

Supporting Information

DFT calculations of pentalenoquinones: towards the interception of 2-bromopentalene-1,5-dione

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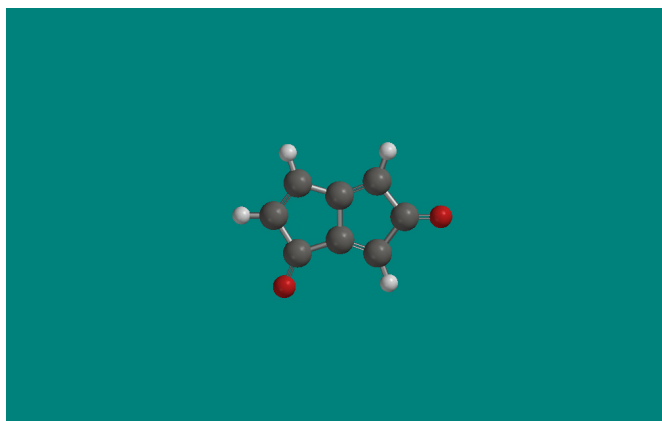
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This paper is dedicated to Professor Udo H. Brinker on the occasion of his 65th birthday

General

Geometry optimizations were performed at the level of B3LYP/6-311+G(d,p)¹⁻³. The nucleus independent chemical shift (NICS)⁴ was used as a descriptor of aromaticity from the magnetic point of view. The index is defined as the negative value of the absolute magnetic shielding computed at ring centers⁵ or another interesting point of the system.⁶ In this study, NICS values were computed with GIAO⁷ B3LYP/6-311G (d,p) // B3LYP/6-311+G(d,p). NICS (0) was calculated at the geometrical center of the ring. For each set of calculations, vibrational analyses were done (using the same basis set employed in the corresponding geometry optimizations). The normal mode analysis for each structure yielded no imaginary frequencies for the $3N-6$ vibrational degrees of freedom, where N is the number of atoms in the system. This indicates that the structure of each molecule corresponds to at least a local minimum on the potential energy surface. All the calculations for the geometry optimizations and energies were performed using Gaussian 98 program package⁷ and Spartan 06 package⁸ programme.

Cartesian Coordinates



Cartesian Coordinates (Angstroms)

Atom	X	Y	Z
1 C C0	-1.1786455	-1.6901633	0.0000000
2 C C1	-2.2035712	-0.7971342	0.0000000
3 C C2	-1.7130855	0.6195372	0.0000000
4 C C3	-0.2304271	0.4821693	0.0000000
5 C C4	0.0828475	-0.9835208	0.0000000
6 C C5	0.8969517	1.1975790	0.0000000
7 C C6	2.0444961	0.1916528	0.0000000
8 C C7	1.4115778	-1.1798929	0.0000000
9 O O8	3.2233182	0.4524232	0.0000000
10 O O9	-2.3891809	1.6259975	0.0000000
11 H H1	-1.2833173	-2.7676437	0.0000000
12 H H2	-3.2592797	-1.0352703	0.0000000
13 H H4	1.9818560	-2.0968913	0.0000000
14 H H3	1.0396131	2.2684724	0.0000000

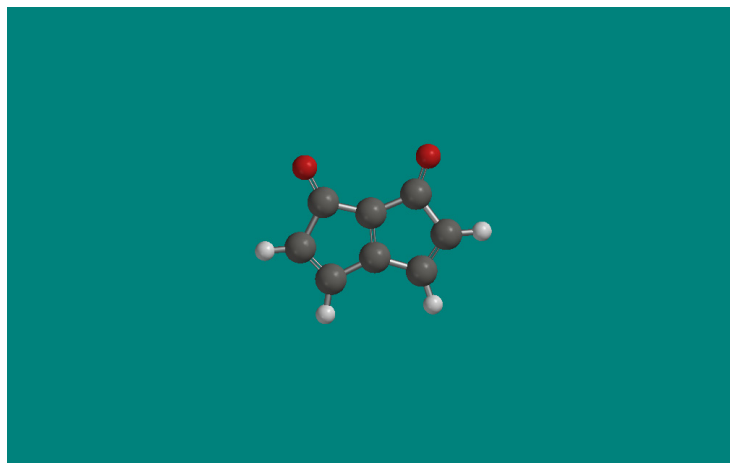
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Cartesian Coordinates (Angstroms)

Atom	X	Y	Z
1 C C0	-0.4564766	-0.6190450	0.0000000
2 C C1	-0.6925611	0.8454554	0.0000000
3 C C2	0.4683747	1.5398599	0.0000000
4 C C3	1.6109302	0.5762951	0.0000000
5 C C4	0.9821874	-0.8707278	0.0000000
6 C C5	-1.6629380	-1.2378700	0.0000000
7 C C6	-2.6947095	-0.1912011	0.0000000
8 C C7	-2.1231342	1.0512166	0.0000000
9 O O8	1.6156440	-1.8976202	0.0000000
10 O O9	2.7862040	0.8343939	0.0000000
11 H H2	-1.8565138	-2.3013387	0.0000000
12 H H3	-3.7582592	-0.3916182	0.0000000
13 H H4	-2.6354963	2.0014815	0.0000000
14 H H1	0.6070974	2.6140018	0.0000000

Point Group = CS



Cartesian Coordinates (Angstroms)

Atom	X	Y	Z
1 C C0	0.0000000	0.0000000	1.0855886
2 C C1	0.0000000	0.0000000	-0.2692092
3 C C2	-1.4114491	0.0000000	-0.7234077
4 C C3	-2.2247684	0.0000000	0.5809421
5 C C4	-1.3806148	0.0000000	1.6245384
6 C C5	1.3806148	0.0000000	1.6245384
7 C C6	2.2247684	0.0000000	0.5809421
8 C C7	1.4114491	0.0000000	-0.7234077
9 O O8	1.8820975	0.0000000	-1.8350410
10 O O9	-1.8820975	0.0000000	-1.8350410
11 H H4	3.3056243	0.0000000	0.5901587
12 H H3	1.6368806	0.0000000	2.6754180
13 H H2	-1.6368806	0.0000000	2.6754180
14 H H1	-3.3056243	0.0000000	0.5901587

