Supplementary Material (ESI) for New Journal of Chemistry

Anodic behaviour of methylidene-cyclopentadiaryl derivatives: Cyclic voltammetry and theoretical study†

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Electronic Supplementary Information

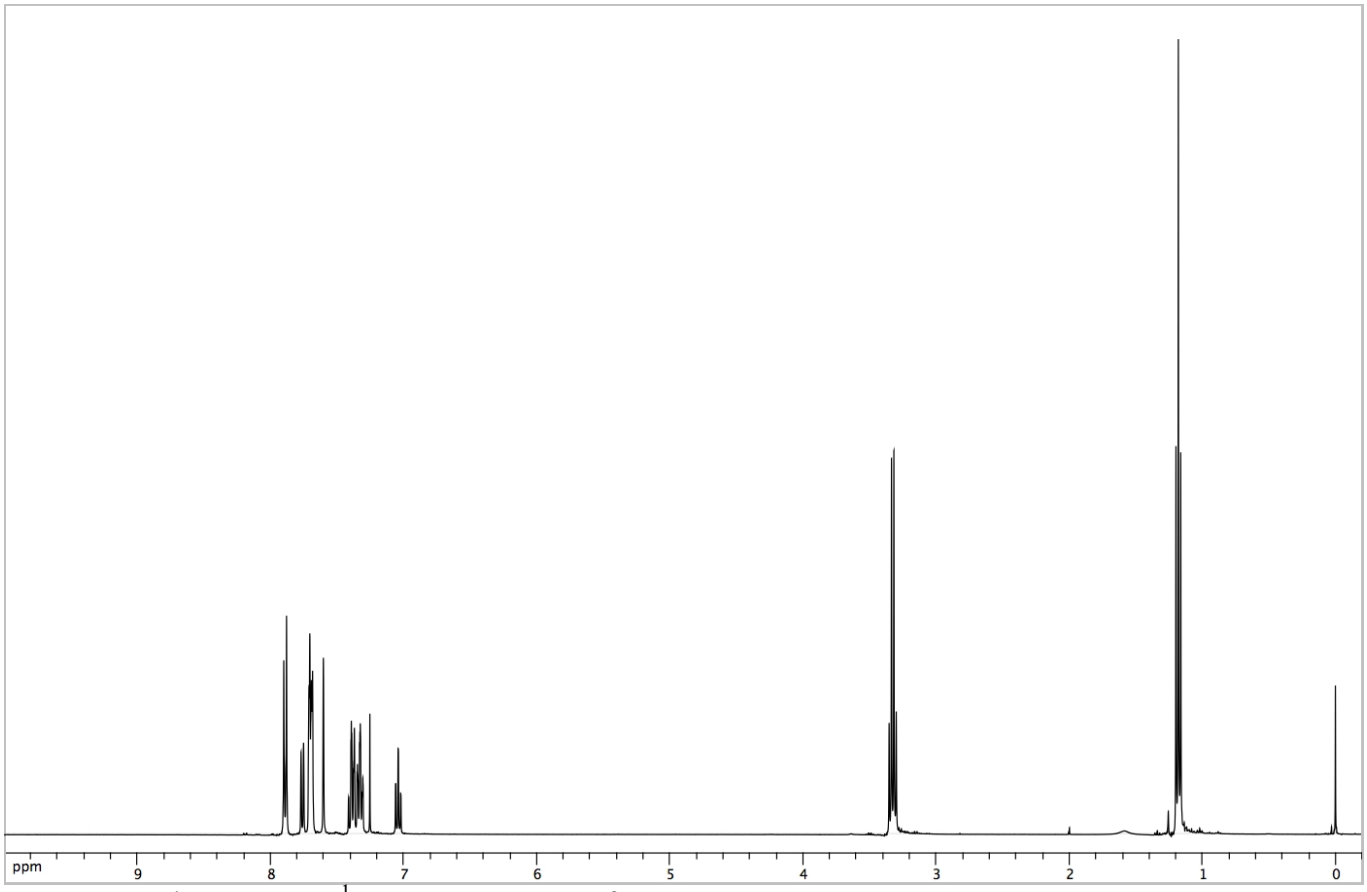

Figure S1. The 400 MHz ^{1}H NMR spectrum of **1**.

