
C(8′)	97%	97%	50%	50%	0%	0%	14%
C(12′)	222%	33%	3%	21%	9%	8%	7%
C(13′)	23%	31%	34%	221%	7%	6%	0%
C(2″)	11%	11%	136%	136%	6%	6%	1%
N(1″)	442%	442%	34%	34%	1%	1%	1%
Compound 2, 2b→2c							
Atom	$\|\Delta q_{ESP}\|$	$\|\Delta q_{ESP*}\|$	$\|\Delta q_{MPA}\|$	$\|\Delta q_{MPA*}\|$	$\|\Delta q_{APT}\|$	$\|\Delta q_{APT*}\|$	$\|\Delta q_{NPA}\|$
N(1)	12%	12%	57%	57%	236%	236%	5%
C(2,2′)	45%	45%	757%	757%	95%	95%	12%
C(3′)	21%	60%	29%	82%	50%	45%	2%
C(4′)	19%	12%	52%	185%	53%	48%	31%
C(10′)	155%	155%	1%	1%	32%	32%	7%
C(9′)	21%	21%	15%	15%	0%	0%	2%
O(1′)	6%	6%	29%	29%	9%	9%	1%
C(5′)	59%	141%	31%	75%	14%	13%	12%
C(6′)	310%	310%	10%	10%	15%	15%	8%
C(7′)	46%	87%	73%	62%	130%	19%	13%
C(8′)	23%	23%	42%	42%	35%	35%	3%
O(2′)	0%	0%	19%	19%	7%	7%	0%
C(12′)	474%	131%	37%	12%	4%	4%	0%
C(13′)	41%	79%	17%	38%	5%	5%	0%
C(2″)	488%	488%	80%	80%	3%	3%	3%
N(1″)	132%	132%	4%	4%	4%	4%	1%

Table S10 The absolute values of the percentage changes of the atomic charge during the transitions from **1c** to **1d** in compound **1** and from **2c** to **2d** in compound **2** according to ESP, MPA, APT and NPA calculation schemas.

Compound 1, 1c→1d							
Atom	$\|\Delta q_{ESP}\|$	$\|\Delta q_{ESP*}\|$	$\|\Delta q_{MPA}\|$	$\|\Delta q_{MPA*}\|$	$\|\Delta q_{APT}\|$	$\|\Delta q_{APT*}\|$	$\|\Delta q_{NPA}\|$
N(1)	68%	68%	11%	11%	35%	35%	2%
C(2,2′)	65%	65%	1678%	1678%	9%	9%	2%
C(3′)	3%	11%	51%	172%	15%	19%	4%
C(4′)	242%	21%	140%	118%	25%	28%	0%
C(10′)	28%	28%	15%	15%	2%	2%	7%
C(9′)	1%	1%	6%	6%	52%	52%	4%
O(1′)	3%	3%	12%	12%	24%	24%	1%
C(5′)	32%	87%	85%	77%	39%	34%	6%
C(6′)	16%	16%	230%	230%	27%	27%	4%
O(2′)	3%	3%	1%	1%	9%	9%	0%
C(7′)	17%	28%	13%	21%	42%	38%	4%
C(8′)	2025%	2025%	231%	231%	8%	8%	1%
C(12′)	23%	6%	52%	45%	7%	6%	1%
C(13′)	11%	30%	1%	58%	6%	6%	1%
C(2″)	25%	25%	6%	6%	5%	5%	0%
N(1″)	35%	35%	11%	11%	3%	3%	1%
Compound 2, 2c→2d							
Atom	$\|\Delta q_{ESP}\|$	$\|\Delta q_{ESP*}\|$	$\|\Delta q_{MPA}\|$	$\|\Delta q_{MPA*}\|$	$\|\Delta q_{APT}\|$	$\|\Delta q_{APT*}\|$	$\|\Delta q_{NPA}\|$
N(1)	31%	31%	37%	37%	18%	18%	1%
C(2,2′)	41%	41%	131%	131%	2%	2%	1%
C(3′)	1%	39%	25%	367%	11%	10%	4%
C(4′)	109%	9%	353%	29%	5%	4%	14%
C(10′)	47%	47%	9%	9%	6%	6%	4%
C(9′)	21%	21%	5%	5%	7%	7%	1%
O(1′)	5%	5%	5%	5%	5%	5%	1%
C(5′)	121%	151%	108%	611%	11%	10%	23%
C(6′)	120%	120%	51%	51%	3%	3%	14%
C(7′)	60%	510%	165%	118%	296%	96%	13%
C(8′)	50%	50%	54%	54%	14%	14%	4%
O(2′)	1%	1%	6%	6%	3%	3%	0%
C(12′)	131%	72%	214%	40%	4%	5%	5%
C(13′)	36%	54%	10%	51%	3%	3%	1%
C(2″)	44%	44%	35%	35%	3%	3%	0%
N(1″)	32%	32%	1%	1%	0%	0%	0%

Table S11 The optimized cartesian coordinates (Å) of the compounds **1** and **2** calculated by B3LYP/6-311++G(d,p) method in DMSO.

Compound 1					
Key	**Structure**	**Geometry**			
g.1a	**1a**	N	2.300210000	2.425767000	1.034977000
		C	2.865302000	2.405951000	-1.277035000
		C	0.862674000	4.031382000	-1.848626000
		H	1.051207000	4.041678000	-2.917097000
		C	-0.174762000	4.810963000	-1.311078000
		H	-0.790694000	5.416859000	-1.965417000
		C	-0.411823000	4.803934000	0.062581000
		H	-1.215311000	5.406500000	0.472048000
		C	0.361246000	4.021000000	0.929874000
		H	0.157377000	4.014355000	1.993516000
		C	1.385665000	3.252891000	0.379184000
		C	1.637792000	3.259214000	-1.000759000
		C	2.090595000	1.991022000	2.409397000
		H	1.181540000	1.389528000	2.521432000
		H	2.018807000	2.863364000	3.062290000
		H	2.948215000	1.400387000	2.731520000
		C	2.758926000	1.516272000	-2.521005000
		H	3.634311000	0.866923000	-2.611493000
		H	2.723610000	2.143239000	-3.415393000
		H	1.863164000	0.896214000	-2.504588000
		C	4.091370000	3.338878000	-1.421988000
		H	5.008352000	2.765424000	-1.579736000
		H	4.223430000	3.974453000	-0.543557000
		H	3.944375000	3.987235000	-2.288454000
		C	2.958403000	1.576339000	0.075085000
		O	2.095597000	0.358805000	-0.074555000
		O	3.965839000	-4.836383000	-0.492557000
		C	4.343487000	1.191446000	0.498897000
		H	4.980950000	2.006222000	0.816570000
		C	4.793568000	-0.065922000	0.478551000
		H	5.813432000	-0.286037000	0.775257000
		C	4.427633000	-2.481393000	-0.013484000
		H	5.476220000	-2.653035000	0.191513000
		C	3.577041000	-3.532873000	-0.363086000
		C	2.235833000	-3.261428000	-0.597956000
		H	1.580135000	-4.082283000	-0.863154000
		C	1.700977000	-1.958266000	-0.497841000
		C	2.585912000	-0.897211000	-0.165508000
		C	3.939036000	-1.173781000	0.083194000
		C	5.337916000	-5.162968000	-0.259867000
		H	5.993797000	-4.640382000	-0.962481000
		H	5.417233000	-6.236077000	-0.420763000
		H	5.632600000	-4.926668000	0.766813000
		C	0.285721000	-1.833070000	-0.756842000
		H	-0.166339000	-2.769448000	-1.057027000
		C	-0.522227000	-0.738458000	-0.655000000
		H	-0.093584000	0.198528000	-0.336299000
		N	-2.661935000	0.333103000	-0.770632000
		C	-1.918002000	-0.756964000	-0.937700000
		C	-2.792187000	-1.901310000	-1.464168000
		C	-5.374369000	-1.689713000	-1.974307000
		H	-5.497562000	-2.714044000	-2.306229000
		C	-6.467681000	-0.817258000	-1.960391000
		H	-7.439452000	-1.171263000	-2.283259000
		C	-6.321229000	0.505619000	-1.535276000
		H	-7.179178000	1.167058000	-1.531918000