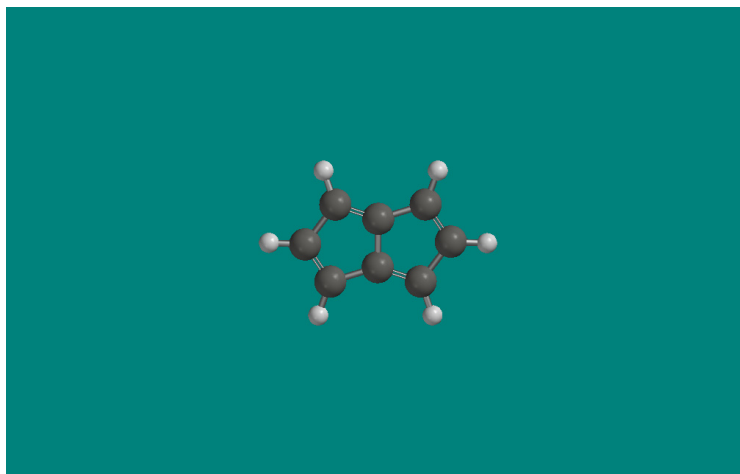
Point Group = C2V



Cartesian Coordinates (Angstroms)

Atom	X	Y	Z
1 C C0	-0.3371613	-0.5794791	0.0000000
2 C C1	0.3371613	0.5794791	0.0000000
3 C C2	-0.5904203	1.7384021	0.0000000
4 C C3	-1.8511675	1.2716087	0.0000000
5 C C4	-1.8092491	-0.2469534	0.0000000
6 C C5	0.5904203	-1.7384021	0.0000000
7 C C6	1.8511675	-1.2716087	0.0000000
8 C C7	1.8092491	0.2469534	0.0000000
9 O O8	2.7465899	1.0068123	0.0000000
10 O O9	-2.7465899	-1.0068123	0.0000000
11 H H3	0.2773691	-2.7735022	0.0000000
12 H H4	2.7751606	-1.8305191	0.0000000
13 H H2	-2.7751606	1.8305191	0.0000000
14 H H1	-0.2773691	2.7735022	0.0000000

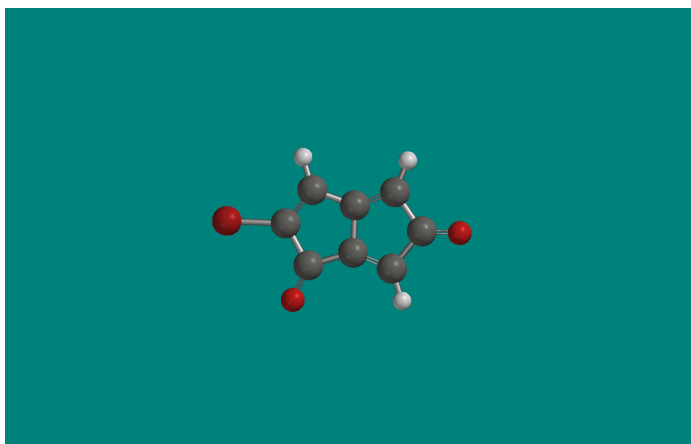
Point Group = C2H



Cartesian Coordinates (Angstroms)

Atom	X	Y	Z
1 C C0	0.0446240	-0.7276712	0.0000000
2 C C1	-0.0446240	0.7276712	0.0000000
3 C C2	-1.4749730	1.0825919	0.0000000
4 C C3	-2.1695116	-0.0796671	0.0000000
5 C C4	-1.2124453	-1.2303833	0.0000000
6 C C5	1.4749730	-1.0825919	0.0000000
7 C C6	2.1695116	0.0796671	0.0000000
8 C C7	1.2124453	1.2303833	0.0000000
9 H H1	-1.8879063	2.0812801	0.0000000
10 H H2	-3.2455823	-0.1859058	0.0000000
11 H H3	-1.5144646	-2.2704609	0.0000000
12 H H4	1.8879063	-2.0812801	0.0000000
13 H H5	3.2455823	0.1859058	0.0000000
14 H H6	1.5144646	2.2704609	0.0000000

Point Group = C2H



Cartesian Coordinates (Angstroms)

Atom	X	Y	Z
1 C C0	-0.0787400	-1.3055841	0.0000000
2 C C1	-0.8885296	-0.2084955	0.0000000
3 C C2	-0.1123501	1.0896556	0.0000000
4 C C3	1.2952826	0.6281602	0.0000000
5 C C4	1.2928018	-0.8708333	0.0000000
6 C C5	2.5482679	1.0904335	0.0000000
7 C C6	3.4578701	-0.1355780	0.0000000
8 C C7	2.5538845	-1.3397641	0.0000000
9 O O8	4.6658196	-0.1239093	0.0000000
10 O O9	-0.5652604	2.2089483	0.0000000
11 H H1	-0.4175649	-2.3329603	0.0000000
12 H H4	2.9191219	-2.3558554	0.0000000
13 H H3	2.9125585	2.1075815	0.0000000
14 Br Br1	-2.7606922	-0.2142645	0.0000000

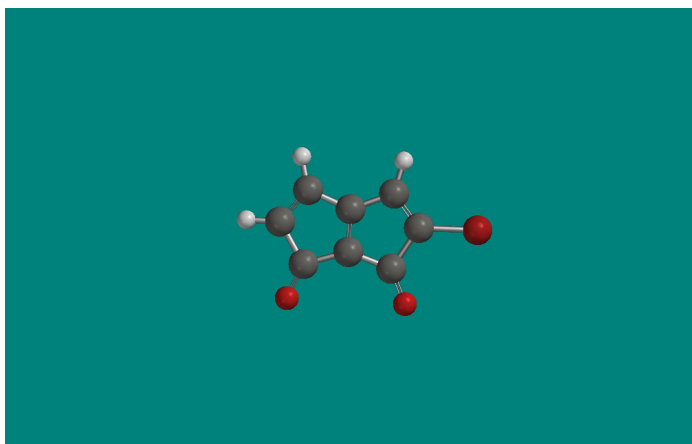
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Cartesian Coordinates (Angstroms)

Atom	X	Y	Z
1 C C0	1.0268969	-0.5358423	0.0000000
2 C C1	0.9318811	0.9452646	0.0000000
3 C C2	2.1585136	1.5217315	0.0000000
4 C C3	3.2009857	0.4551596	0.0000000
5 C C4	2.4388731	-0.9235133	0.0000000
6 C C5	-0.2272741	-1.0443443	0.0000000
7 C C6	-1.1391216	0.1089718	0.0000000
8 C C7	-0.4617794	1.2988573	0.0000000
9 O O8	2.9657288	-2.0074749	0.0000000
10 O O9	4.3962047	0.5959428	0.0000000
11 H H2	-0.5400598	-2.0782017	0.0000000
12 H H4	-0.8891707	2.2890229	0.0000000
13 H H1	2.3994395	2.5774090	0.0000000
14 Br Br1	-3.0123131	-0.0807028	0.0000000

Point Group = CS



Cartesian Coordinates (Angstroms)

