Effect of Intramolecular Paternò-Büchi Reaction on Thermodynamics and Kinetics of Nearly Degenerate [3,3]-Sigmatropic Shift in Fluxional Polycycles.

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Supporting Information

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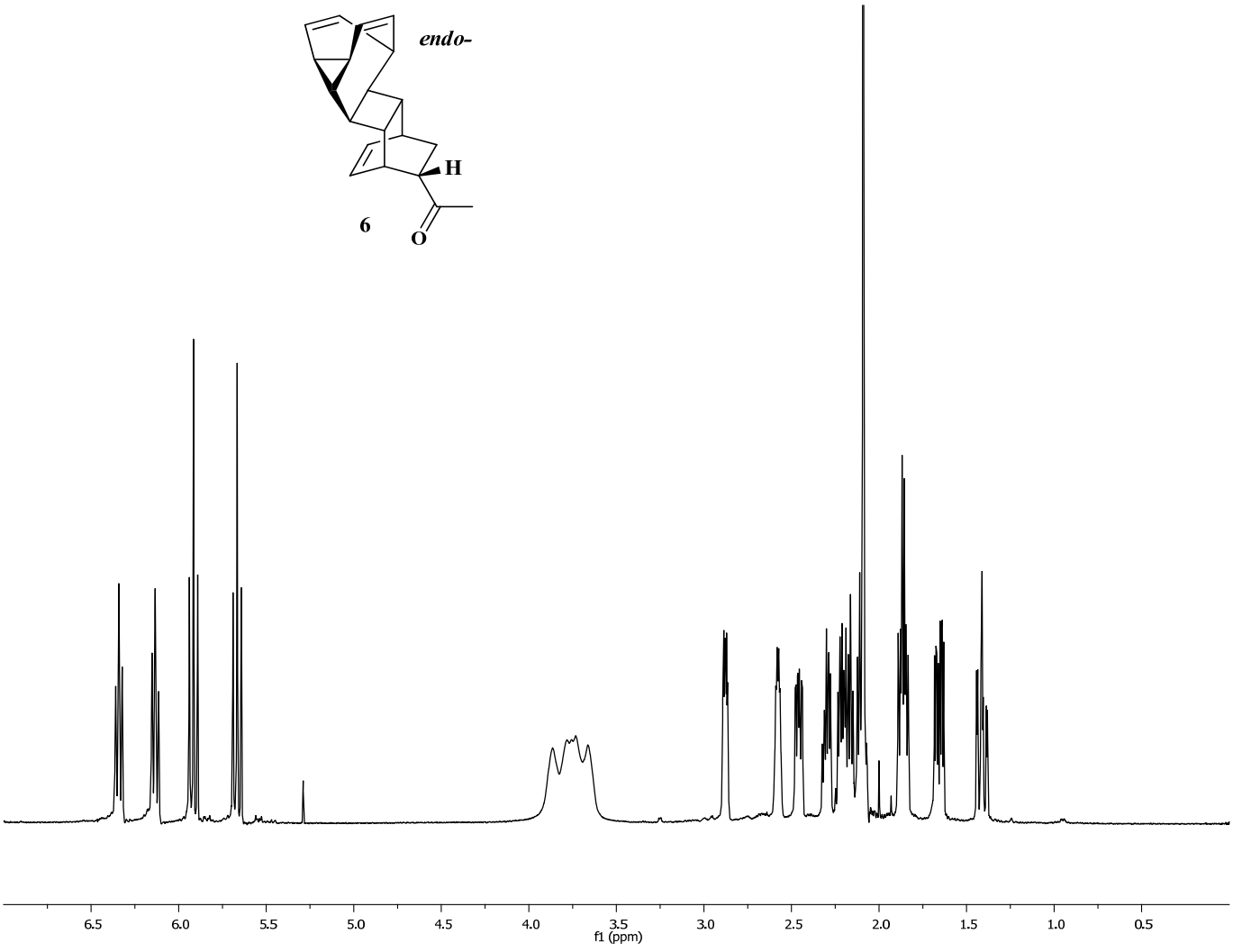
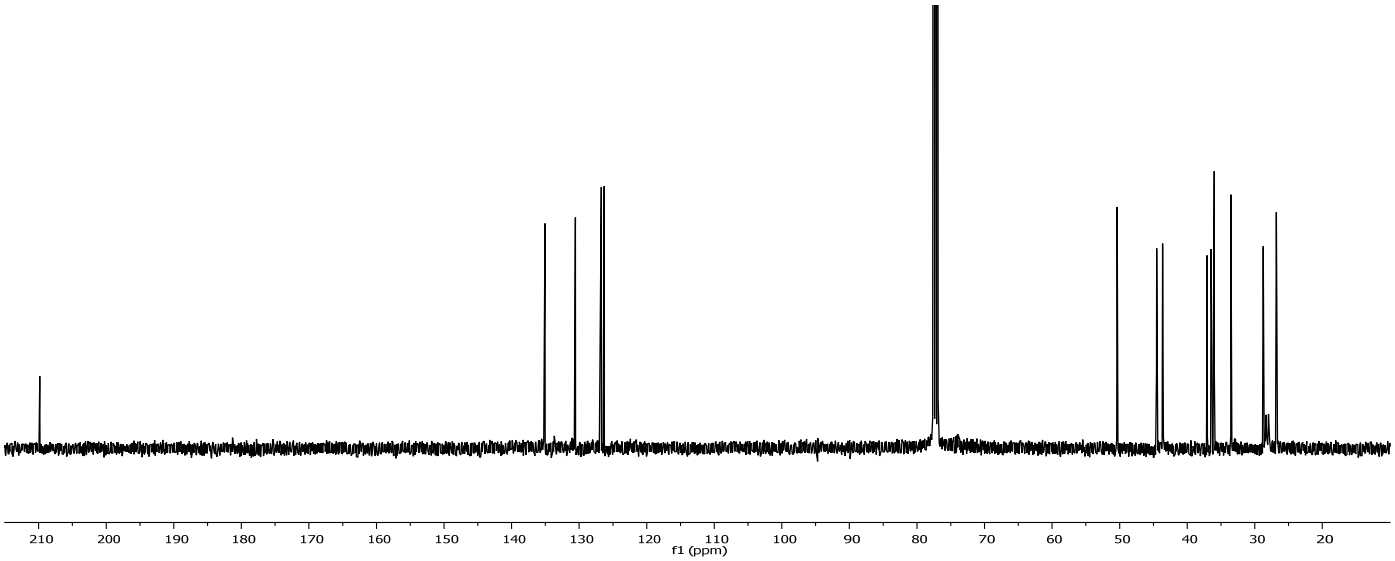
NMR SPECTRA (^{1}H, ^{13}C, COSY)

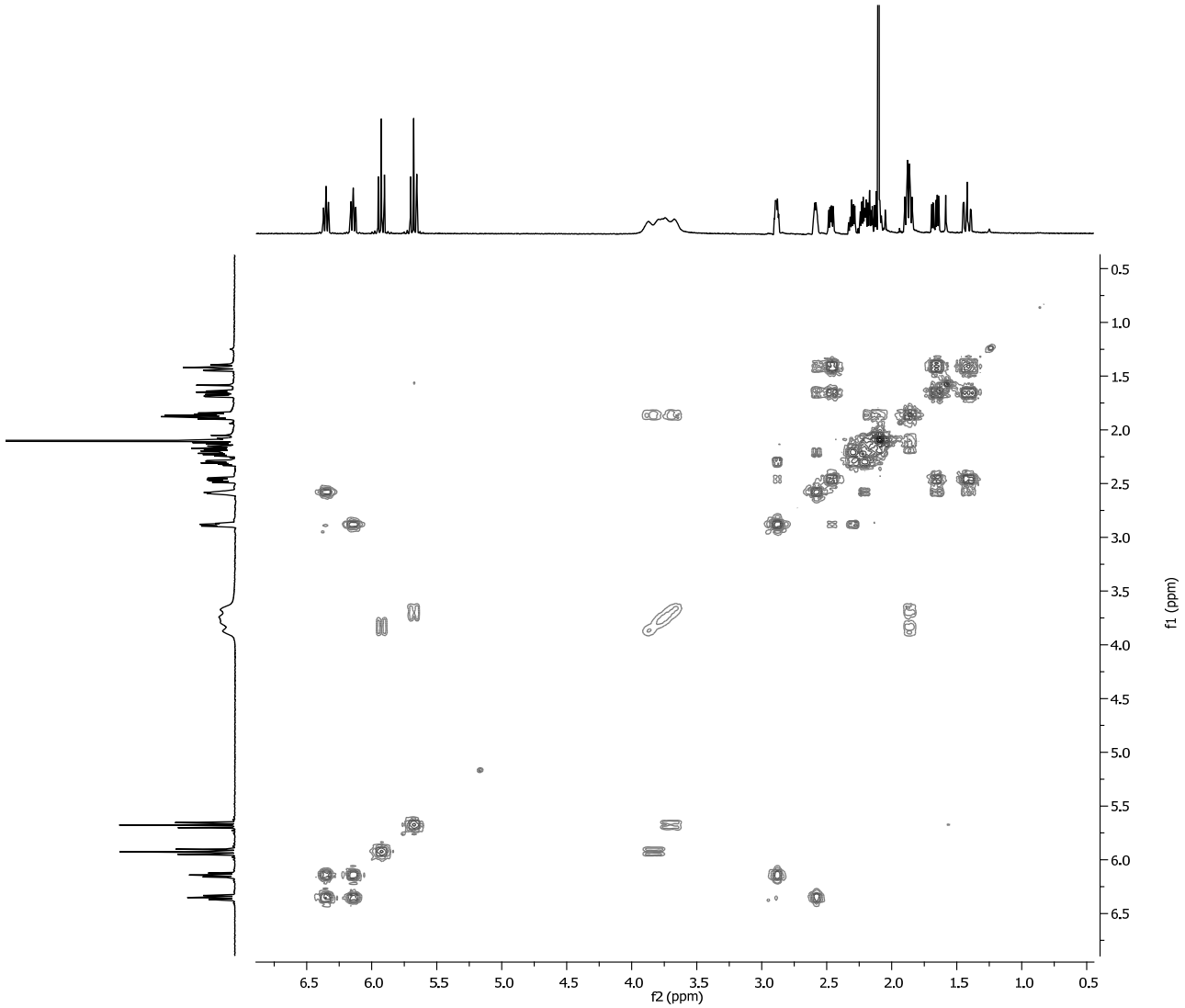
^{1}H NMR (400 MHz, $CDCl_3$):



