

Supporting Information

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

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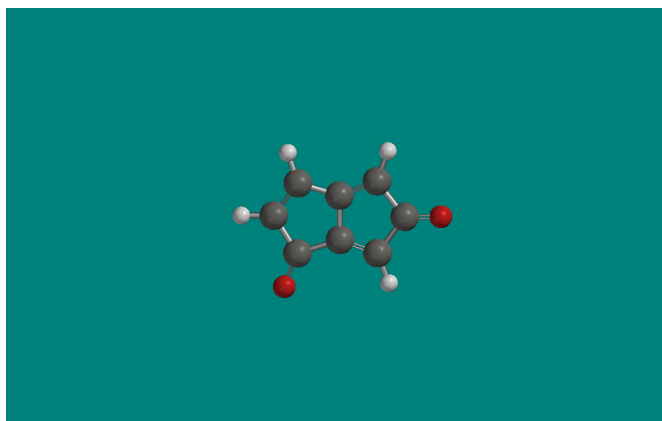
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This paper is dedicated to Professor Udo H. Brinker on the occasion of his 65th birthday

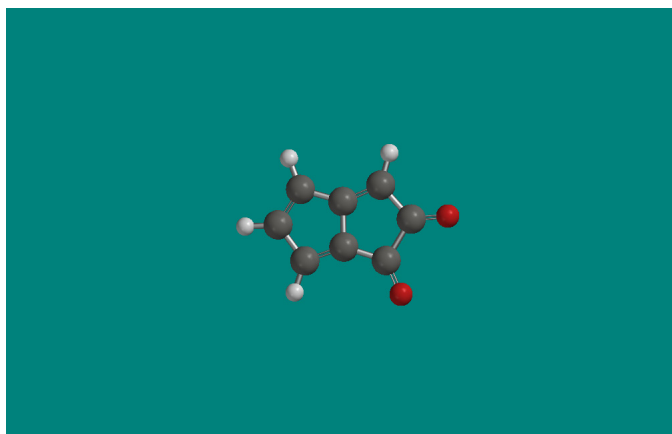
General

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



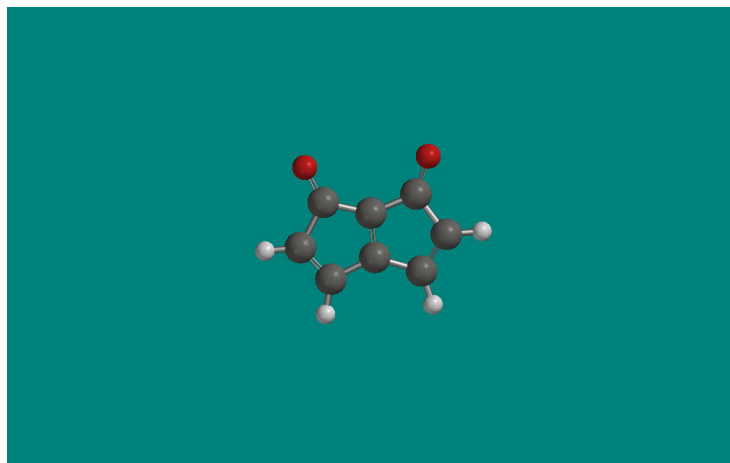
Cartesian Coordinates (Angstroms)				
Atom		X	Y	Z
-----		-----	-----	-----
1	C C0	-1.1786455	-1.6901633	0.0000000
2	C C1	-2.2035712	-0.7971342	0.0000000
3	C C2	-1.7130855	0.6195372	0.0000000
4	C C3	-0.2304271	0.4821693	0.0000000
5	C C4	0.0828475	-0.9835208	0.0000000
6	C C5	0.8969517	1.1975790	0.0000000
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
Point Group = CS				



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

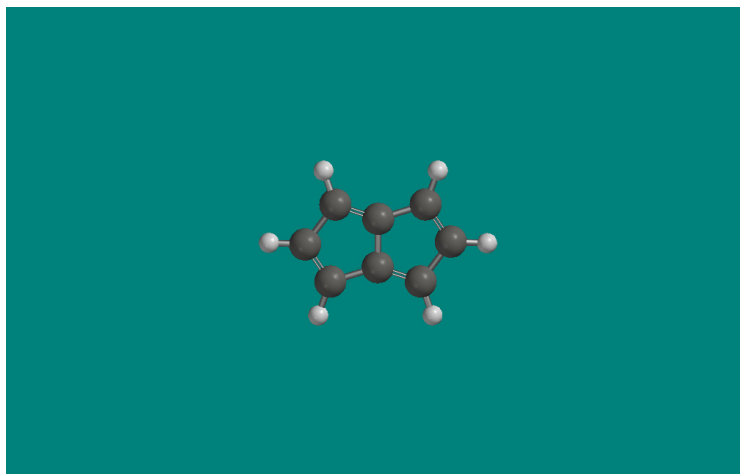
Point Group = C2V



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
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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

