Charge transfer properties of Tröger base derivatives

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Electronic Supporting Information (ESI). Supplementary Material

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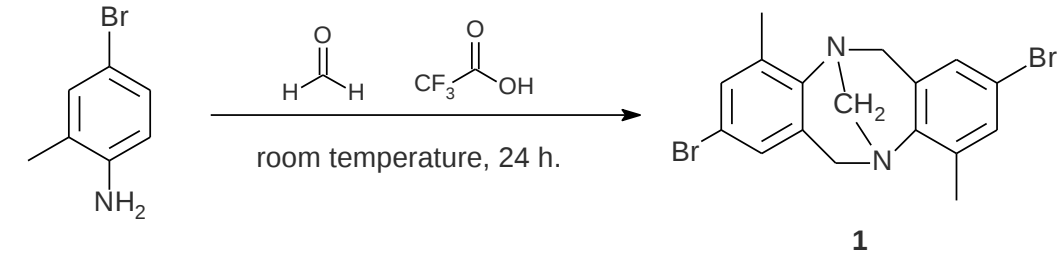
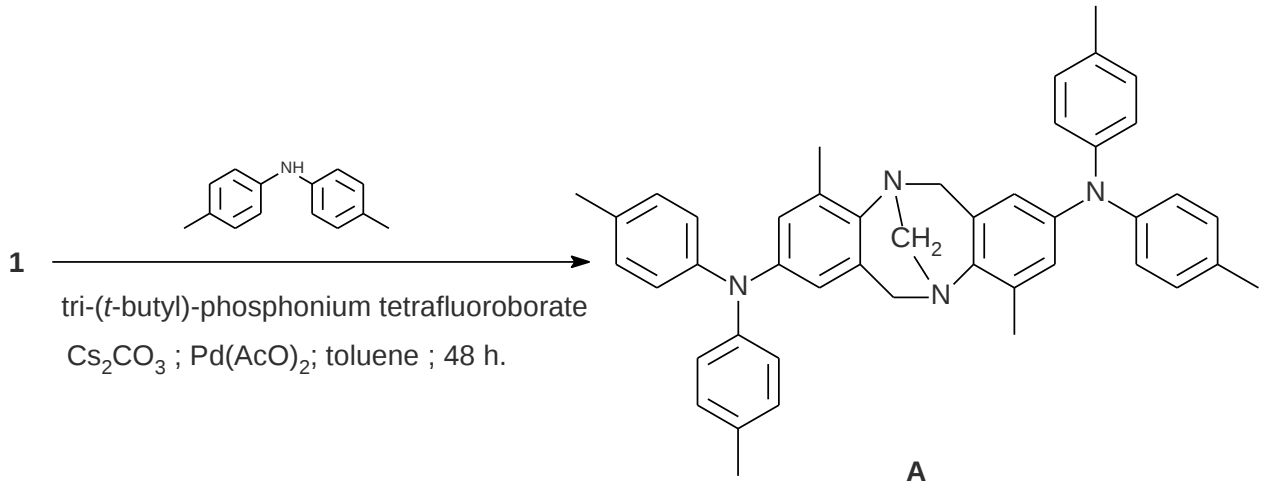
Part 1. Experimental

Synthesis and characterization of compound A

1.1 Synthetic Scheme

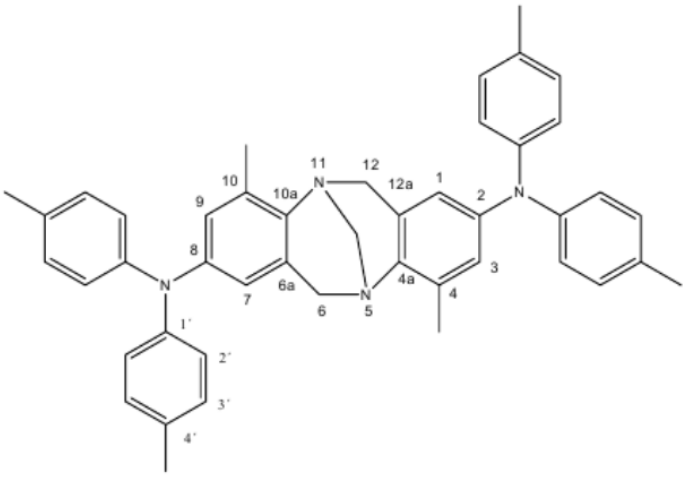


1



A

1.2 NMR Characterization.



NMR spectra for (±)4,10-dimethyl-*N*,*N*,*N'N'*-tetrakis(4-methylphenyl)-6H, 12H-5,11-methanodibenzo[b,f][1,5] diazocine-2,8-diamine.

^{1}H NMR (500 MHz, $CDCl_3$) δ 2.24 (s, 6H, $C^{4/10}$-CH_3); 2.30 (s, 12H, C^4-CH_3); 3.84 (d, *J*=17.0 Hz, H-6α and 12α, 2H); 4.27 (s, H-13, 2H); 4.43 (d, *J*=17.0 Hz, H-6β and H-12β, 2H); 6.45 (d, *J*=2.5 Hz, H-1 and H-7, 2H); 6.77 (d, *J*=2.5 Hz, H-3 and H-9, 2H); 6.93 (d, *J*=8.4 Hz, H-2',

8H); 7.03 (d, *J*=8.4 Hz, H-3', 8H).

^{1}C NMR (125 MHz, $CDCl_3$) δ 17.0 (2C, $C^{4/10}$-CH_3); 20.8 (4C, C4-CH_3); 55.0 (2C, C-6 and C-12); 67.7 (1C, C-13); 119.0 (2C, C-1 and C-7); 124.0 (8C, C-2'); 124.2 (2C, C-3 and C-9); 128.8 (2C, C-4 and C-10); 129.7 (8C, C-3'); 131.8 (4C, C-4'); 133.7 (2C, C-6a and C-12a); 140.8 (2C, C-4a and C-10a); 143.7 (2C, C-2 and C-8); 145.6 (4C, C-1').

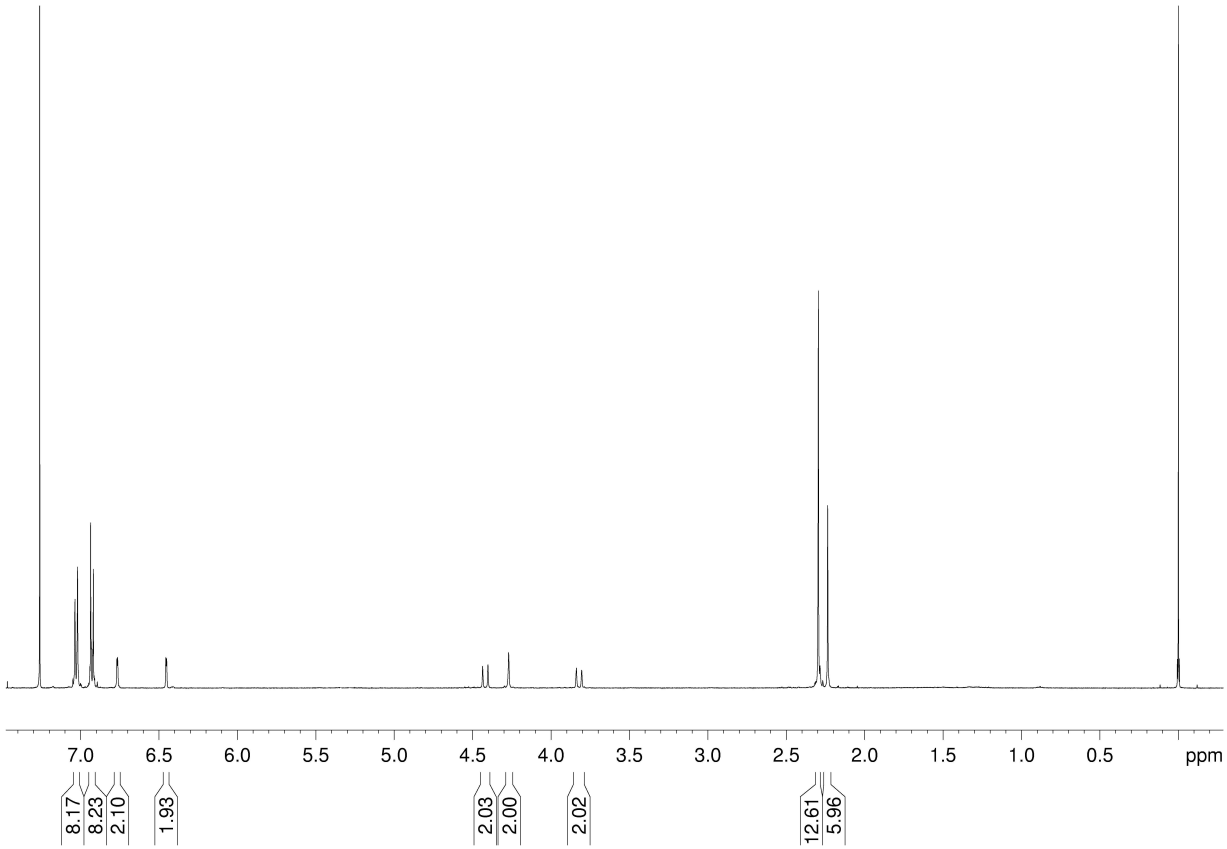


Figure PSI 1: ^{1}H NMR of compound [A]