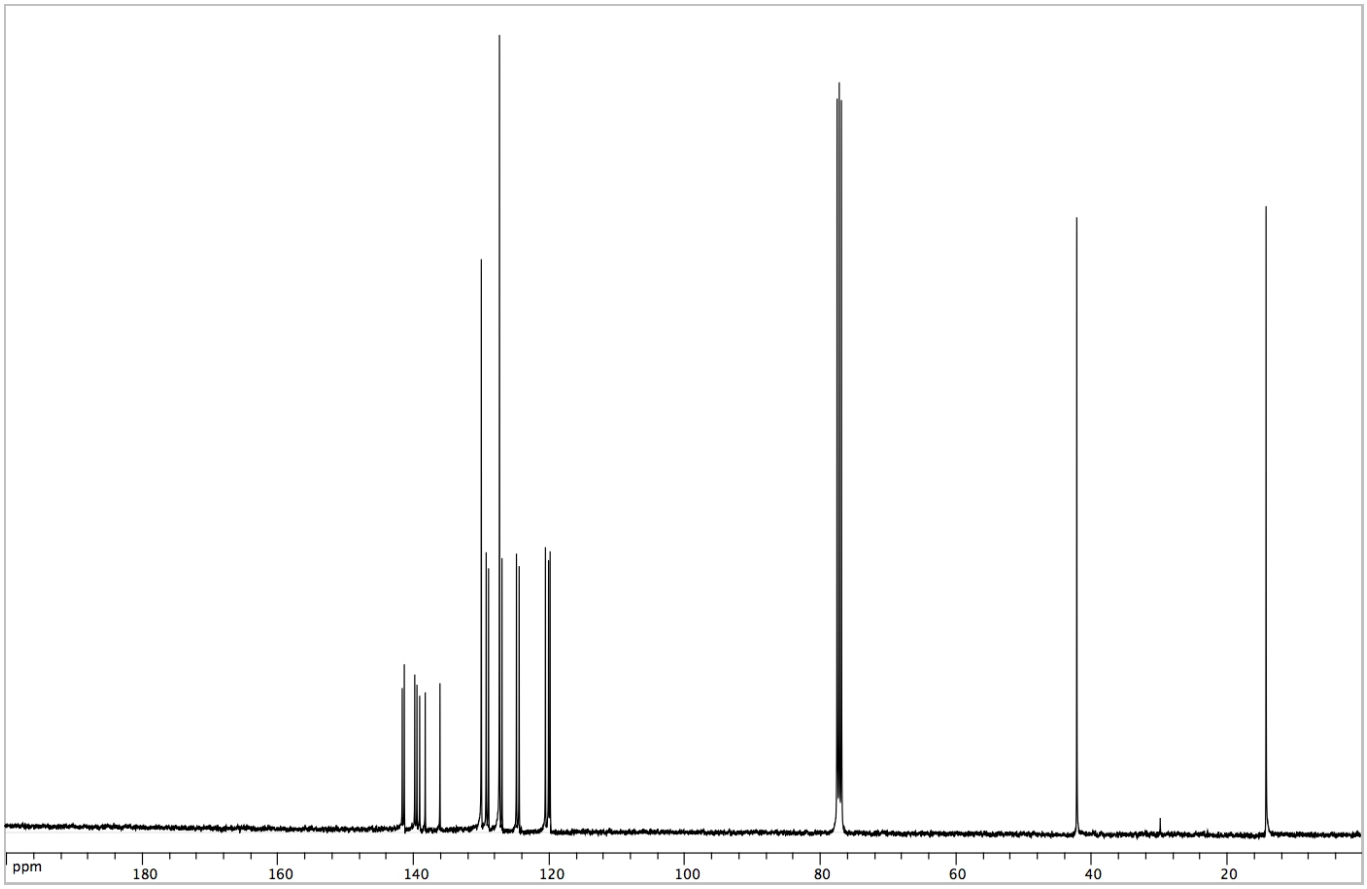

Figure S2. The 100 MHz ^{13}C NMR spectrum of **1**.

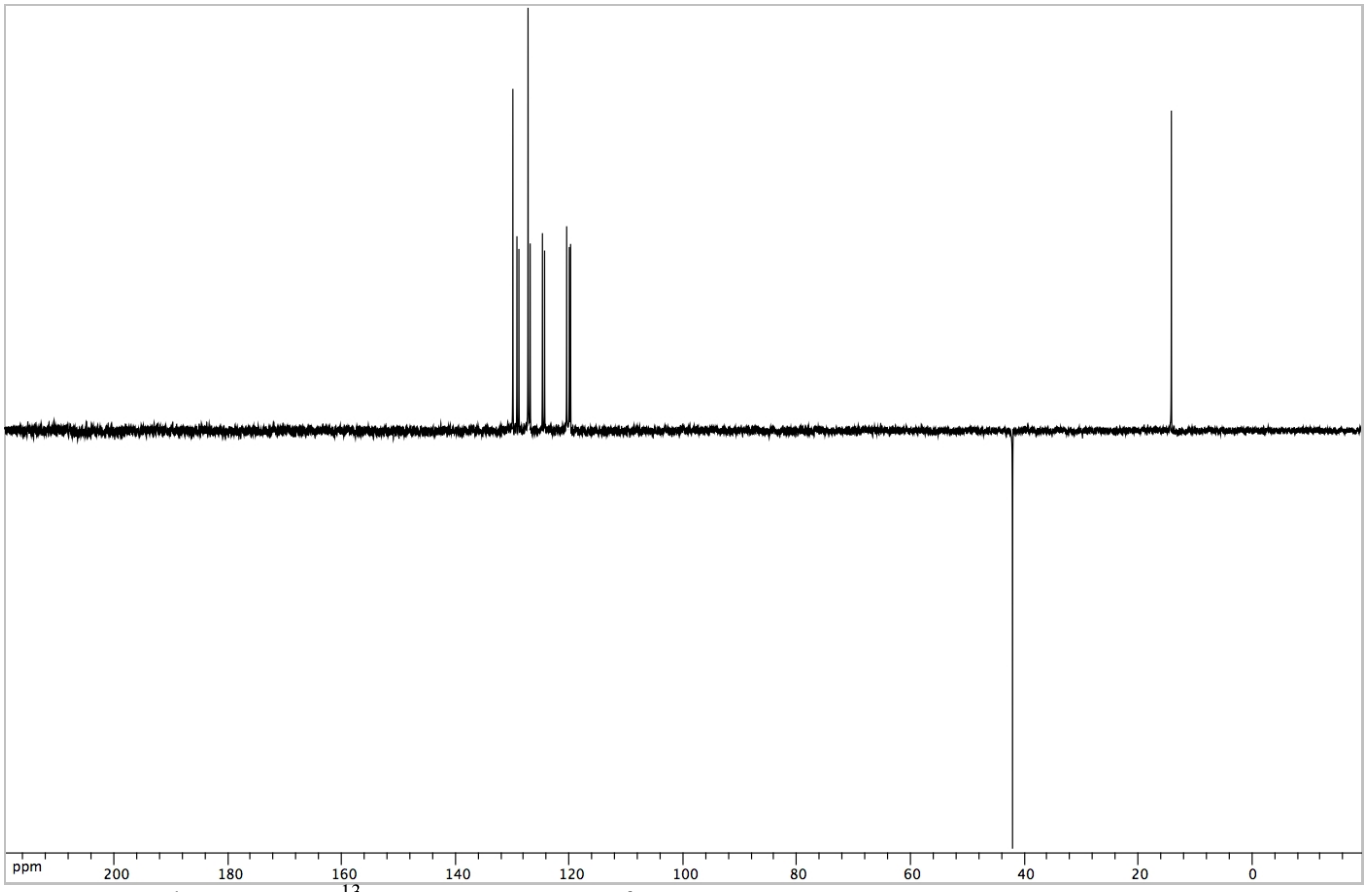

Figure S3. The 100 MHz ^{13}C DEPT spectrum of **1**.