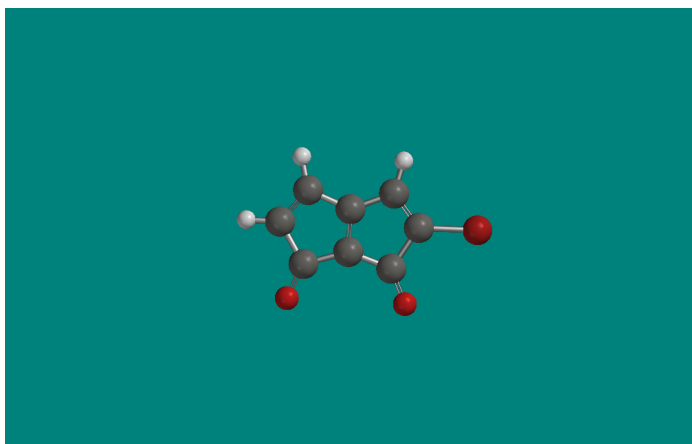
Point Group = CS



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

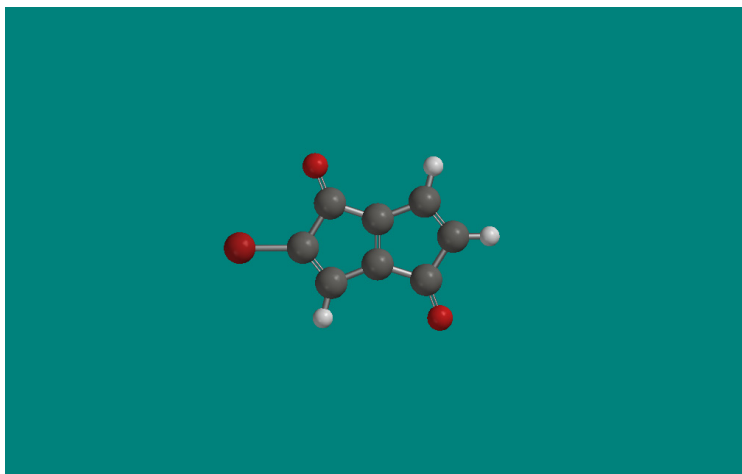
Point Group = CS



Cartesian Coordinates (Angstroms)

Atom		X	Y	Z
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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

Point Group = CS



Cartesian Coordinates (Angstroms)				
Atom		X	Y	Z

1	C C0	1.3314043	-0.8462309	0.0000000
2	C C1	1.4270208	0.4929139	0.0000000
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

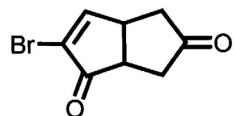
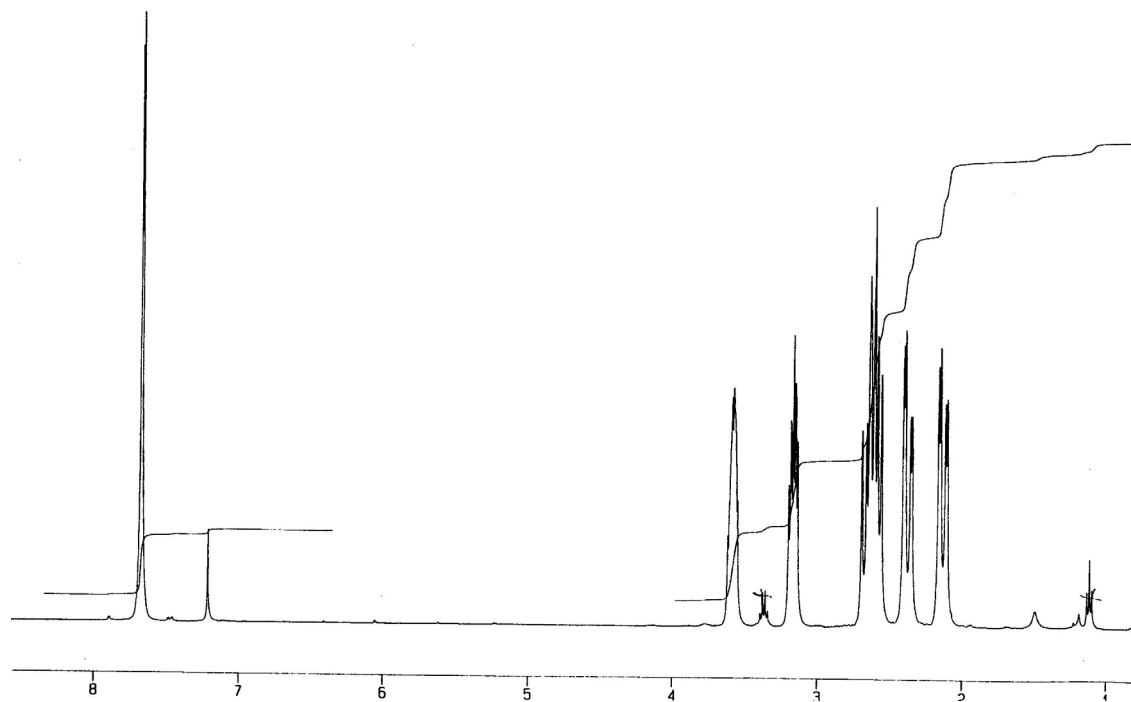
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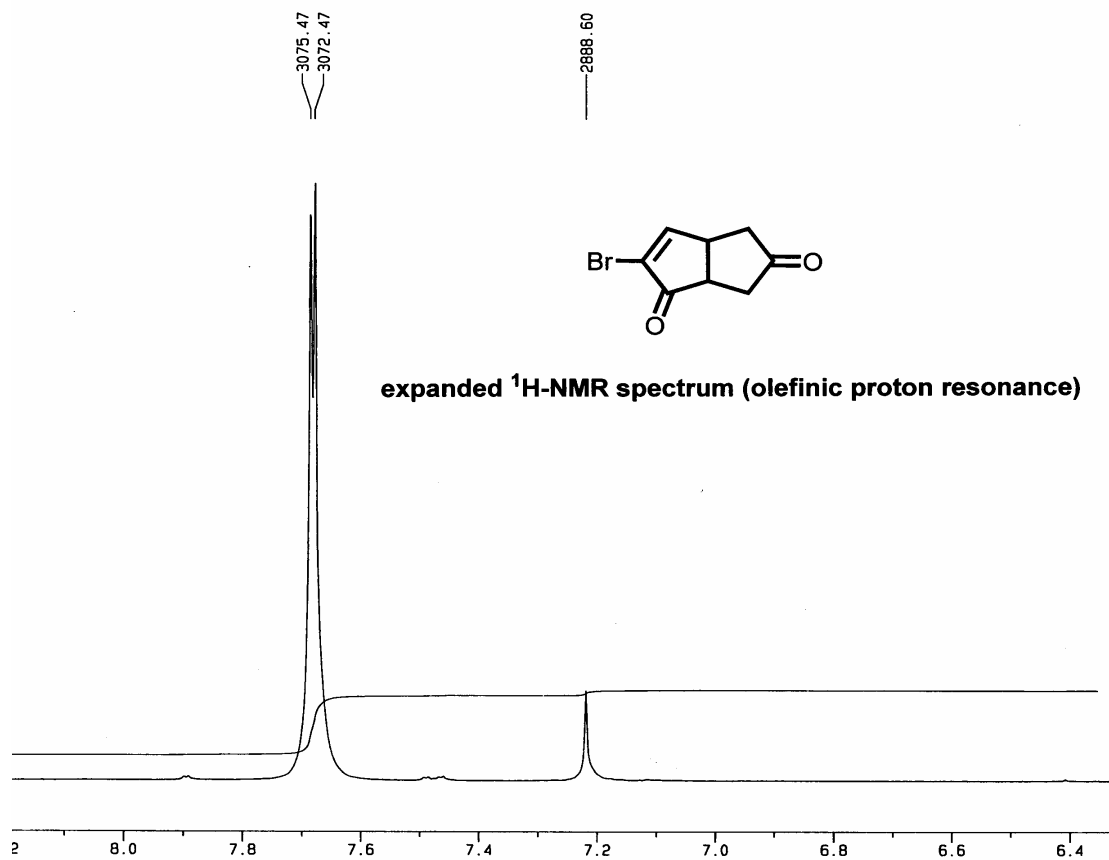