Atom	X	Y	Z
1 C C0	1.2635765	-1.0471875	0.0000000
2 C C1	1.4341301	0.3034156	0.0000000
3 C C2	2.8860557	0.5798311	0.0000000
4 C C3	3.5297362	-0.8168243	0.0000000
5 C C4	2.5656524	-1.7509187	0.0000000
6 C C5	-0.1553880	-1.4342072	0.0000000
7 C C6	-0.8624302	-0.2897114	0.0000000
8 C C7	0.1087634	0.9380456	0.0000000
9 O O8	-0.2384070	2.0886682	0.0000000
10 O O9	3.4948469	1.6226522	0.0000000
11 H H3	-0.5391979	-2.4440534	0.0000000
12 H H2	2.6900590	-2.8251730	0.0000000
13 H H1	4.6014170	-0.9585008	0.0000000
14 Br Br1	-2.7182908	-0.0771605	0.0000000

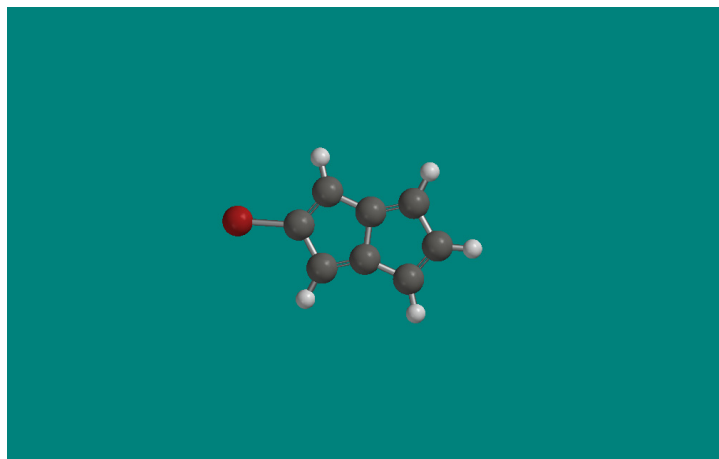
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Cartesian Coordinates (Angstroms)

Atom	X	Y	Z
1 C C0	1.3314043	-0.8462309	0.0000000
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3 C C2	0.1008881	1.1490926	0.0000000
4 C C3	-0.8230152	0.1730952	0.0000000
5 C C4	-0.1229825	-1.2020764	0.0000000
6 C C5	2.6748602	-1.4760533	0.0000000
7 C C6	3.6024528	-0.5023949	0.0000000
8 C C7	2.9020444	0.8407250	0.0000000
9 O O8	3.4031985	1.9373157	0.0000000
10 O O9	-0.6474641	-2.2826505	0.0000000
11 H H3	2.8500452	-2.5430157	0.0000000
12 H H4	4.6777526	-0.5995370	0.0000000
13 H H1	-0.0696213	2.2154476	0.0000000
14 Br Br1	-2.6923012	0.3299951	0.0000000

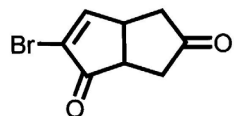
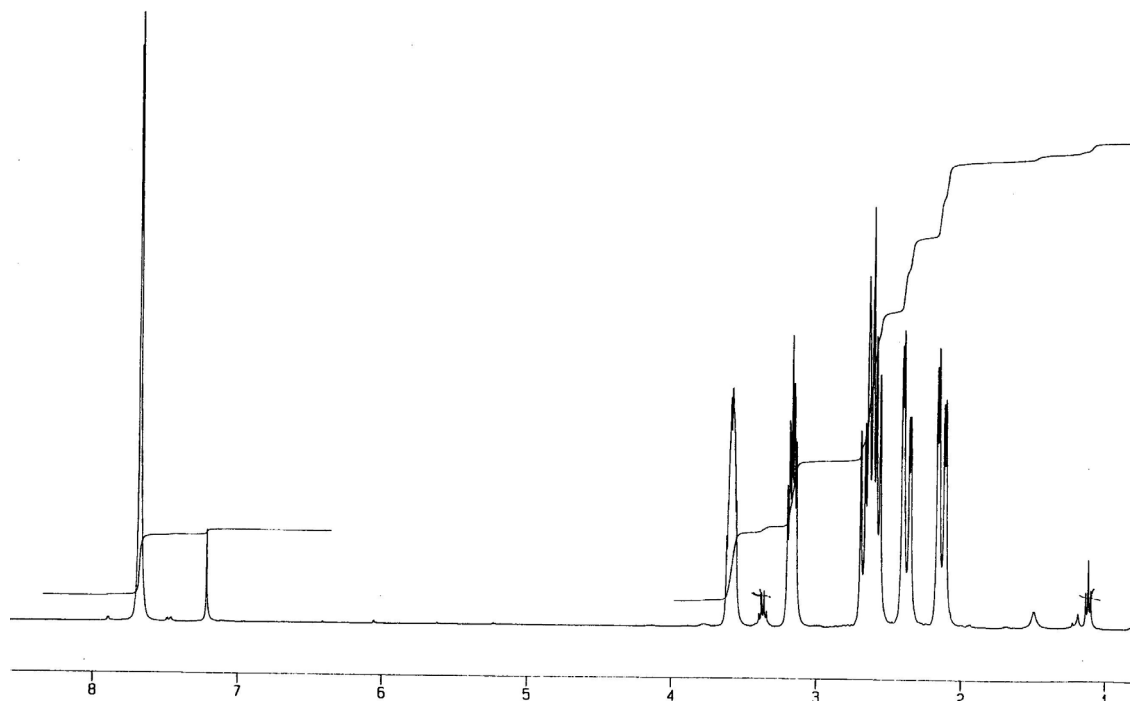
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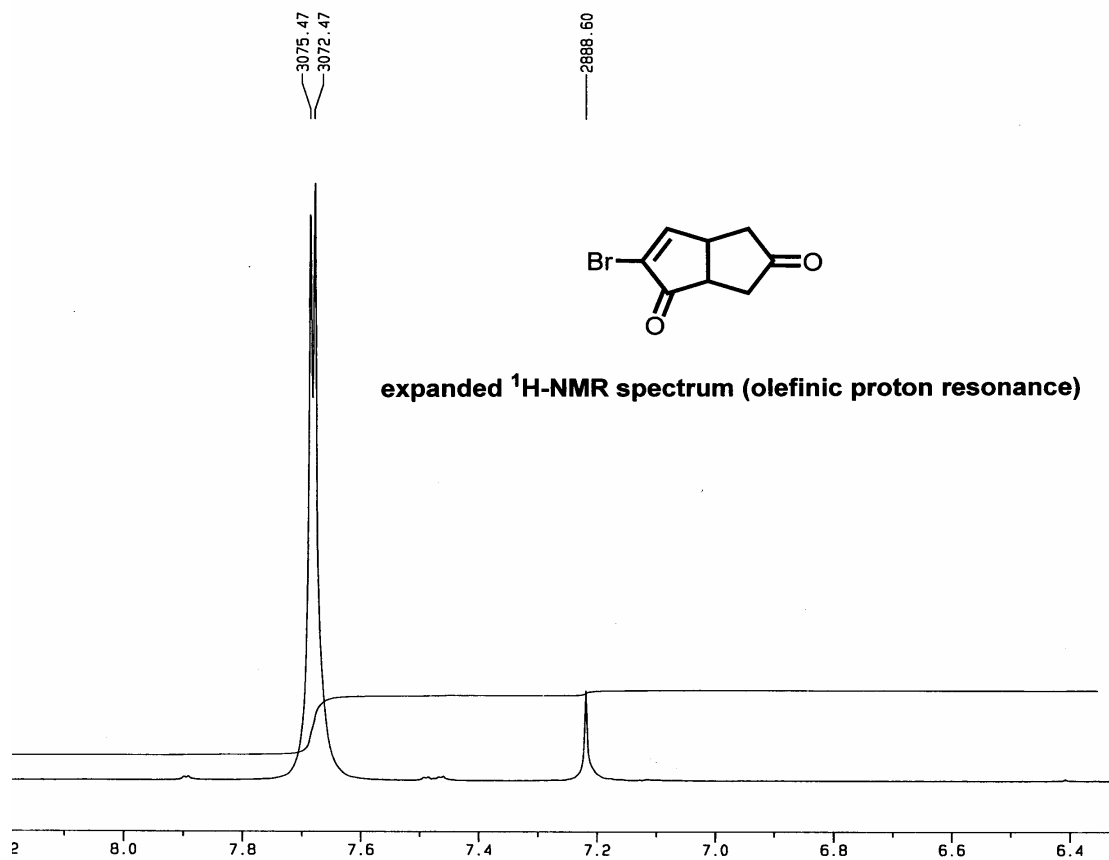