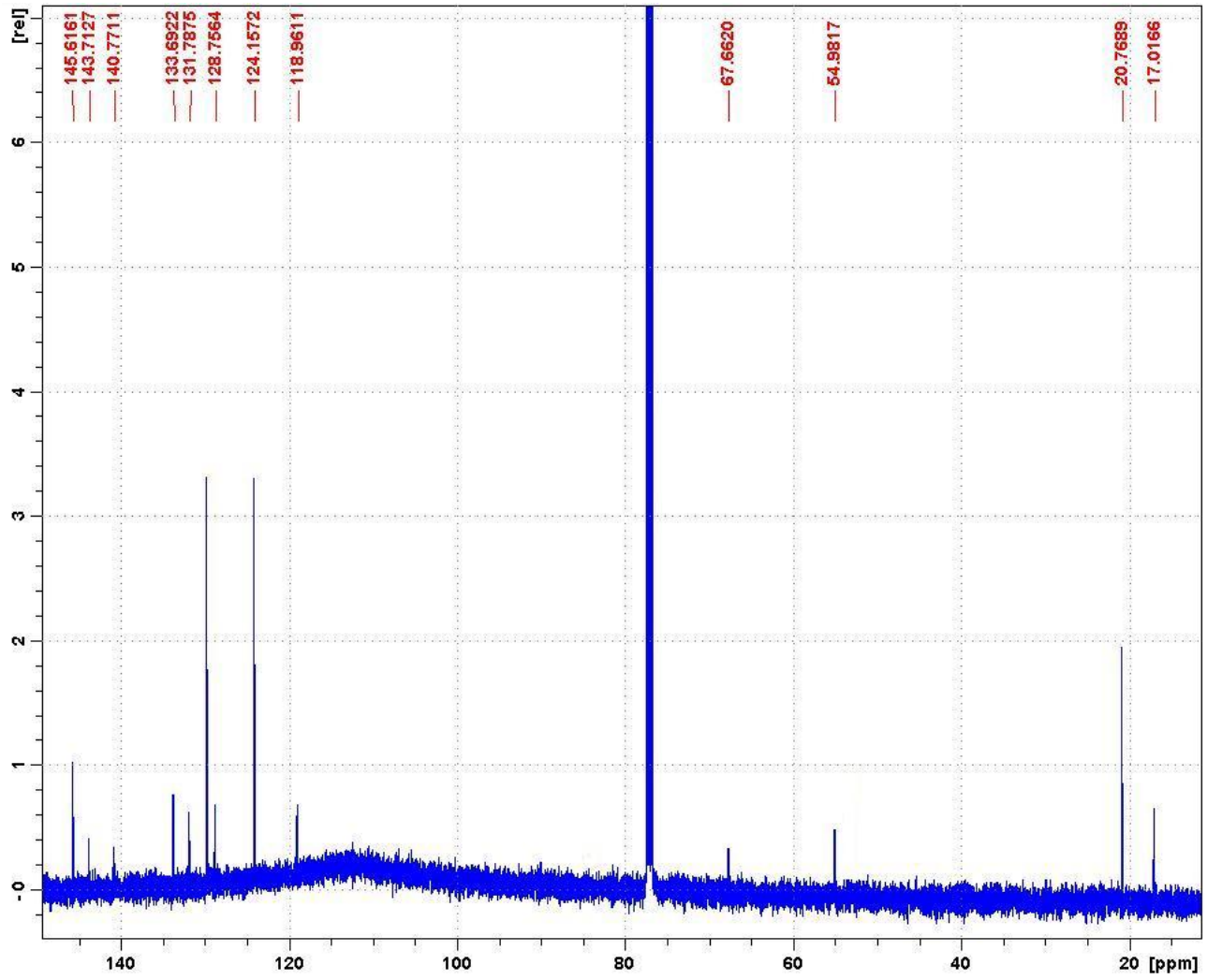


Figure PSI 2: ^{1}C NMR of compound **A**

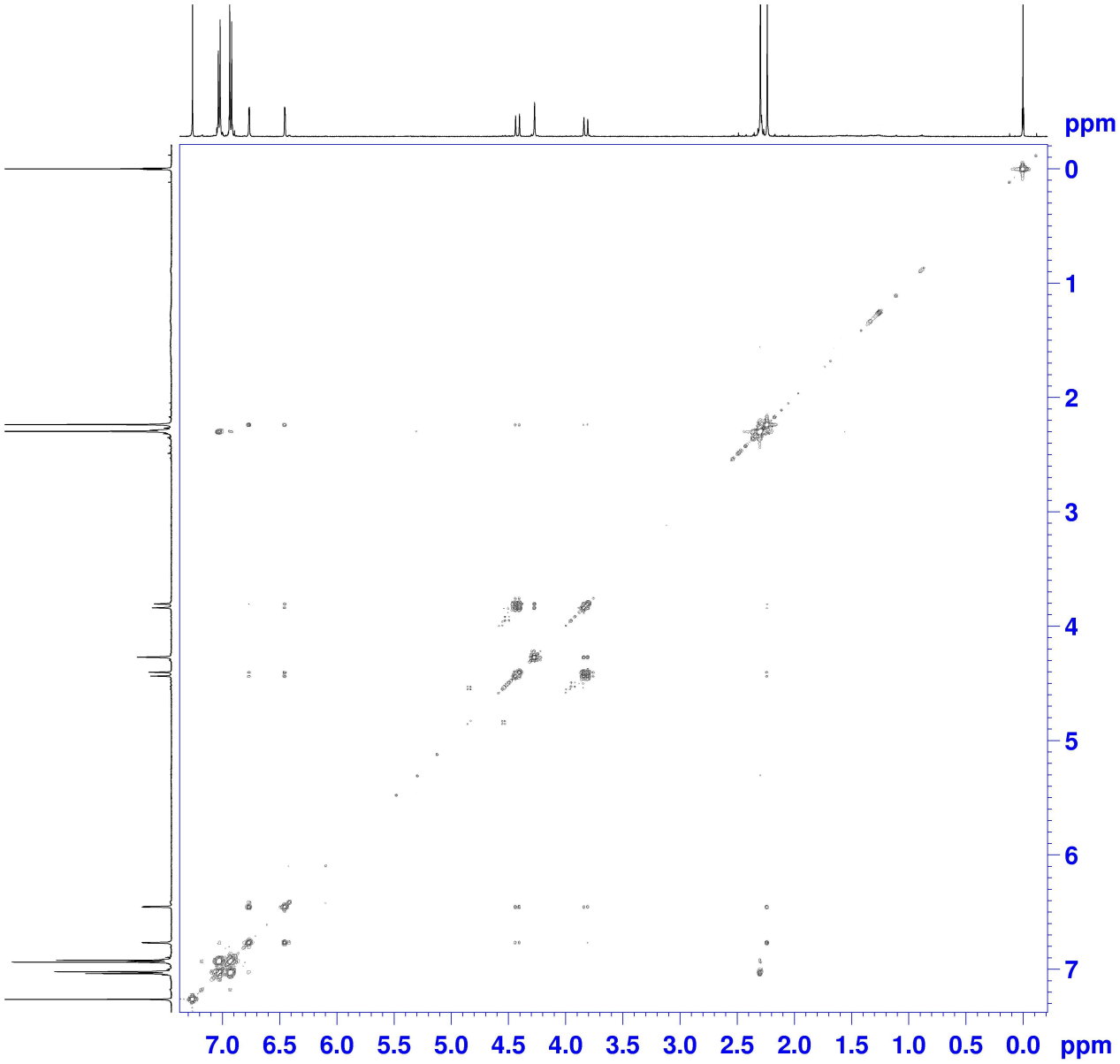


Figure PSI 3: COSY of compound **A**

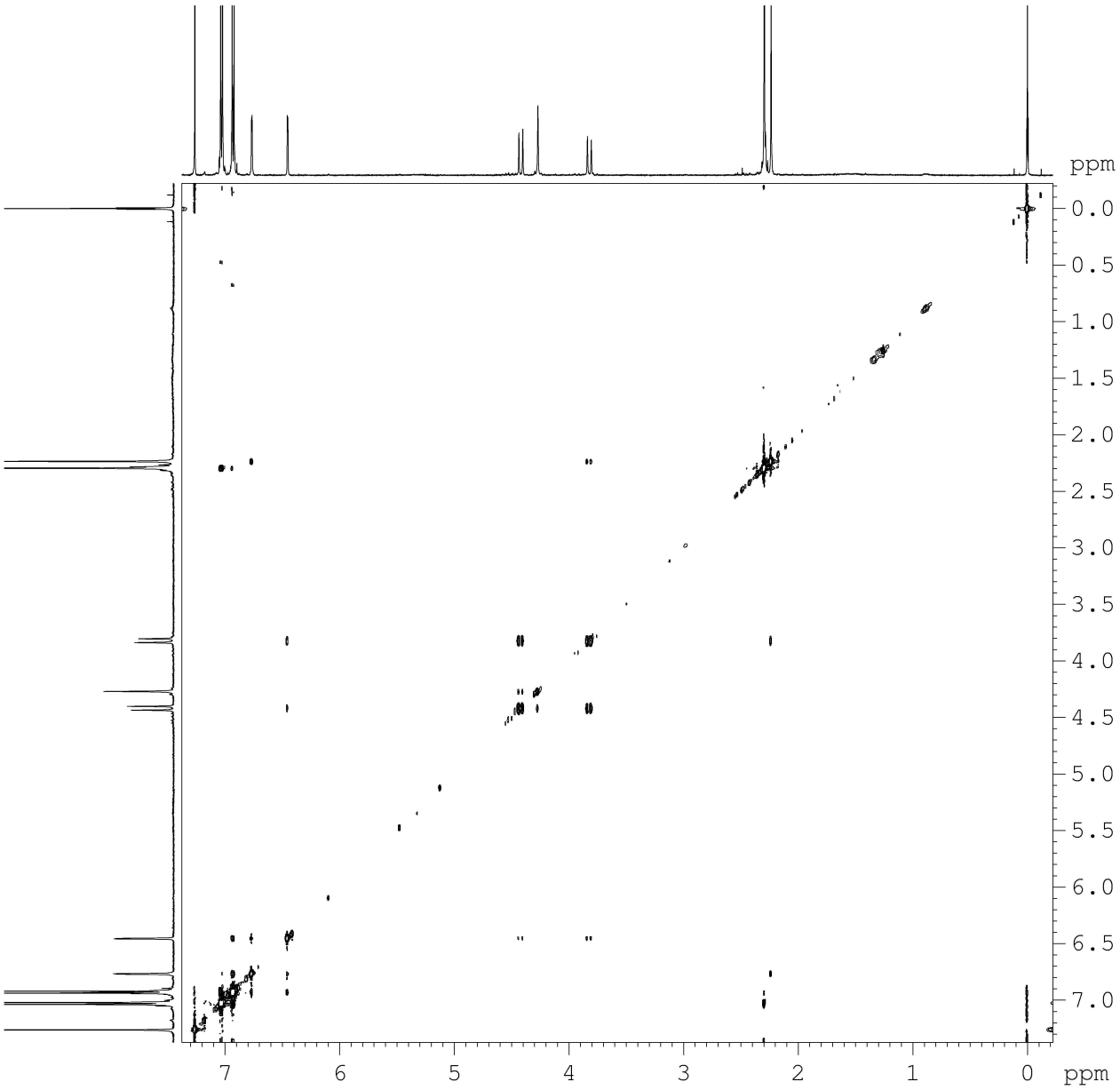


Figure PSI 4: NOESY of compound **A**

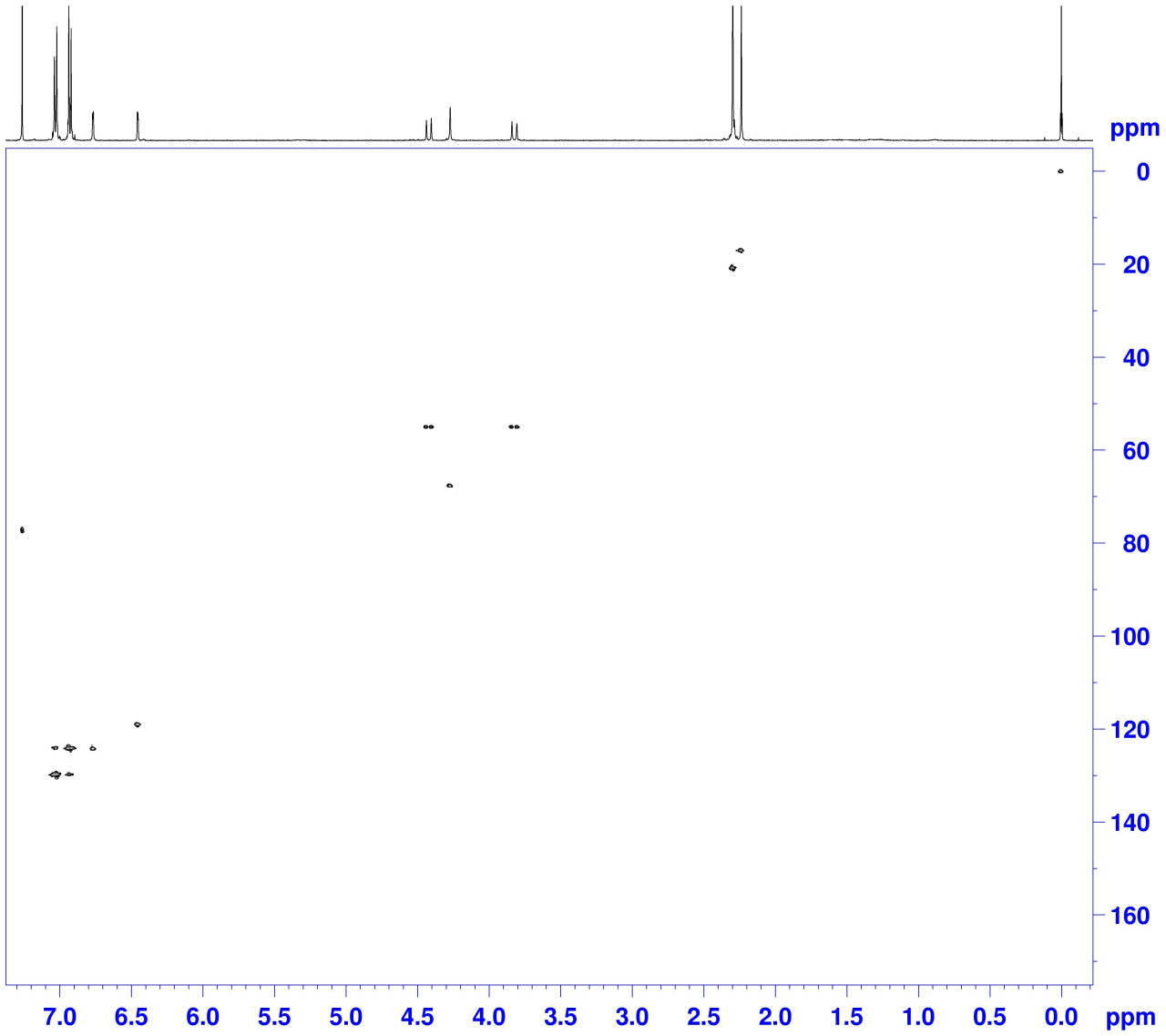


Figure PSI 5: HSQC of compound **A**

1.3 Electronic spectra of A·⁺.

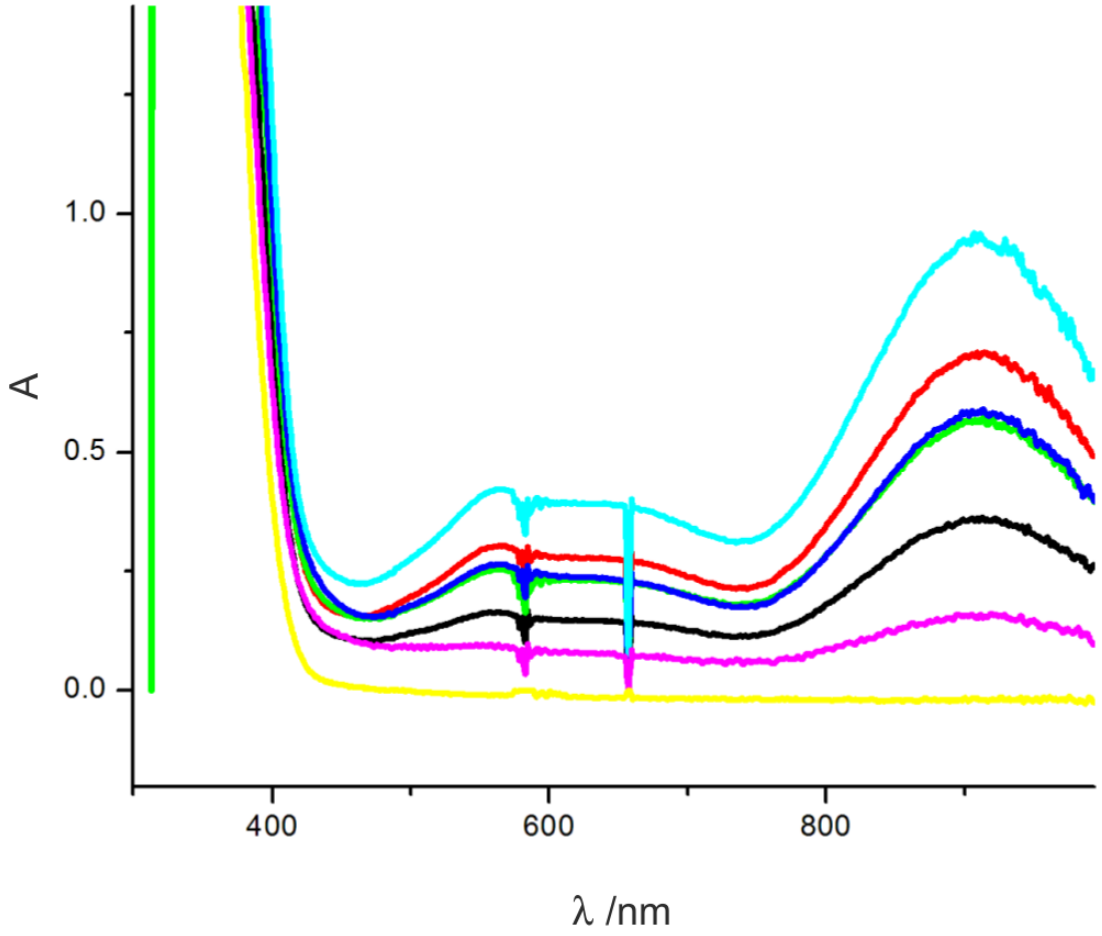


Figure S1. Electronic spectra of a solution of **A**/**A**·⁺ at different concentrations of oxidant, from 0 M (yellow) to 0.5 mM (cyan). The neutral species **A** has no band at wavelenghts longer than 450 nm. (The spikes at 590 and 660 nm are artifacts from the lamp.)
The intervalence band is identified as the peak at 910 nm.

1.4 Electron paramagnetic resonance spectrum of the radical cation of compound B.