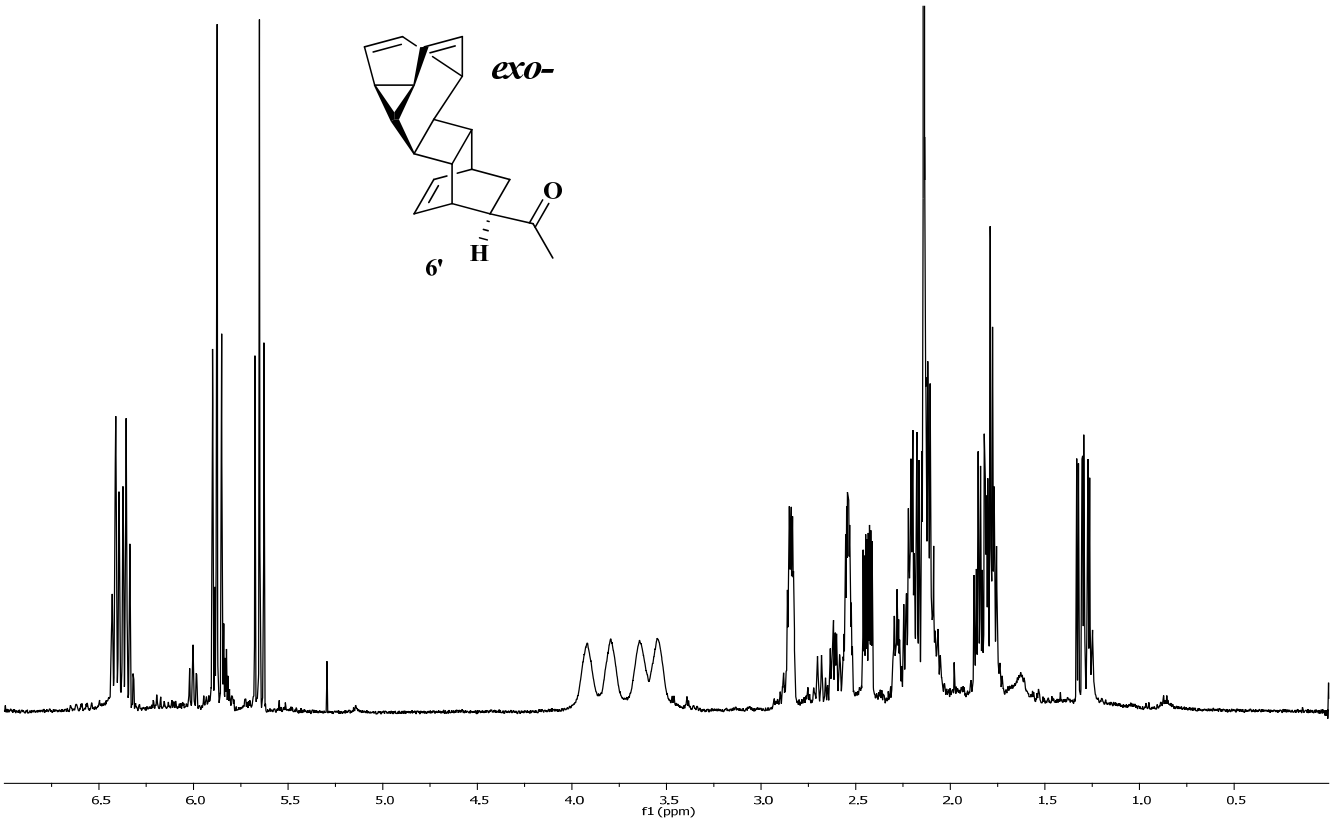
^{13}C NMR (400 MHz, $CDCl_3$):



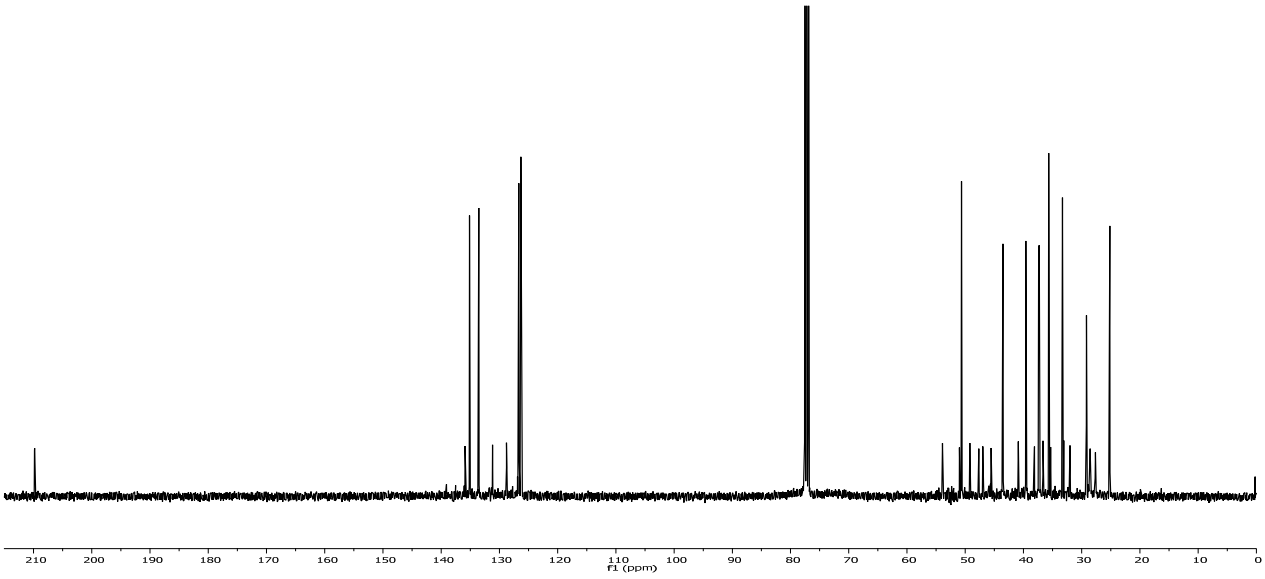
COSY (400 MHz, $CDCl_3$):



^{1}H NMR (400 MHz, $CDCl_3$):



^{13}C NMR (400 MHz, $CDCl_3$) (has the *endo*-**6** as impurity)



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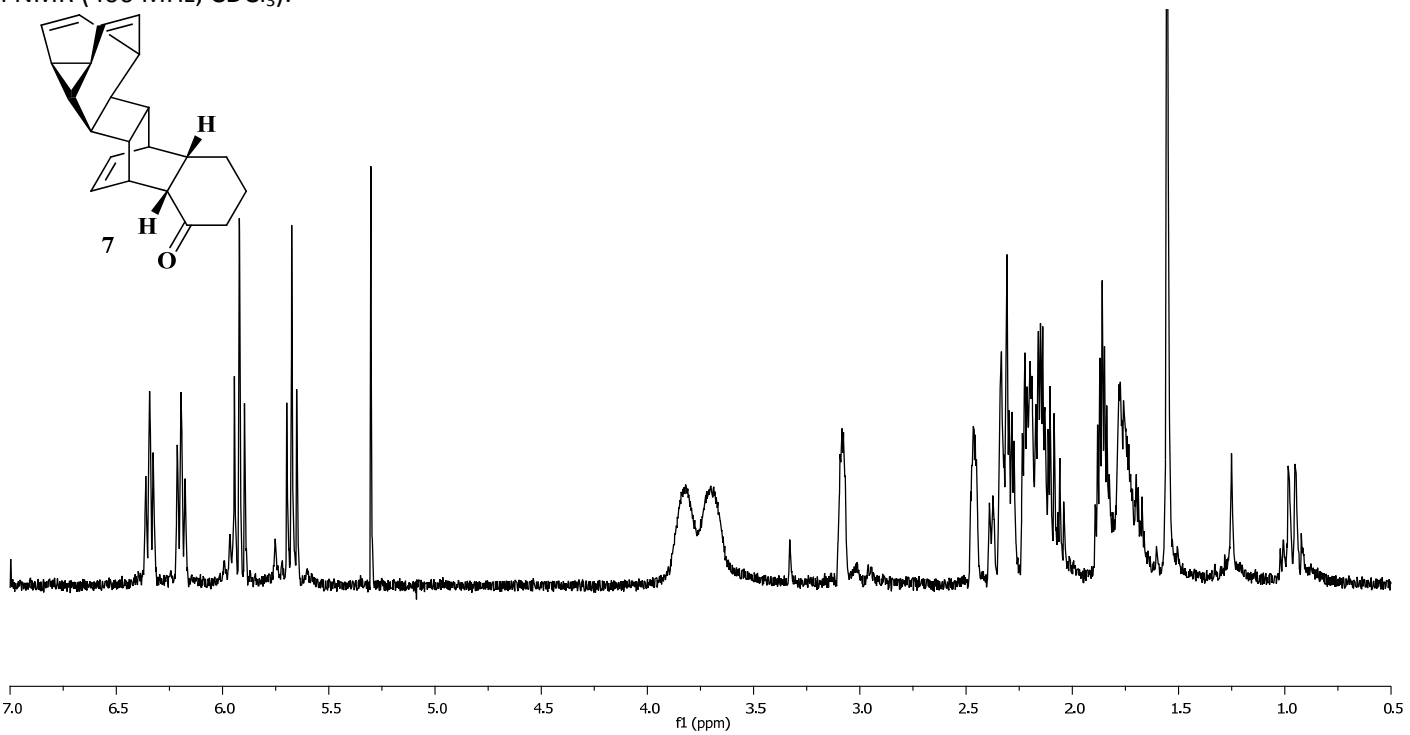

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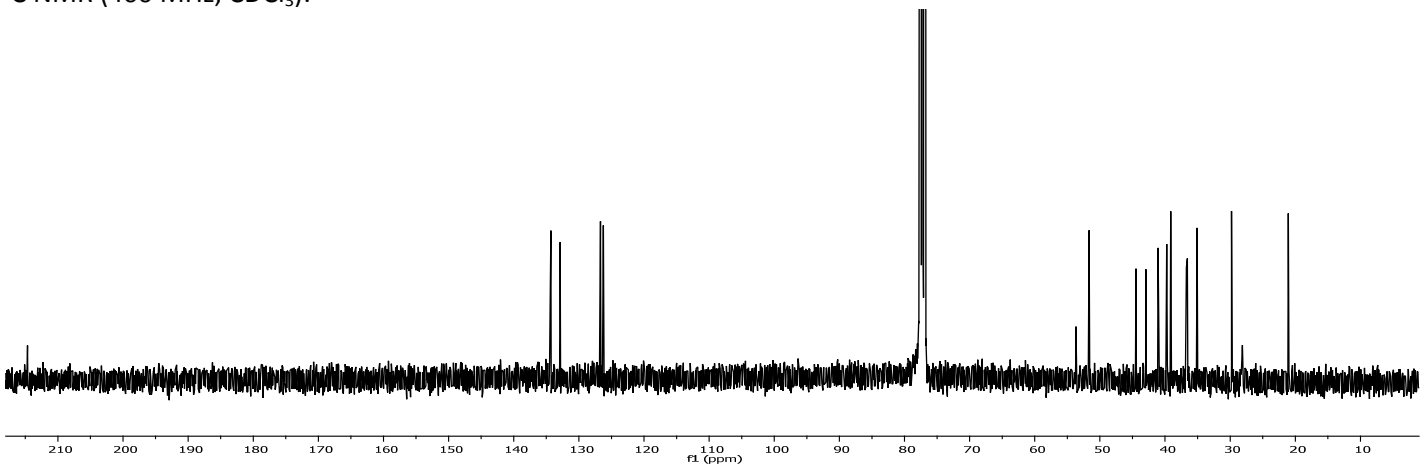
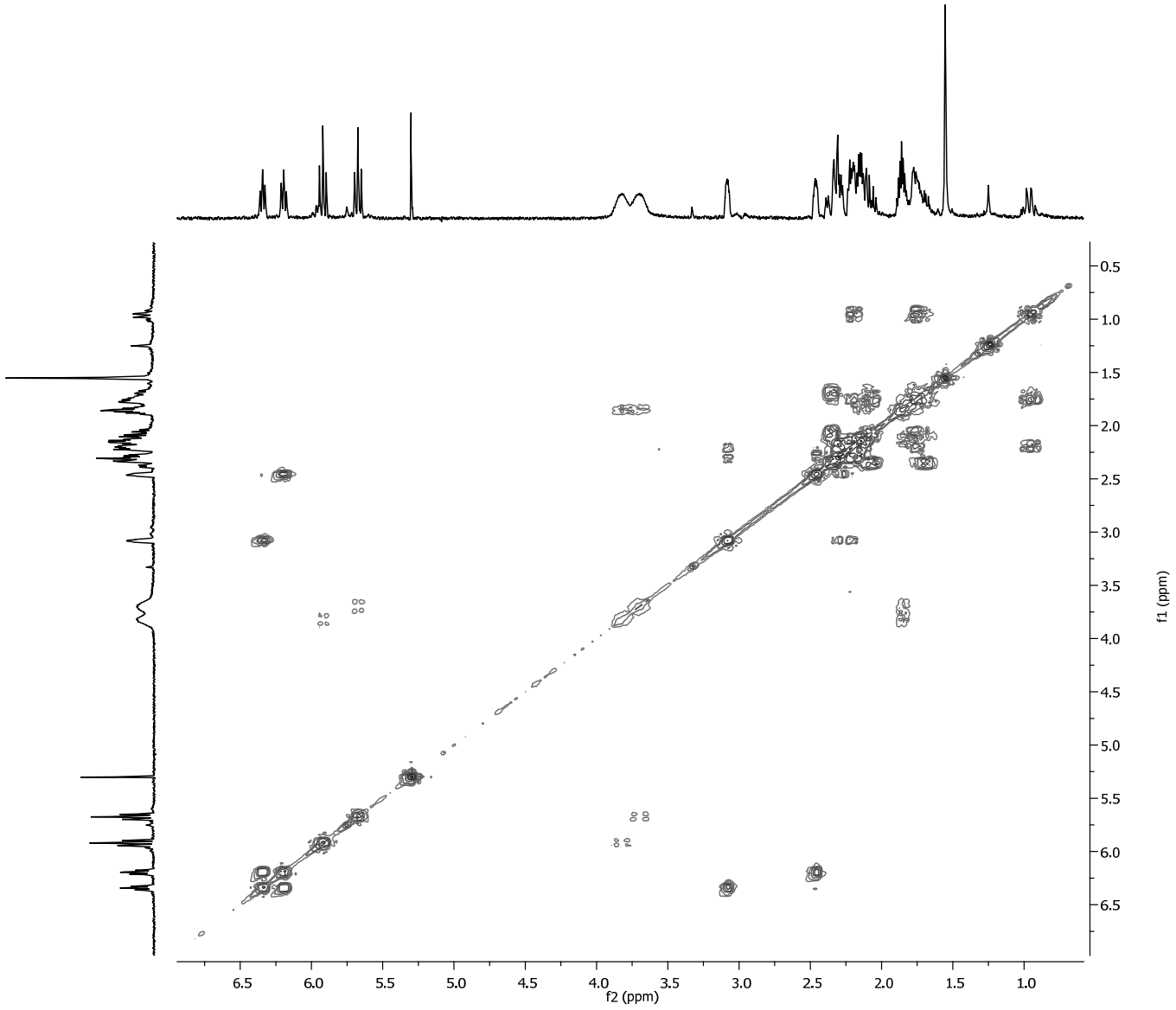