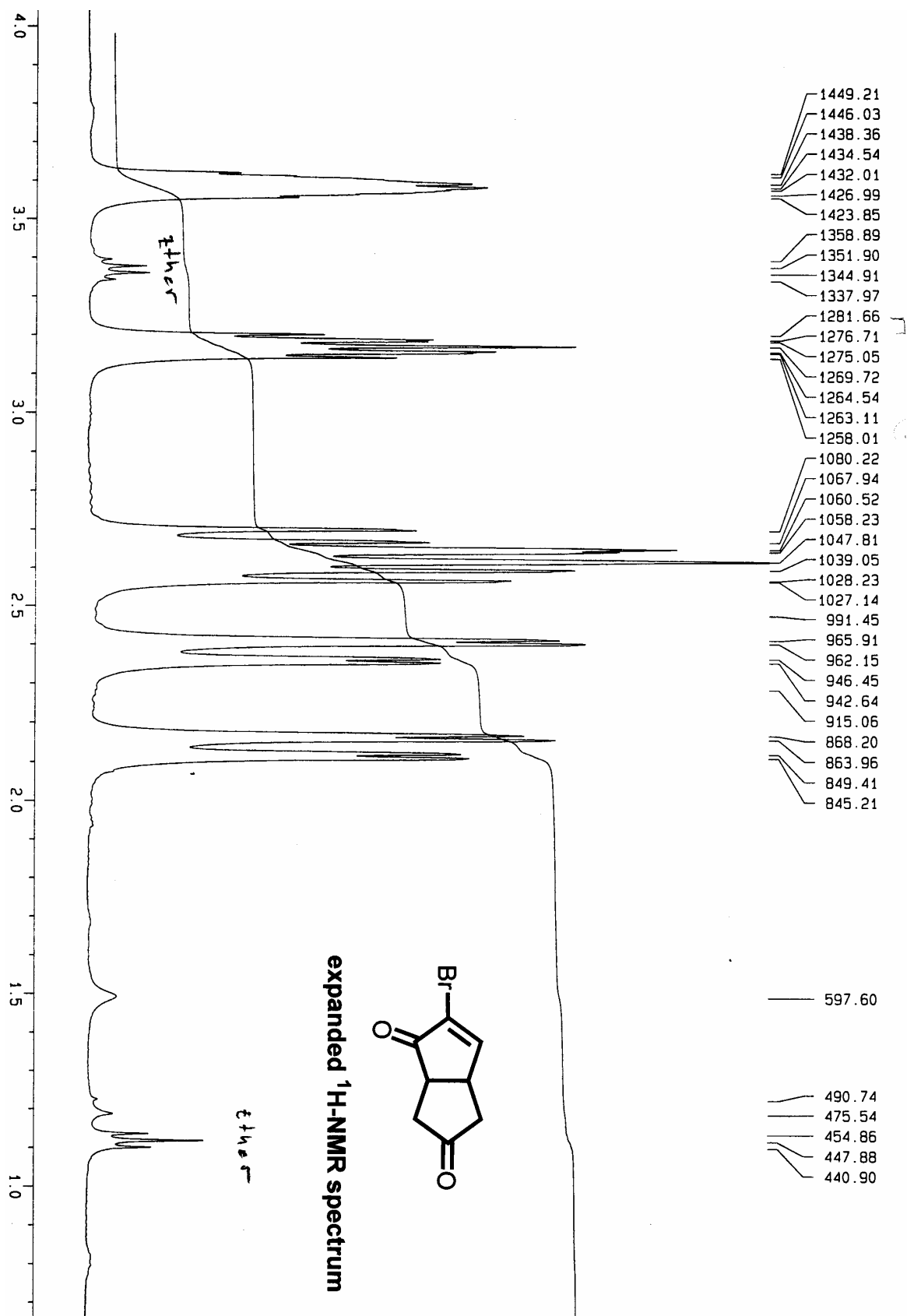
Cartesian Coordinates (Angstroms)