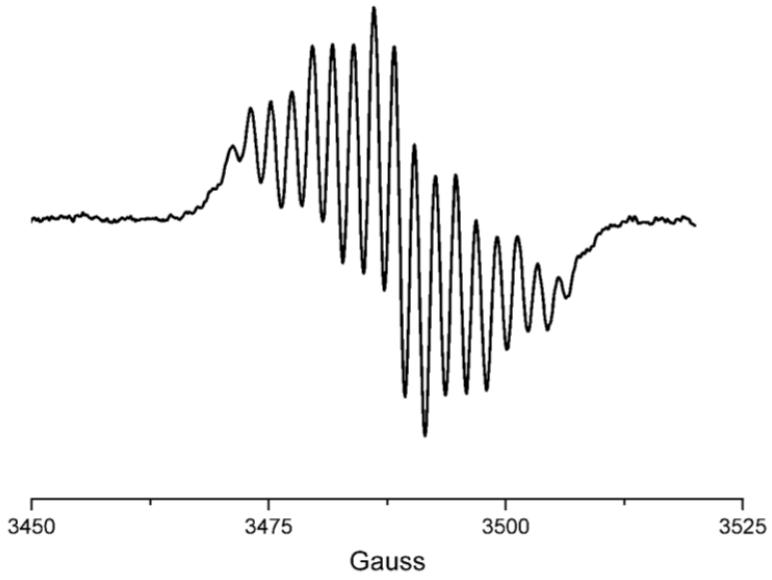


Figure S2. High resolution EPR spectrum of the radical cation of **B** at 298 K, similar conditions to $\mathbf{A}^{\cdot+}$ (See main text figure 2a).

Part 2. Computational

2.1 Additional figures showing the spin and charge distribution of the cationic species in their ground and excited states.

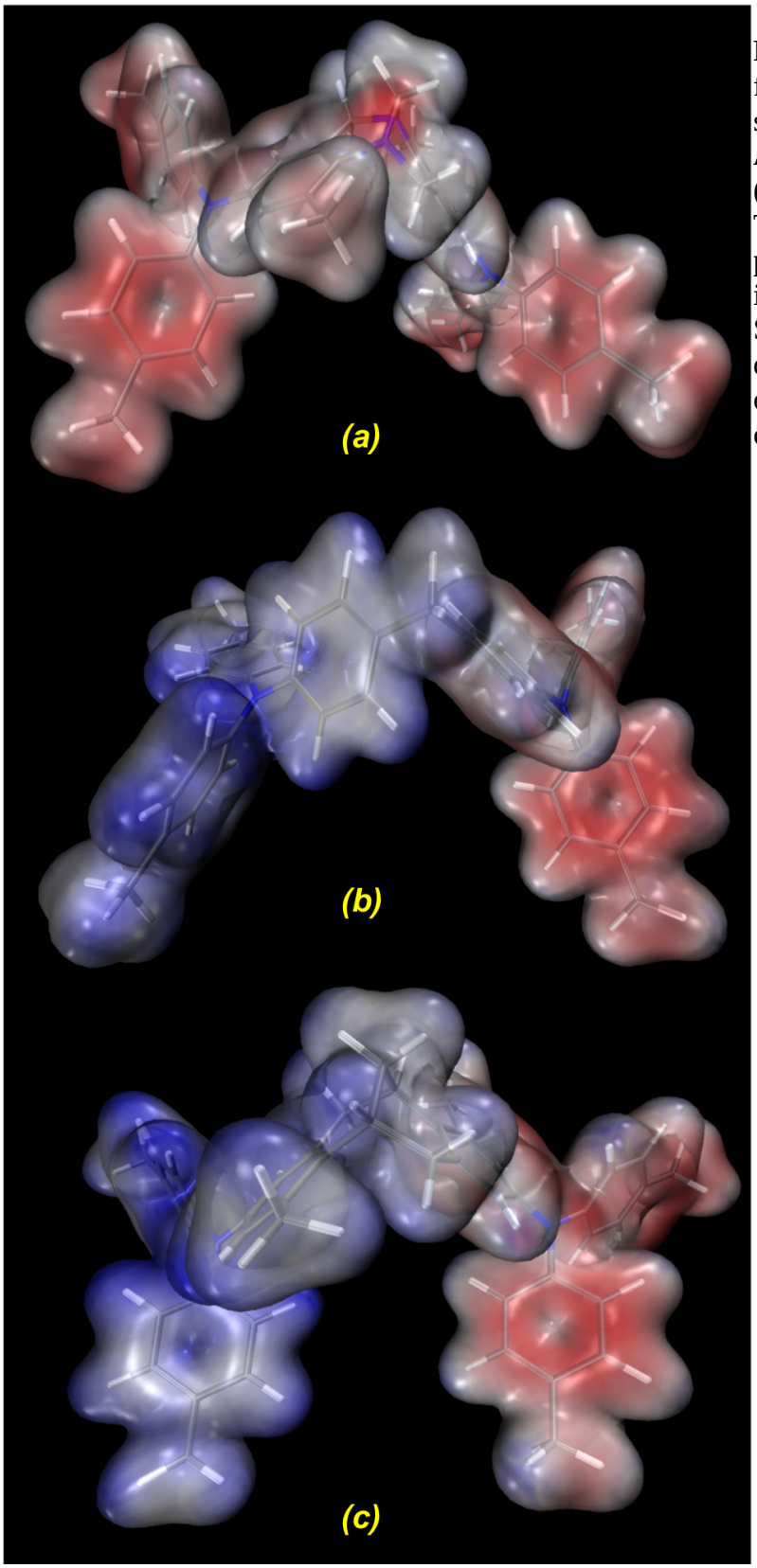


Figure S3. Electrostatic potential from red to blue (blue= more positive) showing the charge delocalization in $\mathbf{A}^{\cdot+}$ (*a*). In sharp contrast, the hole (blue) is localized in $\mathbf{B}^{\cdot+}$ and $\mathbf{C}^{\cdot+}$ (*b*-*c*). The potential (from 0.02 to 0.2 a.u.) is plotted over a 0.02 a.u. electron isodensity translucent surface. See also main text figure 3 for spin density distribution. (Molecules orientation is not the same in all cases)