		C	-5.083668000	0.994191000	-1.112105000
		H	-4.982289000	2.020715000	-0.786794000
		C	-4.014238000	0.107030000	-1.134784000
		C	-4.140459000	-1.214003000	-1.557625000
		C	-2.170835000	1.613510000	-0.248799000
		H	-3.010308000	2.291150000	-0.134527000
		H	-1.453807000	2.051280000	-0.943223000
		H	-1.709502000	1.453934000	0.724919000
		C	-2.864823000	-3.078584000	-0.457877000
		H	-1.918971000	-3.616807000	-0.394692000
		H	-3.629029000	-3.782591000	-0.792931000
		H	-3.128442000	-2.719904000	0.537921000
		C	-2.331512000	-2.373515000	-2.865328000
		H	-1.354441000	-2.855518000	-2.827927000
		H	-2.278234000	-1.536553000	-3.564432000
		H	-3.051792000	-3.097013000	-3.251894000
		Cl	-2.176478000	-0.524429000	3.398813000
		O	-2.947578000	-0.094493000	4.609053000
		O	-1.276708000	0.591133000	2.955489000
		O	-3.126701000	-0.861191000	2.290562000
		O	-1.351112000	-1.728091000	3.735666000
g.1b	**1b**	N	-3.081910000	-1.285688000	0.484663000
		C	-4.243663000	-2.250225000	-1.307049000
		C	-2.880387000	-4.508022000	-1.103956000
		H	-3.386348000	-5.014178000	-1.918263000
		C	-1.866615000	-5.158229000	-0.390062000
		H	-1.588970000	-6.171122000	-0.657185000
		C	-1.202873000	-4.513922000	0.656724000
		H	-0.412430000	-5.029729000	1.189066000
		C	-1.534217000	-3.207527000	1.027721000
		H	-0.992578000	-2.700859000	1.815857000
		C	-2.548679000	-2.591175000	0.307611000
		C	-3.214960000	-3.210184000	-0.748102000
		C	-2.737618000	-0.466987000	1.643079000
		H	-1.770815000	0.013841000	1.500448000
		H	-2.697731000	-1.113700000	2.519548000
		H	-3.505177000	0.288250000	1.785358000
		C	-3.994202000	-1.927038000	-2.796667000
		H	-4.712697000	-1.185969000	-3.153286000
		H	-4.112384000	-2.835038000	-3.392021000
		H	-2.987124000	-1.536855000	-2.950643000
		C	-5.681081000	-2.790613000	-1.103813000
		H	-6.423021000	-2.082266000	-1.477687000
		H	-5.885502000	-2.991984000	-0.050384000
		H	-5.794776000	-3.722731000	-1.661066000
		C	-4.001780000	-1.013274000	-0.435582000
		O	-1.777250000	0.602479000	-1.065502000
		O	-2.401289000	5.768465000	0.744854000
		C	-4.754859000	0.178708000	-0.580109000
		H	-5.762091000	-0.007771000	-0.942116000
		C	-4.464190000	1.509563000	-0.378281000
		H	-5.349476000	2.140984000	-0.419105000
		C	-3.406546000	3.607349000	0.180501000
		H	-4.408759000	3.962882000	0.385491000
		C	-2.320071000	4.461378000	0.335078000
		C	-1.040889000	3.982003000	0.068926000
		H	-0.201922000	4.655203000	0.213619000
		C	-0.802607000	2.670528000	-0.371019000
		C	-1.932138000	1.746330000	-0.579113000
		C	-3.256328000	2.261983000	-0.219769000
		C	-3.690185000	6.306936000	1.038110000

		H	-4.339339000	6.288476000	0.157104000
		H	-3.519396000	7.338885000	1.338463000
		H	-4.169752000	5.764824000	1.859118000
		C	0.558465000	2.296625000	-0.573245000
		H	1.261667000	3.103605000	-0.403700000
		C	1.059254000	1.058312000	-0.912473000
		H	0.345407000	0.262442000	-1.061069000
		N	2.835376000	-0.492898000	-1.323782000
		C	2.428203000	0.758656000	-1.060353000
		C	3.651110000	1.682597000	-0.979042000
		C	6.144875000	0.901613000	-1.363234000
		H	6.581143000	1.883260000	-1.217717000
		C	6.964372000	-0.197019000	-1.647003000
		H	8.036789000	-0.061470000	-1.721289000
		C	6.413001000	-1.466268000	-1.834524000
		H	7.060684000	-2.307006000	-2.052869000
		C	5.034530000	-1.674880000	-1.745203000
		H	4.620186000	-2.663362000	-1.892012000
		C	4.242107000	-0.567886000	-1.463939000
		C	4.775311000	0.706240000	-1.273875000
		C	1.943984000	-1.649993000	-1.428348000
		H	2.535716000	-2.537040000	-1.631039000
		H	1.235610000	-1.504875000	-2.244854000
		H	1.410382000	-1.784362000	-0.486765000
		C	3.822704000	2.270698000	0.445093000
		H	3.037980000	2.990101000	0.681113000
		H	4.782058000	2.789349000	0.502479000
		H	3.806312000	1.479450000	1.196639000
		C	3.602764000	2.796171000	-2.051887000
		H	2.790596000	3.499346000	-1.865383000
		H	3.471767000	2.374345000	-3.050489000
		H	4.542444000	3.352106000	-2.035325000
		Cl	2.148403000	-1.172651000	3.131851000
		O	2.480004000	-2.346967000	4.001199000
		O	1.225234000	-1.609008000	2.033733000
		O	3.406148000	-0.620728000	2.534080000
		O	1.480110000	-0.115061000	3.956033000
g.1c	**1c**	N	-4.825357000	-1.755333000	-0.675572000
		C	-6.074772000	0.139257000	-0.061327000
		C	-8.340061000	-1.214296000	-0.170267000
		H	-8.969625000	-0.377209000	0.109364000
		C	-8.909853000	-2.466445000	-0.429364000
		H	-9.982736000	-2.594947000	-0.349862000
		C	-8.107382000	-3.551309000	-0.787988000
		H	-8.562261000	-4.515012000	-0.984069000
		C	-6.720776000	-3.418880000	-0.898632000
		H	-6.111123000	-4.269026000	-1.174437000
		C	-6.178867000	-2.165216000	-0.637998000
		C	-6.965356000	-1.071456000	-0.277331000
		C	-3.715994000	-2.643581000	-1.020010000
		H	-3.160662000	-2.237506000	-1.866230000
		H	-4.109437000	-3.617171000	-1.294466000
		H	-3.045892000	-2.758704000	-0.166554000
		C	-6.437092000	1.256973000	-1.070060000
		H	-5.801472000	2.134126000	-0.946455000
		H	-7.472751000	1.563948000	-0.910128000
		H	-6.340049000	0.902986000	-2.098404000
		C	-6.192772000	0.637348000	1.399756000
		H	-5.556581000	1.503067000	1.585260000
		H	-5.918760000	-0.149552000	2.105340000
		H	-7.226311000	0.929422000	1.597120000

		C	-4.688395000	-0.455130000	-0.351493000
		O	-0.575801000	0.313330000	-0.557979000
		O	-0.818049000	5.639781000	0.838749000
		C	-3.422579000	0.151924000	-0.317900000
		H	-2.561640000	-0.454459000	-0.553290000
		C	-3.188877000	1.479153000	-0.001756000
		H	-4.043758000	2.100400000	0.239157000
		C	-1.992782000	3.536305000	0.411439000
		H	-2.962696000	3.971491000	0.617985000
		C	-0.847529000	4.311882000	0.499808000
		C	0.391030000	3.726727000	0.228034000
		H	1.274743000	4.352483000	0.302685000
		C	0.532701000	2.381029000	-0.131300000
		C	-0.659717000	1.519848000	-0.237185000
		C	-1.948409000	2.166467000	0.054599000
		C	-2.055599000	6.289938000	1.128718000
		H	-2.724197000	6.274942000	0.262362000
		H	-1.800470000	7.319794000	1.370345000
		H	-2.554818000	5.828373000	1.986316000
		C	1.859891000	1.915894000	-0.384324000
		H	2.617228000	2.682660000	-0.270813000
		C	2.262308000	0.649778000	-0.743306000
		H	1.493985000	-0.101357000	-0.841335000
		N	3.903160000	-0.984385000	-1.355251000
		C	3.599536000	0.267552000	-0.985651000
		C	4.888214000	1.095840000	-0.892439000
		C	7.310855000	0.150394000	-1.357363000
		H	7.824785000	1.084031000	-1.159353000
		C	8.038555000	-0.989499000	-1.717942000
		H	9.117610000	-0.933518000	-1.798547000
		C	7.388177000	-2.199212000	-1.971157000
		H	7.966548000	-3.073446000	-2.245351000
		C	5.998678000	-2.305359000	-1.874768000
		H	5.506825000	-3.249416000	-2.067240000
		C	5.298794000	-1.158274000	-1.519049000
		C	5.931194000	0.056179000	-1.258575000
		C	2.932034000	-2.067001000	-1.531897000
		H	3.417107000	-2.896698000	-2.037327000
		H	2.102882000	-1.722724000	-2.148452000
		H	2.567709000	-2.397363000	-0.557402000
		C	5.128021000	1.611930000	0.548042000
		H	4.397237000	2.370639000	0.829764000
		H	6.120886000	2.062945000	0.605486000
		H	5.072436000	0.792329000	1.266107000
		C	4.900231000	2.252647000	-1.921949000
		H	4.148331000	3.007236000	-1.690467000
		H	4.717570000	1.881387000	-2.932470000
		H	5.879436000	2.735497000	-1.906406000
		Cl	3.310836000	-2.161432000	2.832770000
		O	3.790084000	-3.108444000	3.889997000
		O	2.549088000	-2.923188000	1.789341000
		O	4.484962000	-1.485380000	2.194430000
		O	2.416047000	-1.133066000	3.453493000
g.1d	**1d**	N	-6.625506000	0.364248000	0.043545000
		C	-5.218571000	-1.392487000	-0.644327000
		C	-7.271945000	-3.021430000	-0.967409000
		H	-6.676940000	-3.867142000	-1.292981000
		C	-8.663789000	-3.137245000	-0.871470000
		H	-9.143297000	-4.075570000	-1.123531000
		C	-9.438718000	-2.053928000	-0.452951000
		H	-10.514980000	-2.158037000	-0.382427000