COSY (400 MHz, $CDCl_3$):



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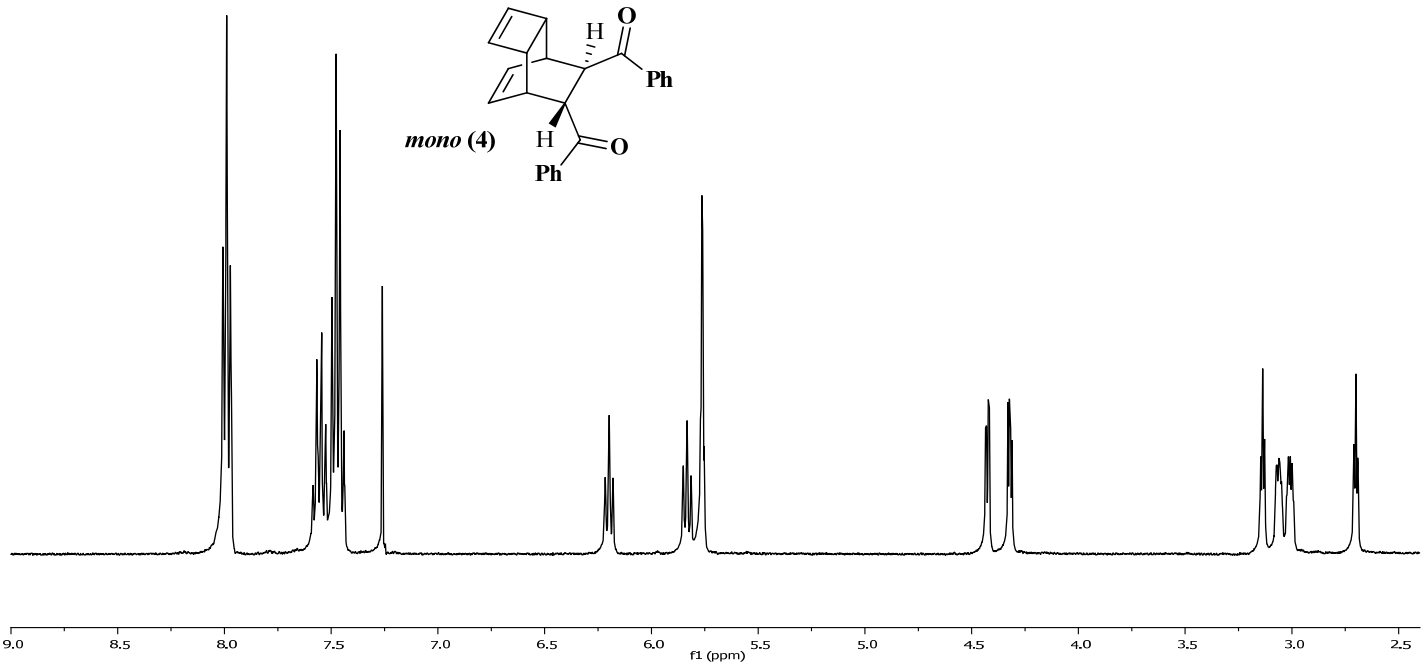

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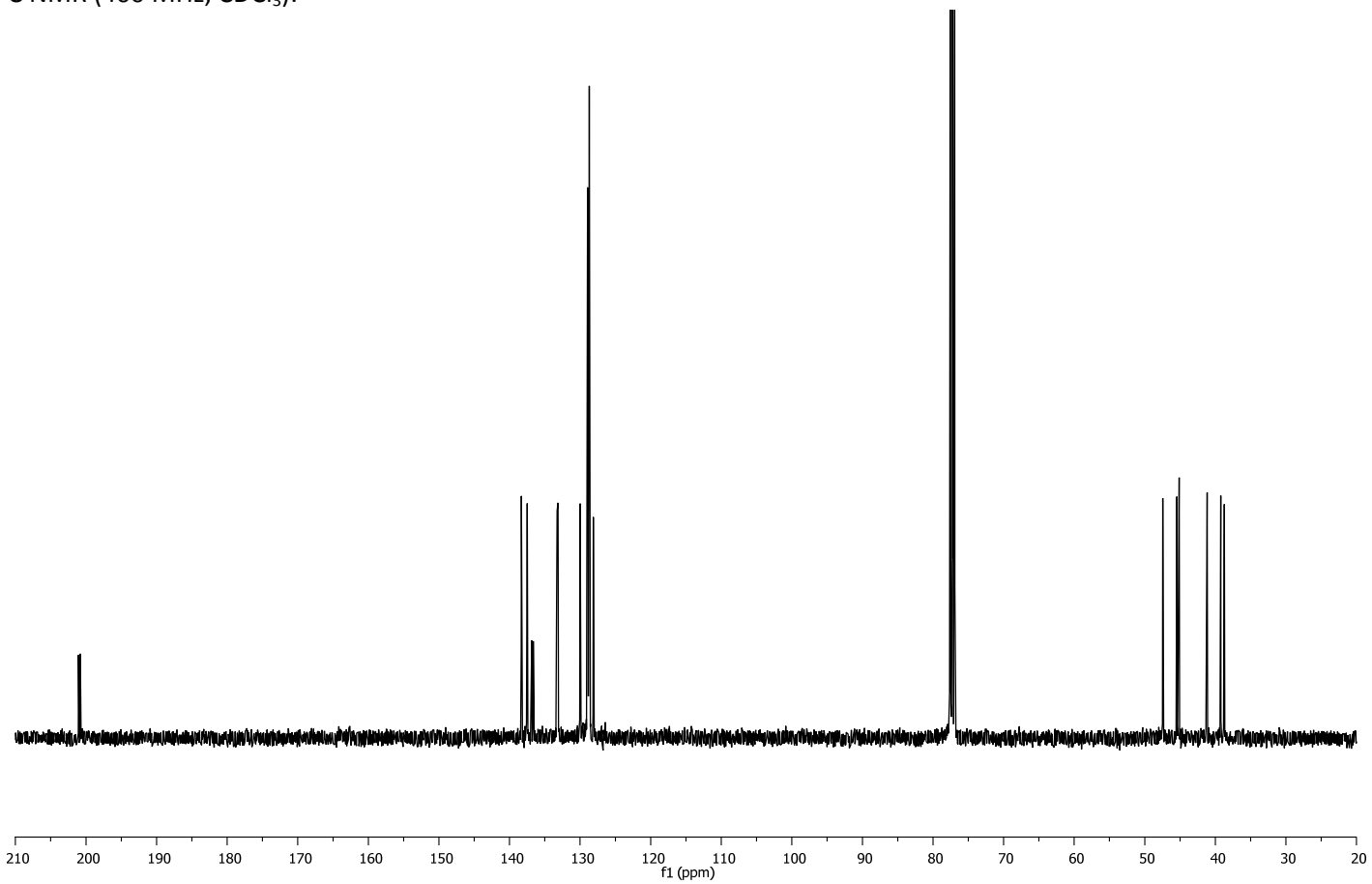

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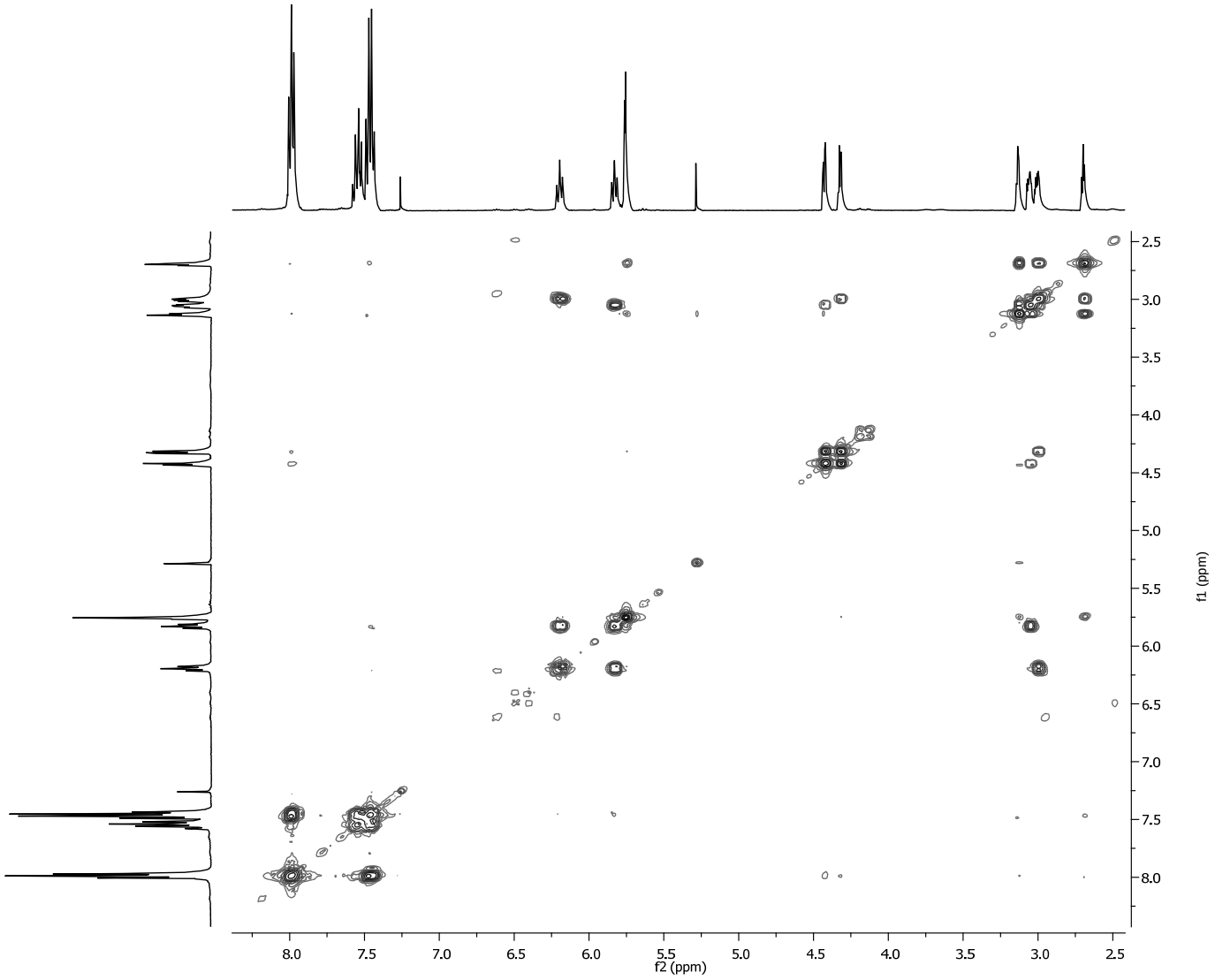