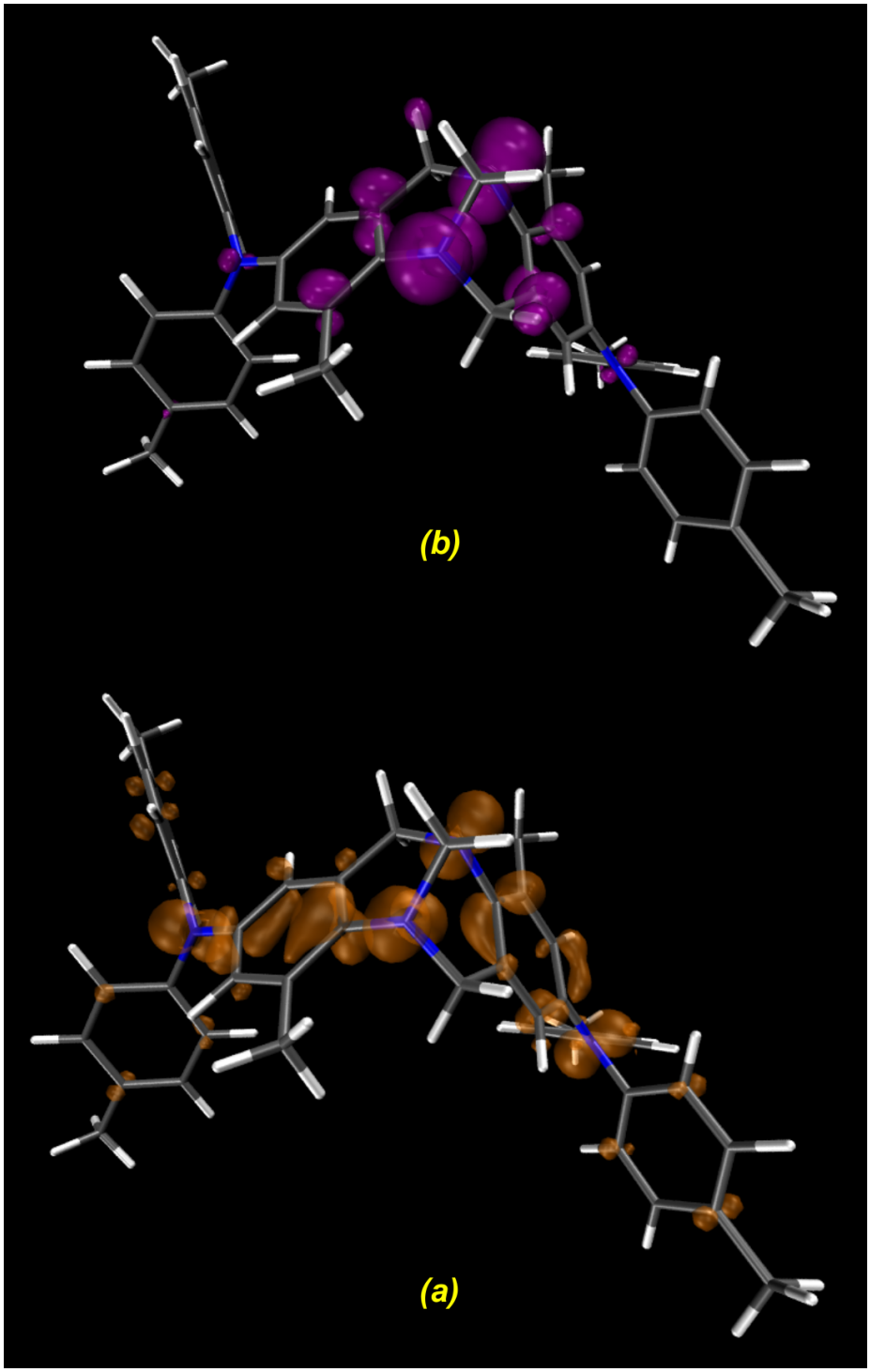


Figure S4. Spin density (0.004 a.u.) of the ground state (*a*) and vertical excited doublet (*b*) corresponding to the NIR absorption band (See ESI Figure S1) obtained by simulating $\mathbf{A}^{\bullet+}$ in dichloromethane.
Dichloromethane: Calculated wavelength of the excited state 1080 nm. Transition Dipole: 4.9 D. Oscillator Strenght : 0.14
(Gas phase: Calculated wavelength of the transition: 1020 nm. Transition Dipole 2.2 D.)

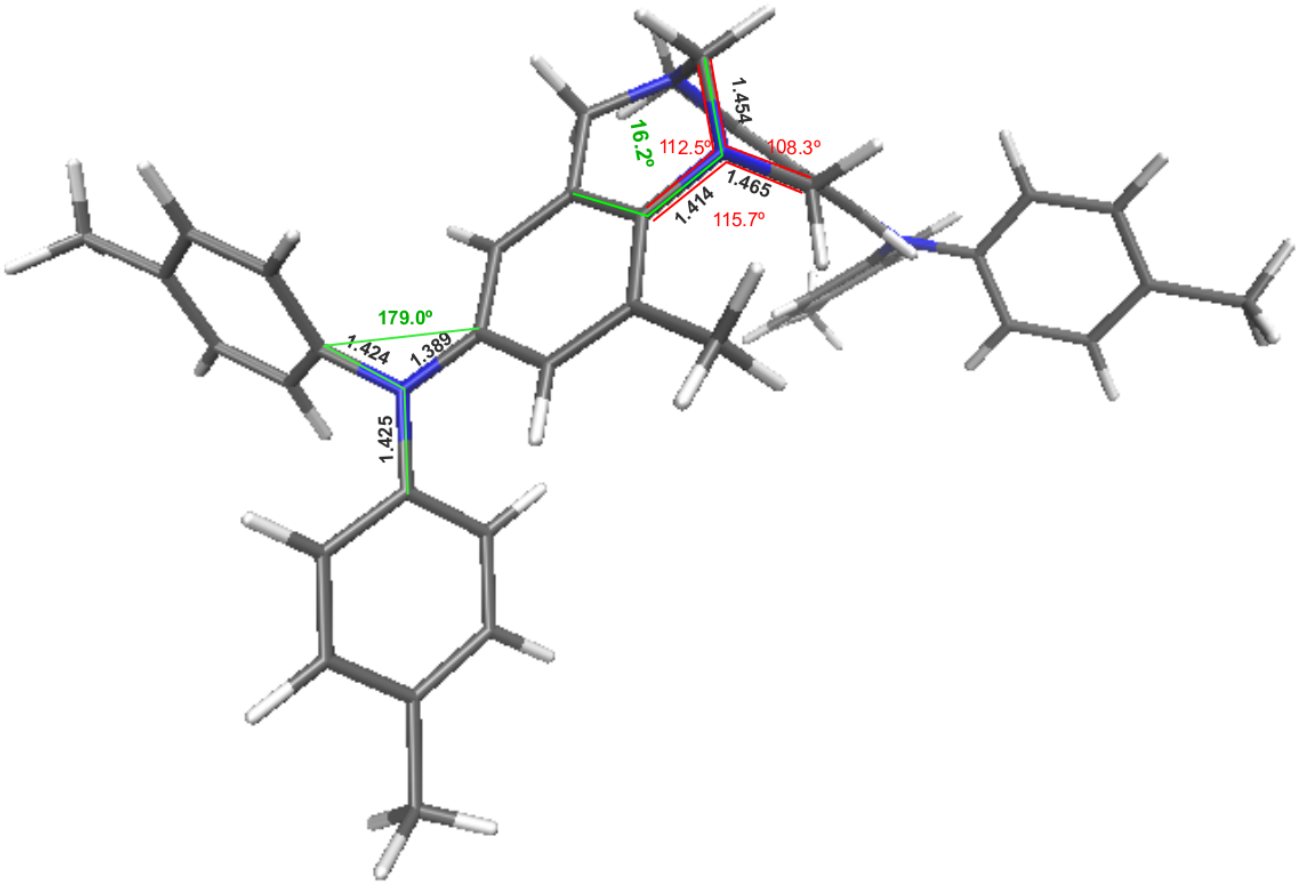


Figure S5. Main geometric parameters for the optimized structure of $\mathbf{A}^{\cdot+}$ in dichloromethane: distances (in Å), angles (red) and dihedrals (green).

2.2 Calculation details

Table S1. CAM-B3LYP / 6-31+G* total energies and total spin expectation value

	gas phase	dichloromethane	ZPE	$<S^2>$
A	-1959.2535	-1959.2690	0.7905	0.0000
A·+	-1959.0295	-1959.0727	0.7927	0.7502
B	-1693.8460		0.6846[(a)]	0.0000
B·+	-1693.6130		0.6853[(a)]	0.7514[(a)]
C	-1927.2002	-1927.2095	0.8144	0.0000
C·+	-1926.9708	-1927.0203	0.8154	0.7518
TTA	-867.1658	-867.1706	0.3646	0.0000
TTA·+	-866.9303	-866.9800	0.3657	0.7517

[(a)]Data obtained from gas-phase calculations

2.3. *XYZ* coordinates of the calculated species.