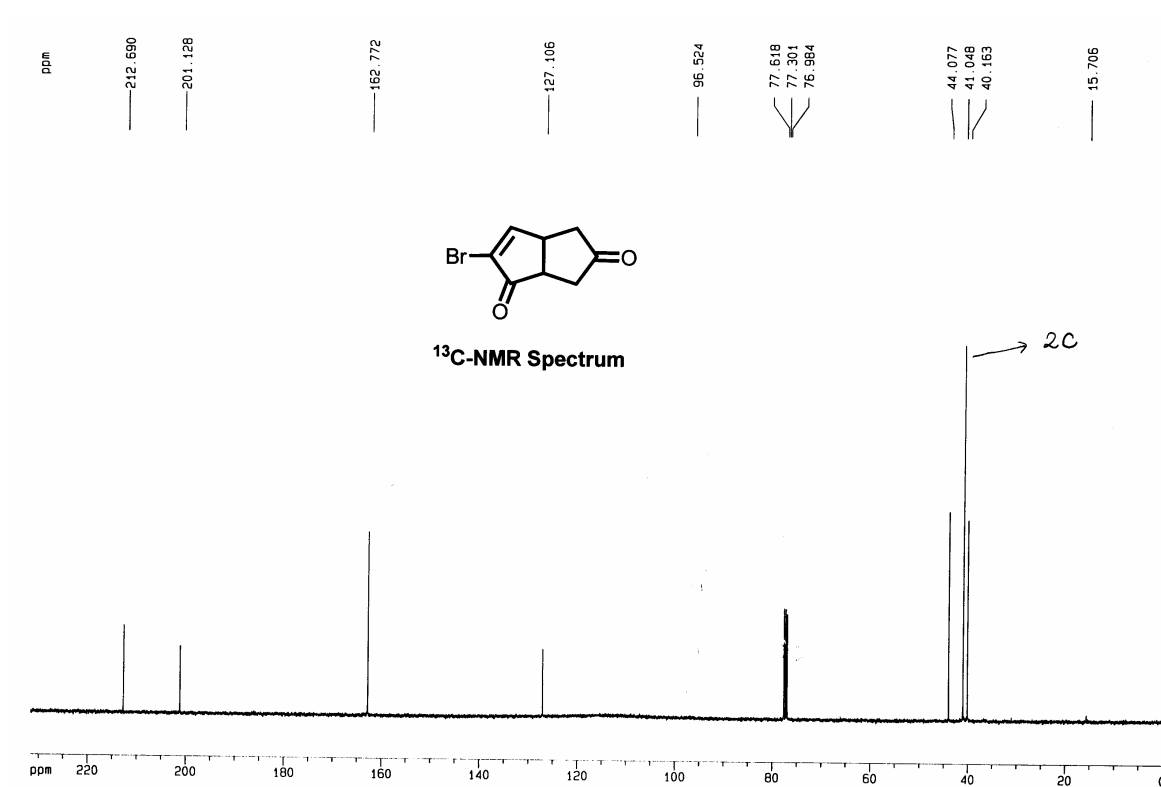
Atom		X	Y	Z
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1	C C0	1.5844728	-0.7487915	0.0000000
2	C C1	1.5917384	0.7151362	0.0000000
3	C C2	3.0028519	1.1500848	0.0000000
4	C C3	3.7565998	0.0283573	0.0000000
5	C C4	2.8665303	-1.1781250	0.0000000
6	C C5	0.1836968	-1.1963051	0.0000000
7	C C6	-0.5567942	-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