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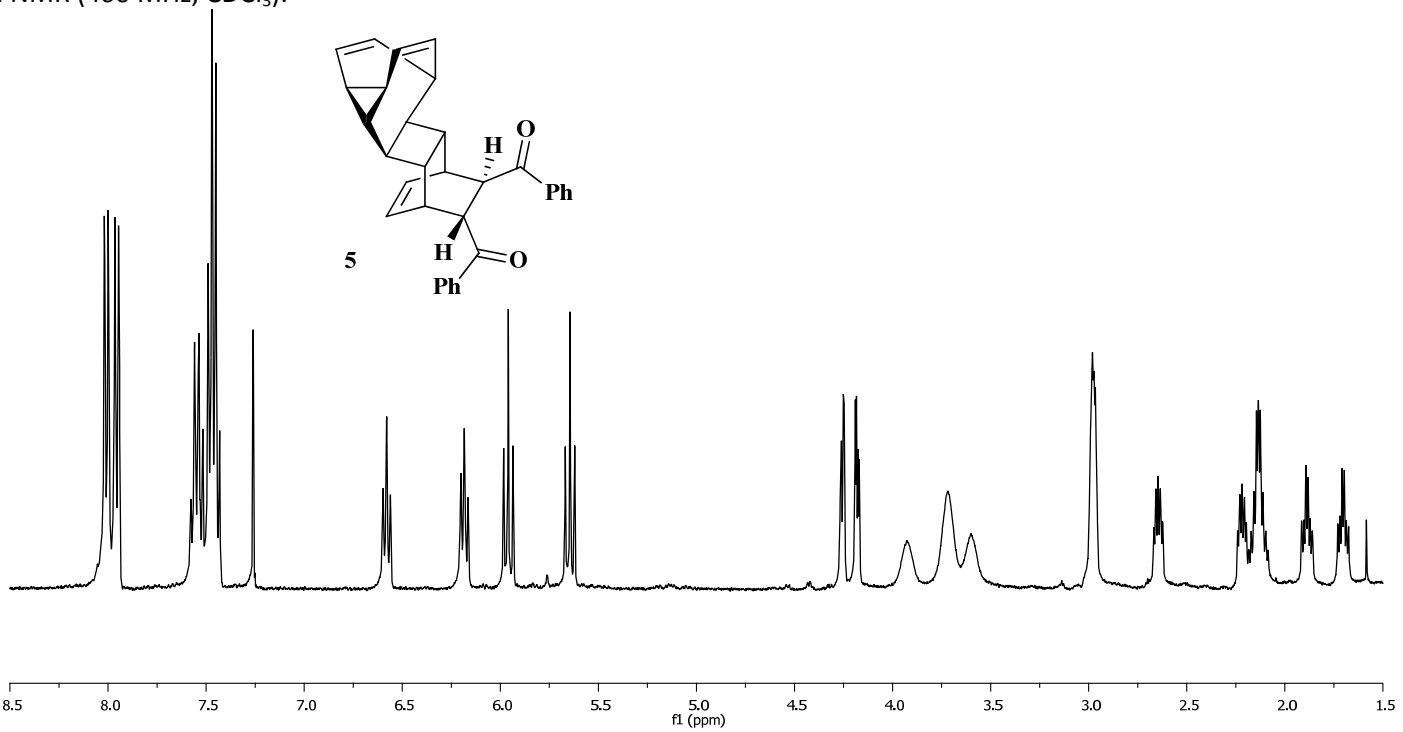

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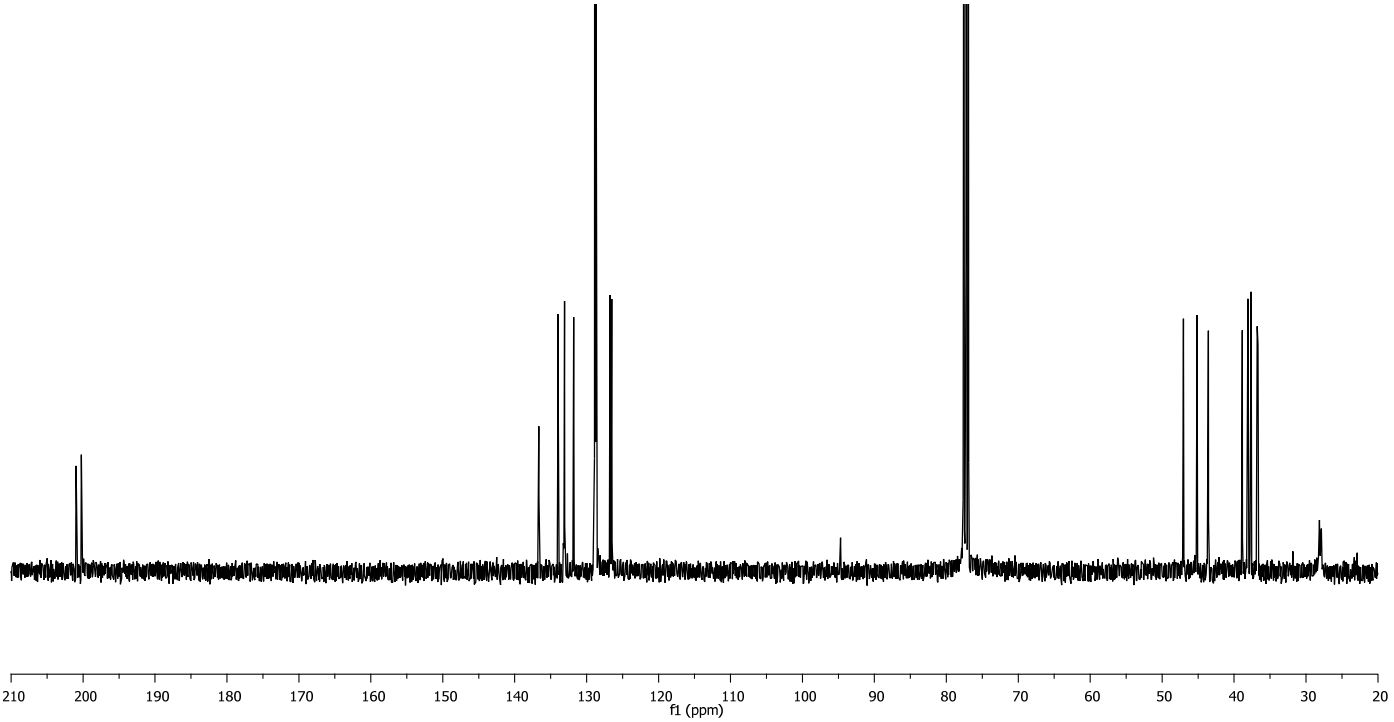

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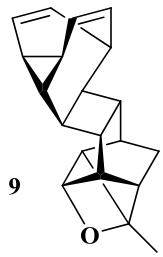

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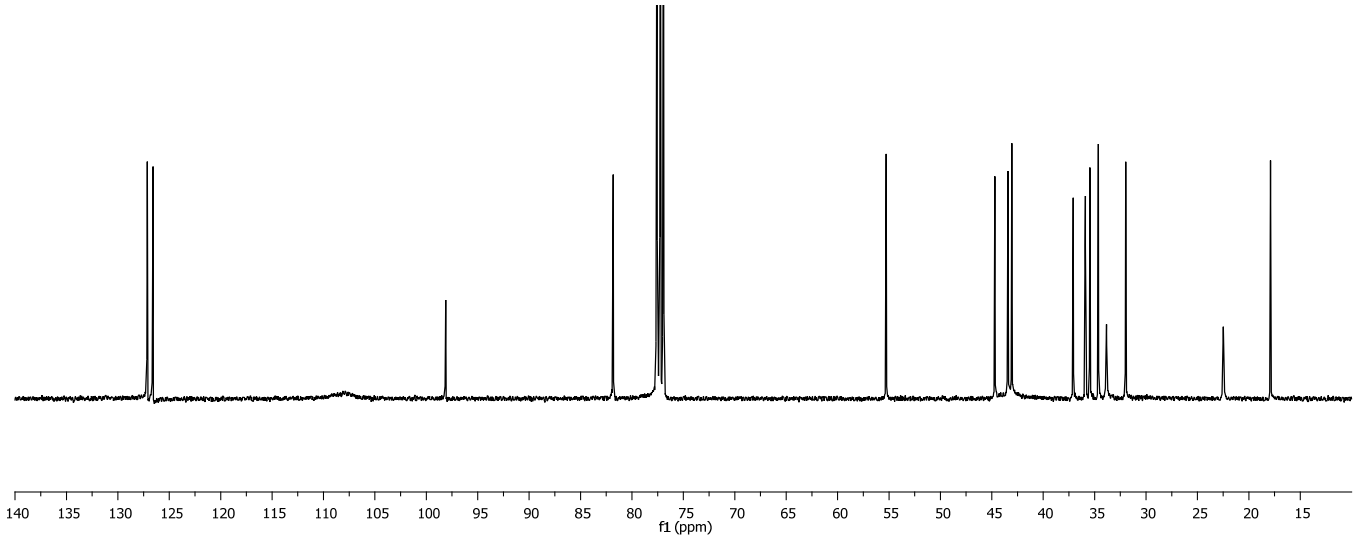