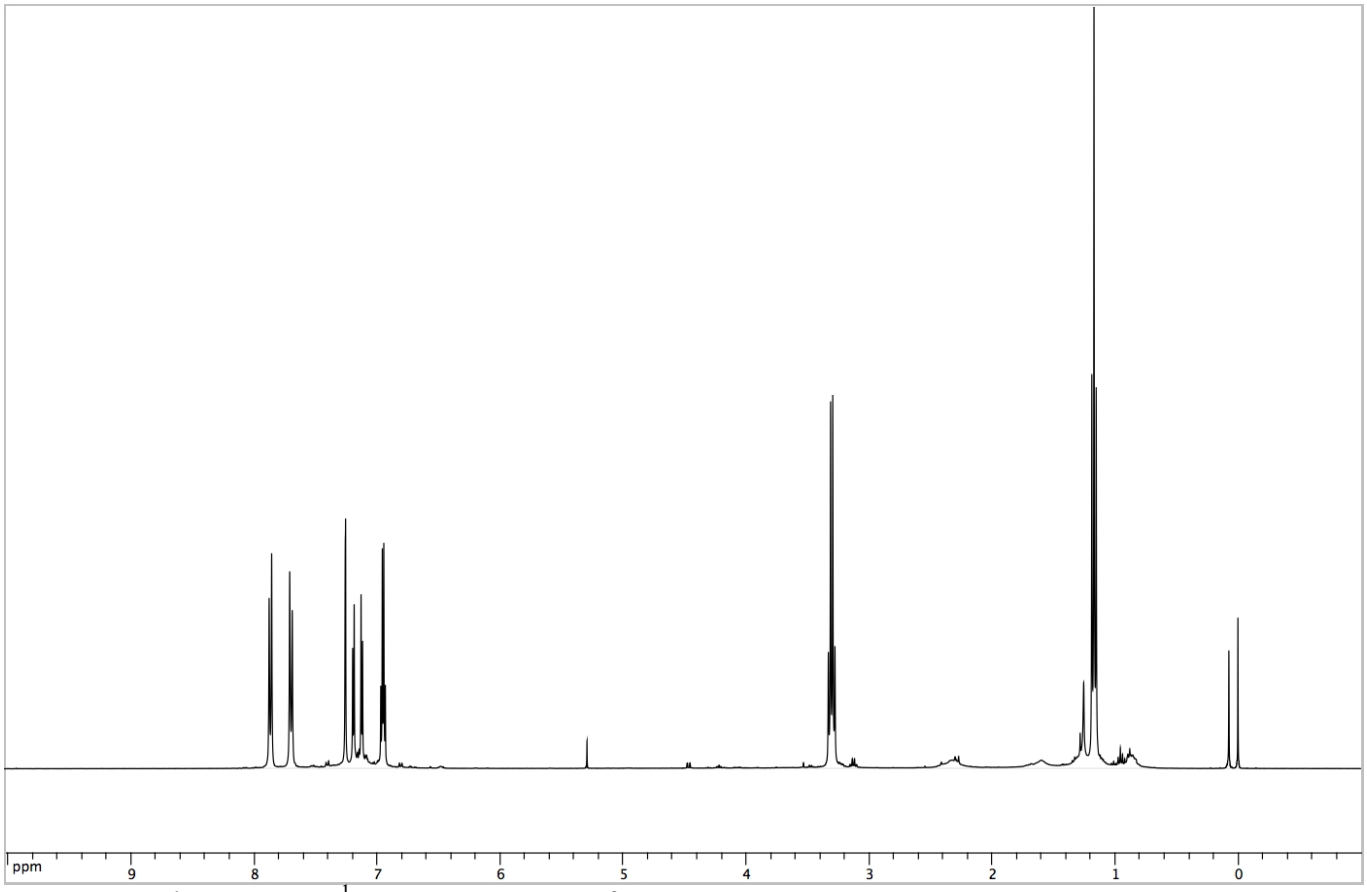

Figure S4. The 400 MHz ^{1}H NMR spectrum of **2**.

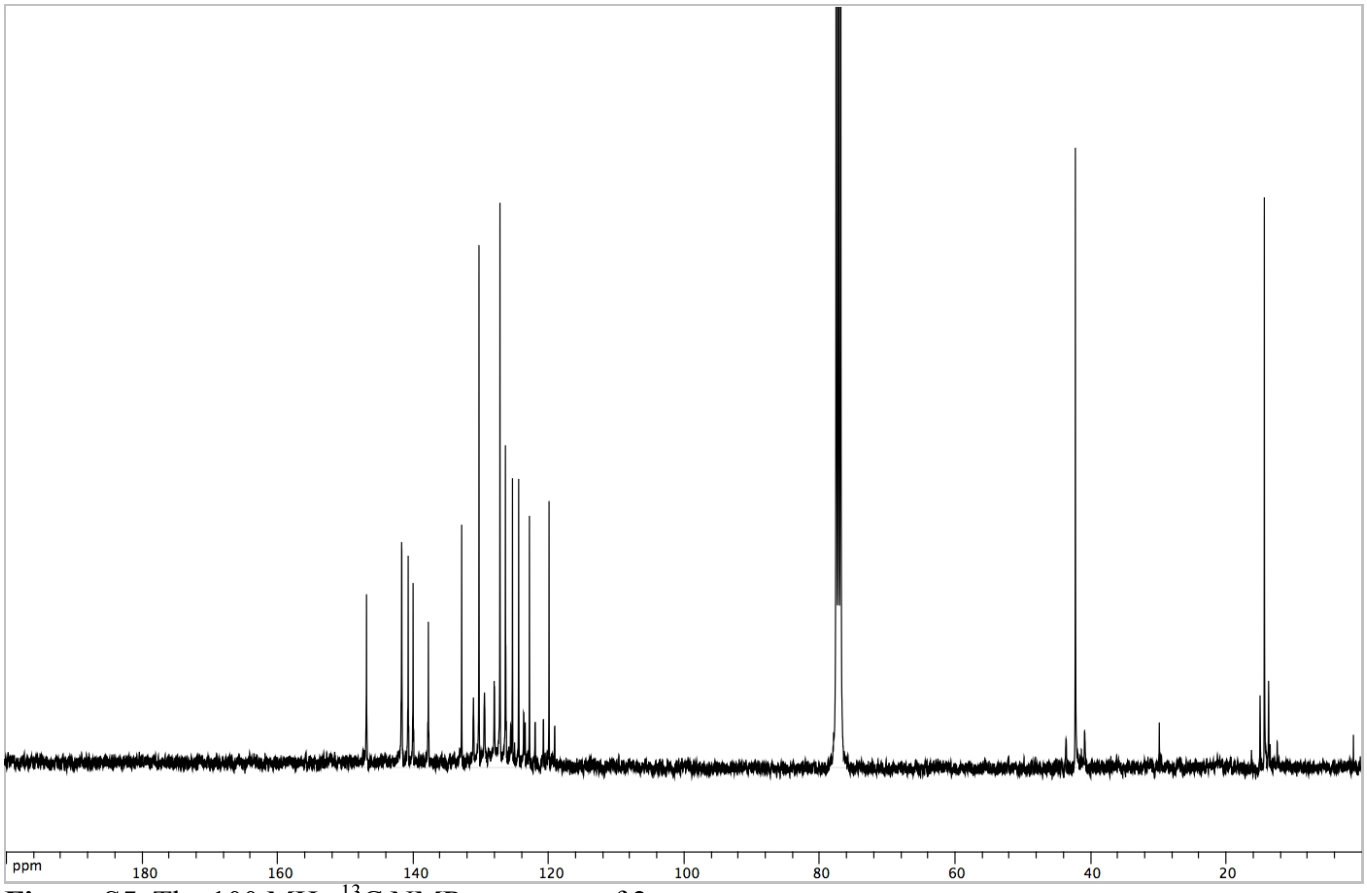

Figure S5. The 100 MHz ^{13}C NMR spectrum of **2**.

