Supplementary Material

Four-directional synthesis of adamantane derivatives

Tao Qu, Andrew J. P. White, and Anthony G. M. Barrett*

Department of Chemistry, Imperial College, Molecular Sciences Research Hub, White City Campus, Wood Lane, London, W12 0BZ, England
Email: agmb@ic.ac.uk

Table of Contents

Appendix 1: X-ray Crystal Structure Determination of Tetra-(*Z*)-allylic Alcohol 21

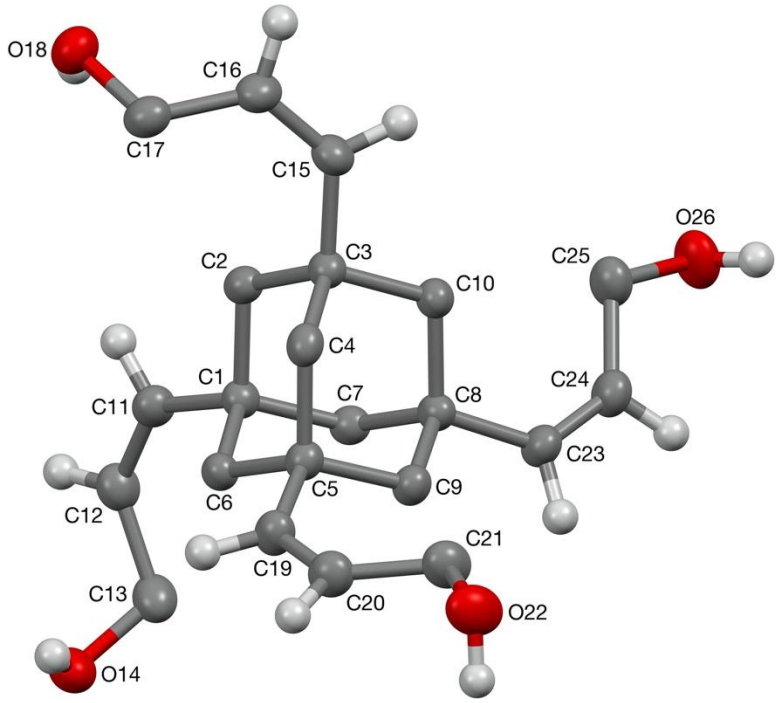


Figure 3. The crystal structure of tetra-(*Z*)-allylic alcohol **21** (50% probability ellipsoids).

*Crystal data for tetra-(Z)-allylic alcohol **21***: $C_{22}H_{32}O_4$, M = 360.47, monoclinic, $P2_1$ (no. 4), a = 7.2942(7), b = 11.5286(12), c = 11.5044(10) Å, β = 92.841(8)°, V = 966.24(16) Å^3, Z = 2, D_c = 1.239 g cm^{-3}, μ(Cu-Kα) = 0.665 mm^{-1}, T = 173 K, colorless needles, Oxford Diffraction Xcalibur PX Ultra diffractometer; 3465 independent measured reflections (R_{int} = 0.0378), F^2 refinement,[51,52] R_1(obs) = 0.0334, wR_2(all) = 0.0826, 2910 independent observed absorption-corrected reflections [$|F_o| > 4\sigma(|F_o|)$, completeness to θ_{full}(67.7°) = 99.7%], 252 parameters. The absolute structure of **21** could not be unambiguously determined [Flack parameter x^+ = –0.01(17)]. CCDC 1982520.

The hydrogen atoms of the O14-, O18-, O22- and O26-based OH groups in the structure of tetra-(Z)-allylic alcohol **21** were all located from ΔF maps and refined freely subject to O–H distance constraints of 0.90 Å.

Appendix 2: X-ray Crystal Structure Determination of Tetra-*syn*-Cyclopropyl Alcohol 35

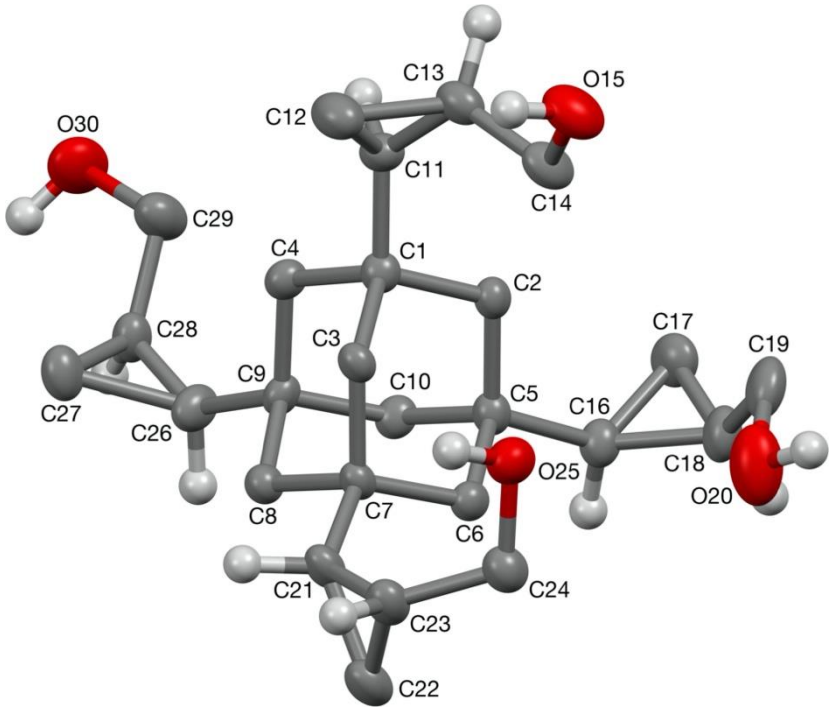


Figure 4. The crystal structure of tetra-*syn*-cyclopropyl alcohol **35** showing the major (*ca*. 64%) occupancy orientation of the C9-bound cyclopropyl alcohol moiety, isomer A (25% probability ellipsoids).

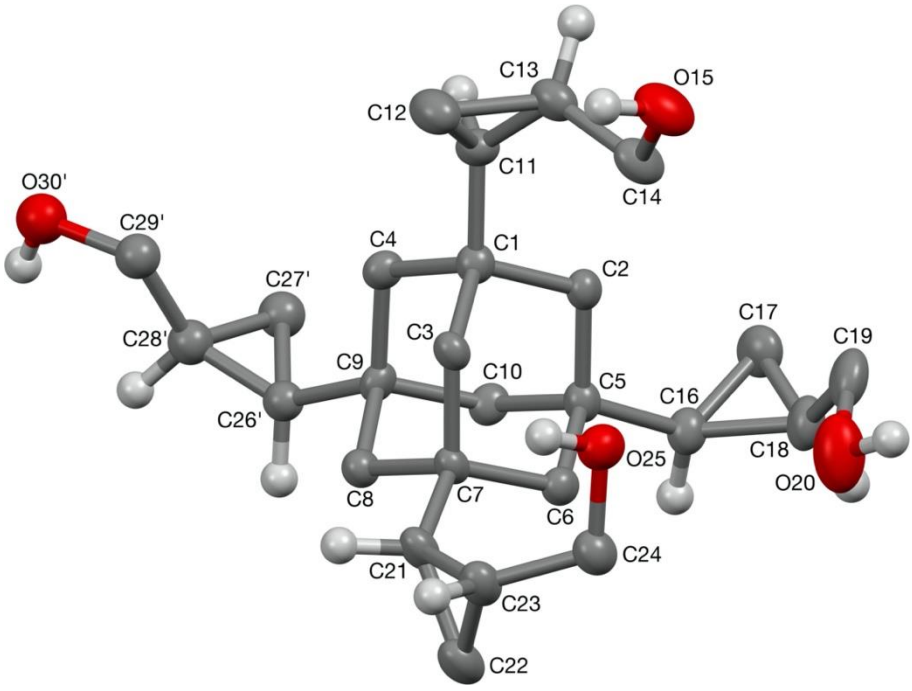


Figure 5. The crystal structure of tetra-*syn*-cyclopropyl alcohol **35** showing the minor (*ca*. 36%) occupancy orientation of the C9-bound cyclopropyl alcohol moiety, isomer B (25% probability ellipsoids).

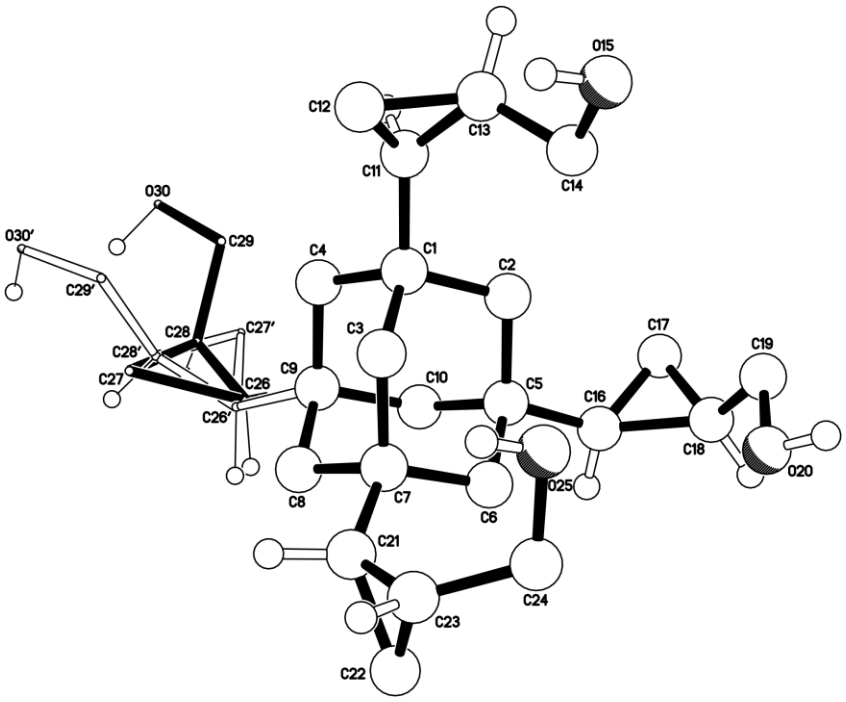


Figure 6. The crystal structure of tetra-*syn*-cyclopropyl alcohol **35** showing an overlay of both the major and minor occupancy orientations of the C9-bound cyclopropyl alcohol moiety. The major (*ca*. 64%) occupancy orientation (isomer A) has been drawn with dark bonds, whilst the minor (*ca*. 36%) occupancy orientation (isomer B) has been drawn with open bonds.