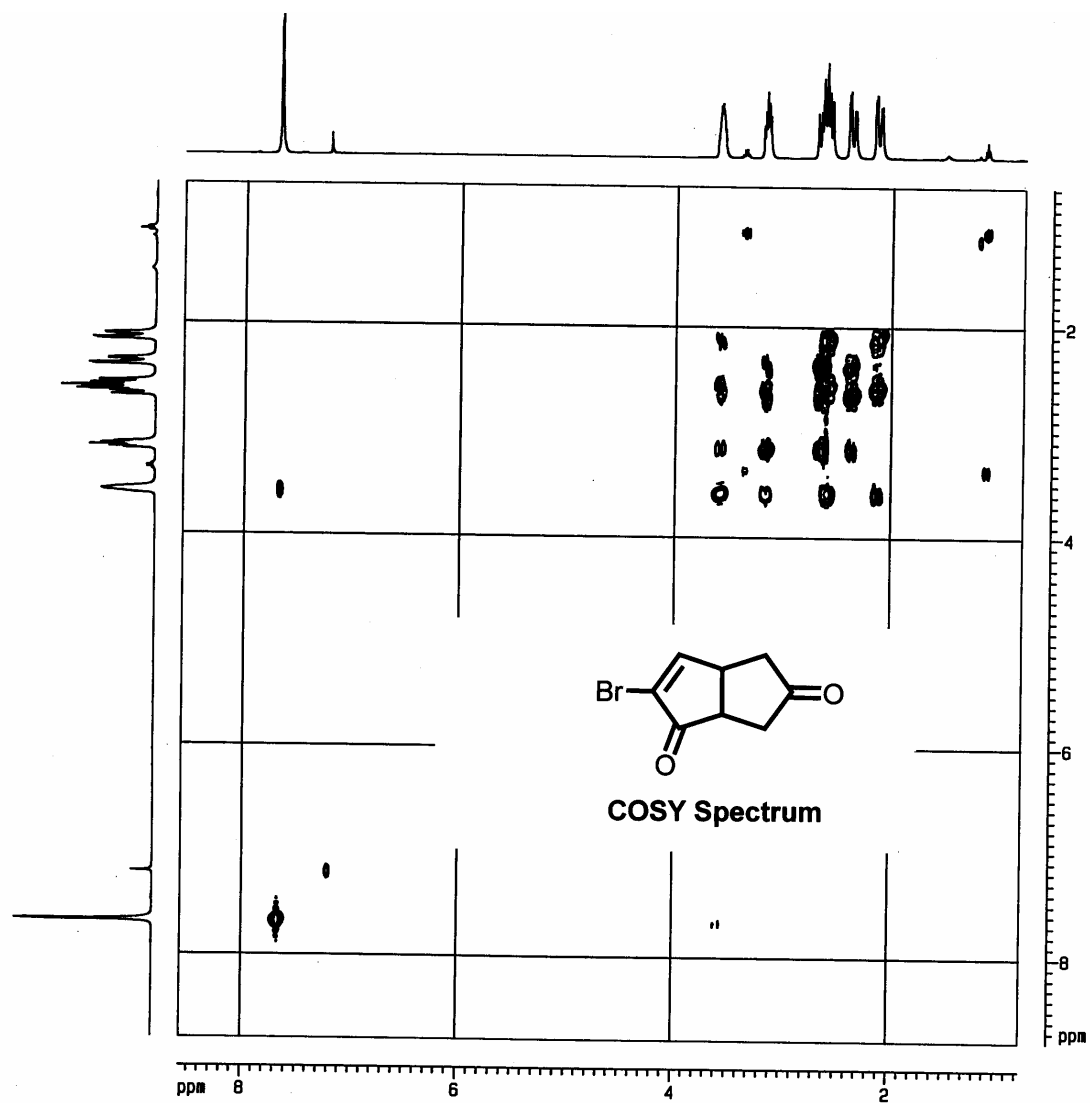
Point Group = CS

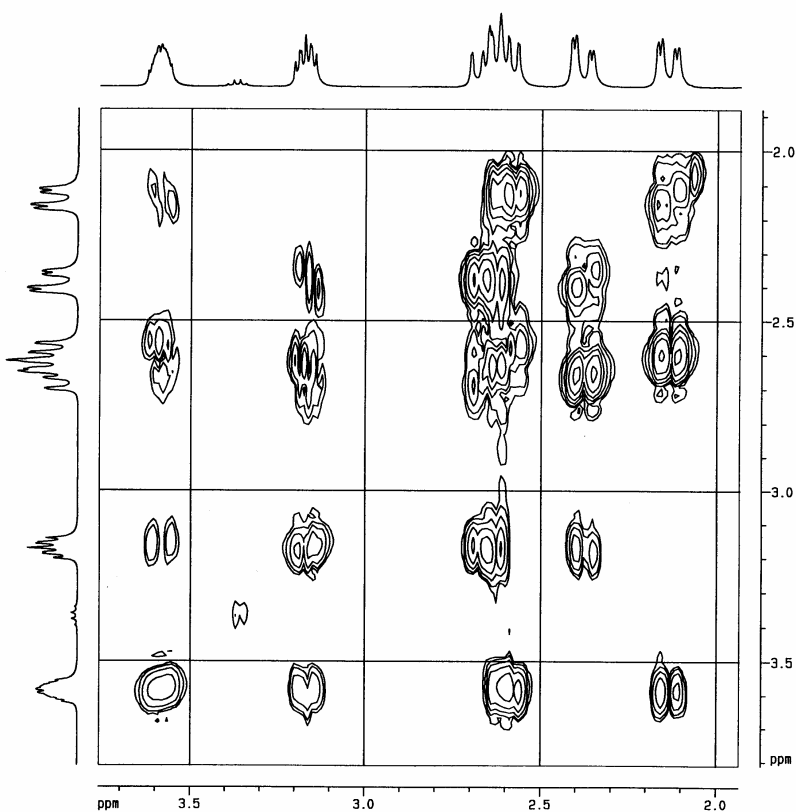
**¹H-NMR Spectrum**



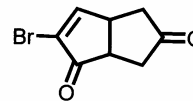








f TA-B4.COSY



expanded COSY Spectrum

```

IN          32
SMH         3541.880 Hz
FIDRES      2.806340 Hz
AQ          0.1817420 sec
RG          64
DS          33.800 mmec
DE          8.00 mmec
TE          300.0 K
D1          1.48889100 sec
P1          13.00 mmec
SFOH        400.1324057 MHz
NUC1        1H
PL1         9.40 dB
DO          0.00000300 sec
PDS         1000.00 mmec
S18         0.00000000 sec
P8          13.00 mmec
S13         0.00000300 sec
S10         0.00018710 sec

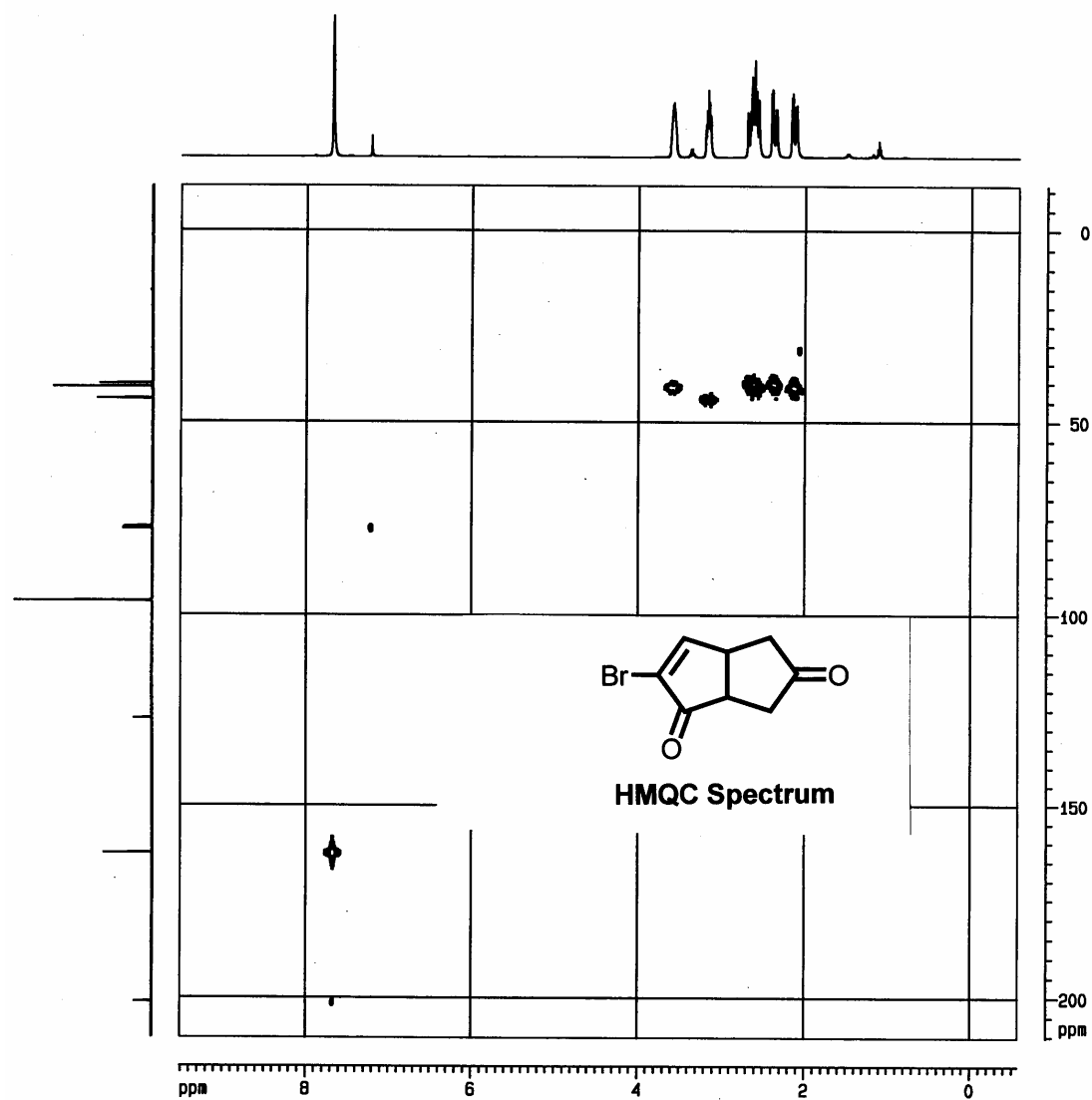
F1 - Acquisition parameters
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TD          128
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FIDRES      41.788745 Hz
DS          13.357 ppm

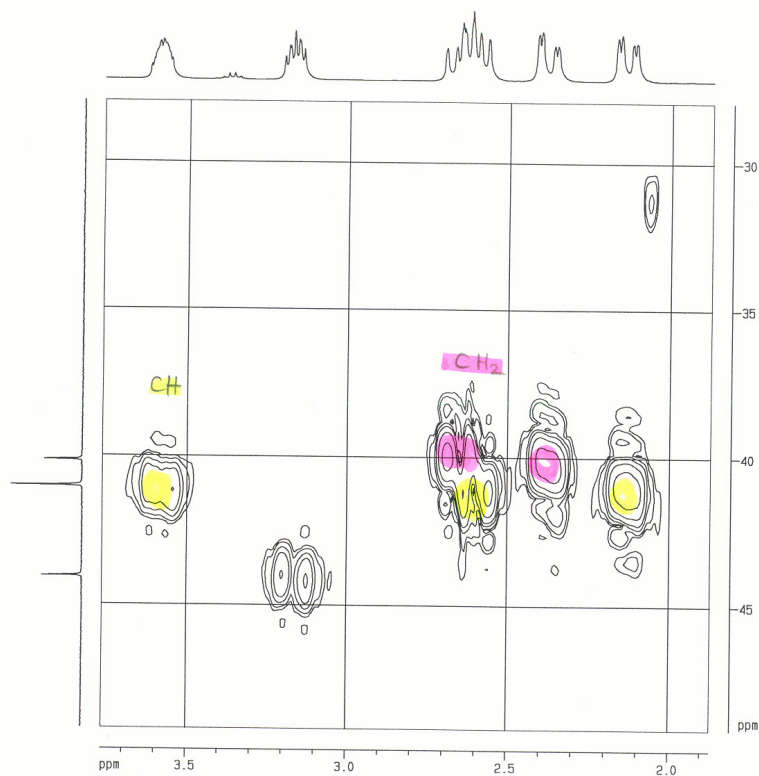
F2 - Processing parameters
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SF          400.1306344 MHz
RG          8192
LB          0
GB          0.00 Hz
GB          0
PC          1.40

F1 - Processing parameters
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RG          8192
LB          0
GB          0.00 Hz
GB          0

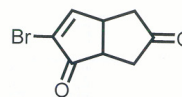
2D NMR plot parameters
CQ2         15.00 cm
CX1         15.00 cm
F2P10       3.781 ppm
F2D1        1504.82 Hz
F2P1C       1.808 ppm
F2D1C       774.88 Hz
F2P1D       3.882 ppm
F2D1D       1505.23 Hz
F2P1H       1.881 ppm
F2D1H       780.74 Hz
F2P1P1C1    0.12188 ppm/cm
F2D1C1      48.88882 Hz/cm
F2P1P1H1    0.13874 ppm/cm
F2D1H1      51.48875 Hz/cm

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f TA-B4.HMGC



expanded HMQC Spectrum