Compound A in methylene chloride

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C	5.88318	1.92823	1.74621
C	4.66723	1.48676	1.21284
C	3.52272	2.25341	1.44657
C	3.59658	3.42347	2.19624
C	4.80681	3.88031	2.72079
C	5.94634	3.10773	2.47779
N	4.59637	0.28740	0.46238
C	5.61131	-0.03459	-0.47231
C	6.16487	0.94837	-1.29970
C	7.16275	0.62413	-2.21089
C	7.63387	-0.68503	-2.34515
C	7.06492	-1.66063	-1.52438
C	6.07798	-1.34586	-0.59559
C	8.72992	-1.02174	-3.32400
C	4.89082	5.16724	3.50169
C	3.49074	-0.58752	0.63307
C	3.05297	-0.93235	1.91466
C	1.97166	-1.78497	2.11286
C	1.31137	-2.31765	0.98974
C	1.74647	-1.98325	-0.29942
C	2.82775	-1.12162	-0.46778
C	1.04992	-2.55942	-1.52068
N	-0.22016	-3.21845	-1.19297
C	-0.00133	-4.04404	-0.01178
N	0.21809	-3.22638	1.17480
C	-1.31271	-2.31010	-1.00195
C	-1.74764	-1.98388	0.28936
C	-1.05152	-2.56859	1.50682
C	-1.97239	-1.76938	-2.12157
C	-3.05284	-0.91699	-1.91783
C	-3.49045	-0.58026	-0.63402
C	-2.82819	-1.12242	0.46333
C	1.55418	-2.15437	3.51218
C	-1.55527	-2.13004	-3.52328
N	-4.59518	0.29461	-0.45759
C	-4.66601	1.49734	-1.20286
C	-3.52248	2.26723	-1.42869
C	-3.59599	3.44072	-2.17355
C	-4.80490	3.89706	-2.70080
C	-5.94405	3.12111	-2.46519
C	-5.88114	1.93873	-1.73878
C	-4.88935	5.18487	-3.48023
C	-5.61155	-0.03404	0.47309
C	-6.17311	0.94384	1.30026
C	-7.17709	0.61328	2.20325
C	-7.64307	-0.69776	2.33163
C	-7.07080	-1.66766	1.50563
C	-6.07841	-1.34681	0.58557
C	-8.70452	-1.05419	3.34121
H	-5.34311	5.98332	-2.88114
H	5.26884	5.98637	2.87817
H	-3.89778	5.52773	-3.78936

H	-5.50230	5.06792	-4.37997
H	3.90929	5.46805	3.87933
H	-2.68907	4.01777	-2.33717
H	5.56805	5.07216	4.35654
H	2.68898	3.99762	2.36626
H	-6.90143	3.43964	-2.87118
H	-5.82463	1.96938	1.23063
H	6.90447	3.42619	2.88198
H	5.80934	1.97136	-1.22786
H	-2.56918	1.94294	-1.02353
H	-7.59945	1.39498	2.83031
H	7.57414	1.40797	-2.84265
H	2.56850	1.92873	1.04396
H	-6.77983	1.34998	-1.58413
H	6.78246	1.34186	1.58617
H	8.60154	-0.48343	-4.26854
H	-9.43959	-0.25062	3.44890
H	-3.57939	-0.51292	-2.77766
H	-8.26738	-1.23006	4.33161
H	3.15317	-0.85792	-1.47091
H	-3.15343	-0.86503	1.46815
H	9.71487	-0.74866	-2.92656
H	3.58007	-0.53454	2.77707
H	0.86986	-1.77049	-2.25351
H	-2.37745	-1.96559	-4.22503
H	8.75055	-2.09283	-3.54493
H	-0.70923	-1.52321	-3.86712
H	-0.87087	-1.78461	2.24479
H	-9.23777	-1.96503	3.05308
H	0.70880	-1.54887	3.85997
H	-5.66165	-2.11965	-0.05253
H	2.37654	-1.99540	4.21498
H	5.66104	-2.12428	0.03557
H	-7.41646	-2.69664	1.57010
H	7.40584	-2.69023	-1.60180
H	1.70216	-3.29807	-2.00357
H	-1.24404	-3.17667	-3.57980
H	-1.70427	-3.30993	1.98486
H	1.24180	-3.20100	3.56187
H	-0.87297	-4.68057	0.16037
H	0.86984	-4.68008	-0.18812

Radical cation of compound A in methylene chloride

93

C	-0.23853	-0.40707	-0.07138
C	-0.05154	-0.28656	1.30758
C	1.24433	-0.29082	1.82484
C	2.33356	-0.42567	0.97142
C	2.16415	-0.54483	-0.40996
C	0.85842	-0.53287	-0.91251
N	-1.17640	-0.14144	2.16993
C	-2.16780	0.82241	1.83069
C	-1.79085	2.10687	1.43360
C	-2.75968	3.04001	1.08742
C	-4.12135	2.72569	1.12947
C	-4.48226	1.43656	1.53199
C	-3.52380	0.49056	1.87283
C	-5.16367	3.73449	0.72436
C	3.34651	-0.65711	-1.33618
C	-1.29262	-0.90558	3.32389

C	-0.72403	-2.19284	3.39536
C	-0.81702	-2.97127	4.53296
C	-1.51777	-2.46220	5.65449
C	-2.06778	-1.16254	5.60242
C	-1.96265	-0.40536	4.45288
C	-2.74097	-0.56821	6.83390
N	-2.50951	-1.41067	8.00936
C	-2.79148	-2.78943	7.64409
N	-1.71491	-3.27409	6.79534
C	-1.24814	-1.26239	8.63098
C	-0.28167	-2.28730	8.53312
C	-0.53243	-3.49032	7.63199
C	-0.96893	-0.10861	9.40487
C	0.23552	-0.03177	10.07712
C	1.19797	-1.05830	10.00287
C	0.91436	-2.18673	9.21550
C	-0.25245	-4.36718	4.52859
C	-1.98867	0.98580	9.57637
N	2.40768	-0.94763	10.67620
C	2.99280	0.32705	10.92540
C	3.08828	1.27682	9.90816
C	3.66651	2.51529	10.16423
C	4.17378	2.83380	11.42558
C	4.07824	1.86637	12.43243
C	3.49588	0.62972	12.19338
C	4.82035	4.16677	11.69689
C	3.10722	-2.10979	11.10969
C	4.47427	-2.24160	10.85740
C	5.15698	-3.36777	11.29822
C	4.50254	-4.39129	11.99088
C	3.13527	-4.24181	12.23921
C	2.44138	-3.11664	11.81140
C	5.24516	-5.62349	12.43620
H	5.90250	4.05816	11.83243
H	3.55355	0.30251	-1.82420
H	4.65635	4.86420	10.87118
H	4.42421	4.62144	12.61061
H	4.24929	-0.95485	-0.79613
H	3.73315	3.24354	9.36060
H	3.16392	-1.39039	-2.12773
H	3.33625	-0.42618	1.39015
H	4.45915	2.08870	13.42582
H	4.99958	-1.46063	10.31706
H	0.69612	-0.63232	-1.98252
H	-0.73939	2.37367	1.40177
H	2.71503	1.04440	8.91587
H	6.22088	-3.45466	11.09425
H	-2.44968	4.03709	0.78633
H	1.39894	-0.18319	2.89380
H	3.42381	-0.10418	12.98964
H	-1.24415	-0.40780	-0.47955
H	-4.83666	4.75509	0.94318
H	6.27181	-5.38610	12.72984
H	0.42767	0.82522	10.71323
H	5.29955	-6.36059	11.62617
H	-2.35105	0.60793	4.44033
H	1.66695	-2.95934	9.09567
H	-5.36307	3.67869	-0.35243
H	-0.23606	-2.60207	2.51757
H	-2.35858	0.43589	7.01523
H	-1.82189	1.52052	10.51447

H	-6.11099	3.55927	1.24200
H	-1.92861	1.72450	8.76892
H	0.33961	-3.66895	7.00364
H	4.74862	-6.10363	13.28403
H	0.76149	-4.39382	4.94399
H	1.38380	-3.01131	12.03156
H	-0.19207	-4.75249	3.50794
H	-3.82512	-0.50999	2.16630
H	2.60379	-5.01272	12.79066
H	-5.53296	1.16158	1.56909
H	-3.82153	-0.48480	6.67217
H	-3.00440	0.58209	9.57927
H	-0.69249	-4.39050	8.23594
H	-0.87085	-5.04515	5.12235
H	-2.85090	-3.41465	8.53657
H	-3.74289	-2.82952	7.11111

Compound A in gas-phase

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C	-0.28837	-0.39378	-0.13660
C	-0.07402	-0.29297	1.24100
C	1.23091	-0.32397	1.73396
C	2.30130	-0.46647	0.85889
C	2.10471	-0.56986	-0.51938
C	0.78983	-0.52935	-0.99740
N	-1.18012	-0.13851	2.12409
C	-2.18195	0.81712	1.79342
C	-1.81774	2.09742	1.37061
C	-2.79695	3.02139	1.03359
C	-4.15635	2.70242	1.10678
C	-4.50381	1.41723	1.53240
C	-3.53559	0.48022	1.86726
C	-5.20948	3.70107	0.70731
C	3.26359	-0.70873	-1.47017
C	-1.27682	-0.89419	3.28637
C	-0.72052	-2.18668	3.35484
C	-0.80655	-2.95983	4.49720
C	-1.48042	-2.43753	5.62766
C	-2.01752	-1.13425	5.57950
C	-1.92218	-0.38257	4.42400
C	-2.67964	-0.53422	6.81384
N	-2.46516	-1.37483	7.99346
C	-2.74071	-2.75359	7.62445
N	-1.66901	-3.24687	6.77516
C	-1.20445	-1.23122	8.62374
C	-0.23428	-2.24923	8.51582
C	-0.48113	-3.44735	7.60762
C	-0.93768	-0.09058	9.41911
C	0.26313	-0.01637	10.09927
C	1.23020	-1.03752	10.01676
C	0.95742	-2.15334	9.20866
C	-0.26499	-4.36484	4.49242
C	-1.96968	0.99042	9.60250
N	2.43115	-0.93822	10.70881
C	3.01431	0.33037	10.98635
C	3.10731	1.30432	9.99118
C	3.68452	2.53598	10.27554
C	4.19177	2.82600	11.54367
C	4.09792	1.83514	12.52744
C	3.51908	0.60376	12.26073

C	4.83791	4.15160	11.84600
C	3.11456	-2.10791	11.14686
C	4.48706	-2.24391	10.92208
C	5.15254	-3.37795	11.36338
C	4.47895	-4.40358	12.03595
C	3.10756	-4.25163	12.25269
C	2.42828	-3.11891	11.82150
C	5.22009	-5.61789	12.52820
H	5.92198	4.04205	11.96377
H	3.34133	0.16495	-2.12663
H	4.66266	4.87441	11.04497
H	4.45241	4.57871	12.77721
H	4.21103	-0.80864	-0.93443
H	3.75242	3.28272	9.48923
H	3.14577	-1.58729	-2.11306
H	3.31200	-0.48398	1.25714
H	4.47865	2.03553	13.52543
H	5.02605	-1.46020	10.39943
H	0.60703	-0.61278	-2.06546
H	-0.76781	2.36542	1.31062
H	2.73534	1.09294	8.99360
H	6.21904	-3.47208	11.17670
H	-2.49817	4.01551	0.71230
H	1.40657	-0.22664	2.80071
H	3.44963	-0.14912	13.03922
H	-1.30110	-0.37004	-0.52577
H	-4.89730	4.72425	0.93513
H	5.84807	-5.37010	13.39157
H	0.44780	0.83016	10.75168
H	5.87903	-6.02347	11.75401
H	-2.30737	0.63234	4.40719
H	1.71317	-2.92388	9.09139
H	-5.40454	3.65141	-0.37046
H	-0.25258	-2.60405	2.46986
H	-2.28265	0.46469	6.99789
H	-1.81081	1.51886	10.54555
H	-6.15640	3.51195	1.22034
H	-1.92192	1.73932	8.80316
H	0.38867	-3.61556	6.97166
H	4.53203	-6.40954	12.83576
H	0.74872	-4.41189	4.90744
H	1.36625	-3.01068	12.01818
H	-0.21126	-4.75373	3.47275
H	-3.82576	-0.51925	2.17559
H	2.56095	-5.02693	12.78237
H	-5.55248	1.13834	1.58951
H	-3.75940	-0.43122	6.65255
H	-2.97940	0.57177	9.60296
H	-0.62665	-4.35388	8.20720
H	-0.89675	-5.03016	5.08652
H	-2.80308	-3.37779	8.51834
H	-3.69319	-2.79652	7.09202