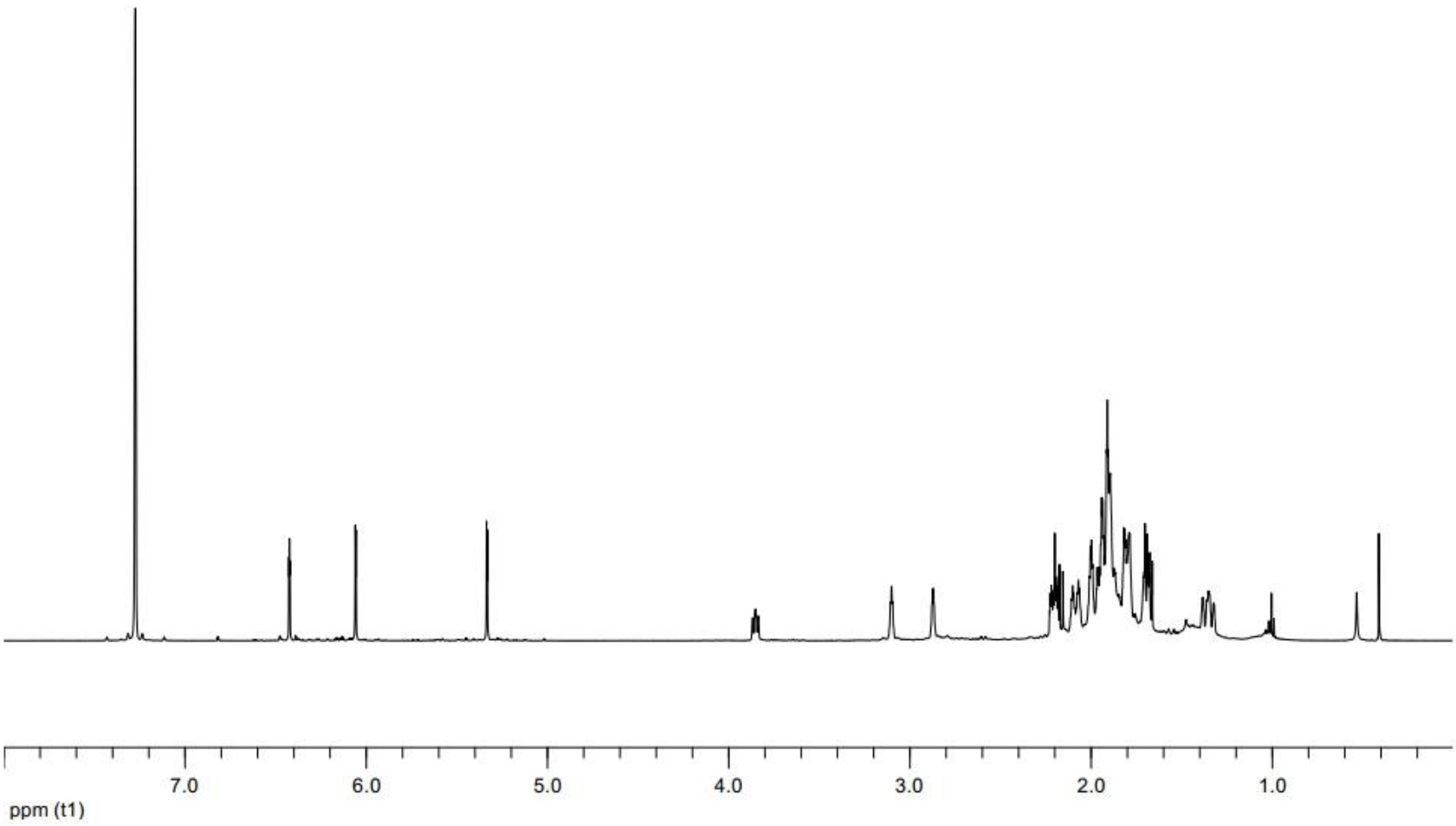
Crystal data for tetra-*syn*-cyclopropyl alcohol **35**: $C_{26}H_{40}O_4$, M = 416.58, monoclinic, $C2$ (no. 5), a = 22.471(3), b = 10.5857(11), c = 9.5321(12) Å, β = 96.404(11)°, V = 2253.3(5) Å^3, Z = 4, D_c = 1.228 g cm^{-3}, μ(Mo-Kα) = 0.081 mm^{-1}, T = 173 K, colorless plates, Oxford Diffraction Xcalibur 3 diffractometer; 6184 independent measured reflections (R_{int} = 0.0833), F^2 refinement,[51,52] R_1(obs) = 0.0905, wR_2(all) = 0.2903, 2785 independent observed absorption-corrected reflections [$|F_o| > 4\sigma(|F_o|)$, completeness to θ_{full}(25.2°) = 99.4%], 294 parameters. The absolute structure of tetra-*syn*-cyclopropyl alcohol **35** could not be determined from the diffraction data [Flack parameter x^+ = 10.0(10)] and so was set by internal reference based on the known stereo-chemistries of the four cyclopropyl alcohol groups. CCDC 1982521.

The C26-based cyclopropyl sidearm in the structure of tetra-*syn*-cyclopropyl alcohol **35** was found to be disordered. Two orientations were identified of *ca*. 64 and 36% occupancy (corresponding to inverted stereo-chemistries at C26 and C28), their geometries were optimized, the thermal parameters of adjacent atoms were restrained to be similar, and only the non-hydrogen atoms of the major occupancy orientation were refined anisotropically (those of the minor occupancy orientation were refined isotropically). The hydrogen atoms of the O15-, O20-, O25- and O30/O30'-based OH groups could not be reliably located from ΔF maps, and adding them in idealized positions with free rotation about the C–O vector to find the best fit with the observed electron density (the SHELX HFIX/AFIX 147 command) gave positions that clashed with adjacent molecules. So, they were added in somewhat arbitrary positions that should be treated with caution.

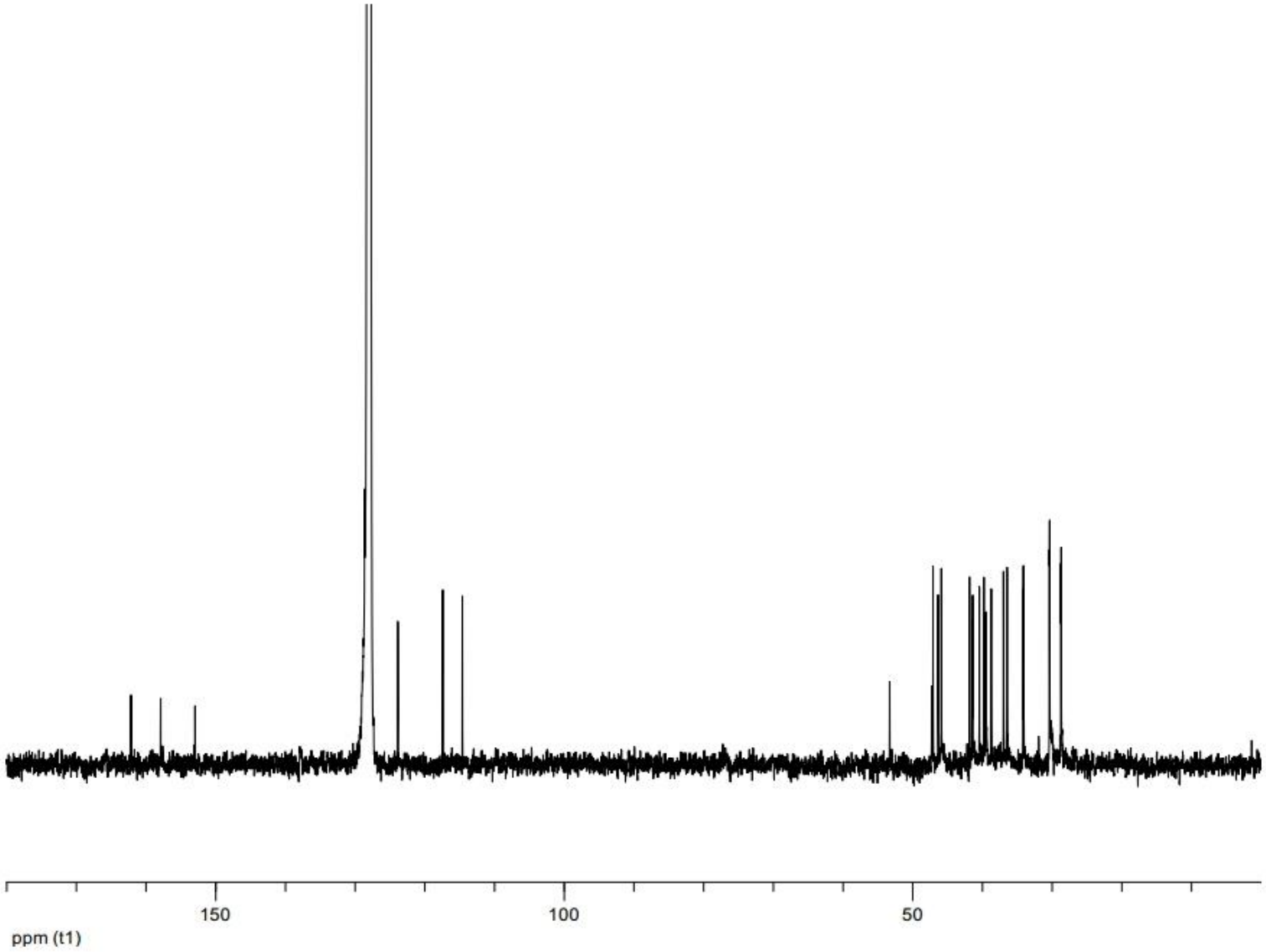
References

51 SHELXTL v5.1, Bruker AXS, Madison, WI, 1998.
52 SHELX-2013, G.M. Sheldrick, *Acta Cryst.*, 2015, **C71**, 3-8.

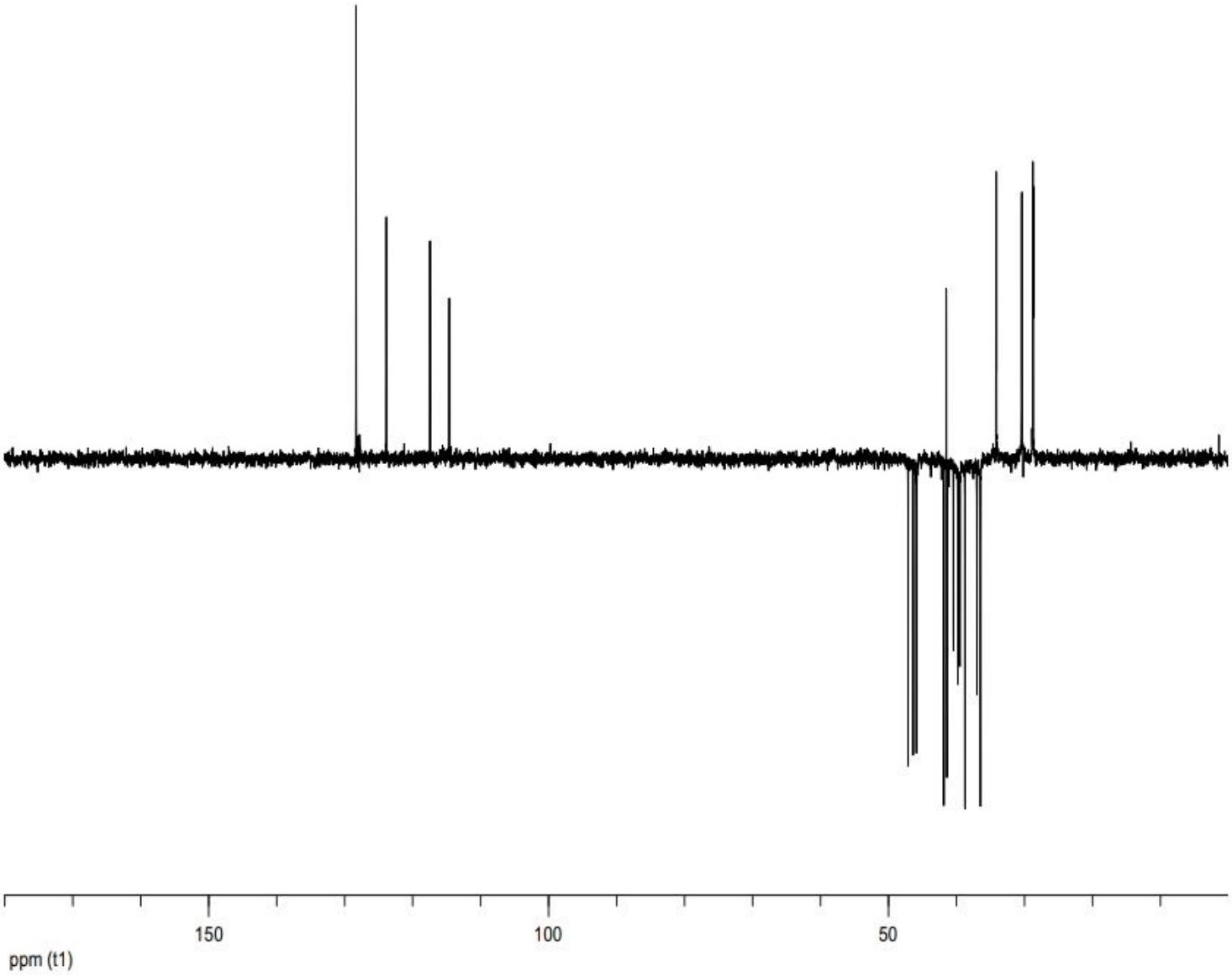
Appendix 3: ^{1}H and ^{13}C spectra of dimer 63.