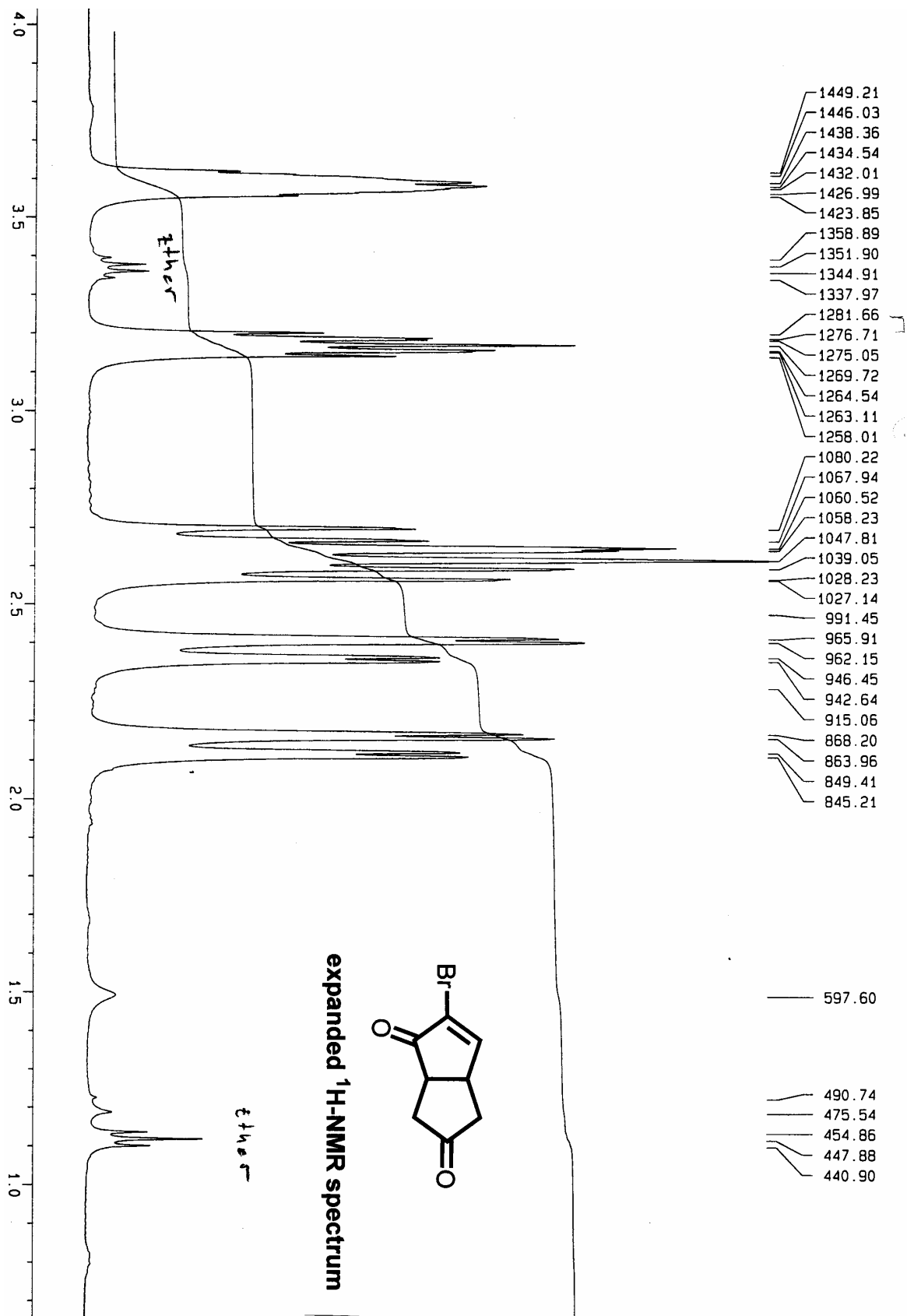
Cartesian Coordinates (Angstroms)