		C	-8.850961000	-0.830413000	-0.120854000
		H	-9.464517000	-0.000104000	0.202824000
		C	-7.467265000	-0.739856000	-0.225096000
		C	-6.677970000	-1.812464000	-0.639800000
		C	-7.112131000	1.665932000	0.496718000
		H	-6.714385000	1.894881000	1.486770000
		H	-8.195821000	1.643250000	0.551395000
		H	-6.813473000	2.444739000	-0.206498000
		C	-4.407373000	-2.259388000	0.349277000
		H	-3.356773000	-1.969111000	0.372788000
		H	-4.462653000	-3.305872000	0.042241000
		H	-4.810941000	-2.178038000	1.360599000
		C	-4.638432000	-1.485573000	-2.076834000
		H	-3.592716000	-1.179011000	-2.108973000
		H	-5.203726000	-0.859161000	-2.769893000
		H	-4.698652000	-2.519566000	-2.422749000
		C	-5.327433000	0.064698000	-0.169889000
		O	-0.349879000	0.018605000	-0.679693000
		O	-1.109689000	5.164155000	1.116303000
		C	-4.312813000	1.007195000	0.040538000
		H	-4.629708000	1.982030000	0.388979000
		C	-2.961252000	0.781249000	-0.162527000
		H	-2.636209000	-0.189443000	-0.513557000
		C	-2.083591000	3.010282000	0.494085000
		H	-3.087625000	3.349793000	0.709112000
		C	-1.015298000	3.871586000	0.675077000
		C	0.283793000	3.426256000	0.396861000
		H	1.099287000	4.126141000	0.549551000
		C	0.564573000	2.136653000	-0.060188000
		C	-0.541881000	1.182997000	-0.269622000
		C	-1.894015000	1.686973000	0.033013000
		C	-2.404728000	5.679598000	1.425972000
		H	-3.053945000	5.674579000	0.544924000
		H	-2.245751000	6.705233000	1.752583000
		H	-2.874948000	5.109193000	2.233026000
		C	1.936512000	1.815075000	-0.303896000
		H	2.617729000	2.633875000	-0.104968000
		C	2.456841000	0.622095000	-0.746475000
		H	1.759341000	-0.180747000	-0.929837000
		N	4.253846000	-0.810404000	-1.425378000
		C	3.830389000	0.374847000	-0.968183000
		C	5.037448000	1.298189000	-0.755087000
		C	7.548074000	0.601944000	-1.192363000
		H	7.971547000	1.556249000	-0.900811000
		C	8.384033000	-0.439993000	-1.609721000
		H	9.456314000	-0.287500000	-1.640182000
		C	7.850878000	-1.675656000	-1.983490000
		H	8.512587000	-2.473224000	-2.299601000
		C	6.473398000	-1.905262000	-1.955125000
		H	6.071950000	-2.868377000	-2.240513000
		C	5.664707000	-0.853035000	-1.541670000
		C	6.179174000	0.384464000	-1.159399000
		C	3.389980000	-1.953411000	-1.733024000
		H	3.954920000	-2.674397000	-2.316533000
		H	2.536978000	-1.623049000	-2.323454000
		H	3.051443000	-2.418513000	-0.805359000
		C	5.181198000	1.710022000	0.731180000
		H	4.377625000	2.378243000	1.042191000
		H	6.128346000	2.236460000	0.865839000
		H	5.172206000	0.831654000	1.378263000
		C	4.983964000	2.534135000	-1.686852000
		H	4.163514000	3.202661000	-1.425556000

		H	4.867121000	2.234919000	-2.730426000
		H	5.917431000	3.092703000	-1.593246000
		Cl	3.590840000	-2.374284000	2.628304000
		O	4.107904000	-3.336522000	3.653358000
		O	3.002733000	-3.137901000	1.479348000
		O	4.714963000	-1.518450000	2.130835000
		O	2.535882000	-1.508402000	3.245208000
g.1a′	**1a′**	N	2.050778000	-2.487047000	-1.192075000
		C	2.233138000	-2.344583000	1.176439000
		C	0.096329000	-3.863386000	1.499844000
		H	0.109661000	-3.815798000	2.583698000
		C	-0.874395000	-4.637370000	0.842996000
		H	-1.613315000	-5.181197000	1.419893000
		C	-0.887334000	-4.704953000	-0.549157000
		H	-1.639983000	-5.303209000	-1.050991000
		C	0.049033000	-4.002955000	-1.319774000
		H	0.020065000	-4.055611000	-2.401204000
		C	1.004969000	-3.240215000	-0.651387000
		C	1.030810000	-3.171079000	0.749412000
		C	2.088394000	-2.129469000	-2.601919000
		H	1.251285000	-1.481898000	-2.889900000
		H	2.058648000	-3.034407000	-3.211424000
		H	3.022396000	-1.609975000	-2.815619000
		C	1.966980000	-1.378275000	2.336417000
		H	2.842098000	-0.751164000	2.528924000
		H	1.766981000	-1.948278000	3.247032000
		H	1.110117000	-0.733659000	2.143379000
		C	3.378585000	-3.308235000	1.569010000
		H	4.280441000	-2.757581000	1.848134000
		H	3.625852000	-3.996230000	0.757533000
		H	3.064061000	-3.901624000	2.430132000
		C	2.578294000	-1.601847000	-0.184539000
		O	1.749411000	-0.351699000	-0.243894000
		O	3.726660000	4.810081000	0.071828000
		C	4.027640000	-1.285168000	-0.394252000
		H	4.677105000	-2.137553000	-0.544777000
		C	4.516222000	-0.042174000	-0.384776000
		H	5.578677000	0.128374000	-0.521033000
		C	4.167565000	2.412797000	-0.141157000
		H	5.241252000	2.540654000	-0.182981000
		C	3.313013000	3.511550000	-0.018366000
		C	1.942377000	3.294936000	0.011270000
		H	1.284444000	4.151175000	0.100335000
		C	1.380806000	2.001135000	-0.073265000
		C	2.266647000	0.893649000	-0.172445000
		C	3.651831000	1.114644000	-0.217209000
		C	5.130404000	5.080411000	0.043974000
		H	5.642322000	4.601175000	0.883616000
		H	5.224468000	6.160717000	0.131714000
		H	5.578119000	4.751753000	-0.898450000
		C	-0.059975000	1.934889000	-0.042845000
		H	-0.516955000	2.907214000	0.087761000
		C	-0.886094000	0.854389000	-0.168786000
		H	-0.449517000	-0.121635000	-0.312443000
		N	-3.063322000	-0.142988000	-0.302052000
		C	-2.306011000	0.937368000	-0.117482000
		C	-3.203372000	2.150970000	0.156486000
		C	-5.840051000	2.059988000	0.281663000
		H	-5.970138000	3.114994000	0.492704000
		C	-6.953672000	1.219549000	0.180702000
		H	-7.947412000	1.629537000	0.315384000