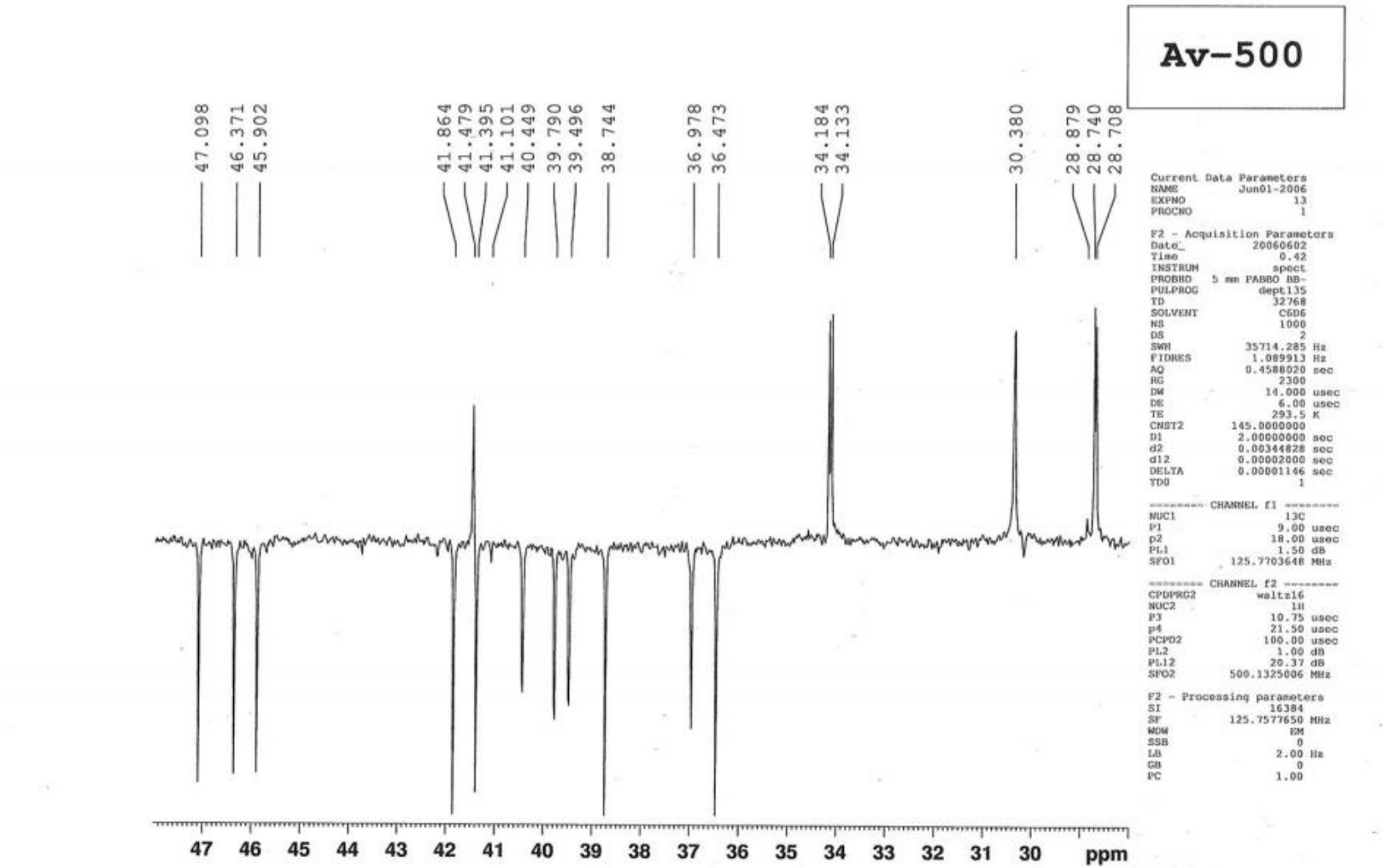
^{1}H NMR of dimer **63** in C_6D_6 (500 MHz).



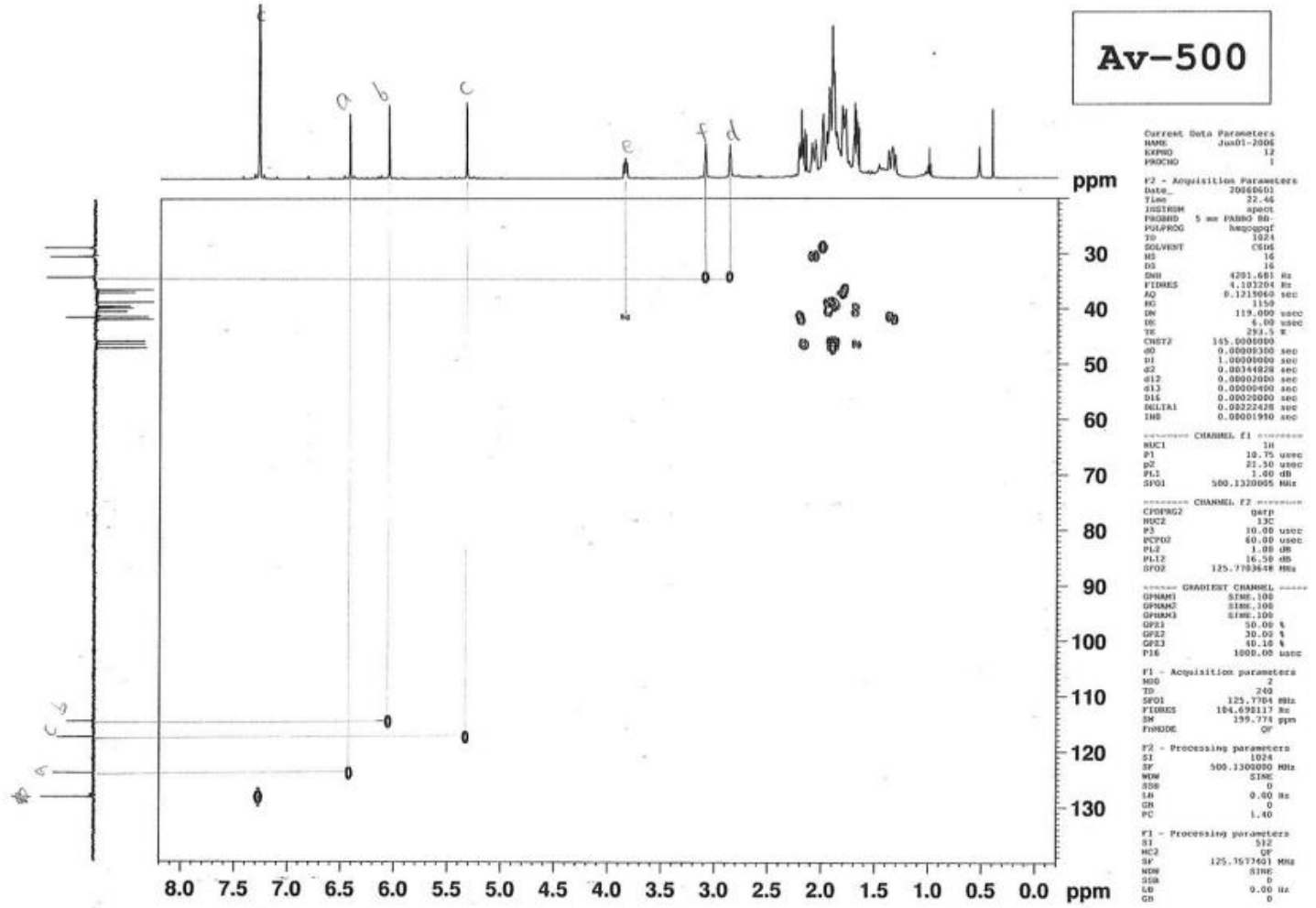
^{13}C NMR of dimer **63** in C_6D_6 (100 MHz).



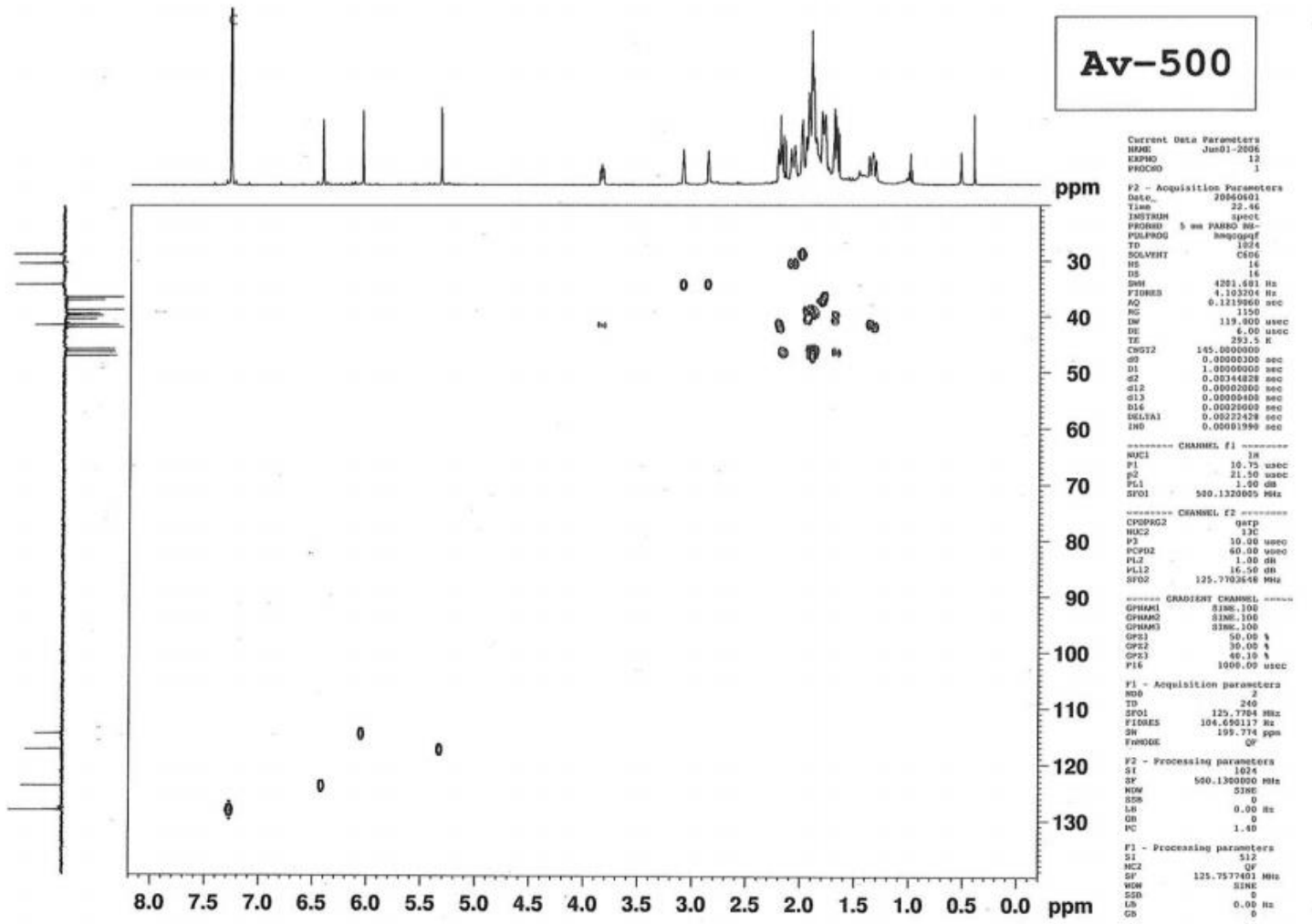
^{13}C DEPT of dimer **63** in C_6D_6 (125 MHz).



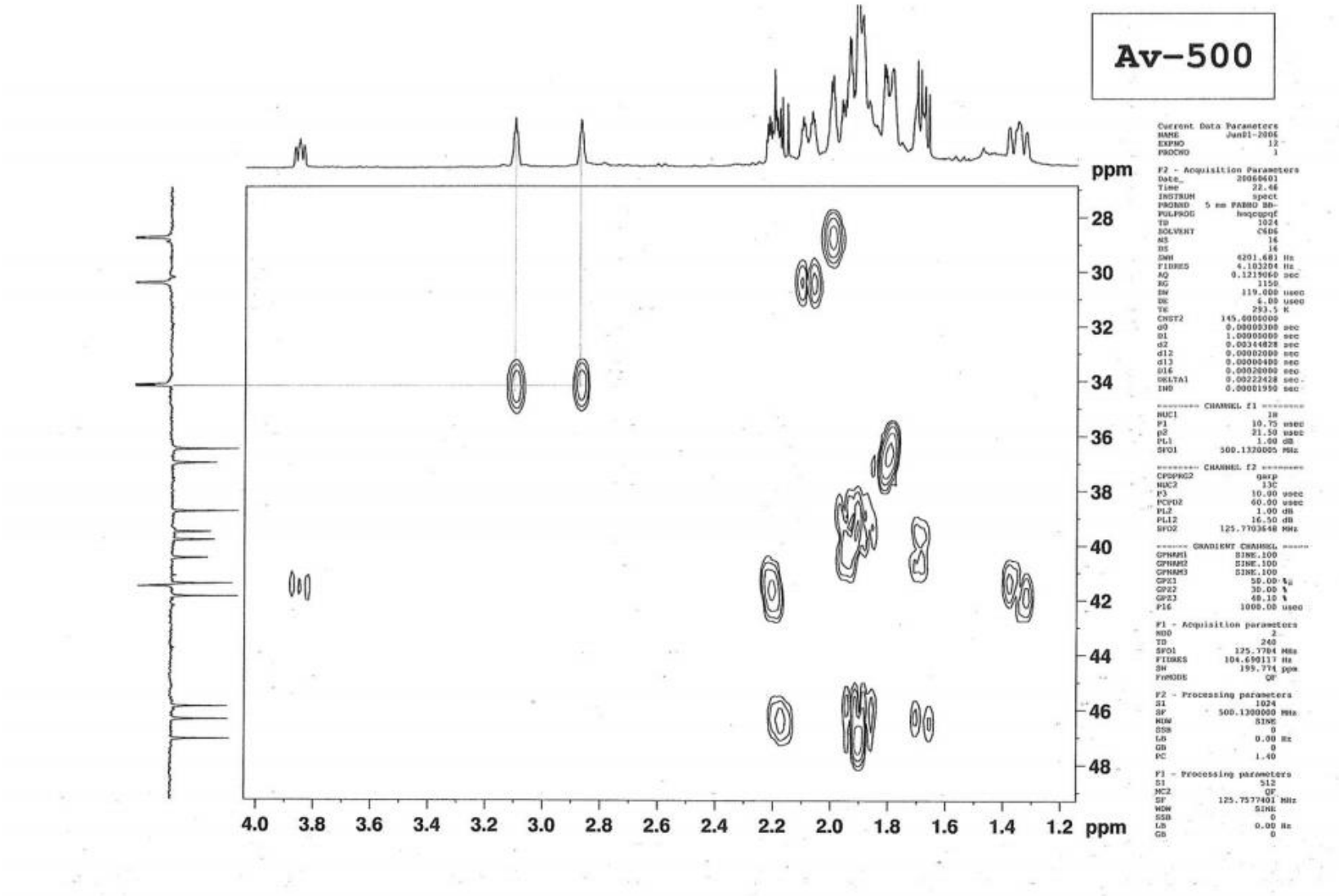
^{13}C DEPT of dimer **63** in C_6D_6 (125 MHz).