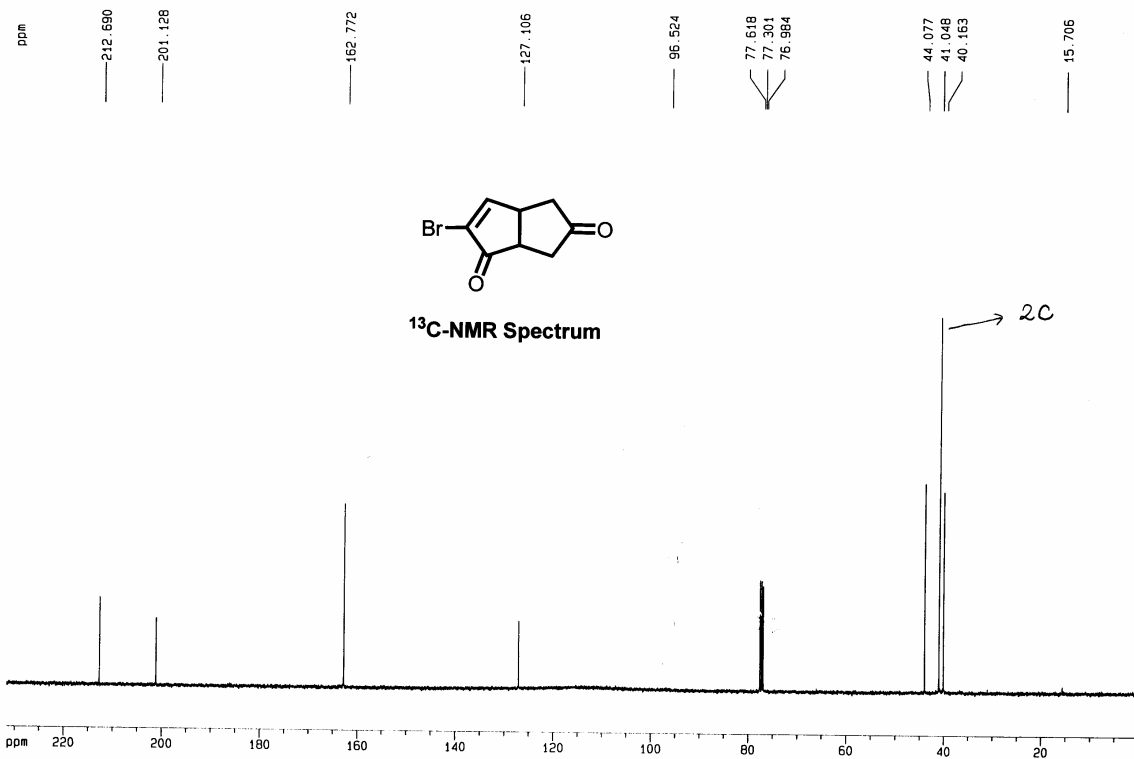
Atom	X	Y	Z
1 C C0	1.5844728	-0.7487915	0.0000000
2 C C1	1.5917384	0.7151362	0.0000000
3 C C2	3.0028519	1.1500848	0.0000000
4 C C3	3.7565998	0.0283573	0.0000000
5 C C4	2.8665303	-1.1781250	0.0000000
6 C C5	0.1836968	-1.1963051	0.0000000
7 C C6	-0.5567942	-0.0663230	0.0000000
8 C C7	0.3151298	1.1527498	0.0000000
9 H H1	3.3582453	2.1701479	0.0000000
10 H H2	4.8368137	-0.0194761	0.0000000
11 H H3	3.2272229	-2.1988837	0.0000000
12 H H4	-0.1814467	-2.2117178	0.0000000
13 H H6	-0.0675419	2.1643707	0.0000000
14 Br Br1	-2.4459246	0.0496761	0.0000000

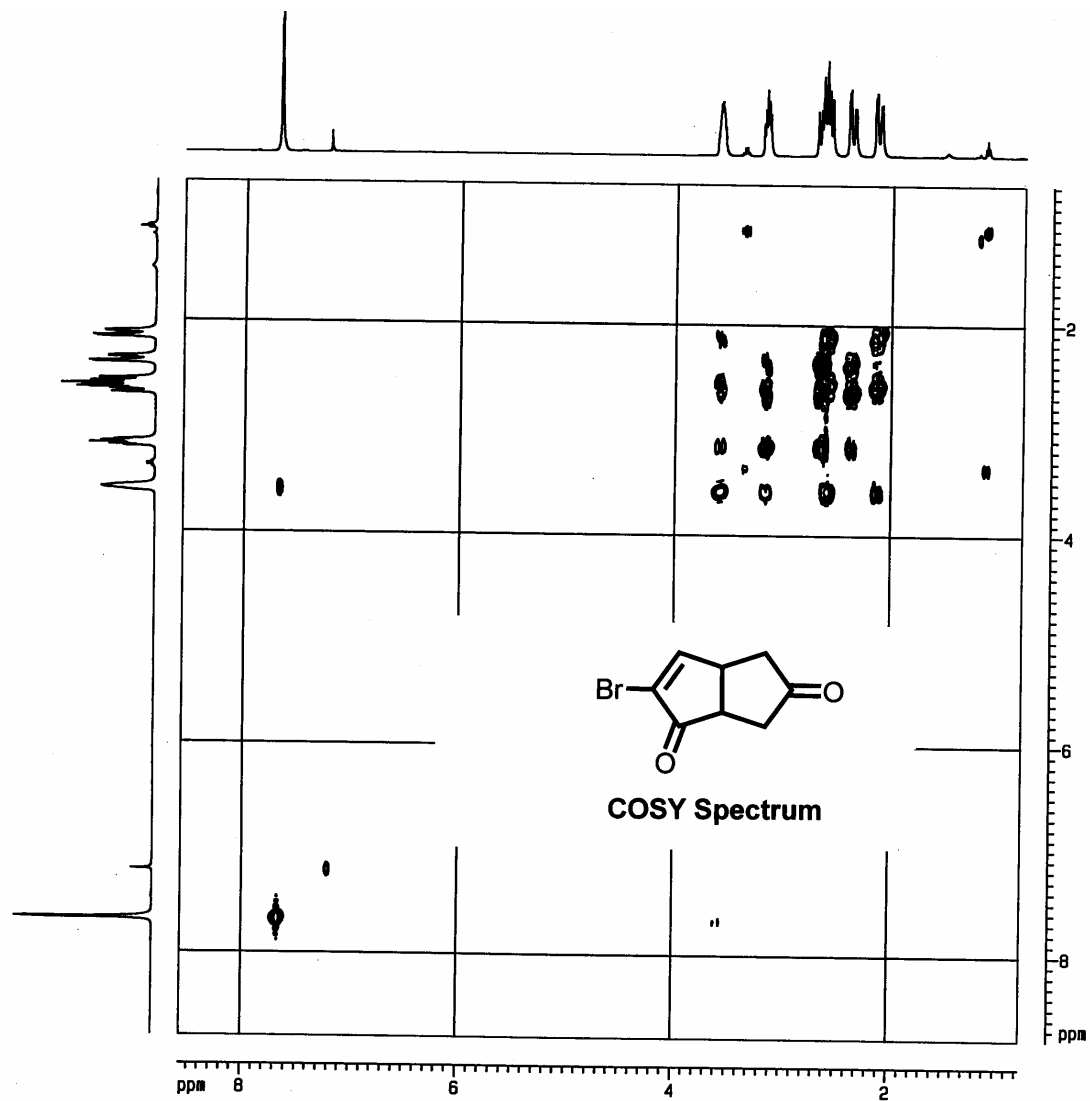
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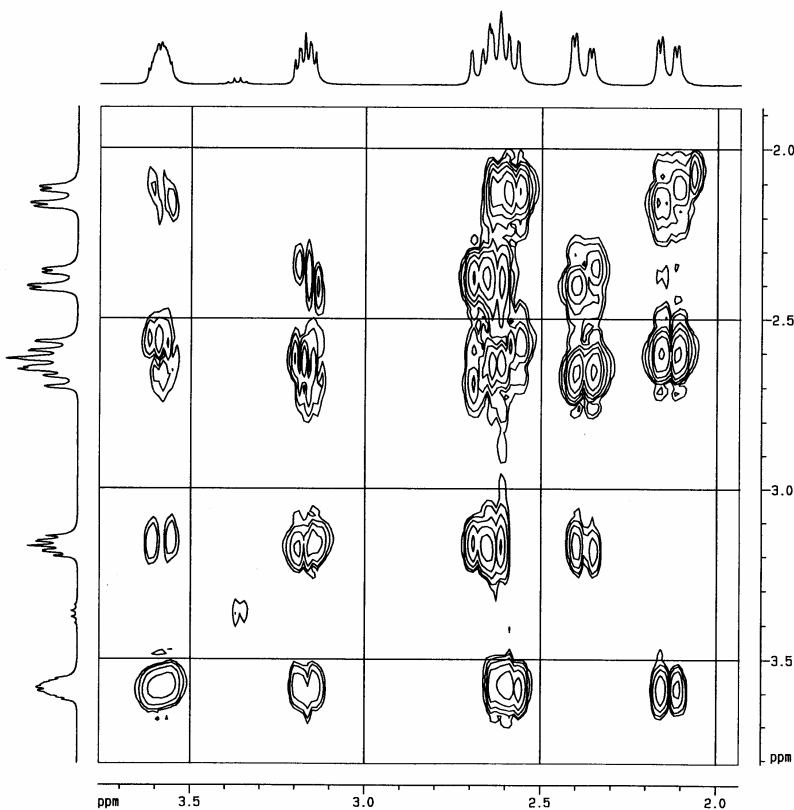
**¹H-NMR Spectrum**