Radical cation of compound A in gas-phase

93

C	-0.28837	-0.39378	-0.13660
C	-0.07402	-0.29297	1.24100
C	1.23091	-0.32397	1.73396
C	2.30130	-0.46647	0.85889
C	2.10471	-0.56986	-0.51938

C	0.78983	-0.52935	-0.99740
N	-1.18012	-0.13851	2.12409
C	-2.18195	0.81712	1.79342
C	-1.81774	2.09742	1.37061
C	-2.79695	3.02139	1.03359
C	-4.15635	2.70242	1.10678
C	-4.50381	1.41723	1.53240
C	-3.53559	0.48022	1.86726
C	-5.20948	3.70107	0.70731
C	3.26359	-0.70873	-1.47017
C	-1.27682	-0.89419	3.28637
C	-0.72052	-2.18668	3.35484
C	-0.80655	-2.95983	4.49720
C	-1.48042	-2.43753	5.62766
C	-2.01752	-1.13425	5.57950
C	-1.92218	-0.38257	4.42400
C	-2.67964	-0.53422	6.81384
N	-2.46516	-1.37483	7.99346
C	-2.74071	-2.75359	7.62445
N	-1.66901	-3.24687	6.77516
C	-1.20445	-1.23122	8.62374
C	-0.23428	-2.24923	8.51582
C	-0.48113	-3.44735	7.60762
C	-0.93768	-0.09058	9.41911
C	0.26313	-0.01637	10.09927
C	1.23020	-1.03752	10.01676
C	0.95742	-2.15334	9.20866
C	-0.26499	-4.36484	4.49242
C	-1.96968	0.99042	9.60250
N	2.43115	-0.93822	10.70881
C	3.01431	0.33037	10.98635
C	3.10731	1.30432	9.99118
C	3.68452	2.53598	10.27554
C	4.19177	2.82600	11.54367
C	4.09792	1.83514	12.52744
C	3.51908	0.60376	12.26073
C	4.83791	4.15160	11.84600
C	3.11456	-2.10791	11.14686
C	4.48706	-2.24391	10.92208
C	5.15254	-3.37795	11.36338
C	4.47895	-4.40358	12.03595
C	3.10756	-4.25163	12.25269
C	2.42828	-3.11891	11.82150
C	5.22009	-5.61789	12.52820
H	5.92198	4.04205	11.96377
H	3.34133	0.16495	-2.12663
H	4.66266	4.87441	11.04497
H	4.45241	4.57871	12.77721
H	4.21103	-0.80864	-0.93443
H	3.75242	3.28272	9.48923
H	3.14577	-1.58729	-2.11306
H	3.31200	-0.48398	1.25714
H	4.47865	2.03553	13.52543
H	5.02605	-1.46020	10.39943
H	0.60703	-0.61278	-2.06546
H	-0.76781	2.36542	1.31062
H	2.73534	1.09294	8.99360
H	6.21904	-3.47208	11.17670
H	-2.49817	4.01551	0.71230
H	1.40657	-0.22664	2.80071
H	3.44963	-0.14912	13.03922

H	-1.30110	-0.37004	-0.52577
H	-4.89730	4.72425	0.93513
H	5.84807	-5.37010	13.39157
H	0.44780	0.83016	10.75168
H	5.87903	-6.02347	11.75401
H	-2.30737	0.63234	4.40719
H	1.71317	-2.92388	9.09139
H	-5.40454	3.65141	-0.37046
H	-0.25258	-2.60405	2.46986
H	-2.28265	0.46469	6.99789
H	-1.81081	1.51886	10.54555
H	-6.15640	3.51195	1.22034
H	-1.92192	1.73932	8.80316
H	0.38867	-3.61556	6.97166
H	4.53203	-6.40954	12.83576
H	0.74872	-4.41189	4.90744
H	1.36625	-3.01068	12.01818
H	-0.21126	-4.75373	3.47275
H	-3.82576	-0.51925	2.17559
H	2.56095	-5.02693	12.78237
H	-5.55248	1.13834	1.58951
H	-3.75940	-0.43122	6.65255
H	-2.97940	0.57177	9.60296
H	-0.62665	-4.35388	8.20720
H	-0.89675	-5.03016	5.08652
H	-2.80308	-3.37779	8.51834
H	-3.69319	-2.79652	7.09202

Compound B in gas-phase

81

C	0.40629	0.15778	0.59470
C	-0.05291	0.47781	1.87355
C	0.79615	1.18783	2.72861
C	2.06202	1.57052	2.30579
C	2.53490	1.24884	1.03073
C	1.68367	0.53140	0.19040
N	-1.34912	0.09094	2.29766
C	-1.84028	-1.20165	1.98940
C	-1.01536	-2.32303	2.08751
C	-1.50419	-3.58686	1.77011
C	-2.82406	-3.77720	1.36519
C	-3.64407	-2.64889	1.27610
C	-3.16516	-1.38174	1.57463
C	-3.35831	-5.15796	1.04141
C	-3.91148	-5.29968	-0.36186
C	-5.24082	-5.65285	-0.58628
C	-5.74756	-5.79911	-1.87421
C	-4.93091	-5.57707	-2.98407
C	-3.59647	-5.21232	-2.76852
C	-3.10028	-5.08465	-1.47949
N	-5.43852	-5.71524	-4.29901
C	-4.65158	-6.33526	-5.30186
C	-3.91443	-7.49022	-5.01917
C	-3.14165	-8.09077	-6.00339
C	-3.08681	-7.57972	-7.30326
C	-3.83342	-6.43411	-7.57635
C	-4.59775	-5.81162	-6.59446
C	-2.24748	-8.24660	-8.36320
C	3.90909	1.67661	0.58210
C	-6.73387	-5.23309	-4.61547

C	-7.60213	-5.99002	-5.40897
C	-8.86561	-5.51013	-5.72507
C	-9.31772	-4.27496	-5.25193
C	-8.44698	-3.53288	-4.45456
C	-7.17127	-3.99401	-4.14525
C	-10.69769	-3.77305	-5.59303
C	-2.15186	0.99776	3.03421
C	-2.21669	2.34784	2.67487
C	-2.99895	3.23363	3.40349
C	-3.75492	2.80997	4.49985
C	-3.69201	1.45924	4.84184
C	-2.89805	0.56468	4.13171
C	-4.59153	3.78482	5.28866
H	-6.78432	-6.08440	-2.02088
H	-5.89736	-5.83324	0.26175
H	-2.06284	-4.79134	-1.33844
H	-2.94926	-5.03039	-3.62051
H	-9.52079	-6.11761	-6.34547
H	-7.27815	-6.95694	-5.78066
H	-6.50900	-3.39092	-3.53224
H	-8.76372	-2.56468	-4.07460
H	-10.87396	-2.77894	-5.17207
H	-10.84279	-3.70612	-6.67706
H	-11.47387	-4.44128	-5.20268
H	-3.94930	-7.91424	-4.02064
H	-3.81109	-6.00713	-8.57603
H	-5.16148	-4.91509	-6.83195
H	-2.86011	-0.47953	4.42526
H	-4.26680	1.09496	5.68988
H	-3.03246	4.27830	3.10241
H	-1.64871	2.69991	1.81960
H	-5.28321	3.26480	5.95786
H	-3.96502	4.43980	5.90582
H	-5.18353	4.42896	4.62981
H	-0.84108	-4.44468	1.85485
H	0.01434	-2.20362	2.40886
H	-3.81840	-0.51932	1.48798
H	-4.67386	-2.76113	0.94598
H	0.45721	1.43945	3.72854
H	2.01842	0.26618	-0.80950
H	-0.23951	-0.39099	-0.08337
H	-2.57745	-8.98751	-5.75696
H	-2.35601	-7.74485	-9.32911
H	-2.53363	-9.29565	-8.49891
H	-1.18382	-8.23222	-8.09920
H	2.70277	2.12132	2.99075
H	4.18805	1.19342	-0.35878
H	4.67074	1.42271	1.32723
H	3.95805	2.76050	0.42424
H	-4.14649	-5.42162	1.75707
H	-2.55469	-5.88857	1.19341

Radical cation of compound B in gas-phase

81

C	0.39896	-0.01605	0.60817
C	-0.08230	0.38821	1.86091
C	0.72672	1.17293	2.69815
C	1.99501	1.53198	2.28243
C	2.49266	1.13870	1.03070
C	1.66943	0.36323	0.20660

N	-1.37692	0.01227	2.27645
C	-1.85696	-1.27562	2.00235
C	-0.98910	-2.37961	2.05866
C	-1.47395	-3.64750	1.79187
C	-2.81572	-3.85806	1.45012
C	-3.66823	-2.74299	1.38726
C	-3.21098	-1.47276	1.66864
C	-3.33900	-5.24063	1.14004
C	-3.88401	-5.34691	-0.26918
C	-5.25056	-5.48114	-0.51346
C	-5.75178	-5.57353	-1.80523
C	-4.89120	-5.52355	-2.91142
C	-3.51459	-5.38187	-2.66924
C	-3.02939	-5.29992	-1.37397
N	-5.38394	-5.62023	-4.21781
C	-4.59026	-6.19008	-5.25584
C	-3.96143	-7.42307	-5.08035
C	-3.19681	-7.97147	-6.10358
C	-3.05388	-7.32356	-7.33239
C	-3.69625	-6.09415	-7.49724
C	-4.44954	-5.52807	-6.47586
C	-2.26141	-7.94306	-8.45437
C	3.87167	1.54675	0.59649
C	-6.70175	-5.18480	-4.53818
C	-7.55889	-6.01159	-5.26769
C	-8.83464	-5.57756	-5.60156
C	-9.30194	-4.31915	-5.21139
C	-8.43743	-3.50532	-4.47860
C	-7.15095	-3.92246	-4.15247
C	-10.68830	-3.86108	-5.58411
C	-2.18620	0.94011	2.96671
C	-2.19991	2.28832	2.57749
C	-2.99945	3.18835	3.25753
C	-3.79285	2.78637	4.34214
C	-3.76265	1.43861	4.71894
C	-2.97633	0.51903	4.04481
C	-4.63547	3.78466	5.08390
H	-6.81723	-5.70041	-1.96068
H	-5.94421	-5.54359	0.32220
H	-1.95702	-5.19564	-1.22291
H	-2.82629	-5.34260	-3.50604
H	-9.48535	-6.23652	-6.17118
H	-7.21754	-6.99464	-5.57663
H	-6.48910	-3.26576	-3.59584
H	-8.76886	-2.51772	-4.16801
H	-10.92713	-2.89802	-5.12445
H	-10.78983	-3.74594	-6.66906
H	-11.44651	-4.58306	-5.26265
H	-4.07187	-7.95237	-4.13870
H	-3.60009	-5.56308	-8.44098
H	-4.93851	-4.56996	-6.62278
H	-2.94874	-0.51712	4.36446
H	-4.35926	1.10637	5.56305
H	-3.01992	4.22598	2.93709
H	-1.60805	2.61251	1.72832
H	-5.34814	3.29392	5.75063
H	-4.00633	4.44355	5.69344
H	-5.19522	4.42147	4.39213
H	-0.80171	-4.49740	1.86242
H	0.04687	-2.23824	2.34645
H	-3.87860	-0.62112	1.59766