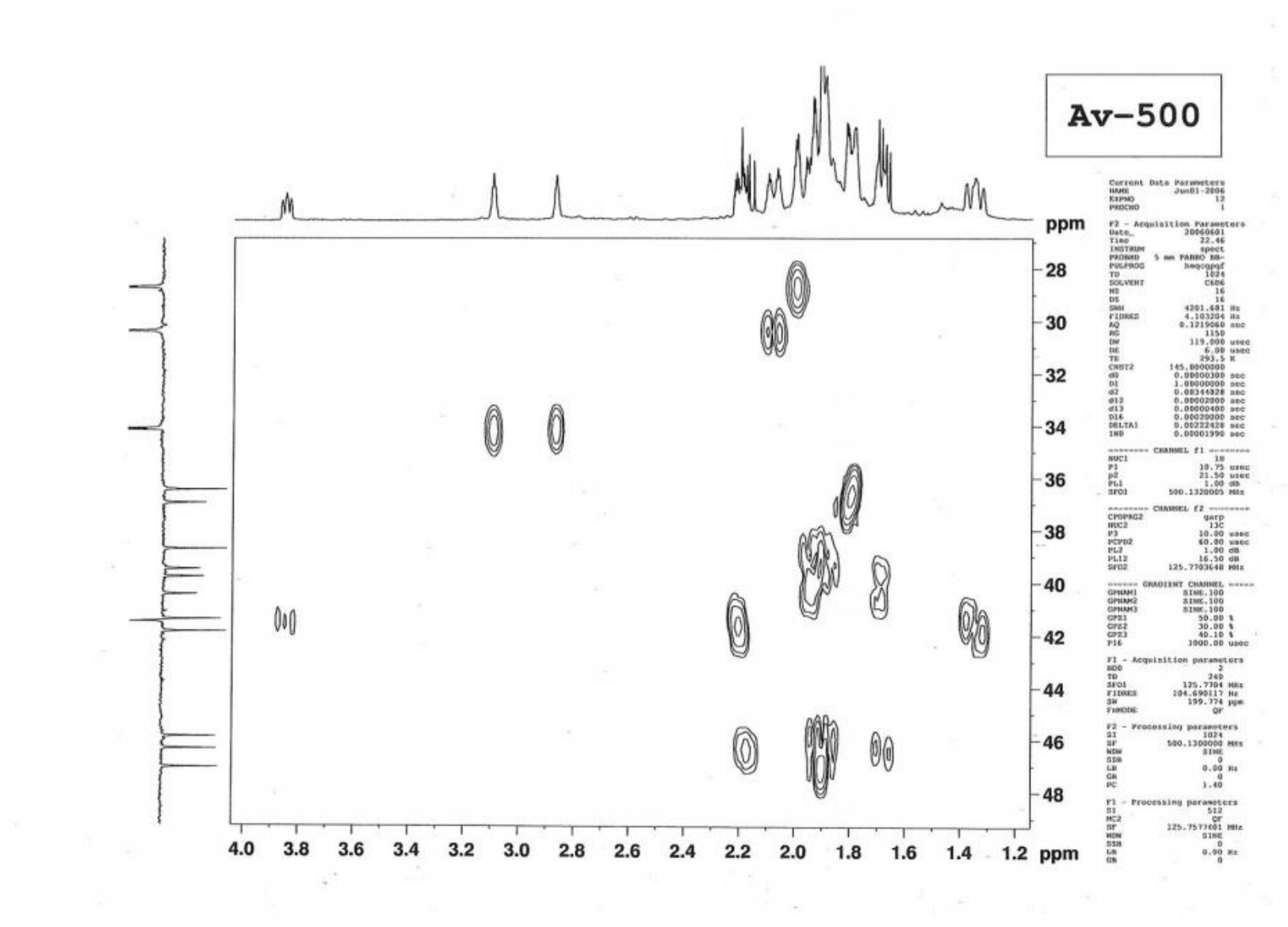
^{1}H and ^{13}C correlation spectrum of dimer **63** in C_6D_6.



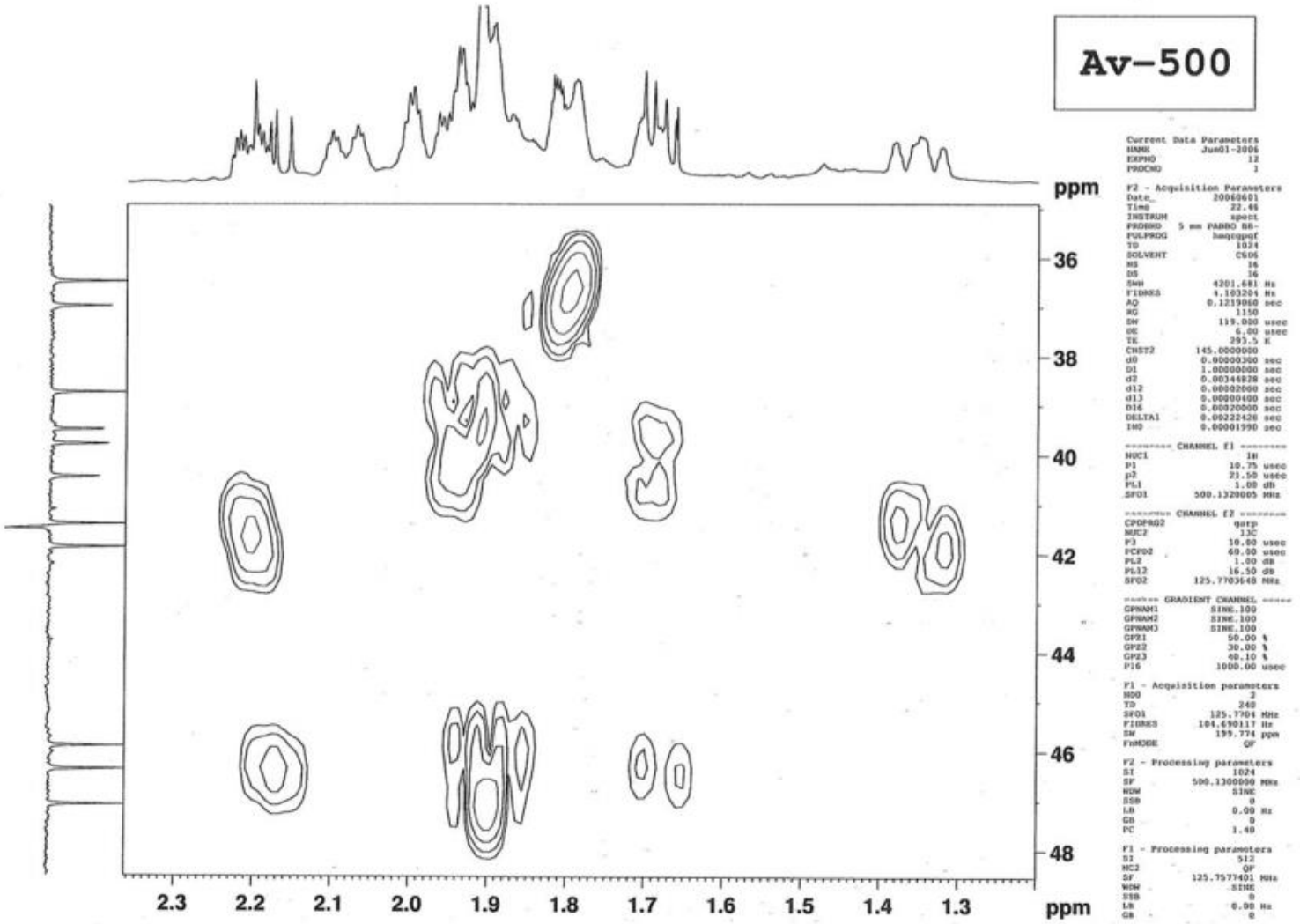
^{1}H and ^{13}C correlation spectrum of dimer **63** in C_6D_6.



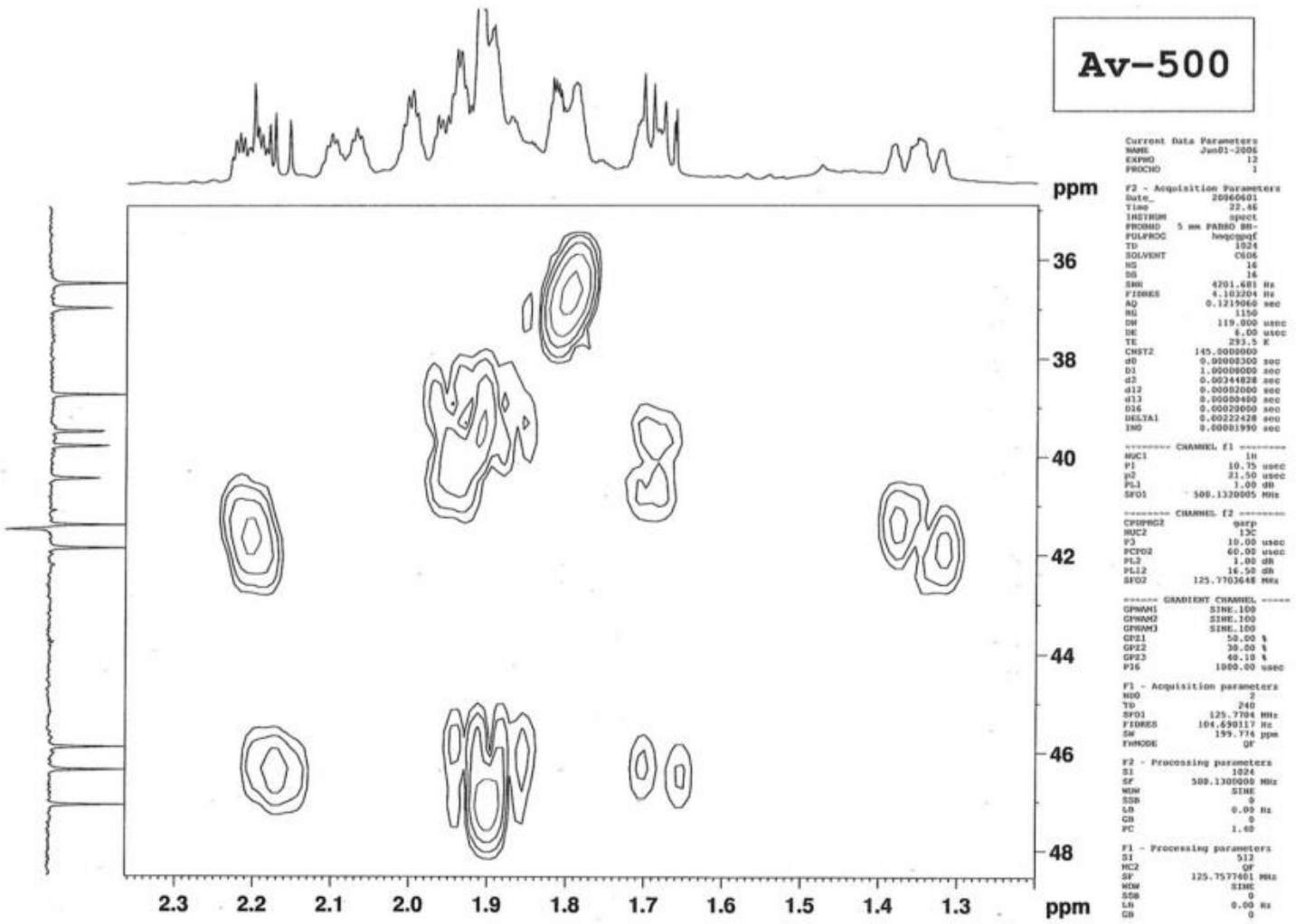
^{1}H and ^{13}C correlation spectrum of dimer **63** in C_6D_6.