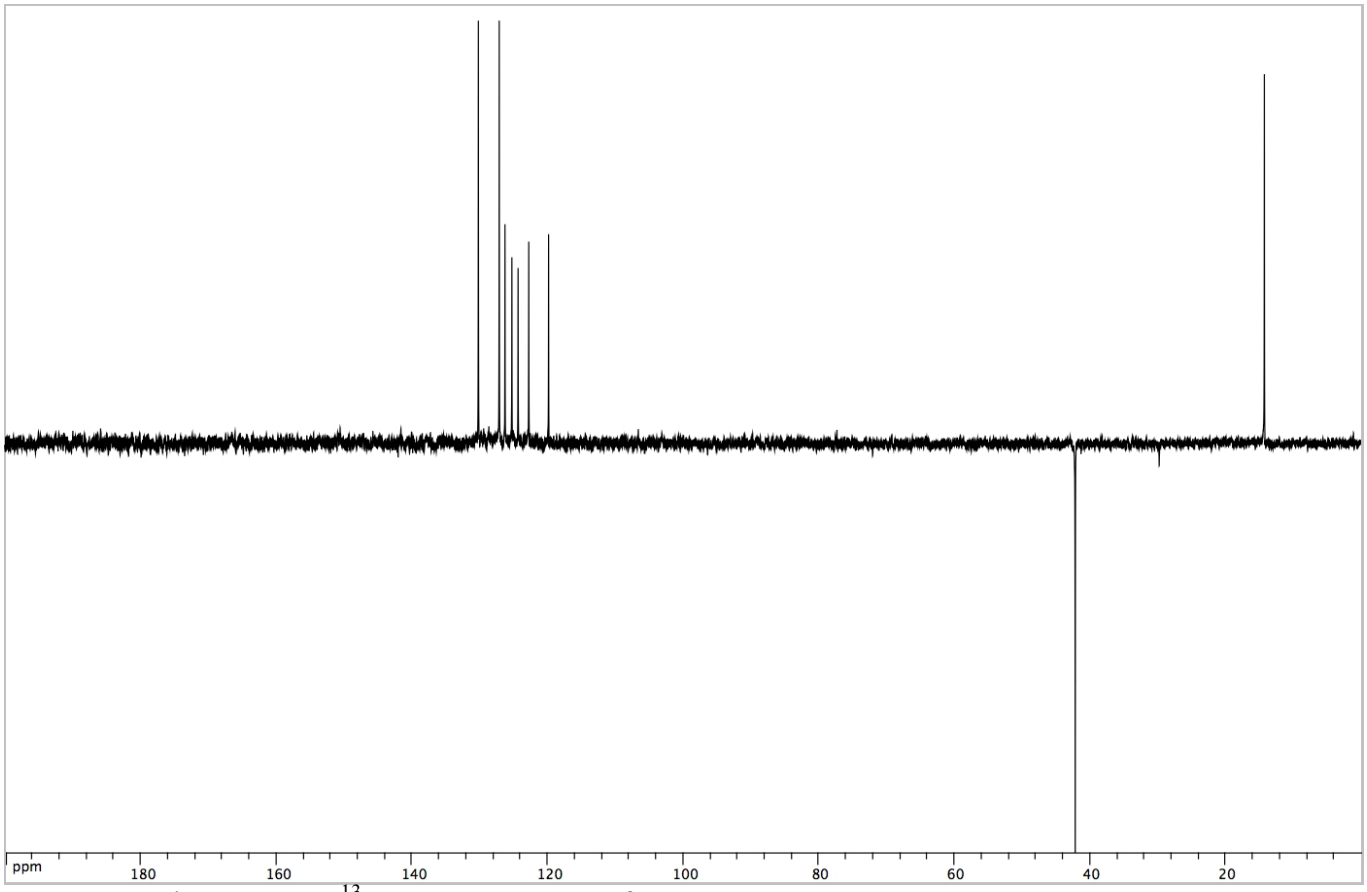

Figure S6. The 100 MHz ^{13}C DEPT spectrum of **2**.

1' neutral rb3lyp/6-31g(d) Energy = -1.453106540464423E+03 au

C	-4.72514282	-0.21930961	0.11437942
C	-3.71100262	-1.19086714	-0.03790421
C	-2.39416315	-0.51116543	-0.13377514
C	-2.69586298	0.94328154	-0.08193395
C	-4.09691719	1.10632500	0.07525864
C	-1.23046076	-1.19261859	-0.27045392
C	0.16347620	-0.72886616	-0.23607069
H	-1.32496860	-2.26736736	-0.42597825
C	2.86631649	0.00393015	-0.15213180
C	1.10146463	-1.31516752	-1.11112989
C	0.62537795	0.21218416	0.70132294
C	1.96787615	0.58353166	0.74387348
C	2.44023055	-0.94522620	-1.08586123
H	0.76451098	-2.05879781	-1.82856657
H	-0.07096663	0.63885100	1.41562041
H	2.32578711	1.31040481	1.46525627
H	3.15150340	-1.38707016	-1.77561801
S	4.58122734	0.53210872	-0.14557803
O	4.98784416	0.84285705	-1.52003190
O	4.72906060	1.53848898	0.91701460
N	5.37462127	-0.92199747	0.26359875
C	6.75385695	-1.01372658	-0.23808023
C	5.23800471	-1.28671695	1.67846944

H	6.77836230	-0.71838646	-1.28684125
H	7.06682513	-2.05912040	-0.15300588
H	4.18538725	-1.25454789	1.97111848
H	5.81272606	-0.62757871	2.34353588
C	-6.05862605	-0.59838288	0.25607211
C	-4.03696049	-2.54619774	-0.04418342
C	-1.88914984	2.07322411	-0.23762342
C	-4.67025209	2.37474368	0.12683619
H	-3.26976234	-3.30896015	-0.15129107
C	-6.37815608	-1.95876996	0.24069719
H	-6.84051364	0.14707429	0.37596535
H	-7.41367615	-2.27016431	0.34794138
C	-5.37591009	-2.92412299	0.09047806
H	-5.63996683	-3.97802821	0.08103316
C	-2.47053906	3.34389436	-0.19303322
H	-0.82224993	1.98232603	-0.40356212
C	-3.84703027	3.49612655	-0.00024142
H	-5.74359752	2.49330114	0.25058571
H	-4.28083827	4.49171461	0.03756411
H	-1.84168374	4.22175906	-0.31241738
H	7.45548338	-0.38684571	0.33207426
H	5.59183250	-2.31570988	1.79499149

1’ radical-cation ub3lyp/6-31g(d) Energy = -1.452845681334502E+03 au

C	-4.65907171	-0.25372882	0.27667831
C	-3.63791698	-1.18428169	-0.05710162
C	-2.39975319	-0.45434247	-0.30599821
C	-2.71431336	0.97296247	-0.19714240
C	-4.08461894	1.09884345	0.16835960
C	-1.20482411	-1.11047066	-0.62086136
C	0.15605790	-0.69045906	-0.52055976
H	-1.32947529	-2.12852804	-0.98716825
C	2.87303058	-0.01902632	-0.36153668
C	1.13545252	-1.41705357	-1.25812649
C	0.59834813	0.35598244	0.33816988
C	1.93911671	0.68494503	0.41637221
C	2.47161366	-1.06994609	-1.20314593
H	0.81495913	-2.22924395	-1.90454181
H	-0.11772566	0.87466733	0.96452537
H	2.27653765	1.49141641	1.05823443
H	3.20597111	-1.58384928	-1.81367006
S	4.61667315	0.44174409	-0.28575396
O	5.18919546	0.07347763	-1.57799482
O	4.65005513	1.80103141	0.24937074
N	5.22395273	-0.60380932	0.87257518
C	6.07228454	-1.72830320	0.46190773
C	5.41270087	-0.12107456	2.24485056
H	5.87299787	-1.99449288	-0.57506492
H	5.85583607	-2.58433704	1.10900230