H	-4.70316	-2.88324	1.09087
H	0.36519	1.46904	3.67697
H	2.02698	0.06060	-0.77284
H	-0.23450	-0.59656	-0.05388
H	-2.71347	-8.93240	-5.94628
H	-1.76212	-7.18072	-9.05996
H	-2.91150	-8.51779	-9.12466
H	-1.49693	-8.62686	-8.07444
H	2.62197	2.12278	2.94409
H	4.11735	1.14870	-0.39046
H	4.62631	1.18828	1.30467
H	3.96143	2.63757	0.55418
H	-4.13271	-5.48927	1.85436
H	-2.53861	-5.97114	1.29835

Compound C in methylene chloride

95

C	-0.00991	-0.00206	0.01705
C	-0.00743	-0.00088	1.41482
C	1.22400	-0.02507	2.07696
C	2.41264	-0.06161	1.35689
C	2.42149	-0.05928	-0.04033
C	1.18657	-0.02084	-0.69167
N	-1.22299	0.02856	2.14236
C	-2.28637	0.86603	1.71535
C	-2.04625	2.17026	1.29697
C	-3.08933	2.99358	0.86836
C	-4.40857	2.52318	0.88149
C	-4.65828	1.19970	1.29952
C	-3.60025	0.39065	1.70099
C	-5.55471	3.43190	0.47007
C	-5.07800	4.55102	-0.45517
C	-3.95673	5.32019	0.24311
C	-2.74338	4.38133	0.36499
C	-4.40218	5.84785	1.59687
C	-5.44541	5.22401	2.29357
C	-6.23553	4.08075	1.68756
C	-3.75965	6.95958	2.17940
C	-4.14663	7.39885	3.44175
C	-5.17619	6.76893	4.14519
C	-5.82241	5.68878	3.55465
C	-6.05122	0.61531	1.28383
N	-5.55029	7.22308	5.43770
C	-5.70514	8.61041	5.67998
C	-5.23081	9.18949	6.86282
C	-5.38880	10.54951	7.09525
C	-6.00522	11.38547	6.15834
C	-6.46473	10.79996	4.97826
C	-6.32861	9.43484	4.74105
C	-2.65846	7.70220	1.45988
C	-6.16684	12.86085	6.42338
C	3.71442	-0.12220	-0.81315
C	-1.37766	-0.77302	3.30088
C	-0.91573	-2.09347	3.32529
C	-1.06893	-2.87387	4.46448
C	-1.69779	-2.37884	5.61092
C	-2.16533	-1.06421	5.57163
C	-2.00237	-0.26656	4.44297
C	-1.84555	-3.23067	6.84605
C	-5.77442	6.28611	6.47632

C	-4.93180	5.17890	6.63142
C	-5.15603	4.25806	7.64615
C	-6.21054	4.40979	8.55264
C	-7.03935	5.52069	8.39403
C	-6.83618	6.44195	7.36980
H	-2.26438	8.50667	2.08619
H	-1.82158	7.05003	1.19124
H	-4.73632	8.56742	7.60227
H	-5.01053	10.97331	8.02278
H	-3.63966	8.24803	3.89051
H	-3.02138	8.15461	0.52964
H	4.51527	0.41491	-0.29556
H	-5.20520	13.33292	6.65282
H	-1.97833	4.81891	1.01443
H	3.60406	0.31276	-1.81091
H	3.35599	-0.07801	1.89774
H	-2.28071	4.28387	-0.62708
H	-1.02977	2.55451	1.29860
H	-3.66058	6.16706	-0.38396
H	4.04888	-1.15865	-0.94293
H	-6.82774	13.04252	7.27861
H	-7.50523	7.29021	7.26521
H	-4.09901	5.04100	5.94915
H	1.24875	-0.01401	3.16205
H	1.15501	-0.01611	-1.77860
H	-6.59420	13.37450	5.55755
H	-2.36897	0.75511	4.44434
H	-0.95483	0.01910	-0.51668
H	-6.70503	9.00586	3.81777
H	-4.70937	4.13987	-1.40258
H	-6.95152	11.41865	4.22833
H	-5.91628	5.21720	-0.69193
H	-6.63300	5.19600	4.08494
H	-2.65989	-0.64613	6.44508
H	-7.21516	4.46558	1.37139
H	-0.43607	-2.50875	2.44453
H	-6.43873	3.33424	2.46208
H	-3.79675	-0.63173	2.01000
H	-6.30766	2.83321	-0.05229
H	-0.89809	-3.30557	7.39299
H	-2.58867	-2.81200	7.53081
H	-0.70276	-3.89791	4.45518
H	-6.74902	1.18763	1.90307
H	-6.04143	-0.41136	1.65869
H	-6.46805	0.59428	0.27024
H	-2.15464	-4.25025	6.59376
H	-4.48598	3.40677	7.74282
H	-7.87270	5.66819	9.07658
C	-6.43449	3.40688	9.65592
H	-7.29790	3.67867	10.26989
H	-6.61291	2.40345	9.25347
H	-5.56273	3.33920	10.31646

Radical cation of compound C in methylene chloride

95

C	-0.03752	-0.03071	-0.01268
C	-0.01925	-0.04999	1.38934
C	1.20680	-0.09497	2.07165
C	2.38788	-0.11190	1.35328
C	2.38860	-0.09938	-0.04925

C	1.15659	-0.05960	-0.71302
N	-1.22771	-0.02444	2.11182
C	-2.29183	0.78165	1.67784
C	-2.03874	2.04045	1.12370
C	-3.08836	2.84633	0.70292
C	-4.41446	2.39584	0.83790
C	-4.67063	1.10970	1.37296
C	-3.61303	0.32228	1.79462
C	-5.56747	3.29162	0.43196
C	-5.13867	4.33586	-0.59802
C	-3.96540	5.13277	-0.02941
C	-2.75917	4.18467	0.07442
C	-4.31167	5.75804	1.31183
C	-5.31319	5.20314	2.11739
C	-6.15432	4.03183	1.64930
C	-3.61908	6.89618	1.77393
C	-3.92030	7.42990	3.02239
C	-4.91436	6.87263	3.83383
C	-5.60719	5.76155	3.36214
C	-6.07001	0.55387	1.45991
N	-5.20475	7.42954	5.10164
C	-5.21538	8.83831	5.27876
C	-4.62118	9.41498	6.40567
C	-4.64205	10.79213	6.58671
C	-5.23759	11.64257	5.64987
C	-5.81714	11.05688	4.52326
C	-5.81845	9.67702	4.33995
C	-2.55649	7.56769	0.93626
C	-5.26555	13.13451	5.86414
C	3.68131	-0.14779	-0.81307
C	-1.36603	-0.81073	3.27275
C	-0.83178	-2.10818	3.31156
C	-0.98109	-2.87412	4.45288
C	-1.64615	-2.37664	5.58298
C	-2.16794	-1.07873	5.52786
C	-2.03878	-0.29872	4.39100
C	-1.77525	-3.21399	6.82364
C	-5.54954	6.58877	6.19139
C	-4.80825	5.43396	6.46590
C	-5.14925	4.61496	7.53413
C	-6.22385	4.92116	8.37633
C	-6.94930	6.08001	8.09945
C	-6.62775	6.89996	7.02073
H	-2.11731	8.41092	1.47512
H	-1.74316	6.88604	0.66800
H	-4.14229	8.77729	7.14236
H	-4.17248	11.21592	7.47133
H	-3.37554	8.30035	3.37444
H	-2.97083	7.95457	-0.00188
H	4.42546	0.52235	-0.37266
H	-4.29000	13.50954	6.19041
H	-1.94267	4.65051	0.63429
H	3.53879	0.13151	-1.85965
H	3.33277	-0.12416	1.88837
H	-2.37103	3.99894	-0.93632
H	-1.01887	2.40470	1.05524
H	-3.70059	5.92768	-0.73285
H	4.10248	-1.15966	-0.79019
H	-5.99316	13.41058	6.63642
H	-7.21588	7.79083	6.82409
H	-3.96153	5.18104	5.83530

H	1.22412	-0.08150	3.15569
H	1.13336	-0.06060	-1.79842
H	-5.54148	13.66255	4.94702
H	-2.42884	0.71283	4.37265
H	-0.98363	-0.02388	-0.54225
H	-6.28665	9.24794	3.45955
H	-4.84231	3.85588	-1.53796
H	-6.28956	11.68864	3.77512
H	-5.98491	4.99517	-0.82101
H	-6.39257	5.32171	3.97011
H	-2.67723	-0.66966	6.39506
H	-7.14853	4.40360	1.36868
H	-0.33548	-2.51643	2.43816
H	-6.31345	3.34434	2.48602
H	-3.80121	-0.67283	2.18246
H	-6.35854	2.66684	0.00718
H	-0.81859	-3.26010	7.35687
H	-2.52048	-2.80253	7.50844
H	-0.58409	-3.88479	4.46752
H	-6.73348	1.19581	2.04601
H	-6.06288	-0.43335	1.92731
H	-6.51812	0.44898	0.46592
H	-2.05883	-4.24187	6.57852
H	-4.55635	3.72368	7.72688
H	-7.79240	6.34741	8.73152
C	-6.57504	4.02883	9.53982
H	-7.44033	4.41347	10.08670
H	-6.81438	3.01299	9.20614
H	-5.74129	3.94874	10.24633

TTA in methylene chloride
43

C	-0.00373	0.01362	0.00936
C	-0.00089	0.00312	1.40552
C	1.23122	-0.01233	2.06892
C	2.41933	-0.02574	1.34990
C	2.42826	-0.00615	-0.04860
C	1.19437	0.01804	-0.69962
N	-1.21581	0.00915	2.13644
C	-1.36360	-0.82727	3.27181
C	-1.97972	-0.35057	4.43430
C	-2.12985	-1.17513	5.54168
C	-1.65944	-2.49236	5.54176
C	-1.03934	-2.95461	4.38041
C	-0.89852	-2.14357	3.25765
C	-1.81661	-3.37130	6.75659
C	3.72608	-0.00763	-0.81588
C	-2.28933	0.83758	1.72279
C	-2.06027	2.14924	1.30158
C	-3.11838	2.95371	0.88875
C	-4.43478	2.49018	0.89683
C	-4.65395	1.17906	1.33051
C	-3.60456	0.36022	1.72814
C	-5.58028	3.36002	0.44485
H	1.25432	-0.01641	3.15412
H	3.36284	-0.03905	1.89077
H	1.16303	0.02820	-1.78632
H	-0.94840	0.02187	-0.52517
H	-2.34409	0.67149	4.46574
H	-2.61375	-0.77991	6.43194