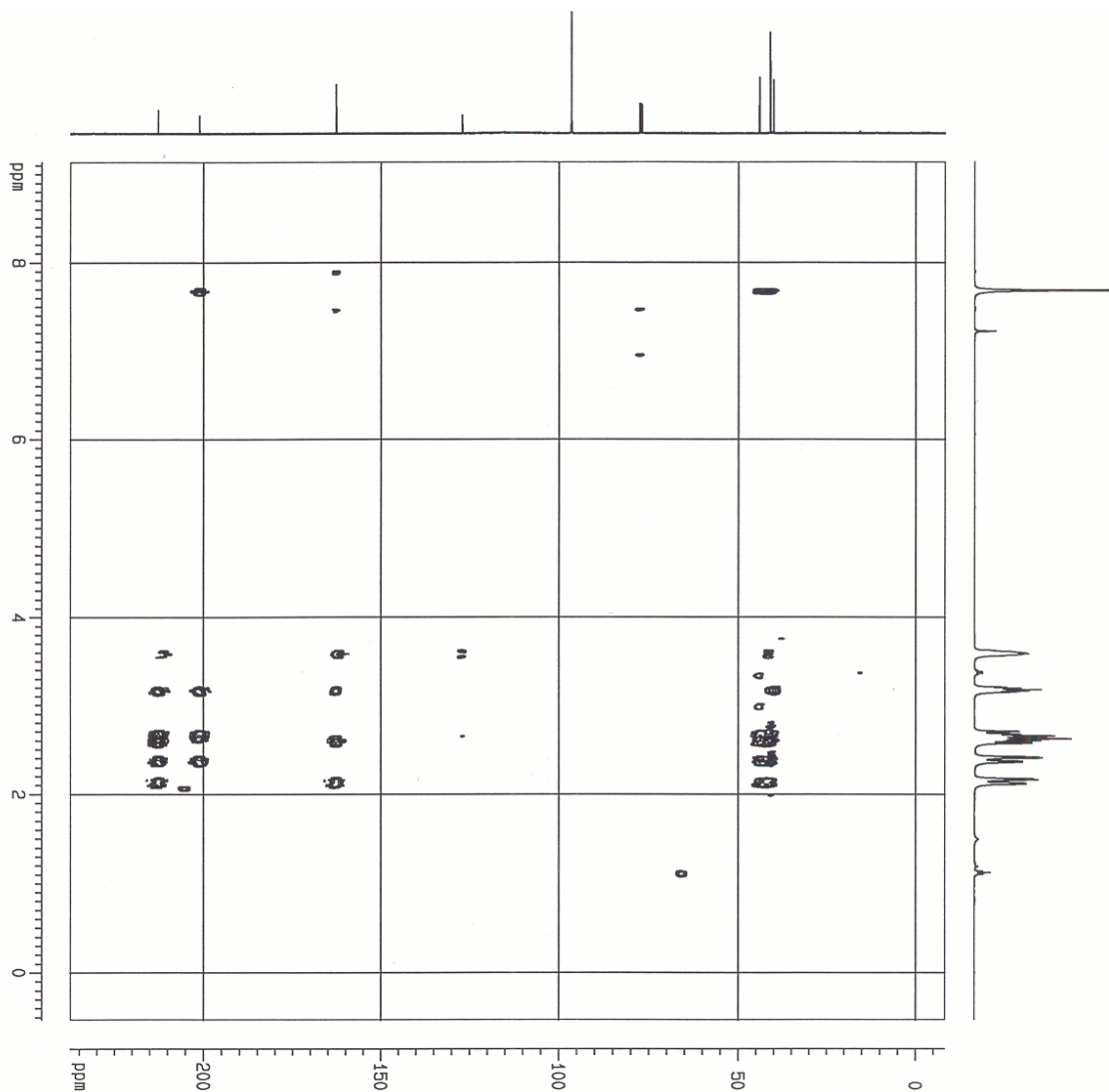
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SM 154.000 uMHC
DE 8.00 uMHC
TE 300.2 K
DZ 0.000000 sec
CZ 0.000000 sec
PZ 1000.00 uMHC
CZ 0.000000 sec
AQ 0.0004700 sec
CZ 0.000000 sec
PZ 53.00 uMHC
SF 400.130000 MHz
NUC1 1H
PL1 0.00 dB
PL2 -1.00 dB
PZ 14.00 uMHC
SF 100.627000 MHz
NUC2 13C
DZ 0.0000000 sec
CZ 0.0000000 sec
PZ 0.00 uMHC
PL1 13.00 dB
CPDPRD 0.00
PCPD 70.00 uMHC
DZ 0.0000000 sec

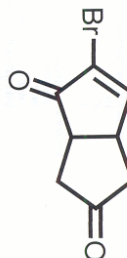
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SF 400.130000 MHz
WDW SINC
SSB 0
LB 0.00 Hz
GB 0
PC 1.40

F3 - Processing parameters
SI 32768
SF 100.627000 MHz
WDW SINC
SSB 0
LB 0.00 Hz
GB 0

2D NMR plot parameters
CZ 10.00 cm
CX 10.00 cm
FOLD 1.700 deg
FOLD 1596.87 Hz
FONE 1.870 deg
FONE 748.30 Hz
FOLD 46.182 deg
FOLD 4966.30 Hz
FONE 27.980 deg
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FIRMOD 1.41548 deg/sec
  
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f TA-84.HMBC



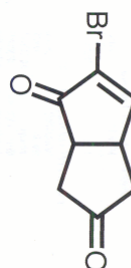
HMBC Spectrum

NAME	5856-204 Hz
PROCESSED	2.327280 Hz
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RG	16384
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DE	8.00 usec
TE	300.2 K
TL	1.50000000 sec
P1	13.00 usec
STOL	400.1284657 MHz
NUC1	13C
NUC2	13C
DE	0.00346000 sec
P2	14.00 usec
STOL	100.6277358 MHz
NUC3	13C
PL2	-1.00 dB
DO	0.00500000 sec
P1B	3.000.00 usec
PLB	0.00000000 sec
P2	28.00 usec
D13	0.00000000 sec
INO	0.00001685 sec

NAME	2
PROCESSED	130
AD	100.6277358 MHz
RG	25648000 Hz
DW	300.018 ppm
DE	0.00 usec
TE	300.2 K
TL	1.50000000 sec
P1	13.00 usec
STOL	400.1284657 MHz
NUC1	13C
NUC2	13C
DE	0.00346000 sec
P2	14.00 usec
STOL	100.6277358 MHz
NUC3	13C
PL2	-1.00 dB
DO	0.00500000 sec
P1B	3.000.00 usec