		C	-6.800120000	-0.142534000	-0.089993000
		H	-7.674440000	-0.777973000	-0.162208000
		C	-5.534365000	-0.703672000	-0.269723000
		H	-5.427195000	-1.760144000	-0.475604000
		C	-4.445323000	0.153320000	-0.166029000
		C	-4.578038000	1.512422000	0.107387000
		C	-2.558296000	-1.486357000	-0.604405000
		H	-3.392747000	-2.122047000	-0.881067000
		H	-2.059803000	-1.908565000	0.268436000
		H	-1.862596000	-1.439576000	-1.439927000
		C	-3.077597000	3.223357000	-0.955817000
		H	-2.102665000	3.710154000	-0.946000000
		H	-3.837788000	3.989584000	-0.793459000
		H	-3.237166000	2.786216000	-1.943180000
		C	-2.938031000	2.751816000	1.559041000
		H	-1.946931000	3.200494000	1.625941000
		H	-3.025512000	1.989366000	2.335317000
		H	-3.676738000	3.530401000	1.757850000
g.1b′	**1b′**	N	-3.088767000	-1.122533000	0.896515000
		C	-3.719613000	-2.307729000	-1.021983000
		C	-2.623778000	-4.541674000	-0.120840000
		H	-2.888200000	-5.147356000	-0.980116000
		C	-1.921928000	-5.106848000	0.950632000
		H	-1.641481000	-6.152890000	0.914468000
		C	-1.577255000	-4.338722000	2.065224000
		H	-1.032162000	-4.793775000	2.883624000
		C	-1.922418000	-2.986594000	2.143296000
		H	-1.648341000	-2.393081000	3.005783000
		C	-2.615966000	-2.451807000	1.065934000
		C	-2.967199000	-3.199671000	-0.056363000
		C	-3.017123000	-0.133426000	1.966257000
		H	-2.031270000	0.331235000	1.992957000
		H	-3.212149000	-0.634151000	2.913828000
		H	-3.773749000	0.627810000	1.796707000
		C	-3.024707000	-2.205816000	-2.397628000
		H	-3.565388000	-1.513709000	-3.046712000
		H	-3.015125000	-3.188182000	-2.874637000
		H	-1.998270000	-1.852711000	-2.292695000
		C	-5.185964000	-2.779366000	-1.191734000
		H	-5.736379000	-2.110903000	-1.856818000
		H	-5.703903000	-2.827067000	-0.231802000
		H	-5.190999000	-3.776561000	-1.636304000
		C	-3.666990000	-0.965689000	-0.288885000
		O	-1.261479000	0.345067000	-0.591235000
		O	-1.728757000	5.742962000	0.431963000
		C	-4.264354000	0.217996000	-0.798004000
		H	-5.159320000	0.022275000	-1.382171000
		C	-3.913359000	1.542655000	-0.701011000
		H	-4.692229000	2.218157000	-1.048949000
		C	-2.799496000	3.610236000	-0.122142000
		H	-3.782634000	4.061190000	-0.176249000
		C	-1.688312000	4.396173000	0.173522000
		C	-0.432439000	3.801899000	0.208766000
		H	0.424925000	4.428093000	0.433880000
		C	-0.236768000	2.433398000	-0.046749000
		C	-1.392236000	1.564638000	-0.333188000
		C	-2.702410000	2.221373000	-0.338017000
		C	-2.992740000	6.404835000	0.384129000
		H	-3.441513000	6.333964000	-0.611556000
		H	-2.789593000	7.448847000	0.614376000
		H	-3.683545000	5.997113000	1.128711000

		C	1.105138000	1.957284000	-0.010302000
		H	1.835201000	2.728869000	0.205535000
		C	1.558506000	0.669743000	-0.215263000
		H	0.814617000	-0.082959000	-0.427510000
		N	3.261611000	-1.005528000	-0.375039000
		C	2.909224000	0.275544000	-0.173088000
		C	4.171504000	1.112685000	0.077057000
		C	6.630939000	0.149884000	0.088588000
		H	7.109414000	1.099768000	0.298120000
		C	7.402842000	-1.007307000	-0.066879000
		H	8.480926000	-0.949341000	0.023989000
		C	6.796670000	-2.235455000	-0.339351000
		H	7.407913000	-3.122115000	-0.458409000
		C	5.409321000	-2.344214000	-0.463229000
		H	4.952707000	-3.301483000	-0.676441000
		C	4.664797000	-1.181226000	-0.303047000
		C	5.253251000	0.053397000	-0.032345000
		C	2.320500000	-2.092254000	-0.647980000
		H	2.864130000	-3.030046000	-0.701486000
		H	1.813017000	-1.920402000	-1.598491000
		H	1.583439000	-2.157596000	0.152615000
		C	4.172906000	1.739088000	1.493153000
		H	3.399245000	2.499734000	1.599459000
		H	5.139708000	2.213029000	1.674396000
		H	4.016025000	0.977271000	2.259309000
		C	4.366118000	2.190565000	-1.017546000
		H	3.591798000	2.956535000	-0.971951000
		H	4.352092000	1.744233000	-2.013854000
		H	5.333113000	2.676813000	-0.873671000
g.1c′	**1c′**	N	4.341348000	-1.899462000	0.079419000
		C	5.479988000	0.152836000	-0.051182000
		C	7.826142000	-1.056334000	-0.138215000
		H	8.406714000	-0.142842000	-0.198958000
		C	8.469644000	-2.299452000	-0.135469000
		H	9.550611000	-2.344514000	-0.193606000
		C	7.730684000	-3.481791000	-0.060110000
		H	8.242513000	-4.436820000	-0.060787000
		C	6.335678000	-3.458211000	0.015384000
		H	5.775848000	-4.382319000	0.070217000
		C	5.720084000	-2.211621000	0.012863000
		C	6.442311000	-1.021330000	-0.064045000
		C	3.284144000	-2.905902000	0.172158000
		H	2.659832000	-2.711119000	1.044543000
		H	3.733783000	-3.888267000	0.276433000
		H	2.667549000	-2.890259000	-0.728079000
		C	5.737689000	1.042330000	1.190065000
		H	5.055990000	1.892303000	1.228349000
		H	6.757978000	1.429237000	1.148767000
		H	5.626570000	0.468863000	2.112525000
		C	5.607258000	0.962664000	-1.364458000
		H	4.913092000	1.802896000	-1.390388000
		H	5.416029000	0.330403000	-2.233835000
		H	6.621674000	1.358398000	-1.445721000
		C	4.128254000	-0.570949000	0.038967000
		O	-0.038305000	-0.101393000	0.102492000
		O	-0.082947000	5.409987000	0.011593000
		C	2.825272000	-0.045429000	0.068461000
		H	1.998278000	-0.737591000	0.104395000
		C	2.517039000	1.302866000	0.047000000
		H	3.337889000	2.010032000	0.019401000
		C	1.205705000	3.329828000	0.034438000

		H	2.154149000	3.852621000	0.023012000
		C	0.015765000	4.043399000	0.027964000
		C	-1.192252000	3.345694000	0.033744000
		H	-2.111910000	3.922090000	0.021058000
		C	-1.260918000	1.945831000	0.053597000
		C	-0.019829000	1.149331000	0.074101000
		C	1.235715000	1.915476000	0.054452000
		C	1.123137000	6.174400000	0.003813000
		H	1.720522000	5.981390000	0.900210000
		H	0.813303000	7.217411000	-0.006350000
		H	1.720260000	5.963962000	-0.888819000
		C	-2.563570000	1.364148000	0.045681000
		H	-3.364374000	2.093745000	0.018572000
		C	-2.900087000	0.027882000	0.066097000
		H	-2.089122000	-0.683353000	0.100124000
		N	-4.460483000	-1.788488000	0.077466000
		C	-4.219194000	-0.468828000	0.037453000
		C	-5.552319000	0.286702000	-0.051685000
		C	-7.926123000	-0.867967000	-0.135255000
		H	-8.486457000	0.058025000	-0.194621000
		C	-8.596272000	-2.096591000	-0.132056000
		H	-9.678041000	-2.117658000	-0.188526000
		C	-7.884217000	-3.295690000	-0.058446000
		H	-8.417630000	-4.238743000	-0.058921000
		C	-6.489233000	-3.303573000	0.015153000
		H	-5.949793000	-4.239732000	0.068629000
		C	-5.847314000	-2.070617000	0.012345000
		C	-6.541611000	-0.864204000	-0.063158000
		C	-3.426770000	-2.821112000	0.168191000
		H	-3.900633000	-3.791193000	0.278561000
		H	-2.794079000	-2.638086000	1.036600000
		H	-2.816241000	-2.822898000	-0.735948000
		C	-5.660151000	1.098498000	-1.365912000
		H	-4.944779000	1.920590000	-1.393177000
		H	-6.664211000	1.519939000	-1.445299000
		H	-5.486660000	0.461034000	-2.235160000
		C	-5.786824000	1.182954000	1.189575000
		H	-5.085461000	2.016763000	1.226125000
		H	-5.688399000	0.607818000	2.112355000
		H	-6.797770000	1.593362000	1.148380000
g.1d′	**1d′**	N	-5.966316000	0.385182000	-0.000533000
		C	-4.649398000	-1.564403000	0.004559000
		C	-6.788649000	-3.111541000	0.023015000
		H	-6.235286000	-4.043767000	0.025520000
		C	-8.188408000	-3.124107000	0.029747000
		H	-8.717003000	-4.069847000	0.037655000
		C	-8.908924000	-1.928107000	0.026437000
		H	-9.992190000	-1.952961000	0.031792000
		C	-8.257580000	-0.691886000	0.016311000
		H	-8.829576000	0.226384000	0.013888000
		C	-6.867194000	-0.705551000	0.009850000
		C	-6.132141000	-1.890711000	0.013204000
		C	-6.385734000	1.785779000	-0.005859000
		H	-6.011718000	2.294681000	0.883835000
		H	-7.469909000	1.834793000	-0.006418000
		H	-6.011355000	2.287754000	-0.899262000
		C	-3.972142000	-2.114408000	1.283500000
		H	-2.907092000	-1.882696000	1.307279000
		H	-4.083913000	-3.200288000	1.310766000
		H	-4.436043000	-1.700167000	2.180955000
		C	-3.984295000	-2.128795000	-1.274469000