H	4.72163350	0.69253408	2.46174130
H	6.43670764	0.24364287	2.39497168
C	-5.92725256	-0.69466060	0.60846459
C	-3.89653345	-2.56216776	-0.04813352
C	-1.96532691	2.11802988	-0.50078929
C	-4.66690632	2.34590112	0.30671694
H	-3.12380361	-3.28591722	-0.29055065
C	-6.18180100	-2.08095706	0.60276944
H	-6.71895432	0.00121198	0.86922911
H	-7.17474961	-2.43847173	0.85829671
C	-5.18110163	-3.00222761	0.27713607
H	-5.40375836	-4.06413811	0.27978719
C	-2.55971376	3.37776777	-0.36291915
H	-0.94570314	2.04619250	-0.86181712
C	-3.88731062	3.49177777	0.04931500
H	-5.70906929	2.45181219	0.59284900
H	-4.33638061	4.47493948	0.15249820
H	-1.98498465	4.26943154	-0.59118554
H	7.13446176	-1.46850005	0.55598051
H	5.22409330	-0.95074535	2.93335687

2’ neutral rb3lyp/6-31g(d) Energy = -2.094598964840660E+03 au

S	-6.10632418	-0.82965269	0.37035396
C	-4.50629883	-0.21999219	0.15573031
C	-3.56837271	-1.23654588	0.04061427
C	-4.14825277	-2.53265882	0.13229153
C	-5.50686420	-2.47472755	0.30498472
C	-2.22043562	-0.64054918	-0.10434959
H	-3.60293940	-3.46856009	0.07158013
H	-6.20541151	-3.29536748	0.39556565
S	-4.23199191	2.72056713	0.00255421
C	-2.55310747	3.14025114	-0.26008440
C	-1.73567754	2.04168843	-0.29443466
C	-2.45437812	0.82508475	-0.09443670
C	-3.82208286	1.04771641	0.06509176
H	-2.27681531	4.18027939	-0.36711419
H	-0.66938586	2.11683128	-0.46626196
C	-1.09413706	-1.38208709	-0.24500036
C	0.30801757	-0.95690016	-0.28775473
H	-1.23962752	-2.45689728	-0.35187123
C	3.01663031	-0.25258664	-0.37599659
C	1.21445999	-1.67202661	-1.09236685
C	0.80372661	0.10200326	0.50005261
C	2.14600837	0.45933091	0.45450711
C	2.55977954	-1.31779792	-1.15238801
H	0.85267834	-2.50414769	-1.69068236
H	0.13176337	0.62425899	1.17228623
H	2.52253399	1.27339686	1.06496453
H	3.25500388	-1.85188743	-1.79112354

S	4.73579210	0.24977658	-0.49315861
O	5.39048558	-0.64321178	-1.46128248
O	4.79135448	1.70430566	-0.67208415
N	5.27859079	-0.05134871	1.09554710
C	5.46954821	-1.47582933	1.39245513
C	6.40683997	0.79419858	1.51392487
H	4.57404824	-2.03754147	1.11449998
H	5.61138962	-1.57657113	2.47284697
H	6.49462365	0.71223778	2.60182290
H	6.20004544	1.83113809	1.25005611
H	7.35924641	0.48621738	1.05761242
H	6.33595398	-1.90518627	0.87088641

2’ radical-cation ub3lyp/6-31g(d) Energy = -2.094351714764352E+03 au

S	-6.13755194	-0.80111257	0.33289792
C	-4.51996626	-0.19557696	0.16065429
C	-3.54584708	-1.24764500	0.07584673
C	-4.13335017	-2.51712166	0.15534733
C	-5.51099512	-2.43090473	0.29196913
C	-2.20563657	-0.66835129	-0.05747278
H	-3.60937982	-3.46501737	0.11980623
H	-6.20610685	-3.25797886	0.37557595
S	-4.26701546	2.70852001	-0.03007096
C	-2.58351859	3.08294714	-0.27985106
C	-1.74038295	1.97961700	-0.28718714
C	-2.44432614	0.78495298	-0.08111748
C	-3.85956738	1.02414495	0.05719011
H	-2.29200537	4.11781465	-0.41481356
H	-0.67395493	2.06746614	-0.44755187
C	-1.06893623	-1.41160293	-0.19903603
C	0.32291071	-0.99380814	-0.22123243
H	-1.22380408	-2.48222047	-0.33176708
C	3.01593434	-0.26682588	-0.33759879
C	1.23184313	-1.73253234	-1.00524103
C	0.80684142	0.08985168	0.54545706
C	2.14568130	0.45045715	0.49093000
C	2.56954580	-1.35516059	-1.08690959
H	0.87819465	-2.58502132	-1.57882553
H	0.13894498	0.61153642	1.22304077
H	2.52232116	1.27671578	1.08441630
H	3.26626788	-1.88793702	-1.72525167
S	4.73154464	0.28467575	-0.50003761
O	5.33544671	-0.54819111	-1.54521729

O	4.69563164	1.74433672	-0.61113344
N	5.34294658	-0.08103763	1.03335743
C	5.70306879	-1.49520211	1.21794304
C	6.34781660	0.86758296	1.54910252
H	4.87831195	-2.13861894	0.90085462
H	5.86829883	-1.65765596	2.28654515
H	6.43282580	0.69844096	2.62628551
H	6.01200305	1.88883863	1.37262107
H	7.33361381	0.72478403	1.08634562
H	6.60688696	-1.77531257	0.66262928

3 neutral rb3lyp/6-31g(d) Energy = -7.239930305131547E+02 au

C	-0.73462841	-1.51033581	-0.00003499
C	-1.18536293	-0.16661933	0.00006019
C	-0.00003265	0.71946603	0.00000673
C	1.18538645	-0.16644488	0.00001531
C	0.73484607	-1.51022520	-0.00000402
C	-0.00017877	2.09414000	-0.00001122
C	-1.63700399	-2.56534432	-0.00015562
C	-2.55460825	0.10980645	0.00007996
C	2.55460312	0.11018879	0.00008575
C	1.63739796	-2.56509147	0.00006160
H	-2.92990815	1.12527262	0.00017344
C	-3.00827002	-2.27944762	-0.00016804
H	-1.29108055	-3.59527986	-0.00022731
H	-3.72650056	-3.09462136	-0.00026158
C	-3.45925711	-0.95829505	-0.00005031
H	-4.52509215	-0.75077737	-0.00005872
C	3.45940907	-0.95776419	0.00013704
H	2.92979473	1.12569945	0.00004840
C	3.00861244	-2.27899416	0.00012800
H	1.29164241	-3.59508544	0.00004362
H	3.72696133	-3.09406300	0.00018299
H	4.52521734	-0.75011082	0.00018274
C	1.19613018	2.87915395	-0.00024180
N	2.15113442	3.54512435	-0.00038860
C	-1.19663242	2.87893211	0.00007592
N	-2.15163423	3.54490624	0.00038994