PLB	0.00000000 sec
P2	28.00 usec
D13	0.00000000 sec
INO	0.00001685 sec

NAME	2
PROCESSED	130
AD	100.6277358 MHz
RG	25648000 Hz
DW	300.018 ppm
DE	0.00 usec
TE	300.2 K
TL	1.50000000 sec
P1	13.00 usec
STOL	400.1284657 MHz
NUC1	13C
NUC2	13C
DE	0.00346000 sec
P2	14.00 usec
STOL	100.6277358 MHz
NUC3	13C
PL2	-1.00 dB
DO	0.00500000 sec
P1B	3.000.00 usec
PLB	0.00000000 sec
P2	28.00 usec
D13	0.00000000 sec
INO	0.00001685 sec

NAME	2
PROCESSED	130
AD	100.6277358 MHz
RG	25648000 Hz
DW	300.018 ppm
DE	0.00 usec
TE	300.2 K
TL	1.50000000 sec
P1	13.00 usec
STOL	400.1284657 MHz
NUC1	13C
NUC2	13C
DE	0.00346000 sec
P2	14.00 usec
STOL	100.6277358 MHz
NUC3	13C
PL2	-1.00 dB
DO	0.00500000 sec
P1B	3.000.00 usec
PLB	0.00000000 sec
P2	28.00 usec
D13	0.00000000 sec
INO	0.00001685 sec



f TA-84.HMBC

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S2	1624	S2	400.1500044 MHz	TD1	1.58
S3	1624	S3	400.1500044 MHz	SFL1	100.02277 MHz
W1	100.81277 MHz	W1	100.81277 MHz	WFL1	235.149000 Hz
W2	100.81277 MHz	W2	100.81277 MHz	WFL2	235.149000 Hz
W3	100.81277 MHz	W3	100.81277 MHz	WFL3	235.149000 Hz
W4	100.81277 MHz	W4	100.81277 MHz	WFL4	235.149000 Hz
W5	100.81277 MHz	W5	100.81277 MHz	WFL5	235.149000 Hz
W6	100.81277 MHz	W6	100.81277 MHz	WFL6	235.149000 Hz
W7	100.81277 MHz	W7	100.81277 MHz	WFL7	235.149000 Hz
W8	100.81277 MHz	W8	100.81277 MHz	WFL8	235.149000 Hz
W9	100.81277 MHz	W9	100.81277 MHz	WFL9	235.149000 Hz
W10	100.81277 MHz	W10	100.81277 MHz	WFL10	235.149000 Hz
W11	100.81277 MHz	W11	100.81277 MHz	WFL11	235.149000 Hz
W12	100.81277 MHz	W12	100.81277 MHz	WFL12	235.149000 Hz
W13	100.81277 MHz	W13	100.81277 MHz	WFL13	235.149000 Hz
W14	100.81277 MHz	W14	100.81277 MHz	WFL14	235.149000 Hz
W15	100.81277 MHz	W15	100.81277 MHz	WFL15	235.149000 Hz