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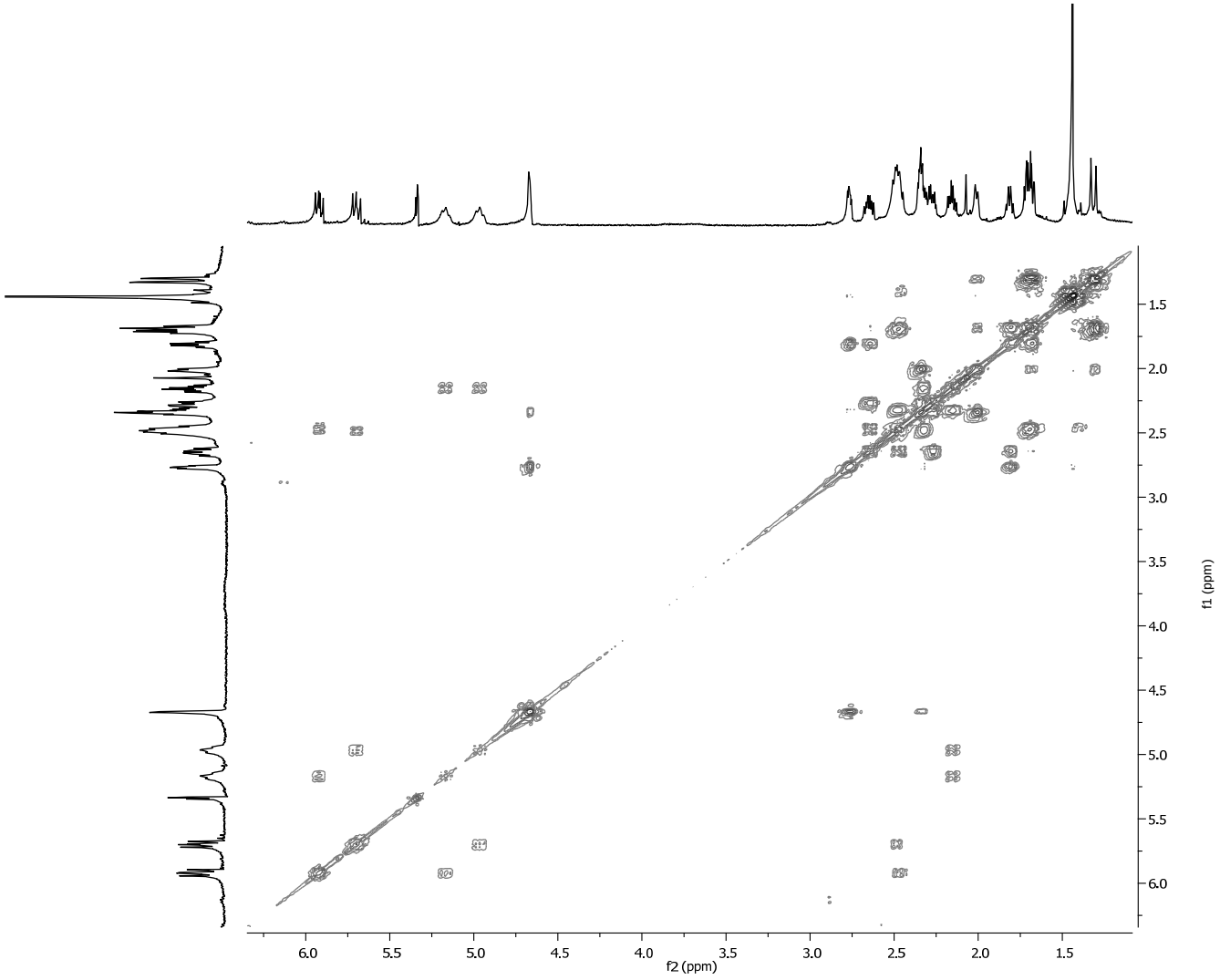

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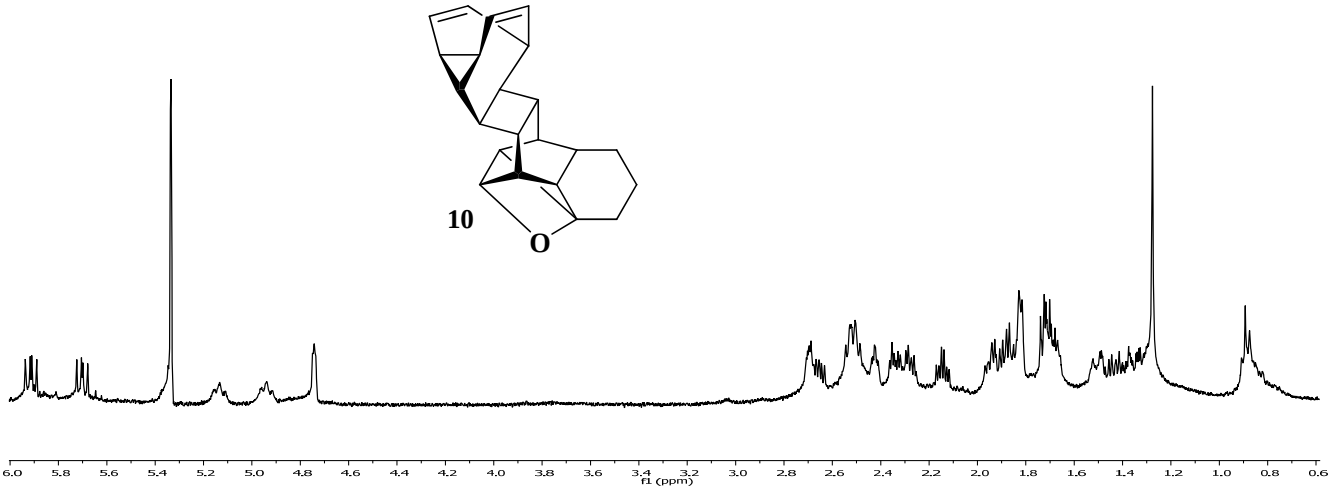

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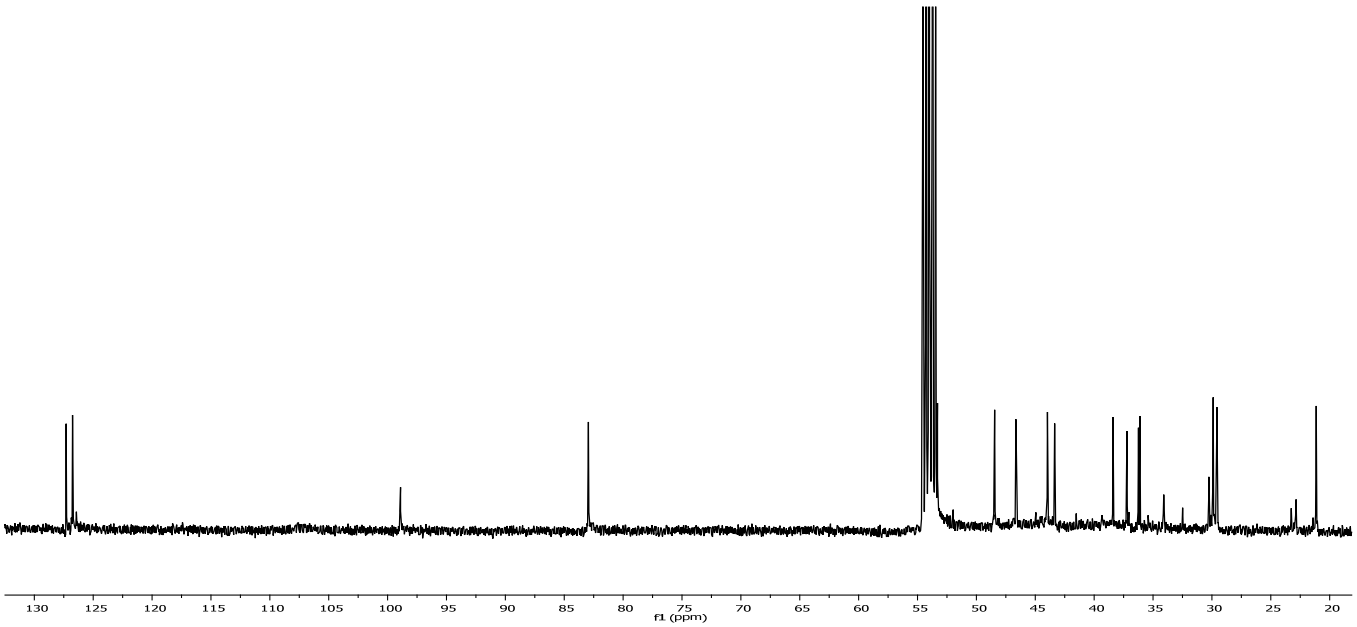

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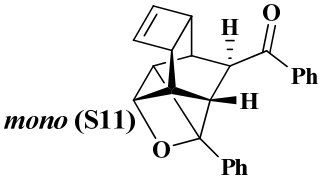
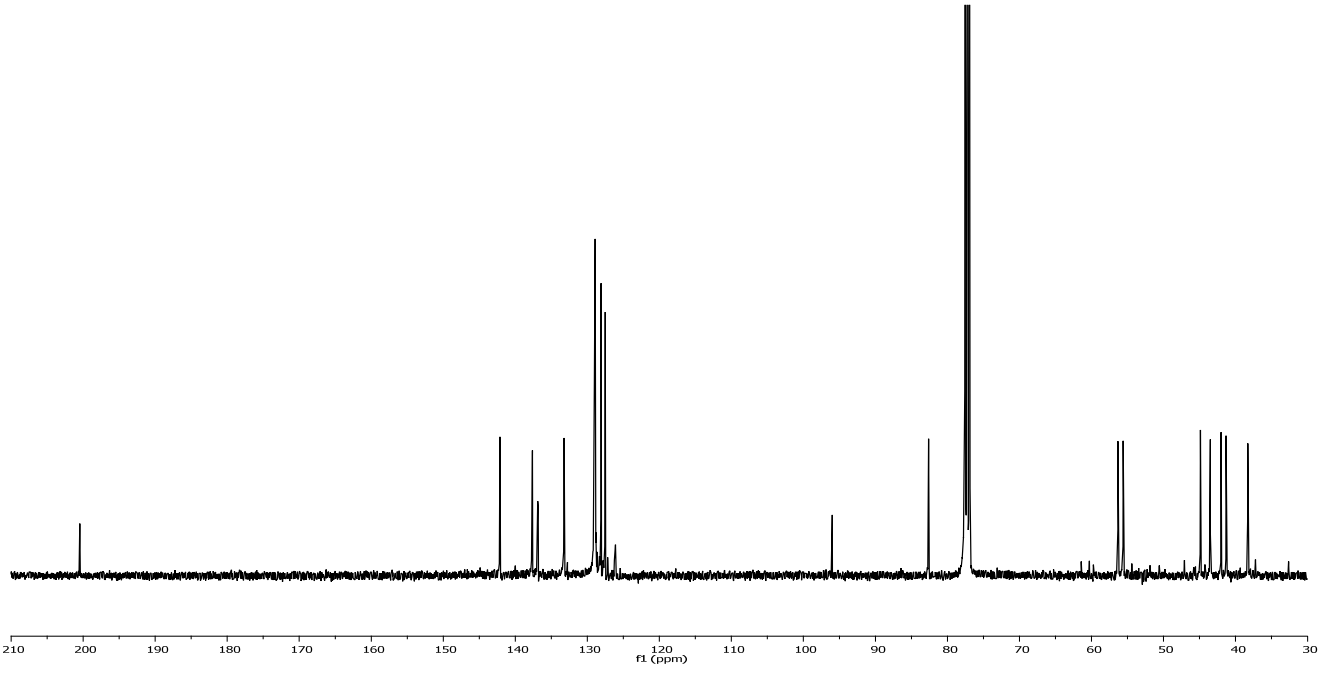
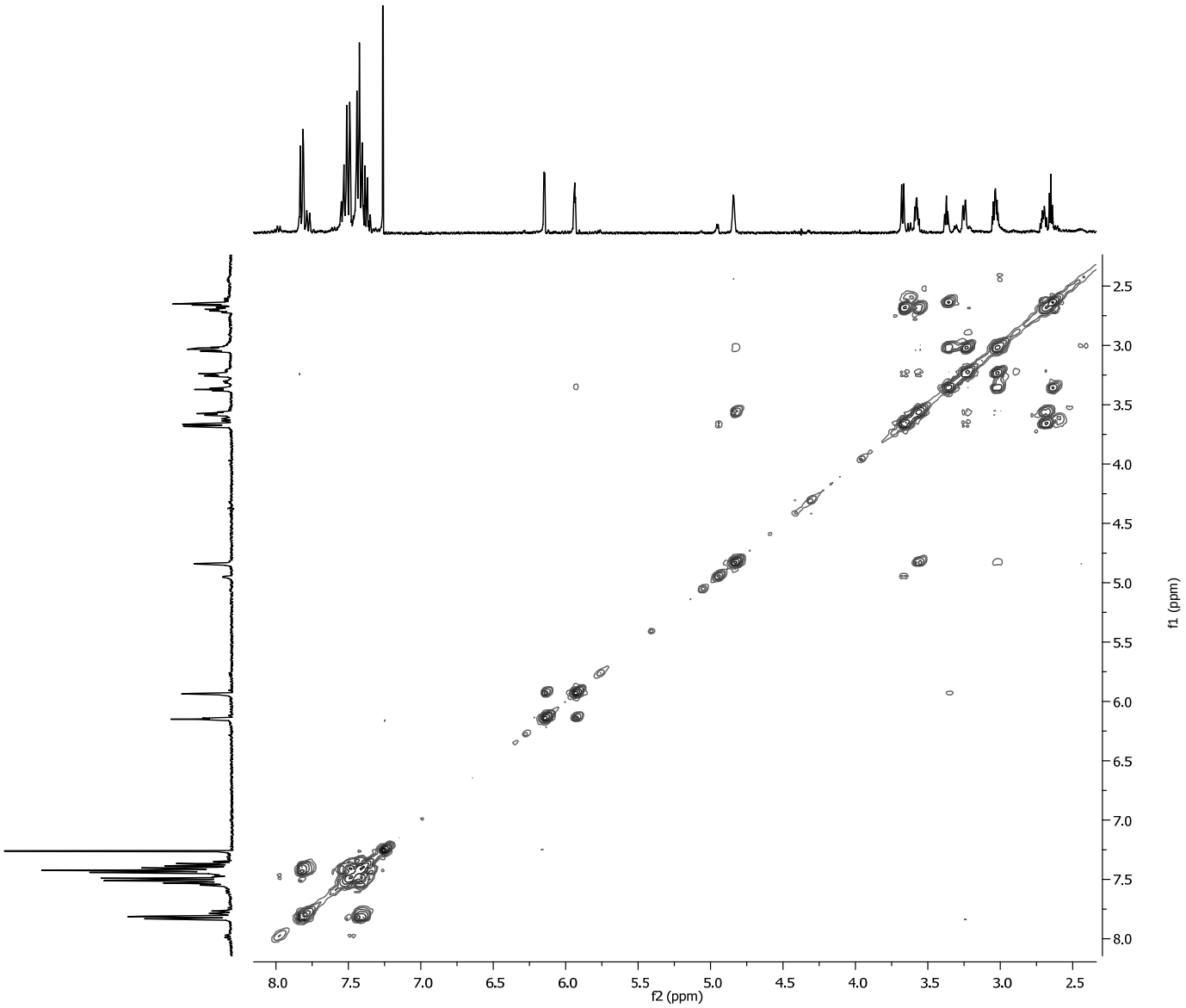