		H	-2.919511000	-1.897602000	-1.311114000
		H	-4.456799000	-1.724686000	-2.172056000
		H	-4.096451000	-3.214919000	-1.288254000
		C	-4.683350000	-0.028981000	-0.003544000
		O	0.300917000	-0.474304000	-0.026588000
		O	-0.201726000	5.005926000	-0.007750000
		C	-3.617846000	0.881901000	-0.011134000
		H	-3.885201000	1.930912000	-0.012769000
		C	-2.277280000	0.537617000	-0.014775000
		H	-2.001441000	-0.508815000	-0.015000000
		C	-1.283163000	2.813797000	-0.014049000
		H	-2.271632000	3.252638000	-0.014124000
		C	-0.168941000	3.637609000	-0.010103000
		C	1.108562000	3.066301000	-0.007075000
		H	1.961378000	3.737564000	-0.001892000
		C	1.324714000	1.684641000	-0.011840000
		C	0.168111000	0.768037000	-0.019498000
		C	-1.160732000	1.406630000	-0.016845000
		C	-1.475397000	5.651900000	-0.013576000
		H	-2.046016000	5.393205000	-0.910841000
		H	-1.266490000	6.719667000	-0.012618000
		H	-2.054370000	5.393299000	0.878339000
		C	2.681097000	1.238175000	-0.009131000
		H	3.405500000	2.044251000	0.004119000
		C	3.142551000	-0.058890000	-0.023557000
		H	2.401507000	-0.843591000	-0.039409000
		N	4.864391000	-1.722134000	-0.047095000
		C	4.503662000	-0.430937000	-0.017405000
		C	5.761814000	0.445924000	0.030294000
		C	8.234618000	-0.483238000	0.055655000
		H	8.709257000	0.490678000	0.089375000
		C	9.014725000	-1.645045000	0.043420000
		H	10.094988000	-1.565752000	0.067840000
		C	8.414971000	-2.905614000	0.000948000
		H	9.033318000	-3.795213000	-0.006896000
		C	7.025315000	-3.042903000	-0.031515000
		H	6.573301000	-4.025151000	-0.063290000
		C	6.272973000	-1.874165000	-0.019742000
		C	6.854064000	-0.607819000	0.024438000
		C	3.928768000	-2.847603000	-0.092883000
		H	4.488910000	-3.773315000	-0.175327000
		H	3.274452000	-2.752799000	-0.959488000
		H	3.329361000	-2.873972000	0.818029000
		C	5.823784000	1.276336000	1.336266000
		H	5.038129000	2.031134000	1.372188000
		H	6.787093000	1.787046000	1.391271000
		H	5.725960000	0.634285000	2.213984000
		C	5.879378000	1.348439000	-1.222854000
		H	5.098145000	2.108159000	-1.249808000
		H	5.817733000	0.757188000	-2.138567000
		H	6.845308000	1.857293000	-1.208350000

Compound 2

Key	Structure	Geometry			
g.2a	**2a**	N	5.259025000	0.388367000	1.133443000
		C	5.471378000	0.303013000	-1.233936000
		C	7.526472000	-1.348864000	-1.060860000
		H	7.661254000	-1.444784000	-2.133116000
		C	8.392194000	-2.019139000	-0.181345000
		H	9.192571000	-2.634695000	-0.575243000
		C	8.219321000	-1.896605000	1.196116000

		H	8.888075000	-2.420329000	1.870458000
		C	7.186670000	-1.115232000	1.732224000
		H	7.056641000	-1.038835000	2.804738000
		C	6.338832000	-0.456122000	0.845045000
		C	6.504579000	-0.572805000	-0.542620000
		C	4.661949000	0.422779000	2.460591000
		H	3.876284000	1.177730000	2.481248000
		H	5.417912000	0.704239000	3.195708000
		H	4.233231000	-0.545132000	2.748805000
		C	4.830482000	-0.323373000	-2.477806000
		H	4.427864000	-1.314698000	-2.273433000
		H	5.579108000	-0.412436000	-3.268953000
		H	4.024053000	0.310256000	-2.858068000
		C	6.137053000	1.644220000	-1.622871000
		H	6.564133000	2.152611000	-0.755569000
		H	5.422732000	2.315559000	-2.106229000
		H	6.945454000	1.446910000	-2.330036000
		O	3.530691000	-0.676748000	-0.074822000
		O	2.230224000	-2.940798000	0.038638000
		N	-5.137261000	-2.448343000	-0.025162000
		C	4.440644000	0.517293000	-0.049109000
		C	3.656573000	1.793779000	-0.084507000
		H	4.243113000	2.702642000	-0.061495000
		C	2.320778000	1.843029000	-0.119632000
		H	1.800835000	2.794662000	-0.139253000
		C	0.089799000	-1.785718000	-0.016093000
		H	-0.459295000	-2.715298000	0.017597000
		C	-0.612034000	-0.552928000	-0.067041000
		C	0.124029000	0.642553000	-0.109924000
		H	-0.396226000	1.591826000	-0.145138000
		C	1.516407000	0.631667000	-0.106333000
		C	2.198327000	-0.593569000	-0.062749000
		C	-4.669720000	-3.837218000	-0.013798000
		H	-4.164389000	-4.056885000	0.927573000
		H	-3.990116000	-4.007585000	-0.848206000
		H	-5.522735000	-4.499145000	-0.121142000
		C	1.565855000	-4.207076000	0.092942000
		H	2.357550000	-4.952141000	0.126361000
		H	0.950443000	-4.365936000	-0.796982000
		H	0.948068000	-4.288030000	0.991713000
		C	-4.343781000	-1.370889000	-0.044942000
		C	-5.205054000	-0.102516000	-0.064568000
		C	-7.845155000	-0.087792000	-0.025793000
		H	-7.940540000	0.991681000	-0.044932000
		C	-8.987624000	-0.894796000	0.008230000
		H	-9.968600000	-0.434935000	0.014983000
		C	-8.877094000	-2.286924000	0.035409000
		H	-9.771934000	-2.896964000	0.063937000
		C	-7.628032000	-2.911862000	0.027729000
		H	-7.556548000	-3.990957000	0.052839000
		C	-6.509430000	-2.087759000	-0.008749000
		C	-6.599935000	-0.697649000	-0.032974000
		C	1.471590000	-1.817500000	-0.009679000
		C	-4.962112000	0.774460000	1.188699000
		H	-5.069400000	0.188769000	2.103908000
		H	-5.700981000	1.578074000	1.208206000
		H	-3.973391000	1.231465000	1.173510000
		C	-4.993364000	0.704381000	-1.370429000
		H	-5.136208000	0.072464000	-2.249296000
		H	-3.999055000	1.147514000	-1.412238000
		H	-5.723508000	1.515122000	-1.409342000
		C	-2.045316000	-0.455246000	-0.073195000

		H	-2.416930000	0.561936000	-0.106487000
		C	-2.935794000	-1.497519000	-0.041780000
		H	-2.548338000	-2.507254000	-0.008467000
		Cl	-1.853590000	4.313736000	0.151656000
		O	-0.412673000	4.239809000	-0.254973000
		O	-2.535303000	3.028128000	-0.216494000
		O	-2.518568000	5.450976000	-0.557512000
		O	-1.947290000	4.521190000	1.631212000
g.2b	**2b**	N	4.735792000	-0.121612000	0.982586000
		C	6.107417000	0.808134000	-0.668847000
		C	8.170521000	-0.676964000	0.068742000
		H	8.859392000	-0.283516000	-0.669845000
		C	8.591944000	-1.658955000	0.972955000
		H	9.610518000	-2.025798000	0.927667000
		C	7.715900000	-2.174598000	1.931093000
		H	8.060653000	-2.936935000	2.619431000
		C	6.395485000	-1.724909000	2.015913000
		H	5.716811000	-2.130889000	2.754687000
		C	6.005153000	-0.751511000	1.106588000
		C	6.860750000	-0.226718000	0.140401000
		C	3.661857000	-0.352431000	1.943769000
		H	2.960972000	0.476361000	1.899323000
		H	4.096830000	-0.408498000	2.940867000
		H	3.143391000	-1.284332000	1.717545000
		C	6.041678000	0.449121000	-2.170387000
		H	5.589073000	-0.531834000	-2.317943000
		H	7.051346000	0.440851000	-2.586532000
		H	5.451162000	1.190110000	-2.713282000
		C	6.710595000	2.222335000	-0.475764000
		H	6.736640000	2.505257000	0.578349000
		H	6.137884000	2.969753000	-1.028304000
		H	7.732409000	2.229456000	-0.859946000
		O	3.272288000	-1.432511000	-1.019573000
		O	1.698434000	-3.556698000	-1.029757000
		N	-5.483654000	-2.163680000	-0.004616000
		C	4.717777000	0.725101000	-0.036102000
		C	3.625868000	1.546670000	-0.443148000
		H	3.936920000	2.542781000	-0.745585000
		C	2.283310000	1.299633000	-0.541196000
		H	1.685709000	2.189713000	-0.726262000
		C	-0.234790000	-2.170568000	-0.614935000
		H	-0.905207000	-3.018452000	-0.628650000
		C	-0.773657000	-0.852809000	-0.412184000
		C	0.116808000	0.233570000	-0.398279000
		H	-0.293825000	1.227949000	-0.262915000
		C	1.499418000	0.090115000	-0.534108000
		C	2.064061000	-1.234900000	-0.793885000
		C	-5.211653000	-3.589580000	-0.171142000
		H	-4.555106000	-3.945017000	0.624803000
		H	-4.743753000	-3.773920000	-1.139577000
		H	-6.145874000	-4.140238000	-0.125038000
		C	0.874682000	-4.722367000	-1.068378000
		H	1.547972000	-5.556443000	-1.255282000
		H	0.138326000	-4.657519000	-1.875249000
		H	0.360499000	-4.873283000	-0.114214000
		C	-4.540066000	-1.197567000	-0.021666000
		C	-5.215367000	0.168107000	0.177505000
		C	-7.809516000	0.523185000	0.516858000
		H	-7.748835000	1.601462000	0.611812000
		C	-9.049714000	-0.121106000	0.601595000
		H	-9.948481000	0.462441000	0.761781000