3 radical-cation ub3lyp/6-31g(d) Energy = -7.236988734029403E+02 au

C	-0.70581001	-1.50425505	0.00010270
C	-1.17781837	-0.13759973	0.00016343
C	-0.00242601	0.75668649	0.00012694
C	1.17912527	-0.12934963	-0.00009146
C	0.71665129	-1.49926911	-0.00017120
C	-0.00774477	2.12728759	0.00011783
C	-1.60727291	-2.59352896	0.00001293
C	-2.54075432	0.11279827	-0.00007980
C	2.54035089	0.13065144	0.00024101
C	1.62578971	-2.58216892	-0.00017492
H	-2.94420651	1.11725186	-0.00004793
C	-2.96284651	-2.32369986	-0.00019831
H	-1.24251777	-3.61556190	0.00011207
H	-3.68336766	-3.13495134	-0.00031980
C	-3.42308450	-0.98510130	-0.00026161
H	-4.49226933	-0.79507055	-0.00046882
C	3.43030073	-0.96096697	0.00040975
H	2.93676027	1.13788963	0.00037247
C	2.97939574	-2.30278953	0.00014717
H	1.26832498	-3.60677333	-0.00045430
H	3.70560109	-3.10896282	0.00023552
H	4.49815445	-0.76359821	0.00073365
C	1.19409412	2.90224922	-0.00056259
N	2.17181936	3.53282358	-0.00075458
C	-1.21555342	2.89293702	0.00027346
N	-2.19765665	3.51667511	0.00068391

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1' neutral rb3lyp/6-31g(d) Charges

		Charges			Charges (H-included)		
		ChelpG	MKS	NPA	ChelpG	MKS	NPA
C	1	-0,0861	-0,1240	-0,2254	0,0057	-0,0022	0,0128
C	2	-0,0754	-0,1193	-0,2348	0,0084	0,0004	0,0033
C	3	-0,1484	-0,1922	-0,2086	-0,0347	-0,0537	0,0240
C	4	0,0226	0,1277	-0,0355	0,0226	0,1277	-0,0355
C	5	0,0682	0,0006	-0,0355	0,0682	0,0006	-0,0355
C	6	-0,1573	-0,1586	-0,2140	-0,0463	-0,0287	0,0228
C	7	0,0005	-0,1311	-0,0186	0,0005	-0,1311	-0,0186
C	8	0,0833	0,1471	-0,0514	0,0833	0,1471	-0,0514
C	9	-0,0211	0,0383	-0,0293	-0,0211	0,0383	-0,0293
C	10	-0,1069	-0,1869	-0,2168	-0,0113	-0,0550	0,0201
C	11	-0,1027	-0,0979	-0,2205	-0,0080	0,0203	0,0181
C	12	-0,0894	-0,1429	-0,2363	0,0059	-0,0176	0,0039
C	13	-0,1003	-0,1736	-0,2046	-0,0376	-0,0411	0,0396
C	14	-0,2047	-0,1656	-0,1758	-0,1101	-0,0592	0,0580
C	15	0,2384	0,1636	-0,0526	0,2384	0,1636	-0,0526
C	16	-0,1530	-0,1537	-0,2197	-0,0731	-0,0346	0,0346
C	17	0,0091	-0,0535	-0,2127	0,1086	0,0668	0,0580
C	18	-0,0600	-0,0212	-0,3338	-0,0600	-0,0212	-0,3338
C	19	-0,0564	-0,1508	-0,1988	0,0500	-0,0081	0,0632
C	20	-0,2061	-0,1489	-0,2081	-0,0794	-0,0141	0,0362
S	21	0,8666	0,7871	2,3430	0,8666	0,7871	2,3430
N	22	-0,3399	-0,2165	-0,7271	-0,3399	-0,2165	-0,7271
C	23	-0,0653	-0,2948	-0,4840	0,1713	0,1203	0,2240
C	24	-0,0442	-0,3006	-0,4849	0,1373	0,0945	0,2142
O	25	-0,4763	-0,4402	-0,9405	-0,4763	-0,4402	-0,9405
O	26	-0,4692	-0,4435	-0,9512	-0,4692	-0,4435	-0,9512

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1' radical-cation ub3lyp/6-31g(d) Charges

		Charges			Charges (H-included)		
		ChelpG	MKS	NPA	ChelpG	MKS	NPA
C	1	0,0233	-0,0213	-0,0253	0,1284	0,1165	0,1036
C	2	-0,1047	-0,1309	-0,1356	0,0162	0,0165	-0,0040
C	3	-0,0739	-0,0969	-0,0355	0,0444	0,0421	0,0867
C	4	-0,0051	0,0040	-0,0297	-0,0051	0,0040	-0,0297
C	5	0,0839	0,0887	0,0106	0,0839	0,0887	0,0106
C	6	-0,1541	-0,1737	-0,0957	-0,0174	-0,0144	0,0330
C	7	0,1225	0,1344	0,0987	0,1225	0,1344	0,0987
C	8	0,0001	0,0220	-0,0421	0,0001	0,0220	-0,0421
C	9	0,0040	-0,0048	-0,0040	0,0040	-0,0048	-0,0040
C	10	-0,0967	-0,1179	-0,0812	0,0247	0,0251	0,0471
C	11	-0,0004	-0,0254	-0,0443	0,1103	0,1111	0,0852
C	12	-0,1401	-0,1507	-0,1302	-0,0090	0,0008	0,0012
C	13	0,0089	-0,0877	-0,0382	0,0787	0,0528	0,0871
C	14	-0,1566	-0,2111	0,0615	-0,0331	-0,0604	0,1867
C	15	0,2086	0,2187	-0,0307	0,2086	0,2187	-0,0307
C	16	-0,0490	-0,1031	-0,0405	0,0144	0,0189	0,0888
C	17	-0,0786	-0,1246	-0,1305	0,0740	0,0424	0,0109
C	18	-0,0416	-0,0147	-0,0564	-0,0416	-0,0147	-0,0564
C	19	-0,0424	-0,1160	-0,1262	0,0970	0,0557	0,0148
C	20	-0,1601	-0,1504	-0,0372	-0,0195	0,0064	0,0906
S	21	0,9262	0,8938	1,1823	0,9262	0,8938	1,1823
N	22	-0,2787	-0,1338	-0,3133	-0,2787	-0,1338	-0,3133
C	23	-0,0966	-0,3192	-0,2403	0,1888	0,1301	0,1337
C	24	-0,0697	-0,3140	-0,2401	0,1866	0,1286	0,1322
O	25	-0,4513	-0,4378	-0,4558	-0,4513	-0,4378	-0,4558
O	26	-0,4530	-0,4428	-0,4572	-0,4530	-0,4428	-0,4572

