Electronic supplementary materials *Mendeleev Commun.*, 2009, **19**, 306–308

Fullerene C_{60} as an effective trap of acenaphthenone carbene generated in the reaction of acenaphthenequinone with hexaethyltriaminophosphine

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Table of contents

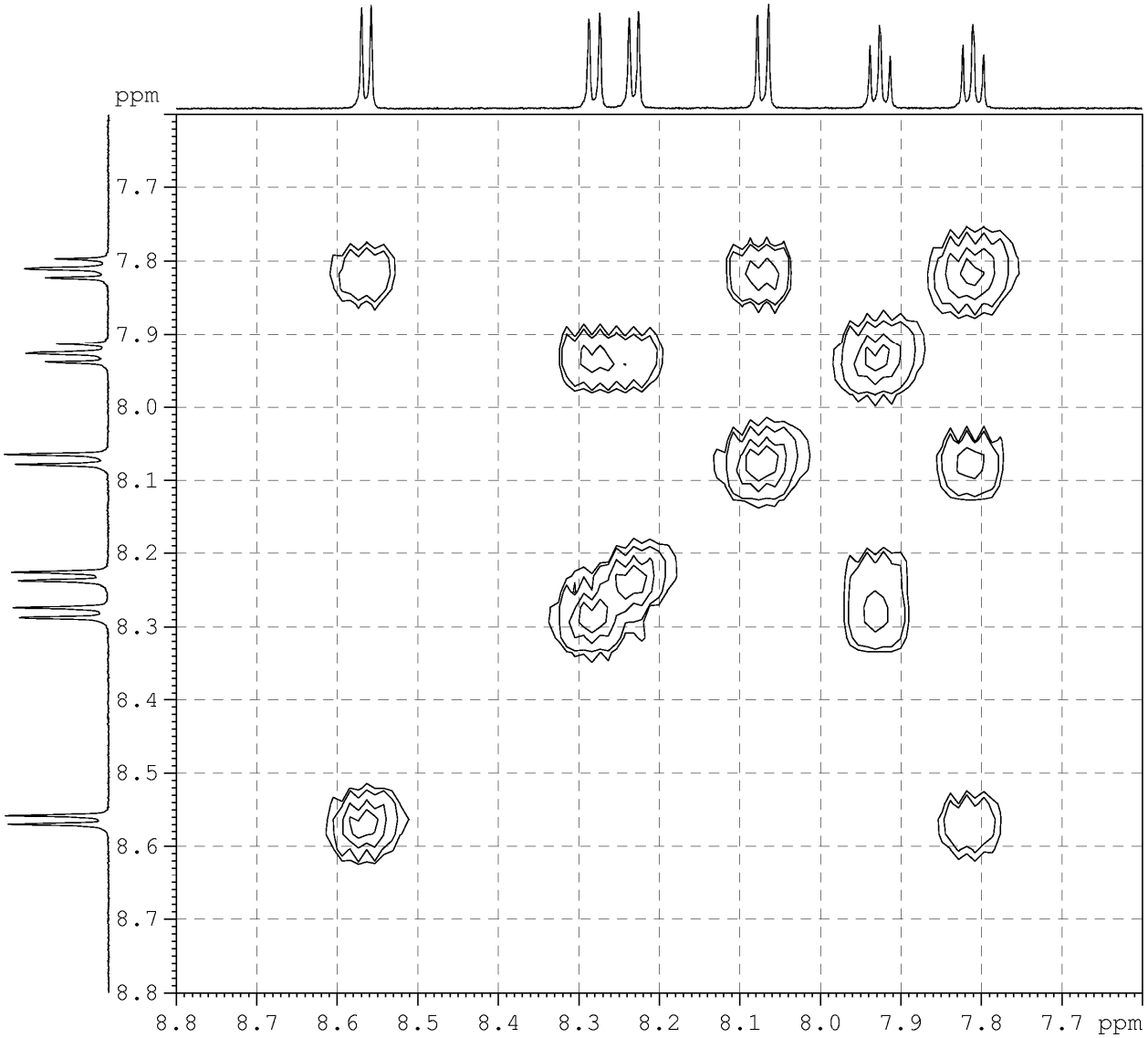

Figure 1 ^{1}H-^{1}H COSY spectrum of compound **5** (600.000 MHz in ^{1}H, 150.864 MHz in ^{13}C, *T* =303K, $CDCl_3$+CS_2).