mono (S11)

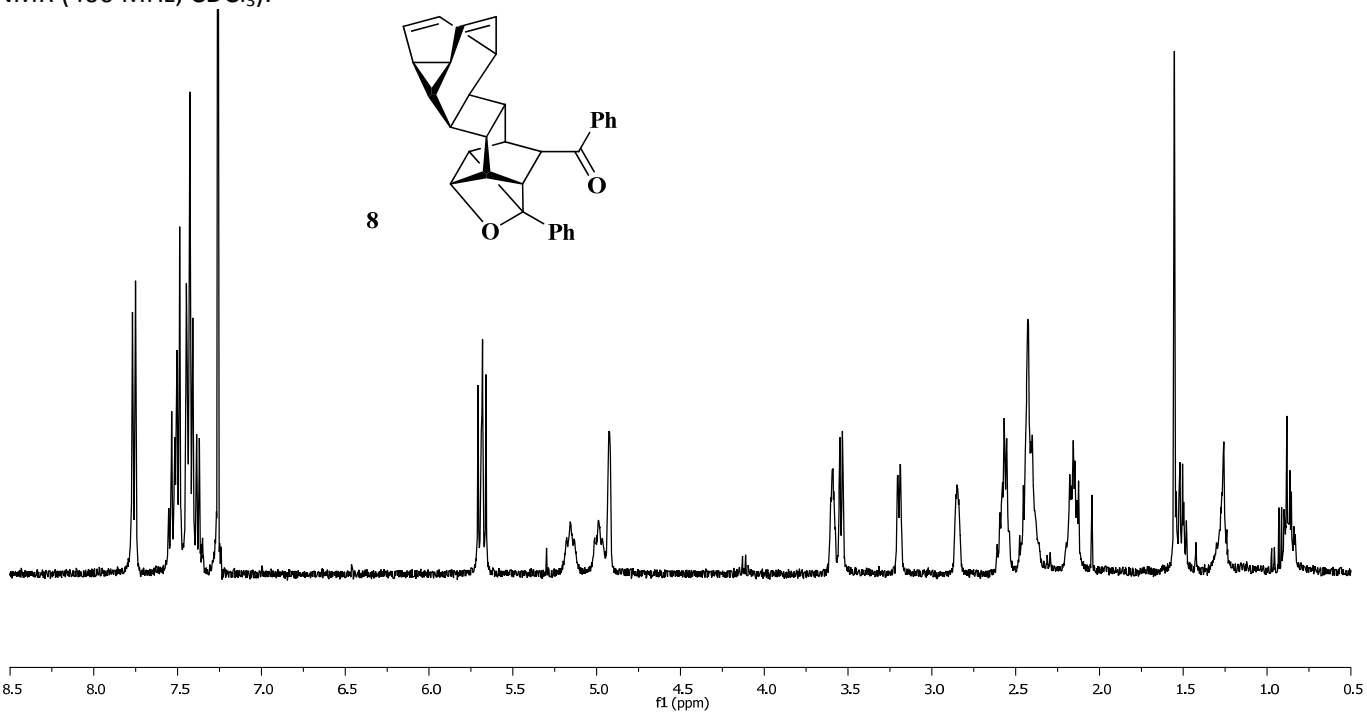
^{13}C NMR (400 MHz, $CDCl_3$):



COSY (400 MHz, $CDCl_3$):



^{1}H NMR (400 MHz, $CDCl_3$):



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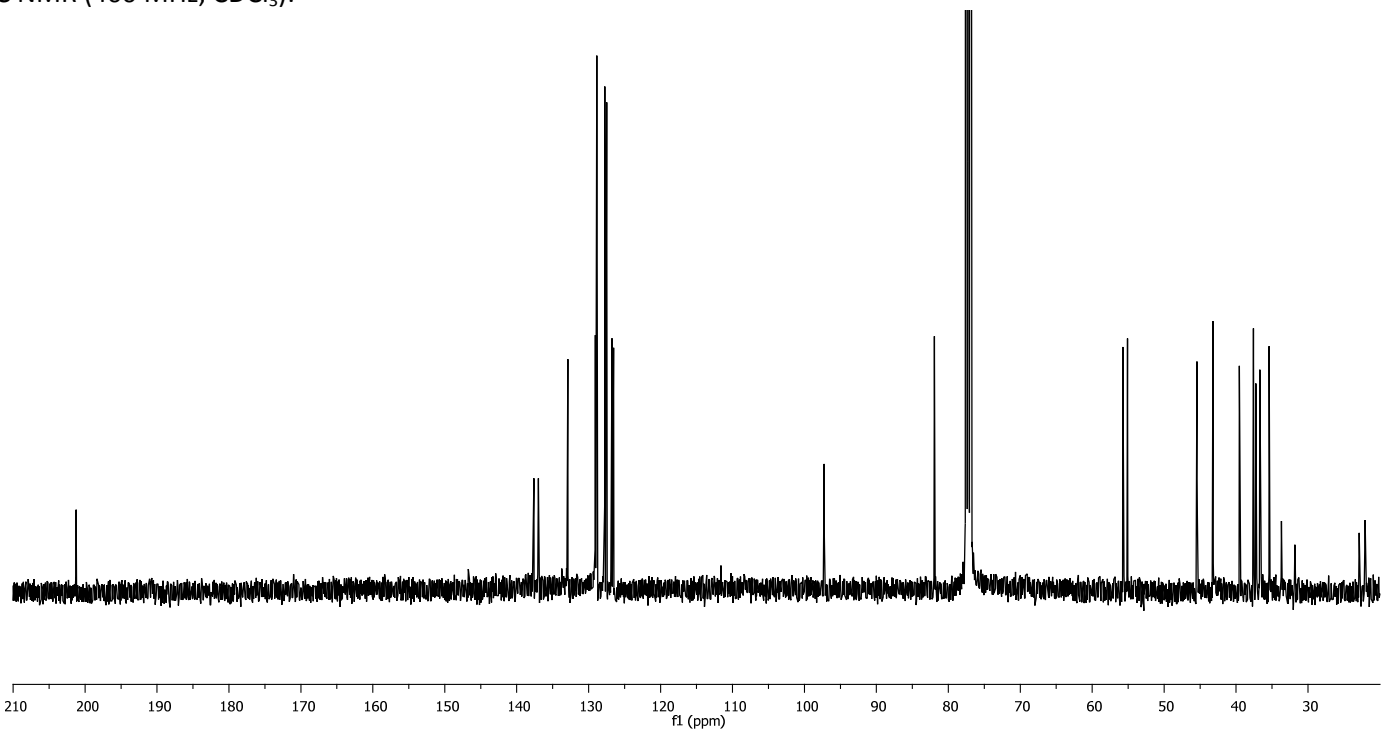
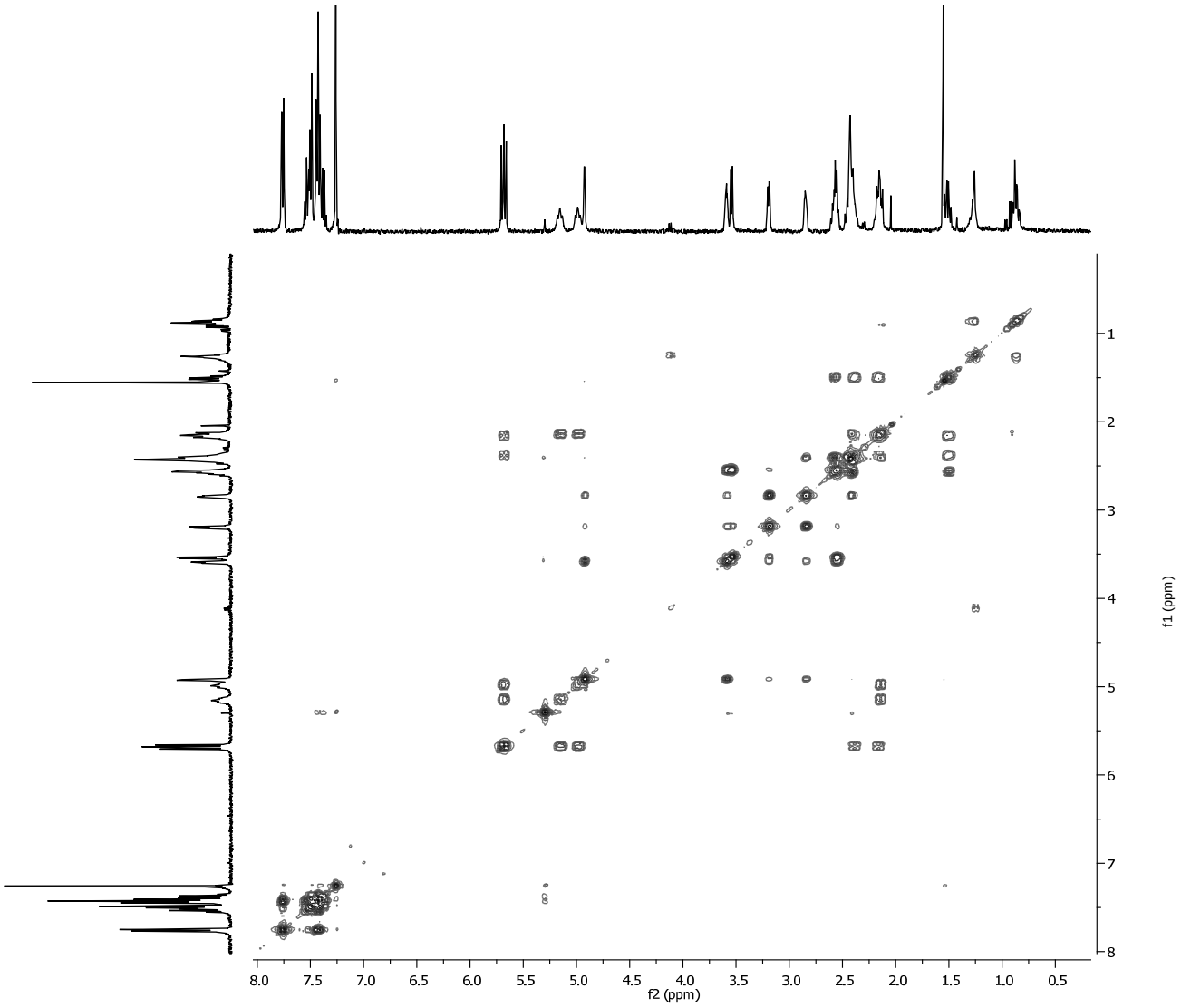
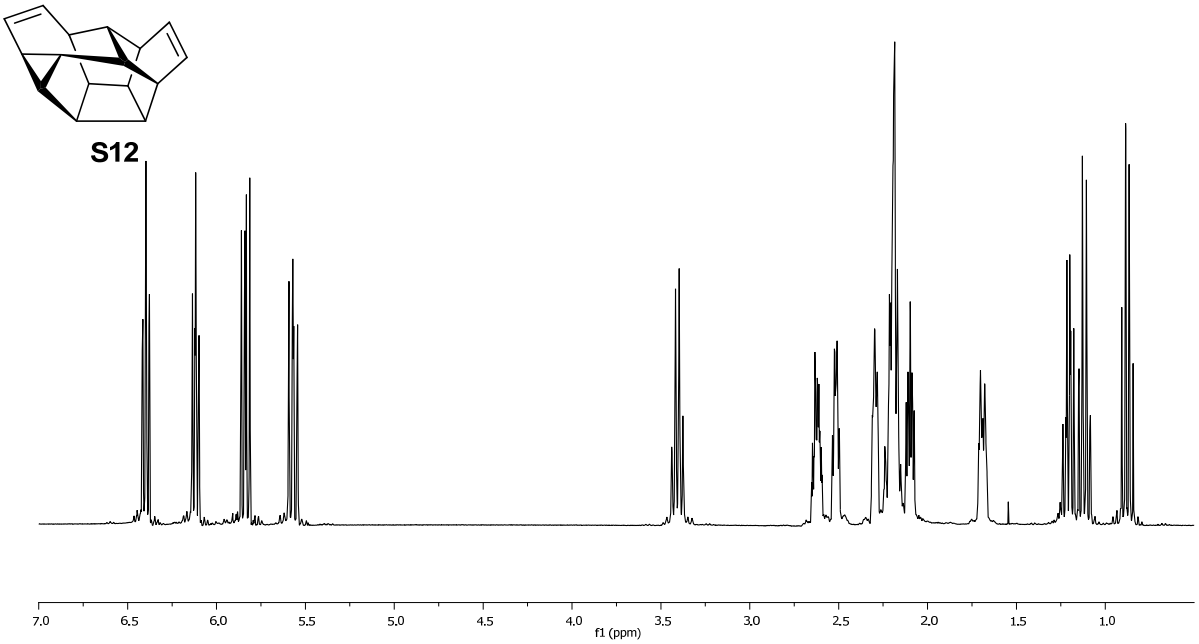