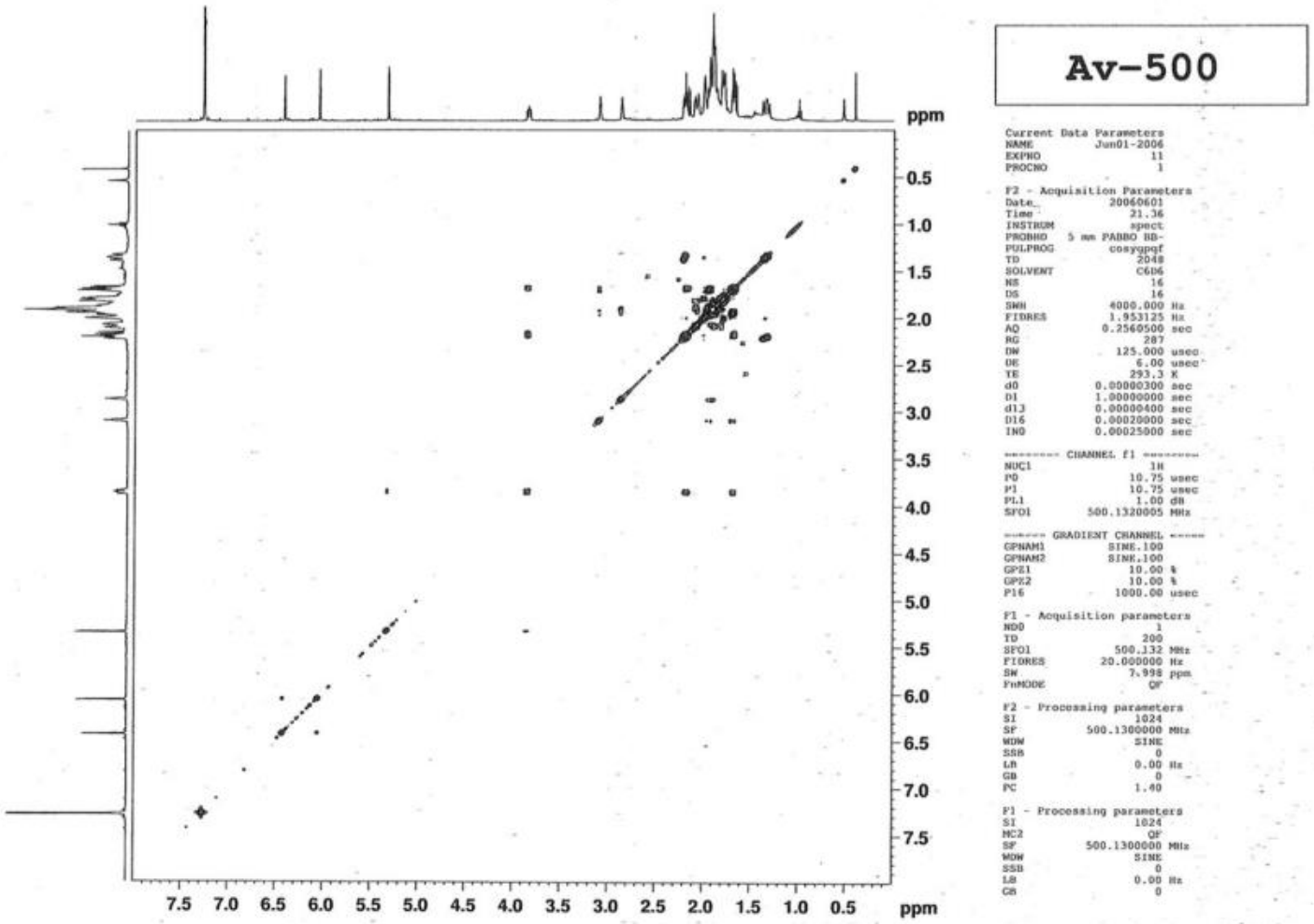
^{1}H and ^{13}C correlation spectrum of dimer **63** in C_6D_6.



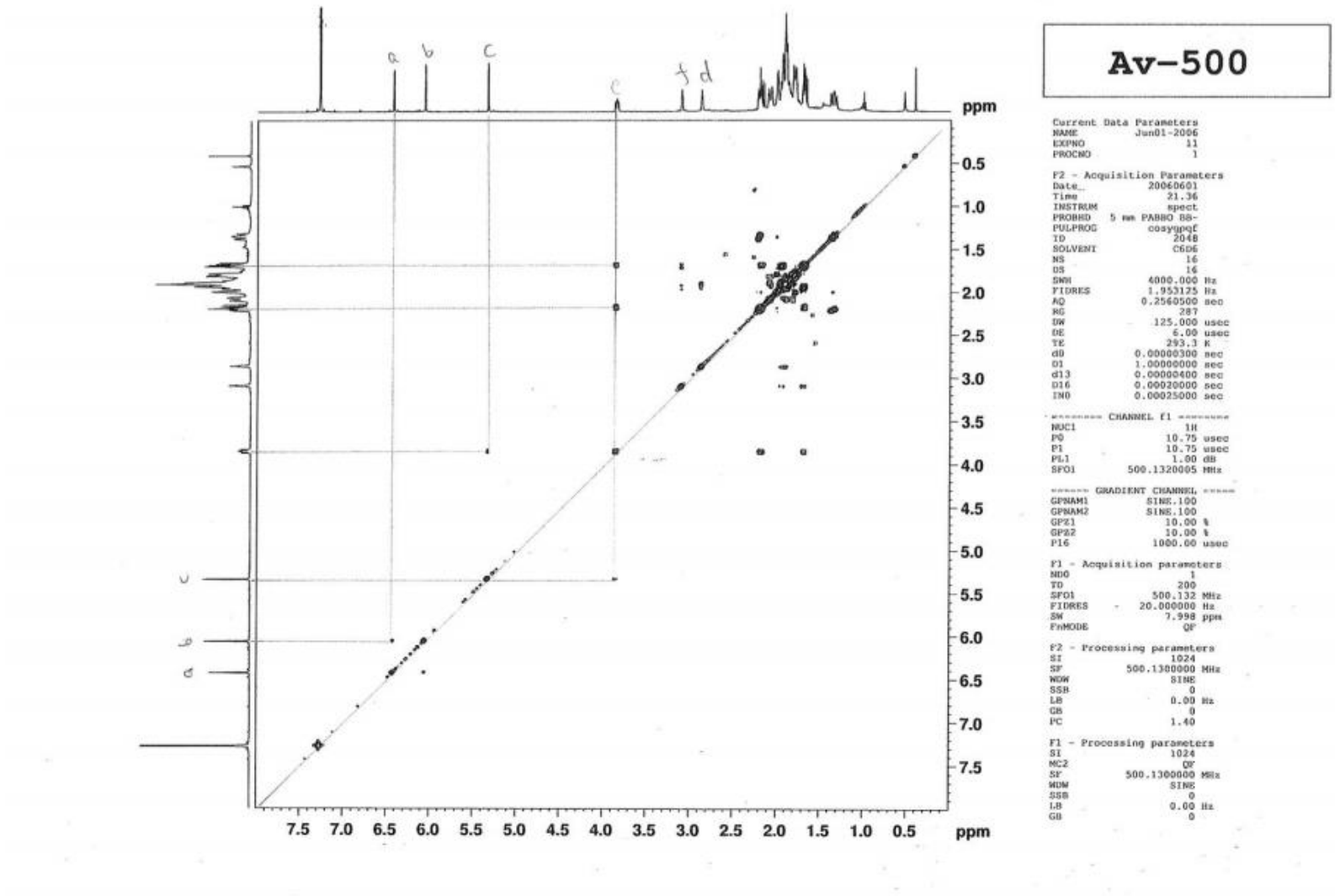
^{1}H and ^{13}C correlation spectrum of dimer **63** in C_6D_6.



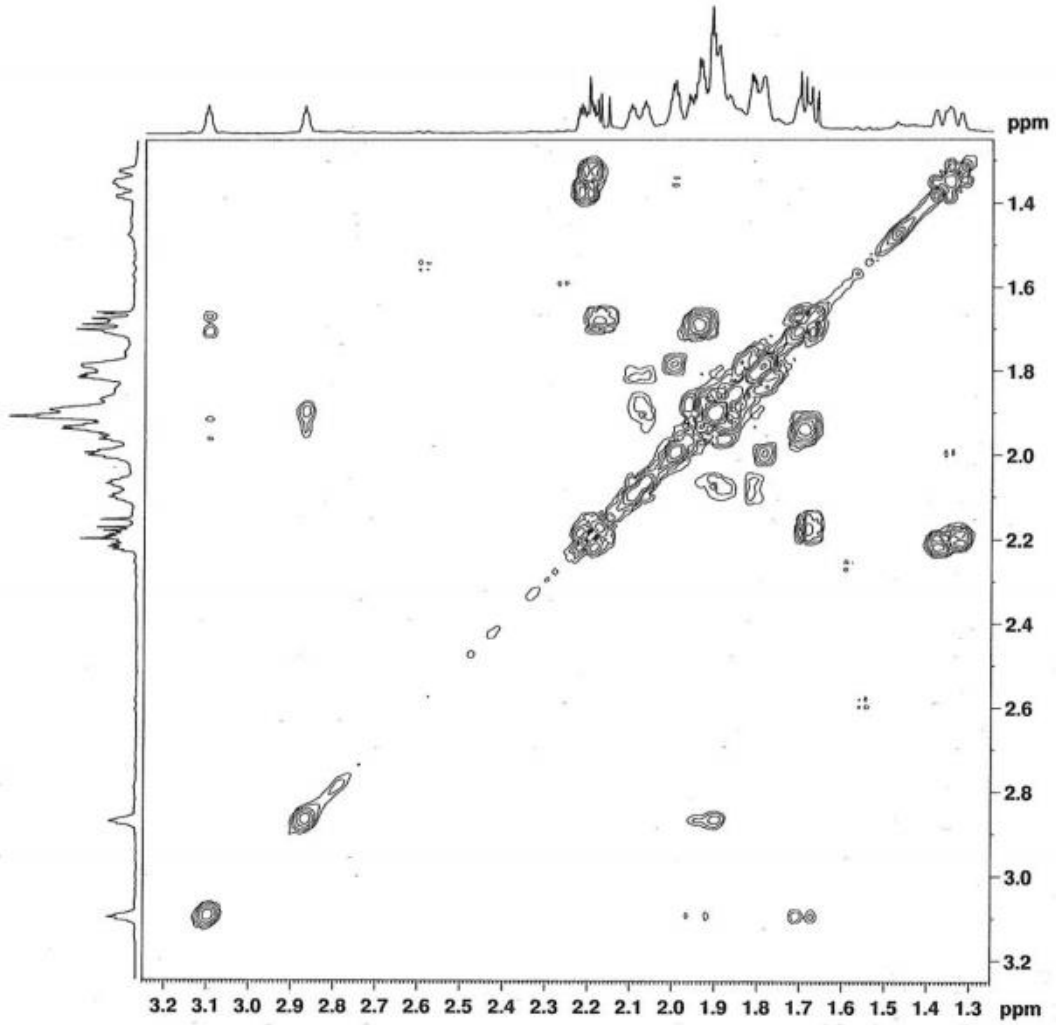
^{1}H and ^{13}C correlation spectrum of dimer **63** in C_6D_6.



^{1}H COSY spectrum of dimer **63** in C_6D_6.