		C	-9.136964000	-1.509205000	0.481545000
		H	-10.103140000	-1.995212000	0.549096000
		C	-7.996200000	-2.289984000	0.275423000
		H	-8.079571000	-3.364985000	0.185505000
		C	-6.776480000	-1.627107000	0.194884000
		C	-6.671623000	-0.241266000	0.311662000
		C	1.101930000	-2.357165000	-0.808902000
		C	-4.731592000	0.867651000	1.470725000
		H	-4.840050000	0.210233000	2.335825000
		H	-5.336020000	1.761080000	1.641773000
		H	-3.690016000	1.179112000	1.394967000
		C	-5.026059000	1.081492000	-1.058527000
		H	-5.342813000	0.574267000	-1.972207000
		H	-3.988413000	1.394514000	-1.172128000
		H	-5.635353000	1.979687000	-0.937160000
		C	-2.150239000	-0.578330000	-0.232438000
		H	-2.381967000	0.472797000	-0.110388000
		C	-3.186017000	-1.500840000	-0.201176000
		H	-2.940222000	-2.547872000	-0.322561000
		Cl	-1.242736000	4.231290000	0.005042000
		O	0.024830000	4.004437000	-0.763057000
		O	-2.096023000	3.000195000	-0.078165000
		O	-1.983172000	5.392461000	-0.580240000
		O	-0.914809000	4.516446000	1.437863000
g.2c	**2c**	N	6.091932000	1.089921000	0.005883000
		C	4.992719000	-0.982078000	-0.102835000
		C	7.283898000	-2.294357000	-0.156948000
		H	6.834189000	-3.279432000	-0.206247000
		C	8.676643000	-2.156950000	-0.146357000
		H	9.303212000	-3.039937000	-0.187436000
		C	9.266488000	-0.892650000	-0.084432000
		H	10.346226000	-0.802663000	-0.078427000
		C	8.487219000	0.265679000	-0.030275000
		H	8.957709000	1.238817000	0.015272000
		C	7.106660000	0.102299000	-0.040501000
		C	6.500706000	-1.151473000	-0.104240000
		C	6.361860000	2.526498000	0.081254000
		H	5.869793000	2.953075000	0.955560000
		H	6.002467000	3.024781000	-0.820192000
		H	7.431786000	2.684300000	0.170151000
		C	4.373957000	-1.662003000	1.143632000
		H	4.777530000	-1.233792000	2.063549000
		H	4.616747000	-2.726561000	1.126236000
		H	3.288885000	-1.567744000	1.153845000
		C	4.386151000	-1.542445000	-1.412719000
		H	4.809777000	-1.041433000	-2.285640000
		H	3.302924000	-1.429505000	-1.432840000
		H	4.614148000	-2.607881000	-1.484925000
		O	2.258580000	3.838973000	0.052965000
		O	-0.028825000	5.154158000	0.086240000
		N	-6.110279000	1.071562000	0.000759000
		C	4.865081000	0.544680000	-0.032348000
		C	3.714113000	1.357202000	-0.010803000
		H	3.855643000	2.426543000	0.025012000
		C	2.413336000	0.899363000	-0.033047000
		H	2.232609000	-0.169548000	-0.066978000
		C	-1.262185000	3.081039000	0.026786000
		H	-2.212676000	3.595194000	0.041509000
		C	-1.244872000	1.641091000	-0.016035000
		C	-0.003623000	0.993676000	-0.037173000
		H	0.016035000	-0.089885000	-0.072416000

		C	1.219347000	1.681898000	-0.013835000
		C	1.223239000	3.151058000	0.030671000
		C	-6.372477000	2.507961000	0.072178000
		H	-6.004409000	3.005740000	-0.826600000
		H	-5.888246000	2.934696000	0.951469000
		H	-7.442247000	2.672807000	0.151245000
		C	-1.247261000	5.898711000	0.105216000
		H	-0.955070000	6.946337000	0.134889000
		H	-1.841595000	5.658425000	0.992051000
		H	-1.838770000	5.708367000	-0.795541000
		C	-4.881126000	0.517665000	-0.034462000
		C	-5.018980000	-1.009693000	-0.099875000
		C	-7.317444000	-2.307931000	-0.151728000
		H	-6.871933000	-3.295202000	-0.197053000
		C	-8.710016000	-2.164966000	-0.142885000
		H	-9.340532000	-3.045260000	-0.181410000
		C	-9.292938000	-0.897583000	-0.085886000
		H	-10.372265000	-0.801725000	-0.081052000
		C	-8.507702000	0.257306000	-0.035093000
		H	-8.974133000	1.232654000	0.006743000
		C	-7.127404000	0.088956000	-0.043470000
		C	-6.528697000	-1.169013000	-0.102314000
		C	-0.105519000	3.800072000	0.047896000
		C	-4.415549000	-1.579781000	-1.406495000
		H	-4.835991000	-1.079948000	-2.281682000
		H	-4.649586000	-2.644266000	-1.474743000
		H	-3.331546000	-1.473753000	-1.427513000
		C	-4.407063000	-1.689919000	1.149242000
		H	-4.811124000	-1.257427000	2.066990000
		H	-3.321485000	-1.601134000	1.162764000
		H	-4.654582000	-2.753531000	1.134320000
		C	-2.418705000	0.843361000	-0.035385000
		H	-2.235734000	-0.224286000	-0.068275000
		C	-3.723510000	1.307976000	-0.013919000
		H	-3.879936000	2.378063000	0.021591000
		Cl	-0.004536000	-3.209534000	0.224211000
		O	1.199271000	-2.423442000	-0.203066000
		O	-1.244022000	-2.469334000	-0.182042000
		O	0.011484000	-3.380572000	1.711137000
		O	0.014718000	-4.551919000	-0.435885000
g.2d	**2d**	N	-4.766408000	-1.322868000	-0.309323000
		C	-5.641382000	0.850710000	-0.135956000
		C	-8.122880000	-0.042746000	-0.319610000
		H	-8.591462000	0.931388000	-0.238983000
		C	-8.908718000	-1.191751000	-0.468379000
		H	-9.987951000	-1.101641000	-0.502208000
		C	-8.317348000	-2.452747000	-0.575792000
		H	-8.941499000	-3.330606000	-0.693157000
		C	-6.928943000	-2.603639000	-0.534897000
		H	-6.474831000	-3.581931000	-0.621699000
		C	-6.173704000	-1.446610000	-0.383373000
		C	-6.743924000	-0.181473000	-0.279304000
		C	-3.908226000	-2.503550000	-0.402189000
		H	-2.888253000	-2.268462000	-0.122385000
		H	-3.925689000	-2.888025000	-1.424333000
		H	-4.288791000	-3.267000000	0.276061000
		C	-5.776135000	1.587799000	1.219350000
		H	-5.726891000	0.885145000	2.053611000
		H	-6.743016000	2.093943000	1.255328000
		H	-4.996638000	2.337736000	1.353231000
		C	-5.687466000	1.838538000	-1.328014000