H	-0.66698	-3.97538	4.34276
H	-0.42188	-2.53416	2.36404
H	-3.80335	-0.65736	2.04942
H	-5.66687	0.78334	1.34726
H	-2.91151	3.97094	0.56542
H	-1.04807	2.54121	1.29524
H	-1.43627	-4.37924	6.56825
H	-1.27204	-2.96414	7.61609
H	-2.86766	-3.45910	7.05280
H	-5.25485	4.39159	0.28300
H	-6.00931	2.99578	-0.49594
H	-6.38810	3.37351	1.18418
H	3.54828	-0.02444	-1.89487
H	4.32401	0.88252	-0.58972
H	4.33849	-0.88029	-0.56339

Radical cation of TTA in methylene chloride
43

C	-0.01387	0.01916	0.00984
C	-0.00739	-0.00032	1.41251
C	1.21413	-0.01713	2.10589
C	2.40092	-0.00817	1.39786
C	2.41334	0.00489	-0.00498
C	1.18646	0.01714	-0.67969
N	-1.22116	0.00026	2.12333
C	-1.35327	-0.77240	3.29201
C	-0.77663	-2.05168	3.35998
C	-0.92022	-2.80442	4.50981
C	-1.62296	-2.31300	5.62061
C	-2.18557	-1.03398	5.53722
C	-2.06275	-0.26705	4.39091
C	-1.75931	-3.14473	6.86394
C	3.71368	-0.01001	-0.75662
C	-2.30353	0.77455	1.66709
C	-3.61236	0.27365	1.75326
C	-4.66888	1.04125	1.29885
C	-4.46277	2.31894	0.75965
C	-3.15105	2.80669	0.69002
C	-2.07830	2.05068	1.12815
C	-5.61766	3.13111	0.24731
H	-3.78685	-0.72206	2.14534
H	-5.67630	0.63994	1.35363
H	-2.97036	3.80204	0.29587
H	-1.07235	2.45343	1.09009
H	-0.25222	-2.45603	2.50136
H	-0.48929	-3.80054	4.54780
H	-2.72096	-0.62837	6.38993
H	-2.48366	0.73143	4.35227
H	1.22180	-0.00124	3.18996
H	3.34125	0.00113	1.94091
H	1.17294	0.01563	-1.76516
H	-0.95480	0.00401	-0.52866
H	-2.37702	-2.64559	7.61387
H	-2.21251	-4.11509	6.63569
H	-0.77759	-3.34393	7.30735
H	3.56775	0.22154	-1.81420
H	4.41944	0.71324	-0.33694
H	4.18447	-0.99764	-0.68974
H	-5.38915	4.19974	0.25482
H	-5.85130	2.85008	-0.78663

H	-6.51888	2.96214	0.84282

Compound C in gas-phase
95

C	0.00087	0.01205	0.01336
C	-0.00037	0.00175	1.41056
C	1.22845	-0.01549	2.07664
C	2.41868	-0.03346	1.36014
C	2.43150	-0.01875	-0.03612
C	1.19917	0.01192	-0.69093
N	-1.21817	0.01260	2.13445
C	-2.28477	0.84899	1.71674
C	-2.04937	2.15397	1.29910
C	-3.09577	2.97630	0.87967
C	-4.41350	2.50465	0.90001
C	-4.65846	1.18094	1.31776
C	-3.59804	0.37247	1.71064
C	-5.56293	3.41212	0.49635
C	-5.09298	4.52891	-0.43504
C	-3.96977	5.30213	0.25567
C	-2.75440	4.36576	0.37832
C	-4.41265	5.83735	1.60695
C	-5.45071	5.21512	2.31092
C	-6.23666	4.06270	1.71714
C	-3.77286	6.95476	2.17988
C	-4.15788	7.40247	3.43872
C	-5.18408	6.77520	4.14897
C	-5.82720	5.68839	3.56804
C	-6.05082	0.59497	1.31017
N	-5.55731	7.23811	5.43734
C	-5.69673	8.62745	5.67506
C	-5.22363	9.20265	6.85971
C	-5.36725	10.56413	7.08803
C	-5.96695	11.40481	6.14581
C	-6.42492	10.82300	4.96432
C	-6.30389	9.45679	4.73043
C	-2.67532	7.69543	1.45275
C	-6.11339	12.88226	6.40730
C	3.72746	-0.06150	-0.80494
C	-1.36736	-0.80261	3.28349
C	-0.88958	-2.11715	3.29456
C	-1.03596	-2.91068	4.42453
C	-1.67345	-2.43589	5.57372
C	-2.15663	-1.12756	5.54742
C	-2.00083	-0.31587	4.42882
C	-1.81351	-3.30274	6.79907
C	-5.79567	6.30825	6.47889
C	-4.96512	5.19395	6.64299
C	-5.20388	4.28144	7.66092
C	-6.26027	4.44885	8.56106
C	-7.07653	5.56663	8.39333
C	-6.85960	6.48002	7.36614
H	-2.27982	8.50318	2.07403
H	-1.83766	7.04402	1.18385
H	-4.74279	8.57426	7.60264
H	-4.99049	10.98550	8.01744
H	-3.65403	8.25668	3.88102
H	-3.04174	8.14527	0.52234
H	4.52079	0.48180	-0.28178
H	-5.14794	13.34543	6.63976

H	-1.99436	4.80587	1.03211
H	3.61676	0.38138	-1.79941
H	3.36087	-0.04476	1.90335
H	-2.28738	4.27034	-0.61236
H	-1.03289	2.53792	1.29519
H	-3.67748	6.14654	-0.37737
H	4.07486	-1.09278	-0.94261
H	-6.77818	13.07432	7.25743
H	-7.51748	7.33569	7.25253
H	-4.13162	5.04573	5.96393
H	1.24712	-0.01416	3.16180
H	1.17151	0.02482	-1.77802
H	-6.52986	13.39974	5.53817
H	-2.37941	0.70125	4.43783
H	-0.94387	0.02789	-0.52070
H	-6.67800	9.02849	3.80605
H	-4.72899	4.11368	-1.38273
H	-6.89926	11.44645	4.21024
H	-5.93261	5.19445	-0.66985
H	-6.63420	5.19760	4.10541
H	-2.65826	-0.72543	6.42445
H	-7.22355	4.43794	1.41082
H	-0.40246	-2.51477	2.40989
H	-6.42296	3.31705	2.49694
H	-3.78996	-0.65054	2.01997
H	-6.31878	2.81168	-0.02082
H	-0.86592	-3.37636	7.34620
H	-2.56049	-2.89901	7.48895
H	-0.65724	-3.93016	4.40570
H	-6.74890	1.17081	1.92611
H	-6.03918	-0.42839	1.69410
H	-6.46996	0.56276	0.29751
H	-2.11637	-4.32180	6.53634
H	-4.54285	3.42390	7.76578
H	-7.91125	5.72572	9.07171
C	-6.49941	3.45430	9.66846
H	-7.36304	3.73771	10.27721
H	-6.68781	2.45028	9.27158
H	-5.63256	3.38199	10.33524

Radical cation of compound C in gas-phase

95

C	0.00887	0.01711	-0.00488
C	0.01140	0.01433	1.39619
C	1.22971	0.01985	2.09117
C	2.41916	0.03850	1.38587
C	2.43681	0.03685	-0.01639
C	1.21147	0.02472	-0.69256
N	-1.20868	-0.00125	2.10811
C	-2.28816	0.77622	1.67862
C	-2.06822	2.03250	1.09646
C	-3.13541	2.81538	0.68279
C	-4.45419	2.34624	0.85116
C	-4.67949	1.06126	1.40833
C	-3.60343	0.29882	1.82399
C	-5.62753	3.21977	0.46255
C	-5.23811	4.26116	-0.58652
C	-4.06424	5.07960	-0.05156
C	-2.84230	4.14966	0.02857
C	-4.38518	5.70900	1.29341

C	-5.35372	5.14539	2.13085
C	-6.19396	3.96267	1.69030
C	-3.70273	6.86321	1.72861
C	-3.98282	7.40360	2.97704
C	-4.94490	6.83727	3.82392
C	-5.62547	5.70524	3.37814
C	-6.06819	0.48437	1.52237
N	-5.21504	7.40307	5.08215
C	-5.13140	8.81236	5.27373
C	-4.44526	9.33263	6.37293
C	-4.37911	10.70527	6.57282
C	-4.97774	11.60078	5.68208
C	-5.65268	11.06813	4.58314
C	-5.74116	9.69432	4.38241
C	-2.67813	7.55063	0.85678
C	-4.91143	13.08769	5.91842
C	3.73957	0.02664	-0.76476
C	-1.32741	-0.81082	3.25990
C	-0.77217	-2.09884	3.27348
C	-0.89899	-2.88622	4.40332
C	-1.56110	-2.41932	5.54801
C	-2.10244	-1.12905	5.51798
C	-1.99580	-0.32820	4.39252
C	-1.66468	-3.27928	6.77567
C	-5.63906	6.59222	6.16918
C	-4.95246	5.41843	6.49485
C	-5.36387	4.63782	7.56633
C	-6.45592	5.00373	8.35962
C	-7.12508	6.18210	8.03171
C	-6.73226	6.96489	6.95007
H	-2.23445	8.40062	1.38052
H	-1.86050	6.88490	0.56066
H	-3.96770	8.65435	7.07345
H	-3.84098	11.08948	7.43601
H	-3.44881	8.28942	3.30440
H	-3.12844	7.93439	-0.06619
H	4.45391	0.73037	-0.32727
H	-3.90019	13.40412	6.19380
H	-2.02021	4.63582	0.56265
H	3.60178	0.28723	-1.81670
H	3.35810	0.06419	1.93126
H	-2.47705	3.95386	-0.98959
H	-1.05600	2.41331	1.00620
H	-3.82805	5.87138	-0.76873
H	4.19864	-0.96806	-0.72524
H	-5.57938	13.38869	6.73384
H	-7.27136	7.87689	6.71406
H	-4.08963	5.12615	5.90392
H	1.23389	0.03946	3.17563
H	1.20048	0.01114	-1.77823
H	-5.20746	13.64703	5.02660
H	-2.40273	0.67729	4.39342
H	-0.93164	-0.01449	-0.54434
H	-6.28357	9.30267	3.52723
H	-4.96154	3.77789	-1.53146
H	-6.13258	11.73820	3.87437
H	-6.09856	4.90678	-0.79221
H	-6.38981	5.25930	4.00743
H	-2.60896	-0.74180	6.39690
H	-7.19829	4.32022	1.42772
H	-0.27294	-2.48224	2.39010

H	-6.32764	3.27861	2.53476
H	-3.76885	-0.69397	2.22809
H	-6.41889	2.57800	0.06310
H	-0.70289	-3.32034	7.30002
H	-2.40890	-2.89317	7.47607
H	-0.48503	-3.89038	4.39849
H	-6.73723	1.13041	2.09698
H	-6.04387	-0.49091	2.01393
H	-6.52292	0.34615	0.53546
H	-1.93678	-4.30716	6.51789
H	-4.81080	3.73196	7.80577
H	-7.97768	6.49636	8.62798
C	-6.88080	4.15569	9.53112
H	-7.75447	4.58044	10.03290
H	-7.14030	3.13857	9.21663
H	-6.07970	4.07236	10.27414