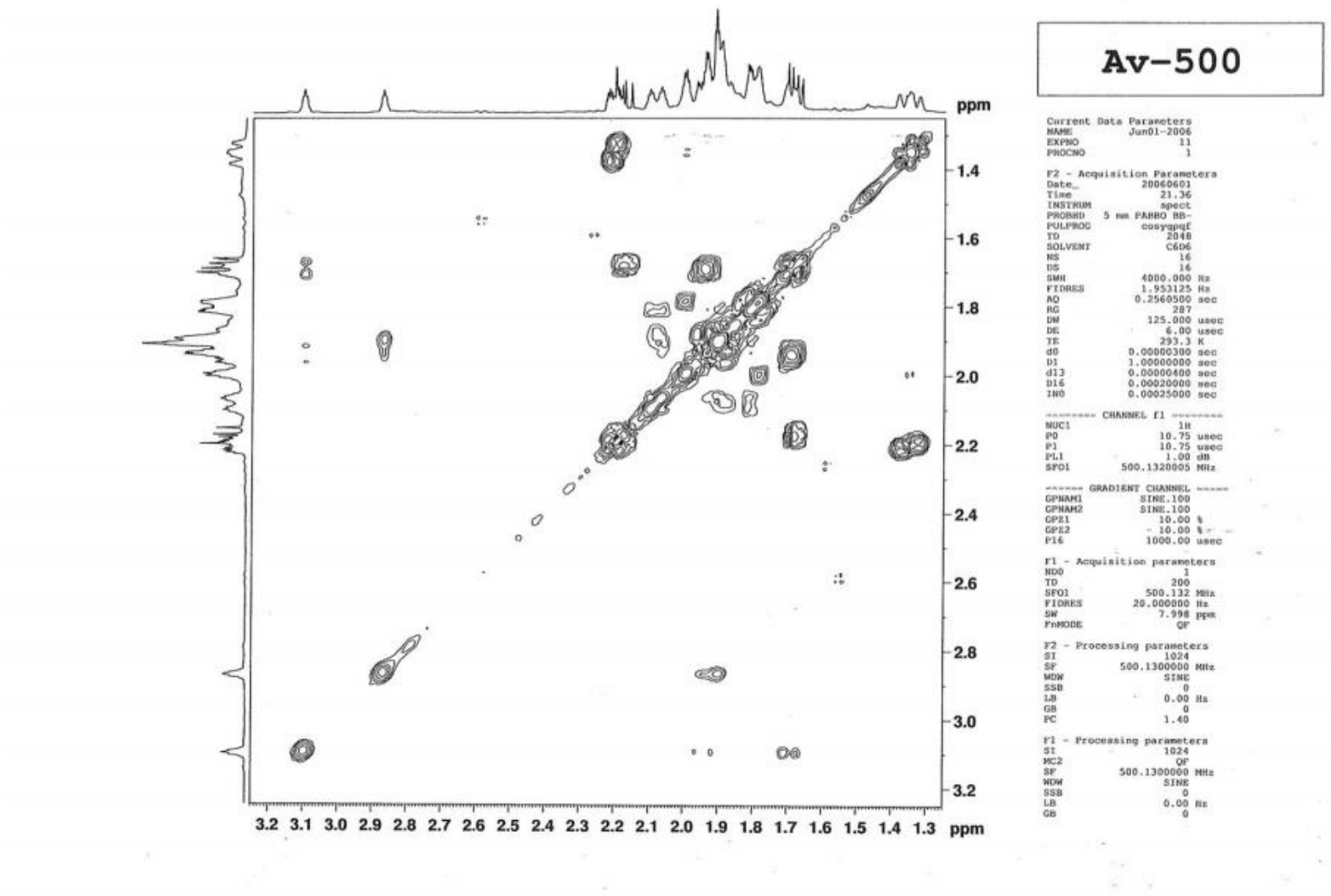
^{1}H COSY spectrum of dimer **63** in C_6D_6.



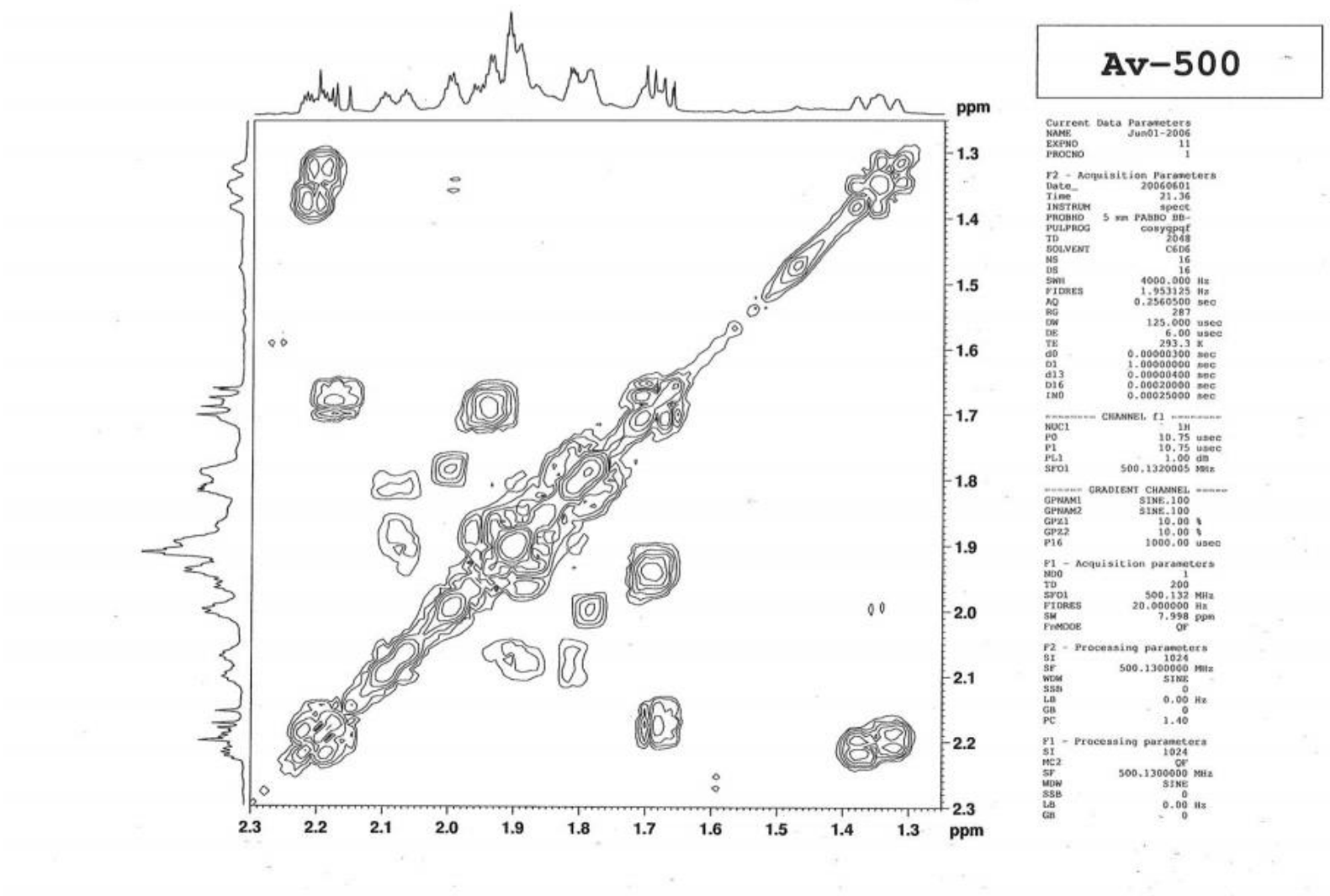
Av–500

```
Current Data Parameters
NAME            Jun01-2006
EXPNO                   11
PROCNO                   1

F2 - Acquisition Parameters
Date_             20060601
Time                 21.36
INSTRUM              spect
PROBHD    5 mm PABBO BB-
PULPROG          cosygpqf
TD                   2048
SOLVENT              C6D6
NS                     16
DS                     16
SWH               4000.000 Hz
FIDRES            1.953125 Hz
AQ                0.2560500 sec
RG                    287
DW                 125.000 usec
DE                   6.00 usec
TE                  293.3 K
d0                0.00000300 sec
D1                1.00000000 sec
d13               0.00000400 sec
D16               0.00020000 sec
IN0               0.00025000 sec

======== CHANNEL f1 ========
NUC1                   1H
P0                  10.75 usec
P1                  10.75 usec
PL1                  1.00 dB
SFO1          500.1320005 MHz

====== GRADIENT CHANNEL =====
GPNAM1             SINE.100
GPNAM2             SINE.100
GPZ1                 10.00 %
GPZ2                 10.00 %
P16                1000.00 usec

F1 - Acquisition parameters
ND0                      1
TD                     200
SFO1            500.132 MHz
FIDRES         20.000000 Hz
SW                 7.998 ppm
FnMODE                QF

F2 - Processing parameters
SI                    1024
SF            500.1300000 MHz
WDW                   SINE
SSB                      0
LB                    0.00 Hz
GB                       0
PC                    1.40

F1 - Processing parameters
SI                    1024
MC2                     QF
SF            500.1300000 MHz
WDW                   SINE
SSB                      0
LB                    0.00 Hz
GB                       0
```

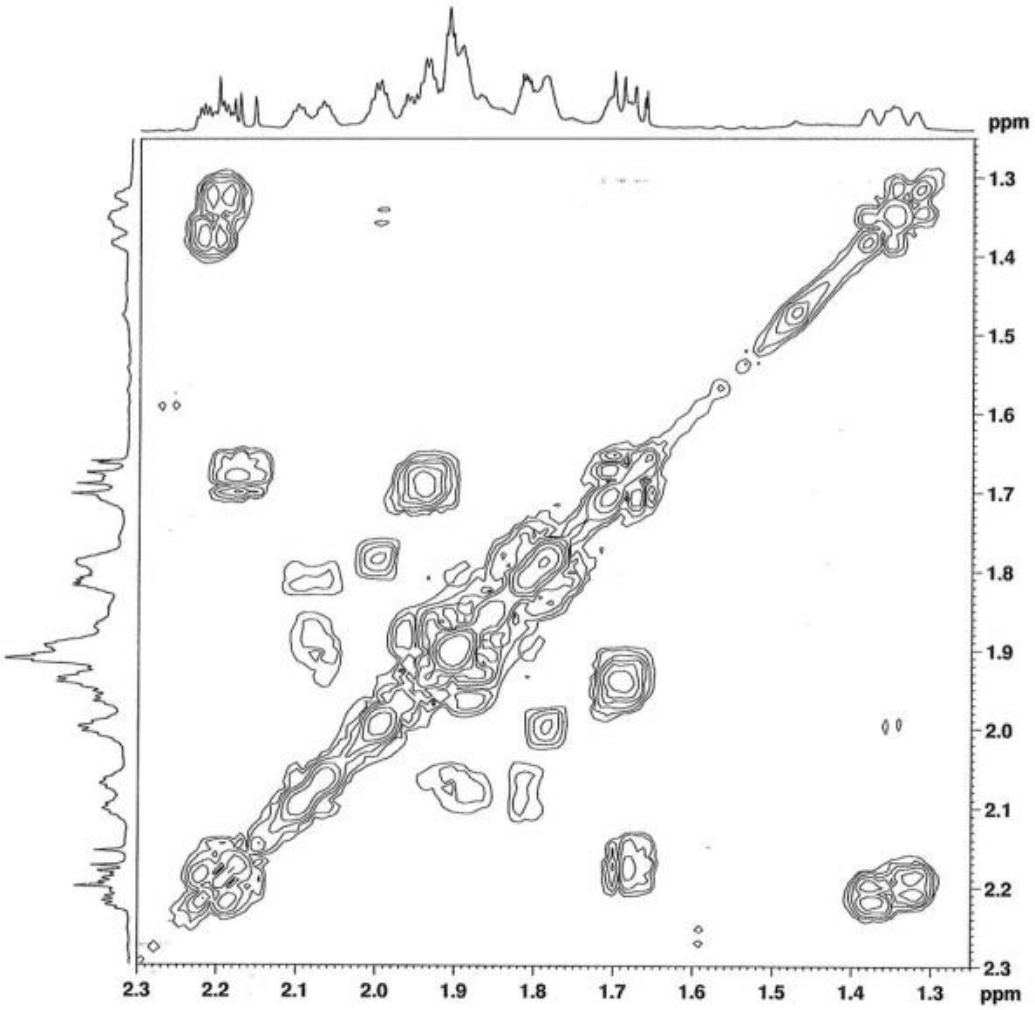
^{1}H COSY spectrum of dimer **63** in C_6D_6.



^{1}H COSY spectrum of dimer **63** in C_6D_6.