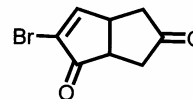








f TA-B4.COSY



expanded COSY Spectrum

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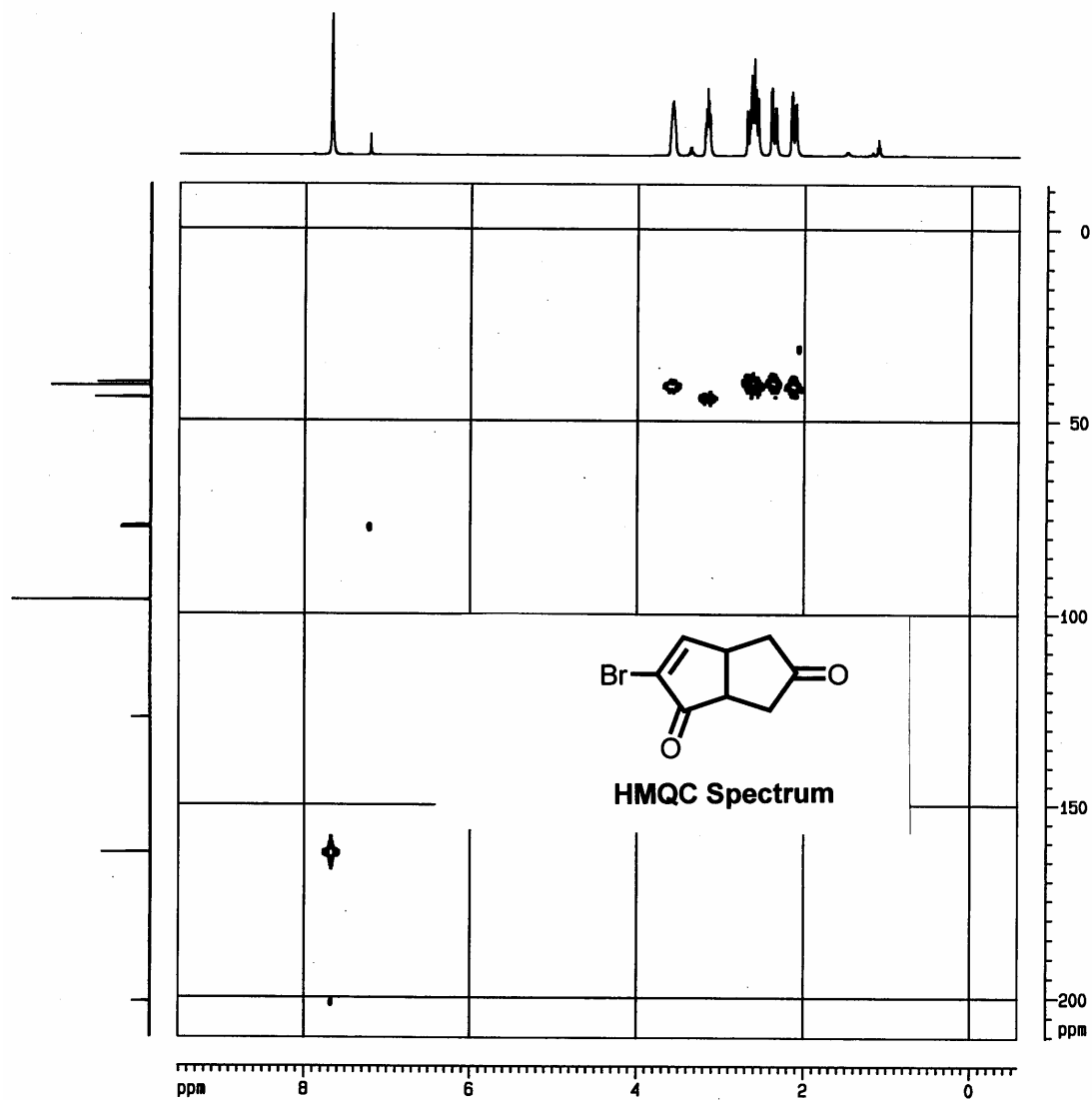
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TE          300.0 K
D1         1.48889100 sec
D11        13.00 mmsec
SFO1       400.1324057 MHz
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PL1        9.40 dB
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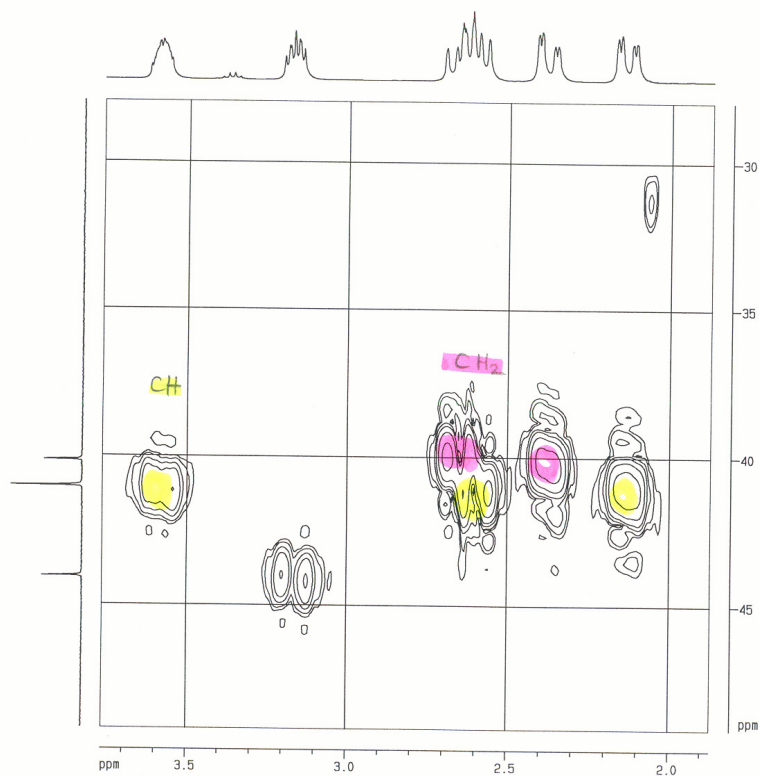
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DM         13.357 mm