COSY (400 MHz, $CDCl_3$):

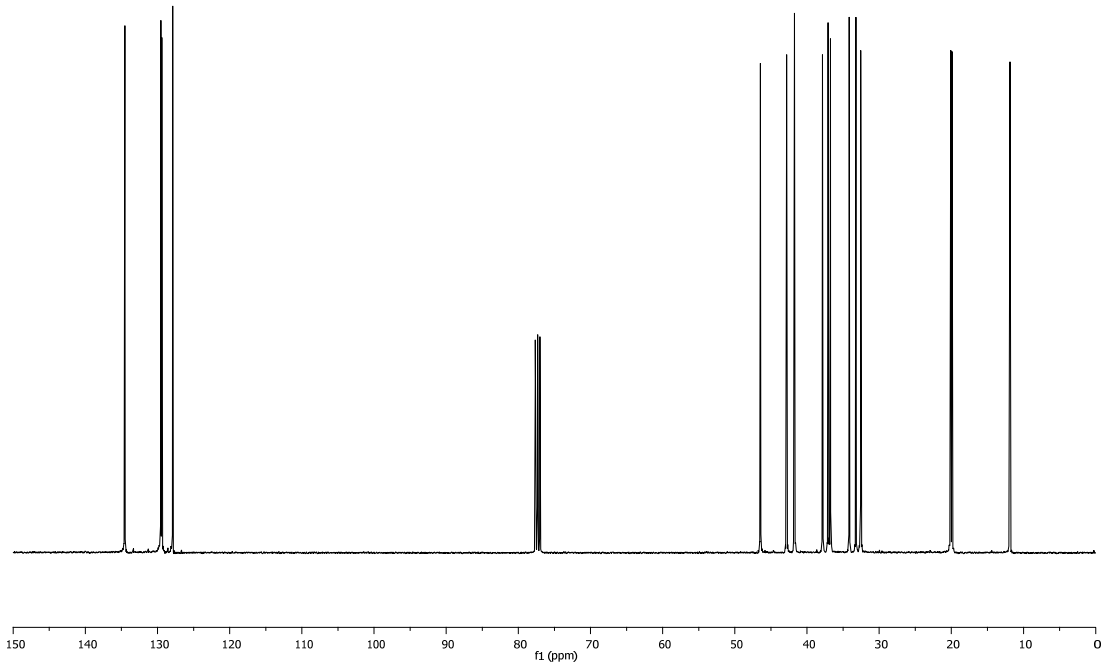


Dimer **2** undergoes secondary intramolecular Diels-Alder reaction into polycycle **S12**
This reaction depletes **2** and is potentially the main side reaction affecting the yield of Diels-Alder adducts of **2** with dienophiles.

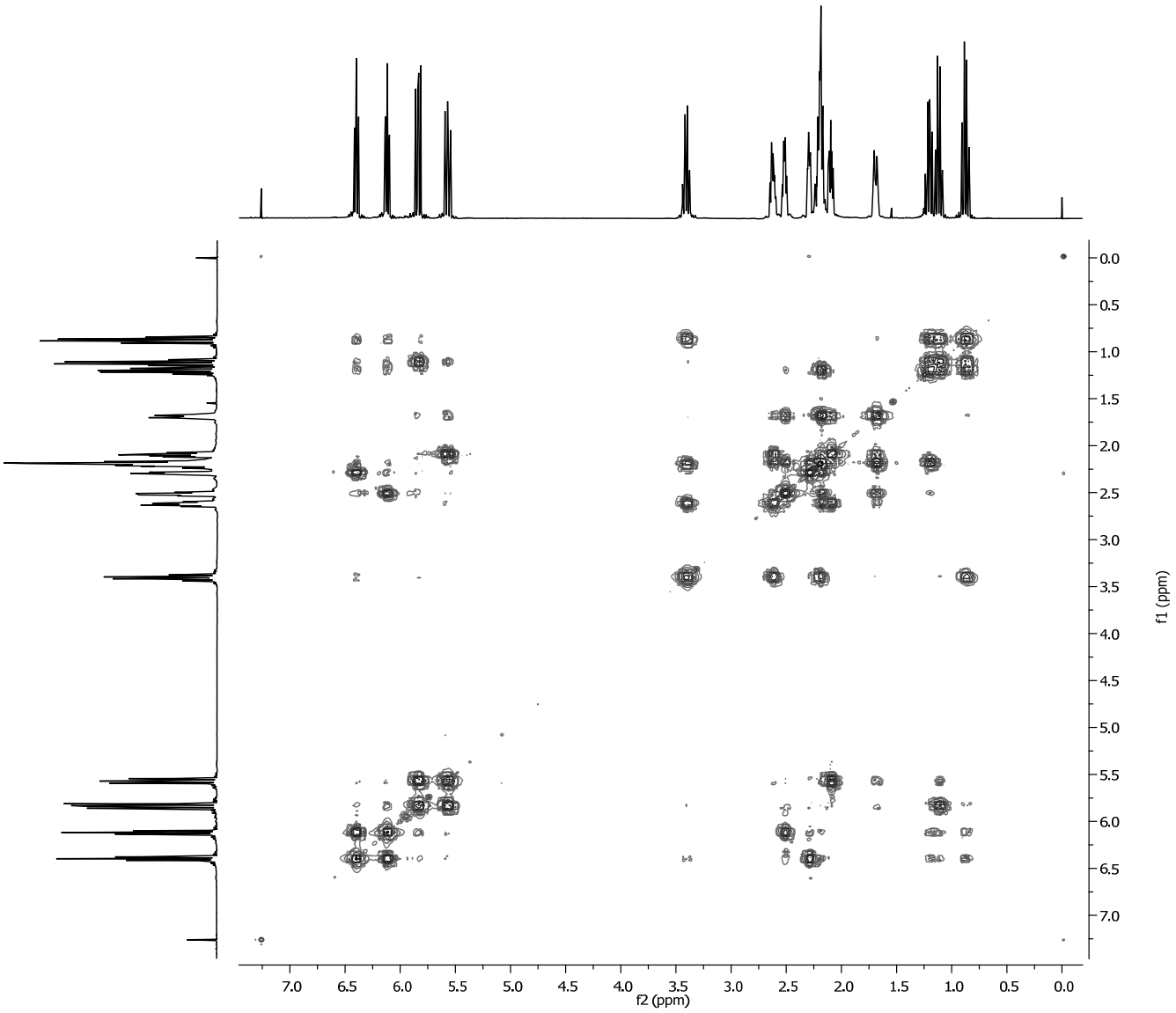
^{1}H NMR (400 MHz, $CDCl_3$):



^{13}C NMR (400 MHz, $CDCl_3$):