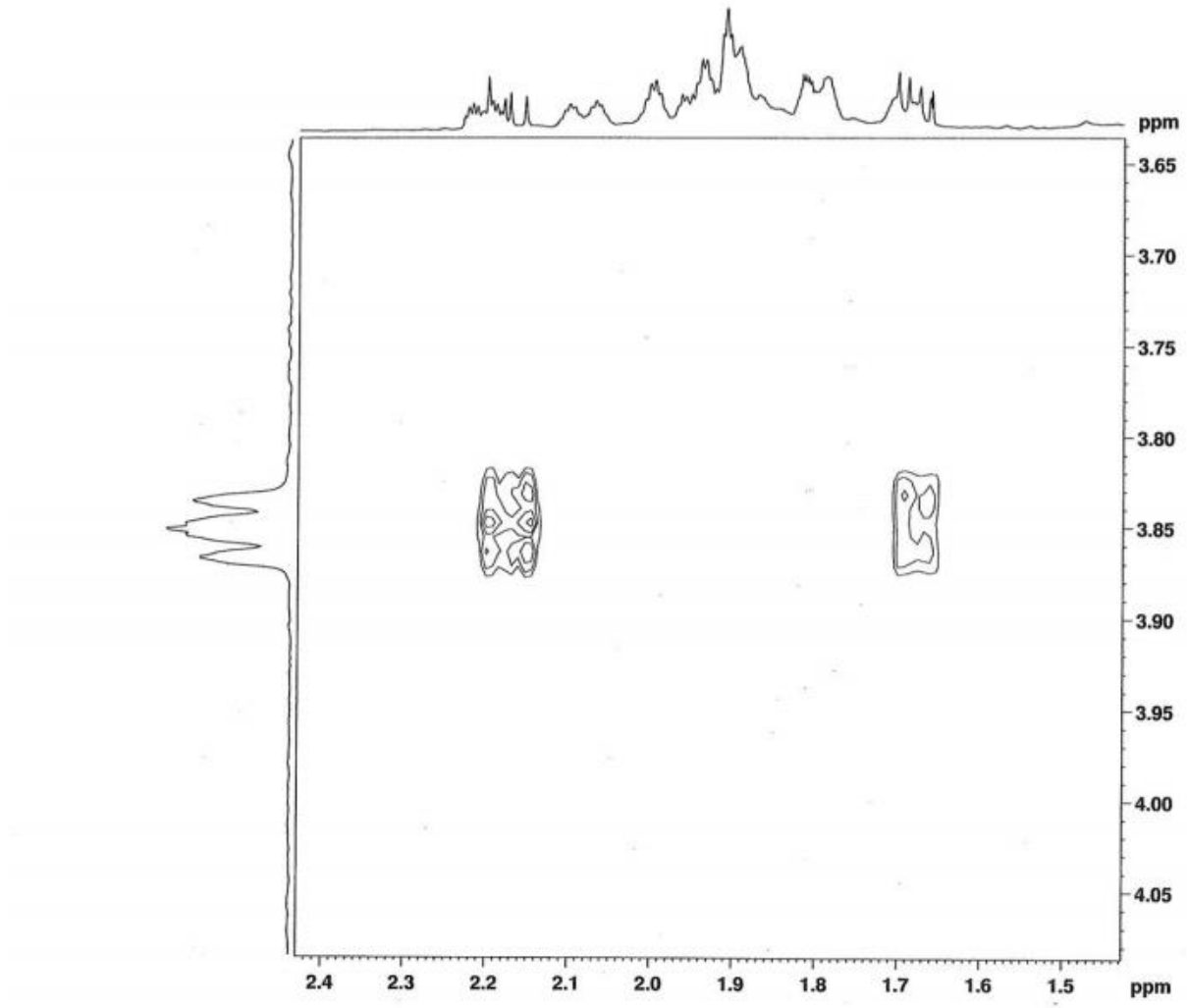
^{1}H COSY spectrum of dimer **63** in C_6D_6.



Av-500

```
Current Data Parameters
NAME            Jun01-2006
EXPNO                   11
PROCNO                   1

F2 - Acquisition Parameters
Date_             20060601
Time                 21.36
INSTRUM              spect
PROBHD   5 mm PABBO BB-
PULPROG          cosygpqf
TD                   2048
SOLVENT              C6D6
NS                     16
DS                     16
SWH               4000.000 Hz
FIDRES            1.953125 Hz
AQ               0.2560500 sec
RG                     287
DW                 125.000 usec
DE                   6.00 usec
TE                  293.3 K
d0               0.00000300 sec
D1               1.00000000 sec
d13              0.00000400 sec
D16              0.00020000 sec
IN0              0.00025000 sec

======== CHANNEL f1 ========
NUC1                   1H
P0                  10.75 usec
P1                  10.75 usec
PL1                  1.00 dB
SFO1           500.1320005 MHz

====== GRADIENT CHANNEL =====
GPNAM1           SINE.100
GPNAM2           SINE.100
GPZ1                10.00 %
GPZ2                10.00 %
P16               1000.00 usec

F1 - Acquisition parameters
ND0                     1
TD                    200
SFO1           500.132 MHz
FIDRES        20.000000 Hz
SW                7.998 ppm
FnMODE                QF

F2 - Processing parameters
SI                    1024
SF           500.1300000 MHz
WDW                   SINE
SSB                      0
LB                    0.00 Hz
GB                       0
PC                    1.40

F1 - Processing parameters
SI                    1024
MC2                     QF
SF           500.1300000 MHz
WDW                   SINE
SSB                      0
LB                    0.00 Hz
GB                       0
```

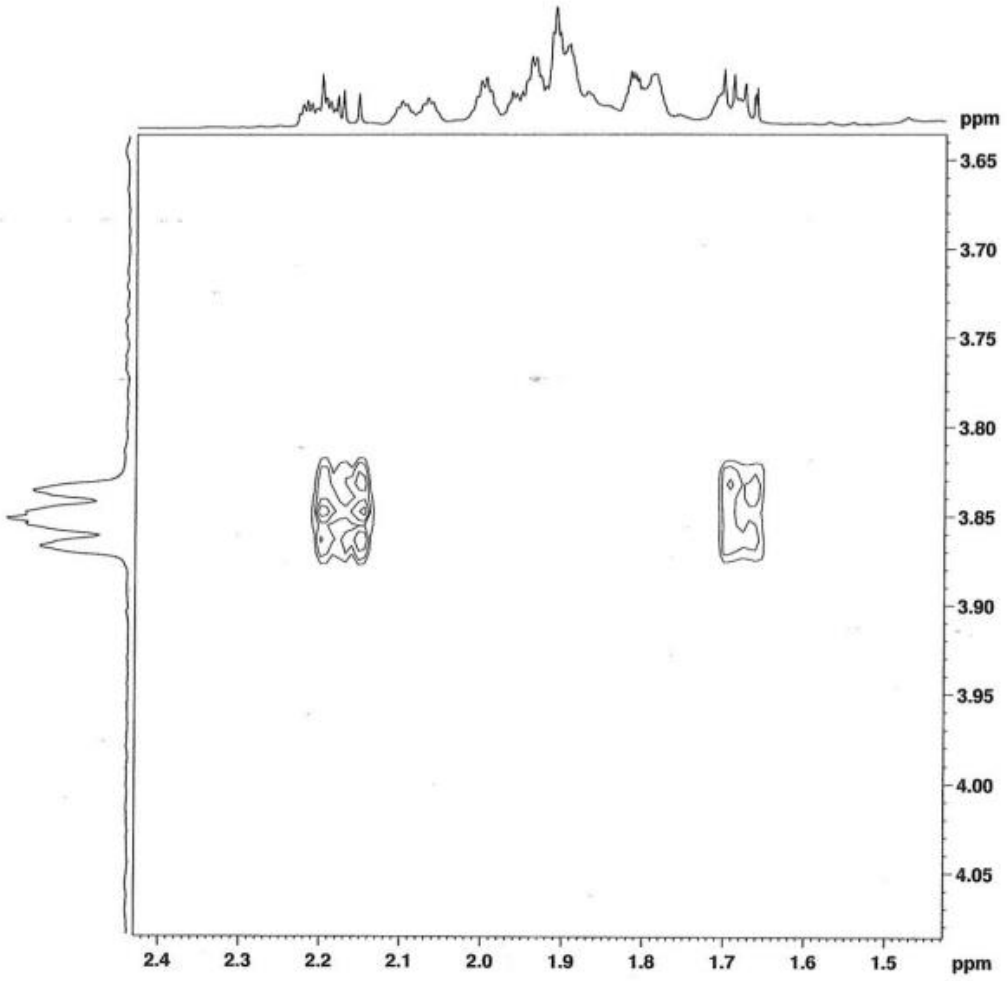
^{1}H COSY spectrum of dimer **63** in C_6D_6.



Av-500

```
Current Data Parameters
NAME            Jun01-2006
EXPNO                   11
PROCNO                   1

F2 - Acquisition Parameters
Date_             20060601
Time                 21.36
INSTRUM              spect
PROBHD   5 mm PABBO BB-
PULPROG          cosygpqf
TD                   2048
SOLVENT              C6D6
NS                     16
DS                     16
SWH               4000.000 Hz
FIDRES            1.953125 Hz
AQ               0.2560500 sec
RG                    287
DW                 125.000 usec
DE                   6.00 usec
TE                  293.3 K
d0               0.00000300 sec
D1               1.00000000 sec
d13              0.00000400 sec
D16              0.00020000 sec
IN0              0.00025000 sec

======== CHANNEL f1 ========
NUC1                   1H
P0                  10.75 usec
P1                  10.75 usec
PL1                  1.00 dB
SFO1          500.1320005 MHz

====== GRADIENT CHANNEL =====
GPNAM1           SINE.100
GPNAM2           SINE.100
GPZ1                10.00 %
GPZ2                10.00 %
P16               1000.00 usec

F1 - Acquisition parameters
NDO                     1
TD                    200
SFO1              500.132 MHz
FIDRES          20.000000 Hz
SW                 7.998 ppm
FnMODE                 QF

F2 - Processing parameters
SI                   1024
SF            500.1300000 MHz
WDW                  SINE
SSB                     0
LB                   0.00 Hz
GB                      0
PC                   1.40

F1 - Processing parameters
SI                   1024
MC2                    QF
SF            500.1300000 MHz
WDW                  SINE
SSB                     0
LB                   0.00 Hz
GB                      0
```

^{1}H COSY spectrum of dimer **63** in C_6D_6.



Av–500

```
Current Data Parameters
NAME                 Jun01-2006
EXPNO                        11
PROCNO                        1

F2 - Acquisition Parameters
Date_              20060601
Time                      21.36
INSTRUM                   spect
PROBHD    5 mm PABBO BB-
PULPROG                cosygpqf
TD                         2048
SOLVENT                    C6D6
NS                           16
DS                           16
SWH                  4000.000 Hz
FIDRES               1.953125 Hz
AQ                  0.2560500 sec
RG                         287
DW                   125.000 usec
DE                     6.00 usec
TE                     293.3 K
d0                  0.00000300 sec
D1                  1.00000000 sec
d13                 0.00000400 sec
D16                 0.00020000 sec
IN0                 0.00025000 sec

======== CHANNEL f1 ========
NUC1                         1H
P0                       10.75 usec
P1                       10.75 usec
PL1                       1.00 dB
SFO1               500.1320005 MHz

====== GRADIENT CHANNEL =====
GPNAM1                SINE.100
GPNAM2                SINE.100
GPZ1                     10.00 %
GPZ2                     10.00 %
P16                    1000.00 usec

F1 - Acquisition parameters
NDO                          1
TD                         200
SFO1                 500.132 MHz
FIDRES              20.000000 Hz
SW                       7.998 ppm
FnMODE                      QF

F2 - Processing parameters
SI                        1024
SF                 500.1300000 MHz
WDW                       SINE
SSB                          0
LB                        0.00 Hz
GB                           0
PC                        1.40

F1 - Processing parameters
SI                        1024
MC2                         QF
SF                 500.1300000 MHz
WDW                       SINE
SSB                          0
LB                        0.00 Hz
GB                           0
```

^{1}H COSY spectrum of dimer **63** in C_6D_6.

checkCIF (basic structural check) running

Checking for embedded fcf data in CIF ...
Found embedded fcf data in CIF. Extracting fcf data from uploaded CIF, please wait . . . . .

checkCIF/PLATON (basic structural check)

Structure factors have been supplied for datablock(s) 21, 35

THIS REPORT IS FOR GUIDANCE ONLY. IF USED AS PART OF A REVIEW PROCEDURE FOR PUBLICATION, IT SHOULD NOT REPLACE THE EXPERTISE OF AN EXPERIENCED CRYSTALLOGRAPHIC REFEREE.