Supplementary Material (ESI) for New Journal of Chemistry

1' radical-cation ub3lyp/6-31g(d) Spin Density

		Spin Density		Spin Density (H included)	
		Mulliken	NPA (β - α)	Mulliken	NPA (β - α)
C	1	0,1171	0,1038	0,1118	0,1007
C	2	-0,0519	-0,0383	-0,0502	-0,0373
C	3	0,0981	0,0859	0,0940	0,0832
C	4	-0,0155	-0,0020	-0,0155	-0,0020
C	5	0,0368	0,0340	0,0368	0,0340
C	6	-0,0017	0,0015	-0,0018	0,0015
C	7	0,1357	0,1248	0,1357	0,1248
C	8	-0,0173	-0,0079	-0,0173	-0,0079
C	9	0,0046	0,0091	0,0046	0,0091
C	10	0,0264	0,0245	0,0254	0,0238
C	11	0,0813	0,0731	0,0775	0,0709
C	12	-0,0372	-0,0265	-0,0361	-0,0258
C	13	0,0942	0,0826	0,0901	0,0800
C	14	0,2218	0,2095	0,2147	0,2068
C	15	-0,0008	0,0115	-0,0008	0,0115
C	16	0,1031	0,0927	0,0982	0,0897
C	17	-0,0593	-0,0432	-0,0572	-0,0419
C	18	0,1595	0,1389	0,1595	0,1389
C	19	-0,0545	-0,0399	-0,0526	-0,0388
C	20	0,0931	0,0838	0,0889	0,0811
S	21	-0,0166	-0,0096	-0,0166	-0,0096
N	22	0,0833	0,0801	0,0833	0,0801
C	23	-0,0033	-0,0014	0,0052	0,0058
C	24	-0,0034	-0,0016	0,0047	0,0054
O	25	0,0086	0,0079	0,0086	0,0079
O	26	0,0089	0,0081	0,0089	0,0081

Supplementary Material (ESI) for New Journal of Chemistry

2' neutral rb3lyp/6-31g(d) Charges

		Charges			Charges (H-included)		
		ChelpG	MKS	NPA	ChelpG	MKS	NPA
C	1	0.0993	0.0423	-0.2418	0.0993	0.0423	-0.2418
C	2	-0.1455	-0.0448	-0.0788	-0.1455	-0.0448	-0.0788
C	3	-0.0381	-0.1455	-0.2563	0.0607	0.0038	-0.0074
C	4	-0.2657	-0.3025	-0.4350	-0.0727	-0.0750	-0.1767
S	5	0.0045	0.0367	0.4855	0.0045	0.0367	0.4855
C	6	0.0200	0.0239	-0.2342	0.0200	0.0239	-0.2342
C	7	-0.0662	-0.0814	-0.0967	-0.0662	-0.0814	-0.0967
C	8	0.1558	0.1244	-0.0147	0.1558	0.1244	-0.0147
S	9	0.0189	0.0477	0.4893	0.0189	0.0477	0.4893
C	10	-0.2626	-0.3167	-0.4366	-0.0657	-0.0910	-0.1769
C	11	-0.0603	-0.0934	-0.2558	0.0390	0.0549	0.0006
C	12	-0.2603	-0.2589	-0.1625	-0.1281	-0.1121	0.0750
C	13	0.2538	0.1760	-0.0555	0.2538	0.1760	-0.0555
C	14	-0.1084	-0.1224	-0.2176	-0.0303	-0.0012	0.0357
C	15	-0.0847	-0.1108	-0.1993	0.0297	0.0179	0.0637
C	16	-0.0674	-0.0826	-0.3310	-0.0674	-0.0826	-0.3310
C	17	0.0432	-0.0320	-0.2123	0.1354	0.0931	0.0587
C	18	-0.2689	-0.1949	-0.2044	-0.1364	-0.0606	0.0400
S	19	0.8700	0.8477	2.3433	0.8700	0.8477	2.3433
N	20	-0.3445	-0.2376	-0.7271	-0.3445	-0.2376	-0.7271
C	21	-0.0560	-0.2633	-0.4849	0.1378	0.1051	0.2146
C	22	-0.0195	-0.2769	-0.4841	0.1801	0.1239	0.2248
O	23	-0.4719	-0.4575	-0.9504	-0.4719	-0.4575	-0.9504
O	24	-0.4764	-0.4537	-0.9402	-0.4764	-0.4537	-0.9402

Supplementary Material (ESI) for New Journal of Chemistry

2' radical-cation ub3lyp/6-31g(d) Charges

		Charges			Charges (H-included)		
		ChelpG	MKS	NPA	ChelpG	MKS	NPA
C	1	0.0816	0.0476	-0.2035	0.0816	0.0476	-0.2035
C	2	0.0204	0.0943	0.0411	0.0204	0.0943	0.0411
C	3	-0.0760	-0.1665	-0.2607	0.0651	0.0214	0.0195
C	4	-0.1325	-0.1676	-0.3053	0.0869	0.0823	-0.0181
S	5	0.1257	0.1539	0.5593	0.1257	0.1539	0.5593
C	6	0.0110	-0.0118	-0.2020	0.0110	-0.0118	-0.2020
C	7	0.0833	0.0858	0.0279	0.0833	0.0858	0.0279
C	8	0.0118	-0.0134	-0.1023	0.0118	-0.0134	-0.1023
S	9	0.1342	0.1718	0.5641	0.1342	0.1718	0.5641
C	10	-0.1414	-0.1890	-0.3074	0.0841	0.0617	-0.0196
C	11	-0.0581	-0.1057	-0.2557	0.0590	0.0670	0.0302
C	12	-0.1213	-0.1347	-0.0620	0.0216	0.0226	0.1899
C	13	0.0994	0.0733	-0.0988	0.0994	0.0733	-0.0988
C	14	0.0001	-0.0342	-0.2114	0.0577	0.0720	0.0369
C	15	-0.1443	-0.1782	-0.1976	-0.0036	-0.0228	0.0764
C	16	-0.0117	-0.0265	-0.2823	-0.0117	-0.0265	-0.2823
C	17	0.0004	-0.0514	-0.2112	0.1175	0.0926	0.0736
C	18	-0.1537	-0.1368	-0.1748	-0.0305	0.0054	0.0786
S	19	0.8901	0.8730	2.3513	0.8901	0.8730	2.3513
N	20	-0.3478	-0.1752	-0.7320	-0.3478	-0.1752	-0.7320
C	21	-0.0759	-0.3867	-0.4846	0.1606	0.0950	0.2296
C	22	-0.0252	-0.3793	-0.4836	0.2056	0.1223	0.2443
O	23	-0.4579	-0.4454	-0.9338	-0.4579	-0.4454	-0.9338
O	24	-0.4640	-0.4470	-0.9301	-0.4640	-0.4470	-0.9301