		H	-5.567909000	1.312493000	-2.277289000
		H	-4.912070000	2.600851000	-1.255837000
		H	-6.656385000	2.341854000	-1.336062000
		O	-2.127973000	4.383725000	0.260286000
		O	0.280470000	5.490034000	0.362547000
		N	5.944215000	0.903156000	-0.234097000
		C	-4.385871000	-0.041483000	-0.177847000
		C	-3.032687000	0.349367000	-0.102899000
		H	-2.287150000	-0.434114000	-0.154203000
		C	-2.618056000	1.655562000	0.024673000
		H	-3.360514000	2.439938000	0.080942000
		C	1.307267000	3.313675000	0.175912000
		H	2.303478000	3.730940000	0.211385000
		C	1.152032000	1.884269000	0.064483000
		C	-0.142698000	1.348231000	0.030744000
		H	-0.246670000	0.271327000	-0.047360000
		C	-1.284868000	2.155021000	0.086316000
		C	-1.152009000	3.617457000	0.202496000
		C	6.330995000	2.312979000	-0.211629000
		H	6.011243000	2.777490000	0.722440000
		H	5.882181000	2.839947000	-1.054914000
		H	7.410957000	2.389145000	-0.287590000
		C	1.564552000	6.113559000	0.417132000
		H	1.373046000	7.180626000	0.508470000
		H	2.134725000	5.919864000	-0.496470000
		H	2.133029000	5.766950000	1.285441000
		C	4.673480000	0.456680000	-0.171868000
		C	4.675074000	-1.077079000	-0.223090000
		C	6.844667000	-2.569888000	-0.407854000
		H	6.313919000	-3.515189000	-0.406326000
		C	8.241843000	-2.547761000	-0.492169000
		H	8.790805000	-3.479635000	-0.556902000
		C	8.933692000	-1.335025000	-0.492925000
		H	10.015282000	-1.332912000	-0.558396000
		C	8.255524000	-0.116055000	-0.409845000
		H	8.805764000	0.815420000	-0.410514000
		C	6.868340000	-0.164223000	-0.327413000
		C	6.161757000	-1.366403000	-0.325858000
		C	0.227988000	4.140365000	0.247226000
		C	4.099371000	-1.686276000	1.078112000
		H	4.615258000	-1.289283000	1.955100000
		H	4.241257000	-2.768857000	1.060026000
		H	3.032454000	-1.491113000	1.184217000
		C	3.936810000	-1.609686000	-1.475149000
		H	4.338858000	-1.161998000	-2.386346000
		H	2.867266000	-1.404625000	-1.432019000
		H	4.069610000	-2.691585000	-1.537830000
		C	2.253039000	0.993733000	-0.026535000
		H	1.983289000	-0.054166000	-0.072625000
		C	3.592381000	1.343467000	-0.071309000
		H	3.843644000	2.395186000	-0.037130000
		Cl	0.005476000	-3.169874000	0.810102000
		O	-0.458819000	-2.068288000	-0.102336000
		O	0.675377000	-2.567713000	2.004168000
		O	0.973082000	-4.045142000	0.078607000
		O	-1.176071000	-3.979288000	1.244388000
g.2a′	**2a′**	N	-4.954225000	-0.702754000	1.248483000
		C	-5.218070000	-0.903595000	-1.106800000
		C	-7.148848000	0.900244000	-1.116036000
		H	-7.301904000	0.869640000	-2.189685000
		C	-7.945212000	1.735951000	-0.316447000

		H	-8.710296000	2.352473000	-0.773806000
		C	-7.749038000	1.775987000	1.062795000
		H	-8.364303000	2.426702000	1.674523000
		C	-6.760182000	0.997053000	1.678922000
		H	-6.610606000	1.047037000	2.750442000
		C	-5.980918000	0.173052000	0.870451000
		C	-6.170985000	0.124810000	-0.517898000
		C	-4.329428000	-0.609544000	2.560064000
		H	-3.600231000	-1.412043000	2.669004000
		H	-5.086258000	-0.735949000	3.336015000
		H	-3.825783000	0.353073000	2.713033000
		C	-4.566144000	-0.488532000	-2.430817000
		H	-4.092474000	0.489996000	-2.363003000
		H	-5.326335000	-0.449649000	-3.214903000
		H	-3.813934000	-1.220746000	-2.738103000
		C	-5.985249000	-2.231618000	-1.309670000
		H	-6.423571000	-2.594469000	-0.377327000
		H	-5.332870000	-3.008403000	-1.716649000
		H	-6.796456000	-2.066559000	-2.021744000
		O	-3.185282000	0.071438000	-0.117383000
		O	-1.737226000	2.239269000	-0.261153000
		N	5.581339000	1.270362000	-0.073578000
		C	-4.176860000	-1.039155000	0.080090000
		C	-3.483444000	-2.362032000	0.196784000
		H	-4.130066000	-3.220316000	0.321181000
		C	-2.154248000	-2.506102000	0.179838000
		H	-1.710165000	-3.490876000	0.275677000
		C	0.319787000	0.949560000	-0.126345000
		H	0.930231000	1.837492000	-0.200322000
		C	0.938214000	-0.322454000	-0.010197000
		C	0.123471000	-1.463023000	0.083066000
		H	0.579021000	-2.442628000	0.177504000
		C	-1.265346000	-1.361829000	0.059973000
		C	-1.863120000	-0.097597000	-0.063530000
		C	5.207063000	2.684975000	-0.162447000
		H	4.648046000	2.979752000	0.726122000
		H	4.604423000	2.856170000	-1.054312000
		H	6.107288000	3.286792000	-0.228549000
		C	-0.990013000	3.456128000	-0.362206000
		H	-1.730688000	4.248728000	-0.439782000
		H	-0.358700000	3.455319000	-1.255063000
		H	-0.375625000	3.614189000	0.528435000
		C	4.716904000	0.251874000	-0.016448000
		C	5.488956000	-1.069709000	0.077126000
		C	8.122487000	-1.262679000	0.111235000
		H	8.144770000	-2.344195000	0.178198000
		C	9.317089000	-0.535233000	0.077690000
		H	10.264595000	-1.058946000	0.119073000
		C	9.301674000	0.858864000	-0.007763000
		H	10.236135000	1.406419000	-0.031608000
		C	8.098158000	1.565030000	-0.063385000
		H	8.100327000	2.644704000	-0.128396000
		C	6.926038000	0.819113000	-0.030242000
		C	6.921730000	-0.571481000	0.056955000
		C	-1.056281000	1.072862000	-0.151516000
		C	5.197035000	-1.805934000	1.408618000
		H	5.371324000	-1.151506000	2.264806000
		H	5.863701000	-2.665989000	1.493978000
		H	4.170448000	-2.169279000	1.454228000
		C	5.216398000	-1.977248000	-1.147835000
		H	5.411145000	-1.444854000	-2.080757000
		H	4.187726000	-2.337540000	-1.163724000

		H	5.877853000	-2.844589000	-1.103861000
		C	2.362450000	-0.504389000	0.017687000
		H	2.675696000	-1.537516000	0.097952000
		C	3.320112000	0.473845000	-0.044405000
		H	3.002736000	1.505502000	-0.118476000
g.2b′	**2b′**	N	-4.530777000	-0.488369000	0.990294000
		C	-5.940086000	-1.313507000	-0.683841000
		C	-7.926678000	0.263457000	0.071820000
		H	-8.630773000	-0.079360000	-0.677484000
		C	-8.301191000	1.248557000	0.992942000
		H	-9.298935000	1.668960000	0.950036000
		C	-7.405072000	1.699198000	1.965301000
		H	-7.713707000	2.464980000	2.666778000
		C	-6.110573000	1.179526000	2.047827000
		H	-5.416318000	1.534654000	2.798143000
		C	-5.766623000	0.205016000	1.121238000
		C	-6.642635000	-0.255910000	0.141111000
		C	-3.446778000	-0.323971000	1.954327000
		H	-2.785011000	-1.183383000	1.895898000
		H	-3.878200000	-0.263706000	2.952643000
		H	-2.886739000	0.586978000	1.741972000
		C	-5.847921000	-0.932632000	-2.178618000
		H	-5.345980000	0.026690000	-2.306713000
		H	-6.853657000	-0.867677000	-2.599025000
		H	-5.292036000	-1.692978000	-2.731185000
		C	-6.616852000	-2.697841000	-0.518148000
		H	-6.657898000	-3.000241000	0.530099000
		H	-6.084612000	-3.462927000	-1.086750000
		H	-7.637522000	-2.642584000	-0.901407000
		O	-3.013398000	0.763407000	-1.009518000
		O	-1.344970000	2.814082000	-1.037343000
		N	5.765337000	1.128148000	-0.010965000
		C	-4.552171000	-1.314694000	-0.043219000
		C	-3.502414000	-2.188455000	-0.460387000
		H	-3.864236000	-3.164506000	-0.771200000
		C	-2.151539000	-2.005639000	-0.561424000
		H	-1.604483000	-2.921935000	-0.772240000
		C	0.523581000	1.344790000	-0.616335000
		H	1.230794000	2.162175000	-0.630373000
		C	1.004667000	0.005701000	-0.408940000
		C	0.066838000	-1.040519000	-0.398660000
		H	0.428534000	-2.054612000	-0.259436000
		C	-1.307029000	-0.837028000	-0.540290000
		C	-1.813678000	0.512941000	-0.793172000
		C	5.551558000	2.562976000	-0.189280000
		H	4.906604000	2.949671000	0.601432000
		H	5.095227000	2.758240000	-1.161048000
		H	6.506859000	3.076024000	-0.142980000
		C	-0.470628000	3.942508000	-1.080981000
		H	-1.106772000	4.804154000	-1.272439000
		H	0.262312000	3.841077000	-1.887051000
		H	0.048763000	4.075056000	-0.127034000
		C	4.783527000	0.202273000	-0.017645000
		C	5.401954000	-1.188089000	0.195364000
		C	7.980993000	-1.648051000	0.525693000
		H	7.876758000	-2.722077000	0.630235000
		C	9.246831000	-1.054447000	0.599171000
		H	10.121656000	-1.672948000	0.760462000
		C	9.390604000	0.327802000	0.466520000
		H	10.376260000	0.774034000	0.525614000
		C	8.282242000	1.153176000	0.258252000