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WDW        RMSE
SSB         0
LB         0.00 Hz
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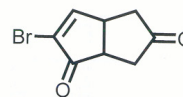
F1 - Processing parameters
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SF         400.1306344 MHz
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LB         0.00 Hz
GB         0

2D NMR plot parameters
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CX1        15.00 cm
F2P10     3.781 ppm
F2D0      1504.82 Hz
F2PC1     1.858 ppm
F2C2      774.48 Hz
F2P1D0    3.882 ppm
F1P1C1    1505.23 Hz
F1P1C2    1.861 ppm
F1C1      782.74 Hz
F2P1PC1H  0.12188 ppm/cm
F2P1DC1H  46.88802 Hz/cm
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f TA-B4.HMGC



expanded HMQC Spectrum

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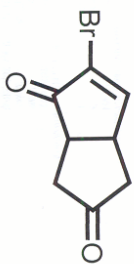
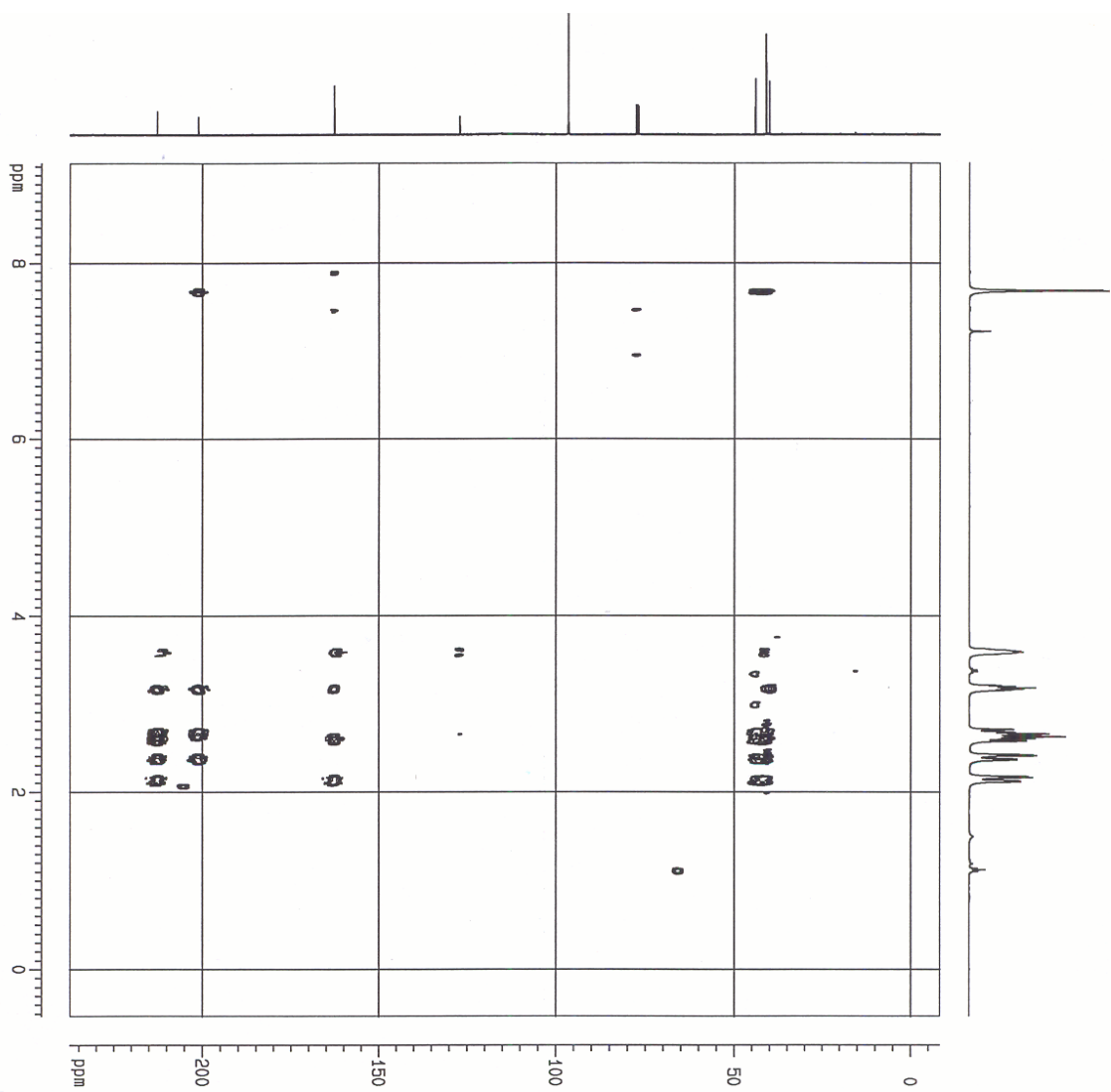
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DZ 0.0002000 sec
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DQ3 0.0001000 sec
AQ2 0.0004000 sec
DQ 2.0000000 sec
P1 53.00 usec
SP2 400.135230 MHz
MAG 30
R1 9.40 dB
R2 -1.00 dB
P3 54.00 usec
SP3 100.627700 MHz
MAG2 130
DQ 0.0002000 sec
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M 0.0000000 sec
R13 13.00 dB
CPDPR0 0
PCP02 70.00 usec
DMS 0.0002200 sec