Supplementary Material (ESI) for New Journal of Chemistry

2' radical-cation ub3lyp/6-31g(d) Spin Density

		Spin Density		Spin Density (H included)	
		Mulliken	NPA (β - α)	Mulliken	NPA (β - α)
C	1	0.1142	0.1177	0.1142	0.1177
C	2	0.2294	0.2056	0.2294	0.2056
C	3	-0.0980	-0.0741	-0.0949	-0.0723
C	4	0.3342	0.3089	0.3182	0.2995
S	5	-0.0416	-0.0379	-0.0416	-0.0379
C	6	0.0985	0.1053	0.0985	0.1053
C	7	0.2332	0.2079	0.2332	0.2079
C	8	-0.0517	-0.0257	-0.0517	-0.0257
S	9	-0.0389	-0.0351	-0.0389	-0.0351
C	10	0.3426	0.3169	0.3262	0.3073
C	11	-0.0925	-0.0701	-0.0896	-0.0684
C	12	0.0037	0.0025	0.0032	0.0020
C	13	-0.0019	-0.0017	-0.0019	-0.0017
C	14	-0.0010	-0.0011	-0.0012	-0.0011
C	15	0.0008	0.0006	0.0008	0.0006
C	16	-0.0028	-0.0024	-0.0028	-0.0024
C	17	0.0010	0.0007	0.0009	0.0007
C	18	-0.0016	-0.0015	-0.0015	-0.0014
S	19	0.0002	0.0001	0.0002	0.0001
N	20	-0.0003	-0.0003	-0.0003	-0.0003
C	21	0.0000	0.0000	0.0000	0.0000
C	22	0.0000	0.0000	0.0000	0.0000
O	23	-0.0001	-0.0001	-0.0001	-0.0001
O	24	-0.0003	-0.0003	-0.0003	-0.0003

3 neutral rb3lyp/6-31g(d) Charges

		Charges			Charges (H-included)		
		ChelpG	MKS	NPA	ChelpG	MKS	NPA
C	1	-0.0783	-0.1106	-0.2009	0.0207	0.0156	0.0428
C	2	-0.0716	-0.0960	-0.2330	0.0270	0.0297	0.0136
C	3	-0.1398	-0.2128	-0.1802	-0.0068	-0.0499	0.0787
C	4	0.0492	0.2231	-0.0693	0.0492	0.2231	-0.0693
C	5	0.0198	-0.0084	-0.0183	0.0198	-0.0084	-0.0183
C	6	-0.1158	-0.1425	-0.2140	-0.0093	-0.0120	0.0277
C	7	0.0762	-0.1643	0.1026	0.0762	-0.1643	0.1026
C	8	0.0492	0.2123	-0.0693	0.0492	0.2123	-0.0693
C	9	0.0199	-0.0079	-0.0182	0.0199	-0.0079	-0.0182
C	10	-0.1157	-0.1433	-0.2140	-0.0092	-0.0118	0.0277
C	11	-0.0787	-0.1031	-0.2009	0.0204	0.0215	0.0428
C	12	-0.0710	-0.1061	-0.2330	0.0275	0.0205	0.0136
C	13	-0.1401	-0.2038	-0.1802	-0.0072	-0.0377	0.0788
C	14	-0.2387	-0.2336	-0.2416	-0.2387	-0.2336	-0.2416
C	15	0.4276	0.4393	0.2794	0.4276	0.4393	0.2794
N	16	-0.4470	-0.4391	-0.2852	-0.4470	-0.4391	-0.2852
C	17	0.4277	0.4410	0.2794	0.4277	0.4410	0.2794
N	18	-0.4471	-0.4382	-0.2852	-0.4471	-0.4382	-0.2852

3 radical-cation ub3lyp/6-31g(d) Charges

		Charges			Charges (H-included)		
		ChelpG	MKS	NPA	ChelpG	MKS	NPA
C	1	-0.0858	-0.1168	-0.1086	0.0540	0.0516	0.0307
C	2	0.1077	0.0790	0.0846	0.2259	0.2221	0.2185
C	3	-0.1815	-0.2173	-0.1268	-0.0253	-0.0411	0.0165

C	4	0.1605	0.2768	0.0731	0.1605	0.2768	0.0731
C	5	0.0461	0.0473	0.0719	0.0461	0.0473	0.0719
C	6	-0.0598	-0.1019	-0.0362	0.0779	0.0621	0.0966
C	7	-0.0447	-0.2359	0.0104	-0.0447	-0.2359	0.0104
C	8	0.1685	0.2845	0.0732	0.1685	0.2845	0.0732
C	9	0.0455	0.0336	0.0719	0.0455	0.0336	0.0719
C	10	-0.0590	-0.0951	-0.0363	0.0792	0.0686	0.0965
C	11	-0.0946	-0.1157	-0.1085	0.0476	0.0522	0.0308
C	12	0.1214	0.0752	0.0846	0.2369	0.2195	0.2185
C	13	-0.1986	-0.2221	-0.1268	-0.0379	-0.0417	0.0165
C	14	-0.1082	-0.1268	-0.0766	-0.1082	-0.1268	-0.0766
C	15	0.3956	0.4123	0.1263	0.3956	0.4123	0.1263
N	16	-0.3571	-0.3496	-0.1005	-0.3571	-0.3496	-0.1005
C	17	0.3906	0.4137	0.1263	0.3906	0.4137	0.1263
N	18	-0.3551	-0.3492	-0.1004	-0.3551	-0.3492	-0.1004

3 radical-cation ub3lyp/6-31g(d) Spin Density

		Spin Density		Spin Density (H included)	
		Mulliken	NPA (b - a)	Mulliken	NPA (b - a)
C	1	-0.0421	-0.0237	-0.0413	-0.0232
C	2	0.2931	0.2600	0.2803	0.2524
C	3	-0.0838	-0.0611	-0.0813	-0.0596
C	4	0.1557	0.1353	0.1557	0.1353
C	5	0.1158	0.1144	0.1158	0.1144
C	6	0.0909	0.0882	0.0862	0.0852
C	7	-0.0405	-0.0174	-0.0405	-0.0174
C	8	0.1559	0.1354	0.1559	0.1354
C	9	0.1157	0.1144	0.1157	0.1144
C	10	0.0908	0.0881	0.0861	0.0852
C	11	-0.0420	-0.0237	-0.0413	-0.0232
C	12	0.2930	0.2599	0.2803	0.2523
C	13	-0.0838	-0.0611	-0.0813	-0.0596
C	14	0.0084	0.0070	0.0084	0.0070
C	15	-0.0021	-0.0017	-0.0021	-0.0017
N	16	0.0026	0.0025	0.0026	0.0025
C	17	-0.0021	-0.0017	-0.0021	-0.0017
N	18	0.0026	0.0025	0.0026	0.0025