		H	8.409466000	2.222925000	0.158372000
		C	7.036072000	0.540335000	0.188712000
		C	6.874811000	-0.838838000	0.318646000
		C	-0.803095000	1.590815000	-0.812379000
		C	4.897077000	-1.847887000	1.501299000
		H	5.049421000	-1.188190000	2.357859000
		H	5.454840000	-2.770255000	1.676249000
		H	3.837980000	-2.100400000	1.444597000
		C	5.170516000	-2.108722000	-1.027514000
		H	5.520102000	-1.634113000	-1.946521000
		H	4.117046000	-2.361649000	-1.149686000
		H	5.727056000	-3.037936000	-0.888837000
		C	2.369502000	-0.318996000	-0.223929000
		H	2.564471000	-1.375708000	-0.089567000
		C	3.442150000	0.559348000	-0.199695000
		H	3.239996000	1.614053000	-0.332420000
g.2c′	**2c′**	N	-6.086780000	0.474211000	0.046833000
		C	-4.937891000	-1.572508000	-0.023171000
		C	-7.196568000	-2.940922000	-0.059535000
		H	-6.723633000	-3.915742000	-0.091039000
		C	-8.592115000	-2.836480000	-0.054131000
		H	-9.197339000	-3.734708000	-0.081366000
		C	-9.212250000	-1.585846000	-0.015386000
		H	-10.293807000	-1.521800000	-0.013377000
		C	-8.461357000	-0.408370000	0.020224000
		H	-8.955259000	0.553695000	0.047253000
		C	-7.077406000	-0.538795000	0.015746000
		C	-6.441520000	-1.778614000	-0.025094000
		C	-6.391458000	1.905550000	0.093847000
		H	-6.058580000	2.391166000	-0.824528000
		H	-5.896560000	2.363284000	0.950354000
		H	-7.463369000	2.039062000	0.197098000
		C	-4.316179000	-2.142291000	-1.321682000
		H	-4.754887000	-1.672998000	-2.204468000
		H	-4.510892000	-3.215386000	-1.371764000
		H	-3.236911000	-1.992164000	-1.351945000
		C	-4.309798000	-2.216889000	1.237344000
		H	-4.742092000	-1.797856000	2.148157000
		H	-3.229800000	-2.072722000	1.270103000
		H	-4.507446000	-3.290637000	1.227027000
		O	-2.262308000	3.289756000	0.017713000
		O	0.023155000	4.613364000	0.004178000
		N	6.110809000	0.455780000	-0.056896000
		C	-4.848223000	-0.041081000	0.019784000
		C	-3.714144000	0.796471000	0.024083000
		H	-3.873109000	1.864017000	0.033658000
		C	-2.408855000	0.355125000	0.012884000
		H	-2.226623000	-0.713357000	0.005989000
		C	1.261896000	2.543022000	-0.003772000
		H	2.212493000	3.057309000	-0.007945000
		C	1.246809000	1.102632000	-0.002446000
		C	0.007397000	0.453173000	0.004492000
		H	-0.008679000	-0.632242000	0.004986000
		C	-1.216627000	1.137688000	0.009891000
		C	-1.224135000	2.607581000	0.010997000
		C	6.409713000	1.886142000	-0.114919000
		H	6.069278000	2.381418000	0.795962000
		H	5.922231000	2.335525000	-0.980804000
		H	7.481904000	2.024142000	-0.210359000
		C	1.239495000	5.362548000	-0.003442000
		H	0.943488000	6.409425000	-0.001505000

		H	1.826931000	5.148840000	-0.901474000
		H	1.838241000	5.148760000	0.887071000
		C	4.869127000	-0.065319000	-0.022022000
		C	4.966166000	-1.597367000	0.027828000
		C	7.230032000	-2.955944000	0.063287000
		H	6.759571000	-3.931808000	0.101764000
		C	8.625674000	-2.848666000	0.052209000
		H	9.233334000	-3.745170000	0.082050000
		C	9.241182000	-1.596412000	0.004470000
		H	10.322578000	-1.528634000	-0.001959000
		C	8.486314000	-0.421157000	-0.034567000
		H	8.977892000	0.541966000	-0.068592000
		C	7.102314000	-0.553865000	-0.024254000
		C	6.471384000	-1.796350000	0.025467000
		C	0.103596000	3.260251000	0.003071000
		C	4.352289000	-2.165427000	1.330309000
		H	4.792394000	-1.690875000	2.209642000
		H	4.551673000	-3.237574000	1.384067000
		H	3.272336000	-2.020475000	1.365075000
		C	4.337902000	-2.251375000	-1.227195000
		H	4.766540000	-1.835568000	-2.141258000
		H	3.257139000	-2.111997000	-1.259031000
		H	4.539377000	-3.324438000	-1.211976000
		C	2.420190000	0.306126000	-0.007467000
		H	2.236406000	-0.760892000	0.002667000
		C	3.729634000	0.752865000	-0.025515000
		H	3.904676000	1.820569000	-0.042219000
g.2d′	**2d′**	N	-4.659442000	-1.892166000	0.074607000
		C	-5.645206000	0.237770000	-0.044689000
		C	-8.075757000	-0.793874000	-0.093848000
		H	-8.588419000	0.159704000	-0.146417000
		C	-8.808376000	-1.986191000	-0.078832000
		H	-9.890476000	-1.951404000	-0.120012000
		C	-8.158095000	-3.220244000	-0.012455000
		H	-8.739447000	-4.134480000	-0.003151000
		C	-6.764458000	-3.300031000	0.042160000
		H	-6.273754000	-4.262896000	0.091587000
		C	-6.059825000	-2.101865000	0.027629000
		C	-6.691965000	-0.861354000	-0.041069000
		C	-3.680524000	-2.977665000	0.151993000
		H	-3.039546000	-2.840863000	1.023047000
		H	-3.071921000	-3.002012000	-0.753098000
		H	-4.204131000	-3.923019000	0.250294000
		C	-5.820194000	1.149899000	1.194566000
		H	-5.742126000	0.574402000	2.119064000
		H	-6.808971000	1.611909000	1.161614000
		H	-5.076094000	1.946195000	1.219261000
		C	-5.724093000	1.049778000	-1.361033000
		H	-5.588899000	0.402282000	-2.229752000
		H	-4.969255000	1.835553000	-1.395351000
		H	-6.706734000	1.519908000	-1.434049000
		O	-2.118630000	3.918814000	0.008829000
		O	0.296852000	5.014982000	0.011106000
		N	5.922950000	0.266839000	-0.009572000
		C	-4.351894000	-0.585646000	0.031790000
		C	-3.015350000	-0.144786000	0.048462000
		H	-2.256569000	-0.916133000	0.080932000
		C	-2.619711000	1.174401000	0.023871000
		H	-3.372015000	1.952162000	0.000173000
		C	1.312201000	2.826015000	0.024265000
		H	2.311362000	3.237606000	0.023778000

		C	1.147340000	1.393210000	0.031686000
		C	-0.149416000	0.868386000	0.036139000
		H	-0.260059000	-0.210176000	0.041297000
		C	-1.289640000	1.679957000	0.028162000
		C	-1.147868000	3.146103000	0.017188000
		C	6.361541000	1.662071000	-0.012376000
		H	5.992028000	2.173913000	0.877263000
		H	5.996382000	2.169911000	-0.906286000
		H	7.446191000	1.695712000	-0.009284000
		C	1.584577000	5.634584000	0.011171000
		H	1.398292000	6.706355000	0.005923000
		H	2.154023000	5.356134000	-0.880616000
		H	2.149975000	5.364229000	0.908008000
		C	4.636680000	-0.130390000	0.004360000
		C	4.581727000	-1.664910000	0.003380000
		C	6.700331000	-3.240257000	-0.024252000
		H	6.135265000	-4.165342000	-0.017572000
		C	8.099669000	-3.270387000	-0.042246000
		H	8.616061000	-4.222828000	-0.049846000
		C	8.835664000	-2.083844000	-0.050728000
		H	9.918390000	-2.122788000	-0.065011000
		C	8.200429000	-0.839346000	-0.041050000
		H	8.783951000	0.071608000	-0.047891000
		C	6.810286000	-0.835847000	-0.022969000
		C	6.059868000	-2.010985000	-0.015169000
		C	0.237291000	3.662006000	0.017875000
		C	3.919543000	-2.213921000	1.290606000
		H	4.406215000	-1.813822000	2.182276000
		H	4.015414000	-3.301481000	1.307121000
		H	2.858519000	-1.967630000	1.337358000
		C	3.887682000	-2.211185000	-1.268247000
		H	4.350947000	-1.807866000	-2.170864000
		H	2.825439000	-1.966320000	-1.287435000
		H	3.984308000	-3.298548000	-1.290618000
		C	2.237170000	0.483425000	0.028769000
		H	1.948902000	-0.560259000	0.036247000
		C	3.583708000	0.797647000	0.014771000
		H	3.866417000	1.842061000	0.008015000