F1 - Acquisition parameters
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DE 8.000000 sec

F2 - Processing parameters
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SSB 0
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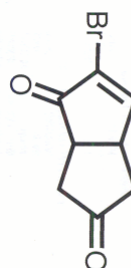
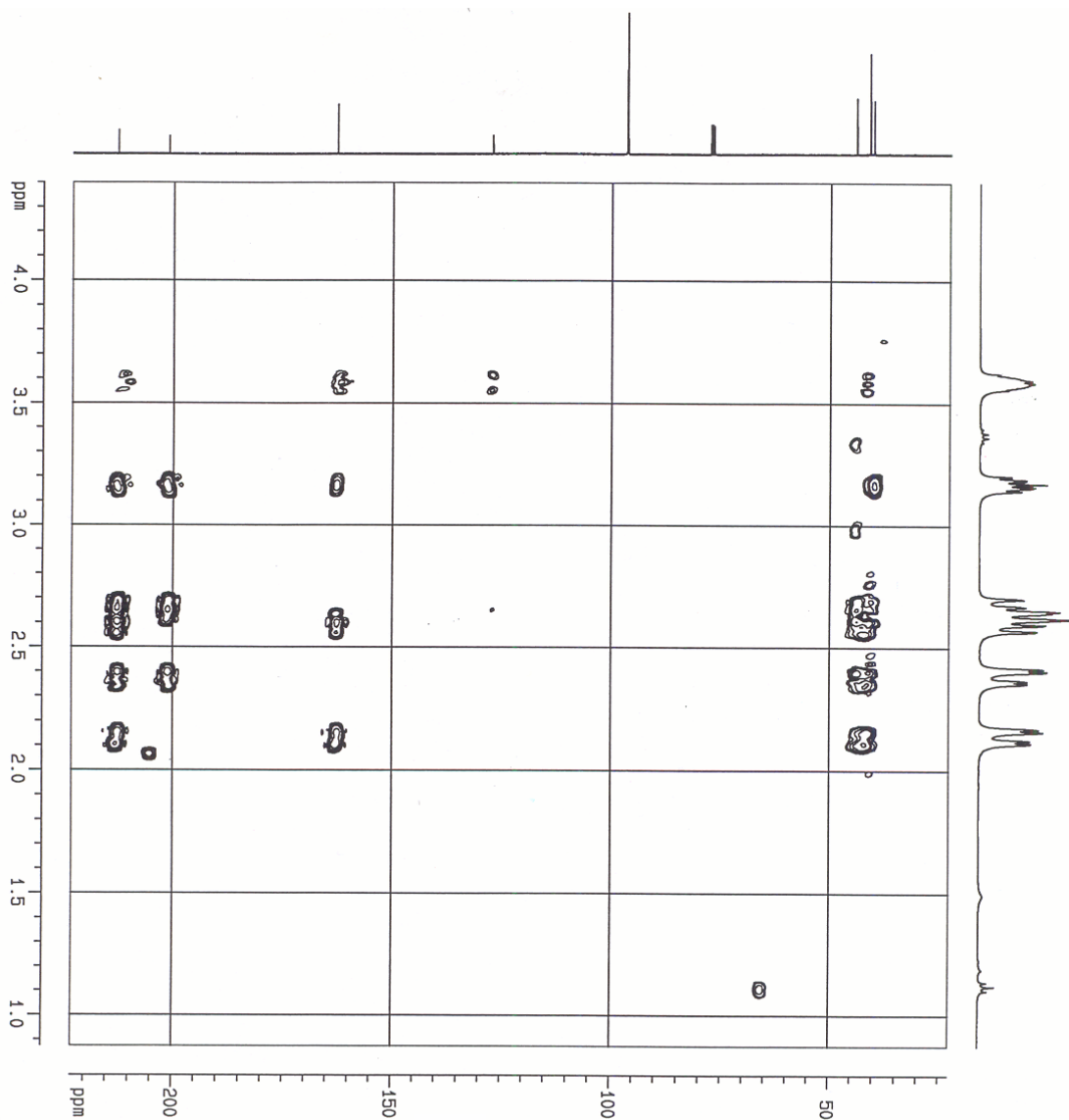
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FPLH 4060.00 Hz
FPHC 27.0000 ppm
FPHS 200.00 Hz
FORMC 0.100000 usec/c
FORMH 80.0000 Hz/c
FORMW 1.415000 usec/c
    
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f TA-84.HMBC

HMBC Spectrum

SIH 52961.264 Hz
 SIH2 2327.268 Hz
 SIH3 0.141899 Hz
 SIH4 1.6884 Hz
 SIH5 1.6884 Hz
 SIH6 1.6884 Hz
 SIH7 1.6884 Hz
 SIH8 1.6884 Hz
 SIH9 1.6884 Hz
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 SIH12 1.6884 Hz
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 SIH33 1.6884 Hz
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 SIH100 1.6884 Hz



f TA-84.HMBC

expanded HMBC Spectri

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 PULPROG: zgpg30
 PROCNO: 1
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 SF: 400.1500044 MHz
 SFO: 400.1500044 MHz
 SWH: 100.8127250 MHz
 FIDRES: 0.1871981 Hz
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 SFO2: 100.6262626 MHz
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 F2CH2PRG2: zgpg30
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 F2F2SFRES: 0.2500000 MHz
 F2F2AQ: 1.50000000 sec
 F2F2SFO2: 100.6262626 MHz
 F2F2CH2PRG2: zgpg30
 F2F2F2PULPROG: zgpg30
 F2F2F2SI: 400.1500044 MHz
 F2F2F2SF: 400.1500044 MHz
 F2F2F2SFO: 400.1500044 MHz
 F2F2F2SWH: 100.8127250 MHz
 F2F2F2FIDRES: 0.1871981 Hz
 F2F2F2SFRES: 0.2500000 MHz
 F2F2F2AQ: 1.50000000 sec
 F2F2F2SFO2: 100.6262626 MHz
 F2F2F2CH2PRG2: zgpg30

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