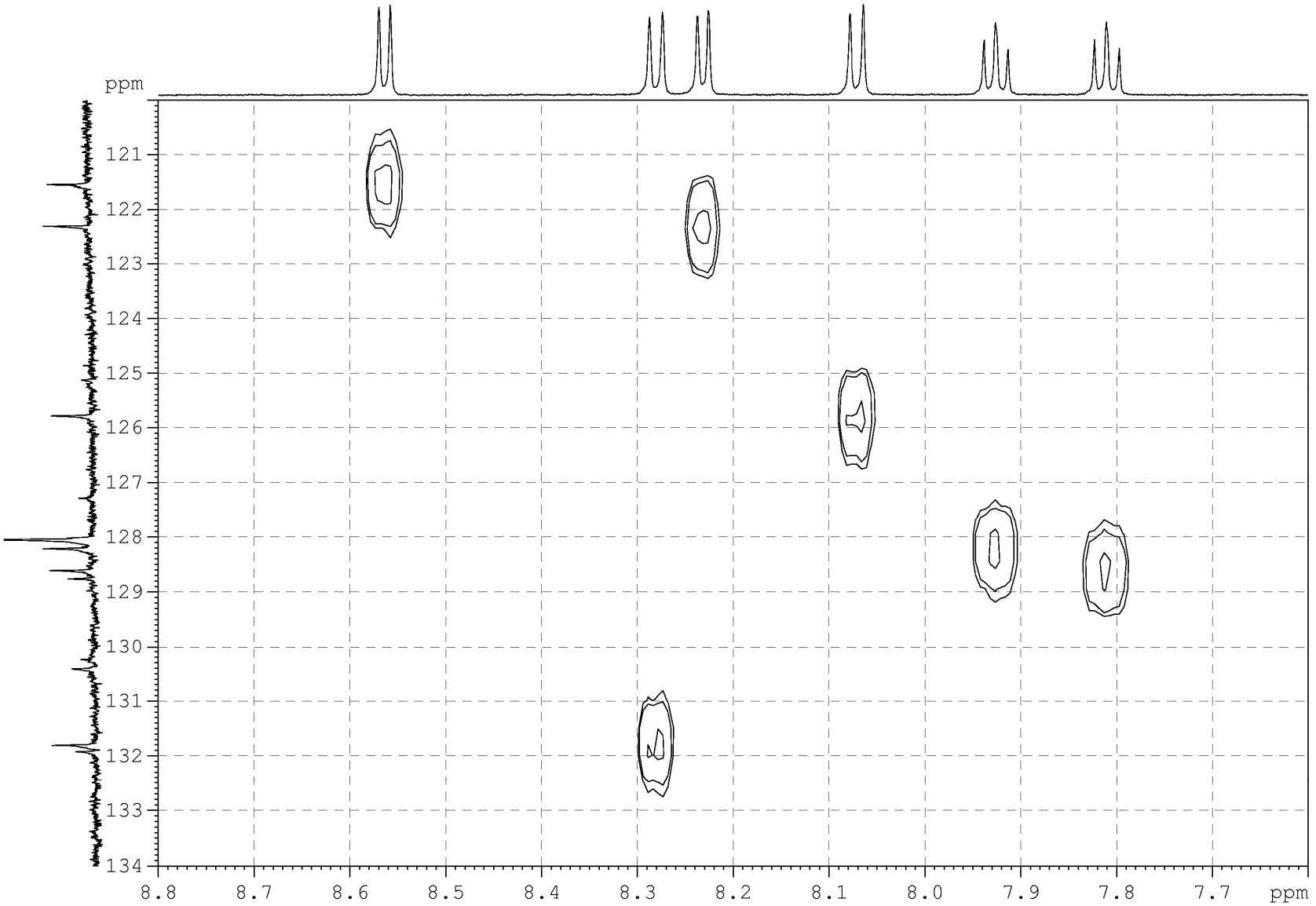

Figure 2 ^{1}H-^{13}C HSQC spectrum of compound **5** (600.000 MHz in ^{1}H, 150.864 MHz in ^{13}C, T = 303K, $CDCl_3$+CS_2).