W16	100.81277 MHz	W16	100.81277 MHz	WFL16	235.149000 Hz
W17	100.81277 MHz	W17	100.81277 MHz	WFL17	235.149000 Hz
W18	100.81277 MHz	W18	100.81277 MHz	WFL18	235.149000 Hz
W19	100.81277 MHz	W19	100.81277 MHz	WFL19	235.149000 Hz
W20	100.81277 MHz	W20	100.81277 MHz	WFL20	235.149000 Hz
W21	100.81277 MHz	W21	100.81277 MHz	WFL21	235.149000 Hz
W22	100.81277 MHz	W22	100.81277 MHz	WFL22	235.149000 Hz
W23	100.81277 MHz	W23	100.81277 MHz	WFL23	235.149000 Hz
W24	100.81277 MHz	W24	100.81277 MHz	WFL24	235.149000 Hz
W25	100.81277 MHz	W25	100.81277 MHz	WFL25	235.149000 Hz
W26	100.81277 MHz	W26	100.81277 MHz	WFL26	235.149000 Hz
W27	100.81277 MHz	W27	100.81277 MHz	WFL27	235.149000 Hz
W28	100.81277 MHz	W28	100.81277 MHz	WFL28	235.149000 Hz
W29	100.81277 MHz	W29	100.81277 MHz	WFL29	235.149000 Hz
W30	100.81277 MHz	W30	100.81277 MHz	WFL30	235.149000 Hz
W31	100.81277 MHz	W31	100.81277 MHz	WFL31	235.149000 Hz
W32	100.81277 MHz	W32	100.81277 MHz	WFL32	235.149000 Hz
W33	100.81277 MHz	W33	100.81277 MHz	WFL33	235.149000 Hz
W34	100.81277 MHz	W34	100.81277 MHz	WFL34	235.149000 Hz
W35	100.81277 MHz	W35	100.81277 MHz	WFL35	235.149000 Hz
W36	100.81277 MHz	W36	100.81277 MHz	WFL36	235.149000 Hz
W37	100.81277 MHz	W37	100.81277 MHz	WFL37	235.149000 Hz
W38	100.81277 MHz	W38	100.81277 MHz	WFL38	235.149000 Hz
W39	100.81277 MHz	W39	100.81277 MHz	WFL39	235.149000 Hz
W40	100.81277 MHz	W40	100.81277 MHz	WFL40	235.149000 Hz
W41	100.81277 MHz	W41	100.81277 MHz	WFL41	235.149000 Hz
W42	100.81277 MHz	W42	100.81277 MHz	WFL42	235.149000 Hz
W43	100.81277 MHz	W43	100.81277 MHz	WFL43	235.149000 Hz
W44	100.81277 MHz	W44	100.81277 MHz	WFL44	235.149000 Hz
W45	100.81277 MHz	W45	100.81277 MHz	WFL45	235.149000 Hz
W46	100.81277 MHz	W46	100.81277 MHz	WFL46	235.14

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