No syntax errors found. CIF dictionary
Please wait while processing .... Interpreting this report

Structure factor report

Datablock: 21

Bond precision: C–C = 0.0040 A Wavelength=1.54248
Cell: a=7.2942(7) b=11.5286(12) c=11.5044(10)
alpha=90 beta=92.841(8) gamma=90
Temperature: 173 K

	Calculated	Reported
Volume	966.24(16)	966.24(16)
Space group	P 21	P 21
Hall group	P 2yb	P 2yb
Moiety formula	C22 H32 O4	C22 H32 O4
Sum formula	C22 H32 O4	C22 H32 O4
Mr	360.48	360.47
Dx,g cm-3	1.239	1.239
Z	2	2
Mu (mm-1)	0.665	0.665
F000	392.0	392.0
F000'	393.15	
h,k,lmax	8,14,14	8,13,13
Nref	3709[1952]	3465
Tmin,Tmax	0.946,0.967	0.880,0.969
Tmin'	0.858	

Correction method= # Reported T Limits: Tmin=0.880 Tmax=0.969
AbsCorr = ANALYTICAL
Data completeness= 1.78/0.93 Theta(max)= 70.874
R(reflections)= 0.0334(2910) wR2(reflections)= 0.0826(3465)
S = 0.981 Npar= 252

The following ALERTS were generated. Each ALERT has the format
test-name_ALERT_alert-type_alert-level.
Click on the hyperlinks for more details of the test.

Alert level C

RADNW01_ALERT_1_C The radiation wavelength lies outside the expected range for the supplied radiation type. Expected range 1.54175-1.54180 Wavelength given = 1.54248
PLAT222_ALERT_3_C NonSolvent Resd 1 H Uiso(max)/Uiso(min) Range 4.1 Ratio
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.600 6 Report
PLAT915_ALERT_3_C No Flack x Check Done: Low Friedel Pair Coverage 88 %
PLAT978_ALERT_2_C Number C-C Bonds with Positive Residual Density. 0 Info

Alert level G

PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite 8 Note

PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records 1 Report
PLAT860_ALERT_3_G Number of Least-Squares Restraints ..... 5 Note
PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary . Please Do !
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600 20 Note
PLAT961_ALERT_5_G Dataset Contains no Negative Intensities ..... Please Check

0 **ALERT level A** = Most likely a serious problem - resolve or explain
0 **ALERT level B** = A potentially serious problem, consider carefully
5 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
6 **ALERT level G** = General information/check it is not something unexpected

2 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
2 ALERT type 2 Indicator that the structure model may be wrong or deficient
4 ALERT type 3 Indicator that the structure quality may be low
2 ALERT type 4 Improvement, methodology, query or suggestion
1 ALERT type 5 Informative message, check

Datablock: 35

Bond precision: C-C = 0.0076 A Wavelength=0.71073
Cell: a=22.471(3) b=10.5857(11) c=9.5321(12)
alpha=90 beta=96.404(11) gamma=90
Temperature: 173 K

	Calculated	Reported
Volume	2253.3(5)	2253.3(5)
Space group	C 2	C 2
Hall group	C 2y	C 2y
Moiety formula	C26 H40 O4	C26 H40 O4
Sum formula	C26 H40 O4	C26 H40 O4
Mr	416.58	416.58
Dx,g cm-3	1.228	1.228
Z	4	4
Mu (mm-1)	0.081	0.081
F000	912.0	912.0
F000'	912.41	
h,k,lmax	34,16,14	34,15,13
Nref	8399[4395]	6184
Tmin,Tmax	0.987,0.996	0.987,0.996
Tmin'	0.984	

Correction method= # Reported T Limits: Tmin=0.987 Tmax=0.996
AbsCorr = ANALYTICAL
Data completeness= 1.41/0.74 Theta(max)= 32.843
R(reflections)= 0.0905(2785) wR2(reflections)= 0.2903(6184)
S = 1.003 Npar= 294

The following ALERTS were generated. Each ALERT has the format
test-name_ALERT_alert-type_alert-level.
Click on the hyperlinks for more details of the test.

Alert level B
PLAT910_ALERT_3_B Missing # of FCF Reflection(s) Below Theta(Min). 13 Note

Alert level C
STRVA01_ALERT_2_C Chirality of atom sites is inverted?
From the CIF: _refine_ls_abs_structure_Flack 10.000
From the CIF: _refine_ls_abs_structure_Flack_su 1.000
PLAT026_ALERT_3_C Ratio Observed / Unique Reflections (too) Low .. 45% Check
PLAT084_ALERT_3_C High wR2 Value (i.e. > 0.25) ..... 0.29 Report
PLAT241_ALERT_2_C High MainMol Ueq as Compared to Neighbors of C12 Check
PLAT340_ALERT_3_C Low Bond Precision on C-C Bonds ..... 0.00763 Ang.
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ..... 3.764 Check
PLAT907_ALERT_2_C Flack x > 0.5, Structure Needs to be Inverted? . 10.00 Check
PLAT915_ALERT_3_C No Flack x Check Done: Low Friedel Pair Coverage 53 %

Alert level G
PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite 11 Note
PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ... 10 Report

PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms ..... 5 Report
PLAT032_ALERT_4_G Std. Uncertainty on Flack Parameter Value High . 1.000 Report
PLAT033_ALERT_4_G Flack x Value Deviates > 3.0 * sigma from Zero . 10.000 Note
PLAT066_ALERT_1_G Predicted and Reported Tmin&Tmax Range Identical ? Check
PLAT072_ALERT_2_G SHELXL First Parameter in WGHT Unusually Large 0.12 Report
PLAT111_ALERT_2_G ADDSYM Detects New (Pseudo) Centre of Symmetry . 84 %Fit
PLAT113_ALERT_2_G ADDSYM Suggests Possible Pseudo/New Space Group C2/m Check
PLAT175_ALERT_4_G The CIF-Embedded .res File Contains SAME Records 1 Report
PLAT176_ALERT_4_G The CIF-Embedded .res File Contains SADI Records 1 Report
PLAT178_ALERT_4_G The CIF-Embedded .res File Contains SIMU Records 5 Report
PLAT301_ALERT_3_G Main Residue Disorder .....(Resd 1) 17% Note
PLAT410_ALERT_2_G Short Intra H...H Contact H4B ..H29A . 2.12 Ang.
x,y,z = 1_555 Check
PLAT417_ALERT_2_G Short Inter D-H..H-D H25 ..H30 . 2.05 Ang.
-1/2+x,1/2+y,z = 3_455 Check
PLAT789_ALERT_4_G Atoms with Negative _atom_site_disorder_group # 24 Check
PLAT791_ALERT_4_G Model has Chirality at C11 (Chiral SPGR) S Verify
And 9 other PLAT791 Alerts
Less ...

PLAT791_ALERT_4_G Model has Chirality at C13 (Chiral SPGR) R Verify
PLAT791_ALERT_4_G Model has Chirality at C16 (Chiral SPGR) S Verify
PLAT791_ALERT_4_G Model has Chirality at C18 (Chiral SPGR) R Verify
PLAT791_ALERT_4_G Model has Chirality at C21 (Chiral SPGR) S Verify
PLAT791_ALERT_4_G Model has Chirality at C23 (Chiral SPGR) R Verify
PLAT791_ALERT_4_G Model has Chirality at C26 (Chiral SPGR) S Verify
PLAT791_ALERT_4_G Model has Chirality at C28 (Chiral SPGR) R Verify
PLAT791_ALERT_4_G Model has Chirality at C26' (Chiral SPGR) R Verify
PLAT791_ALERT_4_G Model has Chirality at C28' (Chiral SPGR) S Verify

PLAT860_ALERT_3_G Number of Least-Squares Restraints ..... 40 Note
PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary . Please Do !
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600 259 Note
PLAT916_ALERT_2_G Hooft y and Flack x Parameter Values Differ by . 7.70 Check
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density. 1 Info
PLAT992_ALERT_5_G Repd & Actual _reflns_number_gt Values Differ by 1 Check

---

0 **ALERT level A** = Most likely a serious problem - resolve or explain
1 **ALERT level B** = A potentially serious problem, consider carefully
8 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
32 **ALERT level G** = General information/check it is not something unexpected

2 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
12 ALERT type 2 Indicator that the structure model may be wrong or deficient
8 ALERT type 3 Indicator that the structure quality may be low
17 ALERT type 4 Improvement, methodology, query or suggestion
2 ALERT type 5 Informative message, check

It is advisable to attempt to resolve as many as possible of the alerts in all categories. Often the minor alerts point to easily fixed oversights, errors and omissions in your CIF or refinement strategy, so attention to these fine details can be worthwhile. In order to resolve some of the more serious problems it may be necessary to carry out additional measurements or structure refinements. However, the purpose of your study may justify the reported deviations and the more serious of these should normally be commented upon in the discussion or experimental section of a paper or in the "special_details" fields of the CIF. checkCIF was carefully designed to identify outliers and unusual parameters, but every test has its limitations and alerts that are not important in a particular case may appear. Conversely, the absence of alerts does not guarantee there are no aspects of the results needing attention. It is up to the individual to critically assess their own results and, if necessary, seek expert advice.

Publication of your CIF in IUCr journals

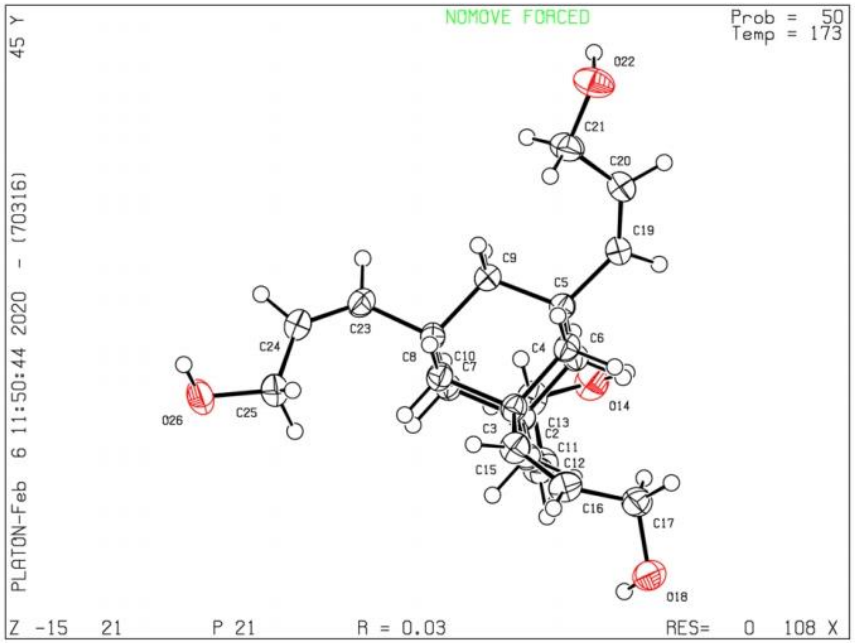
A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica*, *Journal of Applied Crystallography*, *Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section C* or *E* or *IUCrData*, you should make sure that full publication checks are run on the final version of your CIF prior to submission.

Publication of your CIF in other journals

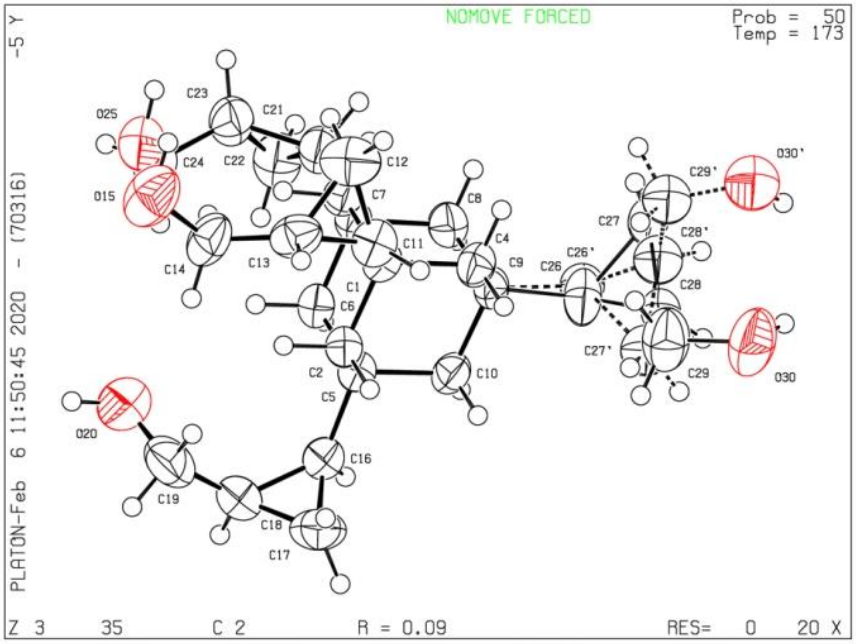
Please refer to the *Notes for Authors* of the relevant journal for any special instructions relating to CIF submission.

PLATON version of 22/12/2019; check.def file version of 13/12/2019

Datablock 21 - ellipsoid plot



Datablock 35 - ellipsoid plot



Download CIF editor (publCIF) from the IUCr
Download CIF editor (enCIFer) from the CCDC
Test a new CIF entry