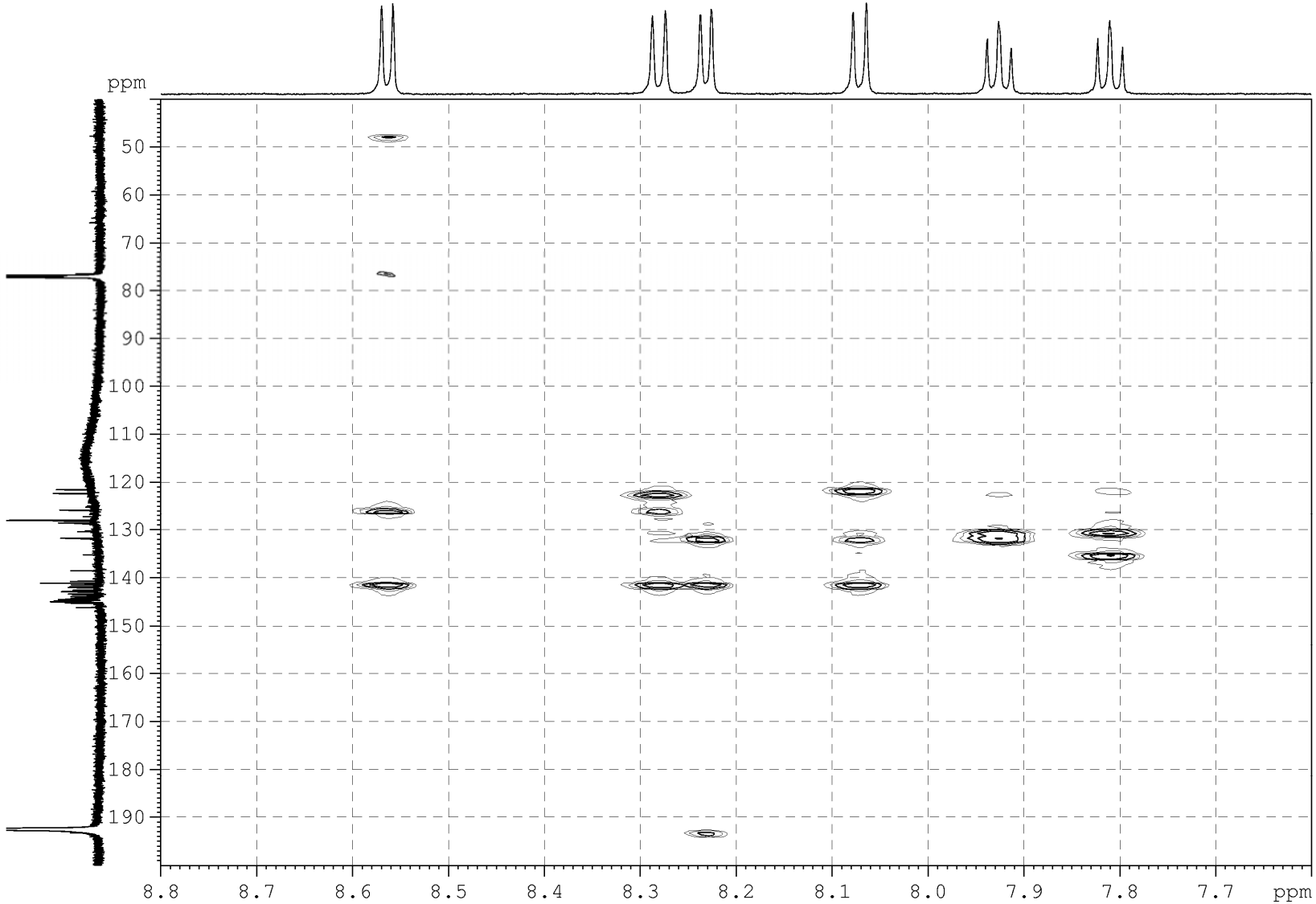

Figure 3 ^{1}H-^{13}C HMBC spectrum of compound **5** (600.000 MHz in ^{1}H, 150.864 MHz in ^{13}C, T = 303K, $CDCl_3$+CS_2).

Cartesian coordinates of the optimized geometry of **5a** in gas phase (RHF/6-31G)

C	2.953064	2.918320	-0.585510
C	2.228088	2.197678	-1.615051
C	2.824783	2.178146	0.655640
C	1.541367	2.893372	-2.585480
C	1.655716	1.010147	-1.025635
C	2.031494	0.997894	0.404663
C	2.706741	2.855209	1.849380
C	0.234726	2.440002	-2.989838
C	0.433762	0.557571	-1.431396
C	1.165024	0.533646	1.351364
C	1.765732	2.389847	2.836472
C	-0.595139	3.607880	-3.232407
C	-0.306885	1.312332	-2.410477
C	-0.532639	-0.109100	-0.502518
C	-0.136063	-0.122131	1.006851
C	1.004471	1.269318	2.580063
C	1.167252	3.550171	3.474365
C	-1.922318	3.587708	-2.881912
C	-1.709427	1.290985	-2.040024
C	-1.854568	0.520737	-0.830933
C	-1.123108	0.496811	1.952911
C	-0.399124	1.248016	2.946609
C	-0.160843	3.530075	3.821335
C	-0.305756	-1.427979	0.233261
C	-2.496094	2.399246	-2.273438
C	-0.964691	2.349136	3.554382
C	-2.728394	0.943710	0.127319
C	-2.353317	0.931473	1.554916
C	-1.513214	-2.316147	0.542679
C	0.811722	-2.400970	-0.069016
C	-3.445419	2.819733	-1.275772
C	-3.545319	2.111969	-0.098175
C	-2.948868	2.092514	2.171692
C	-2.280014	2.781662	3.159180
C	-1.077393	-3.714813	0.415161
C	0.276398	-3.707062	0.059586
C	2.126083	-2.290298	-0.412598
O	-2.626175	-1.930862	0.838730
C	-3.690918	2.821030	1.159653
C	1.003265	-4.876678	-0.141266
C	2.895889	-3.471161	-0.625214
C	-1.747879	-4.891052	0.581024
C	2.370209	-4.723862	-0.498505
C	-1.032181	-6.095993	0.381912
C	0.296478	-6.094254	0.034027
H	2.950928	4.292007	-0.573120
H	1.532074	4.345596	-2.569107
H	2.696747	4.307465	1.863068
H	0.208466	4.787582	-2.969559
H	1.742859	4.737350	2.869431
H	-2.525574	4.747513	-2.250809
H	-0.991470	4.697342	3.587021
H	-3.469055	4.272079	-1.255463
H	-2.304413	4.234039	3.176498
H	-3.722458	4.193512	1.179703
H	2.613464	-1.349700	-0.531555
H	3.927612	-3.355515	-0.894974
H	-2.784958	-4.908554	0.852859
H	2.981140	-5.590118	-0.666809
H	-1.543167	-7.030289	0.507614
H	0.810379	-7.026077	-0.109283

Calculated ^{13}C chemical shifts (ppm) of **5a** (B3LYP/6-31G(d)//RHF/6-31G)

nuclei	**δ**
C1	187.66
C2	33.52
C2a	130.44
C3	115.59
C4	121.12
C5	117.81
C5a	121.70
C6	124.13
C7	120.45
C8	115.11
C8a	124.58
C8b	133.96
C1/6 (C_{60})	68.26