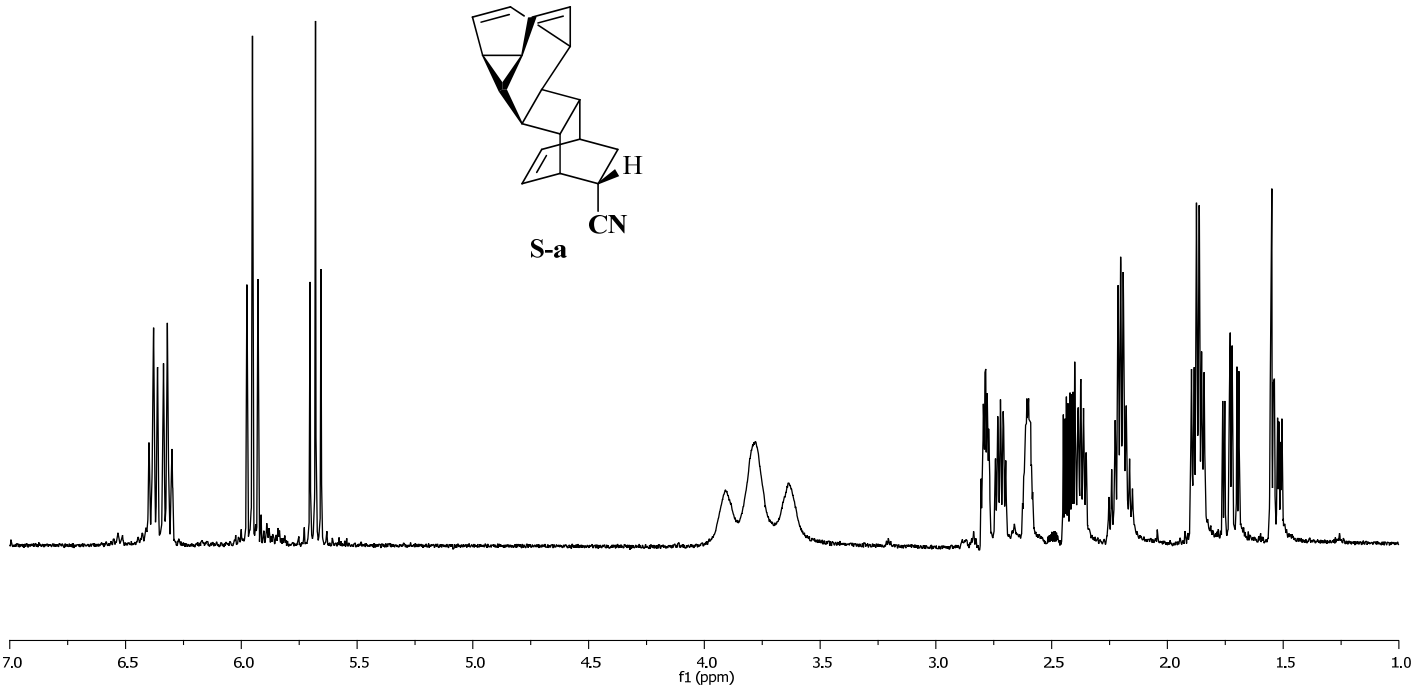


COSY (400 MHz, $CDCl_3$):

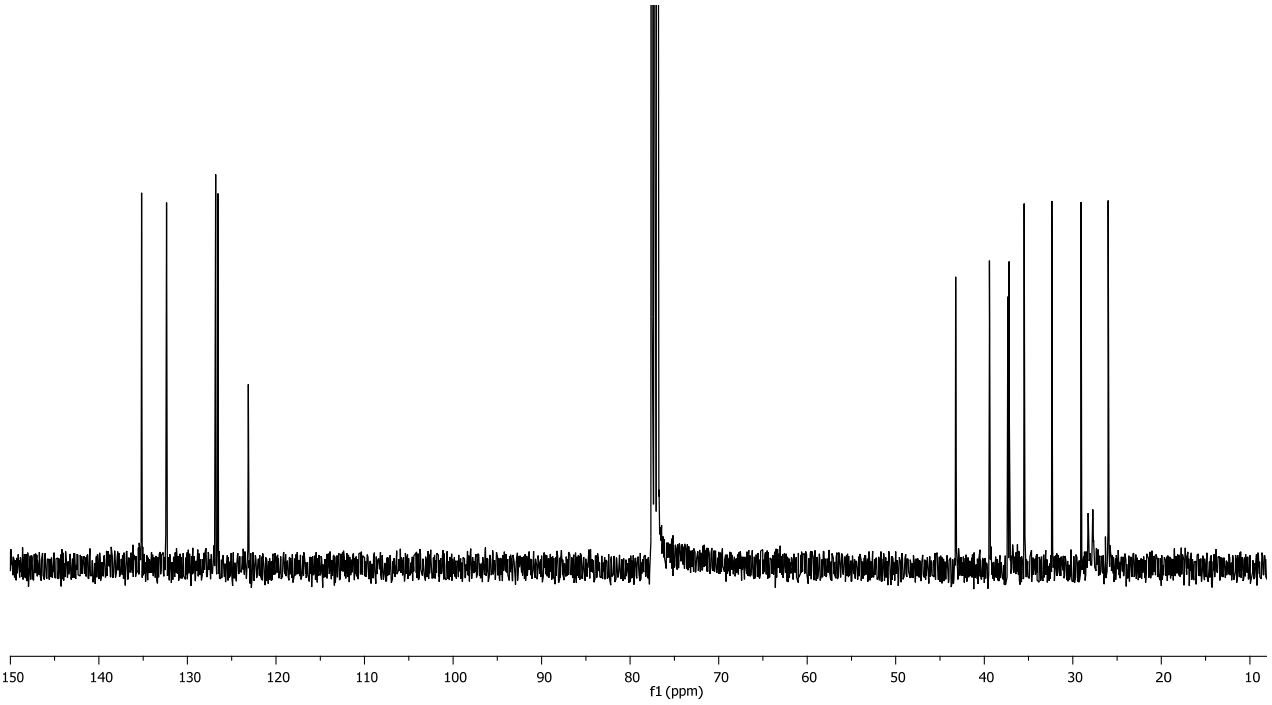


OTHER POLYCYCLES WHICH, ACCORDING TO NMR, EXPERIENCE COMPLETE AVERAGING IN THE COPE MOIETY

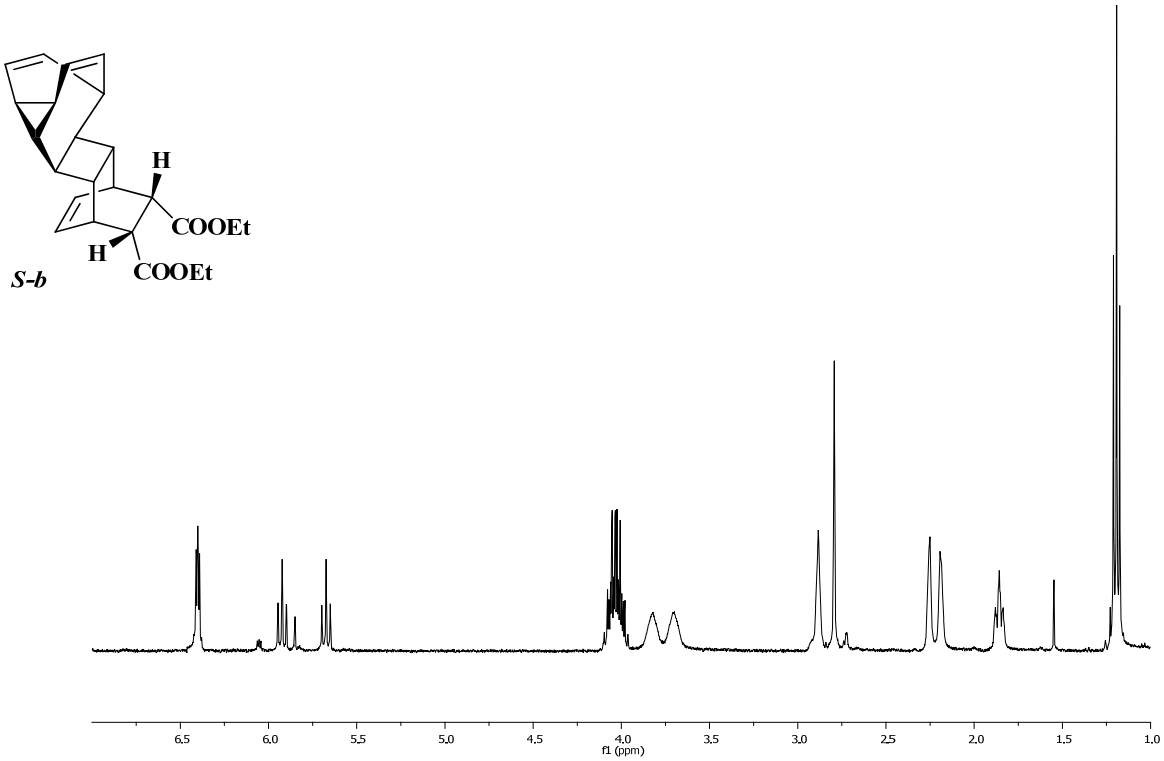
^{1}H NMR (400 MHz, $CDCl_3$):



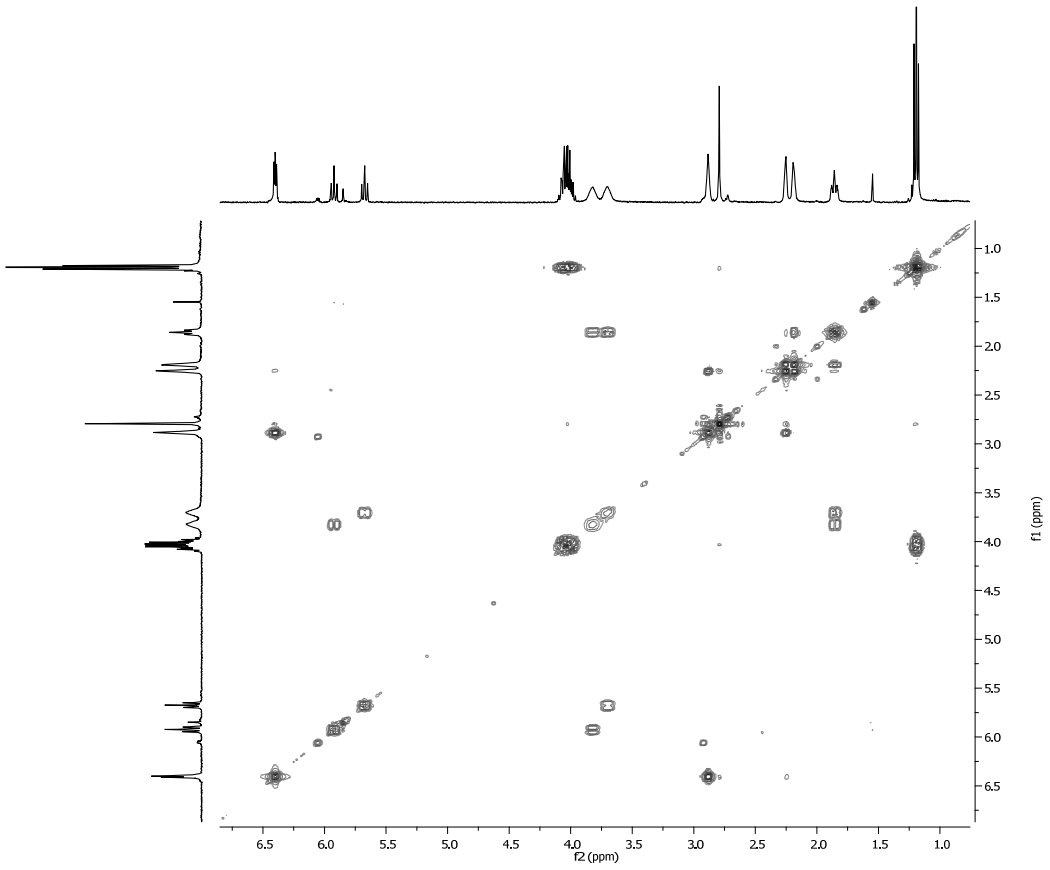
^{13}C NMR (400 MHz, $CDCl_3$):



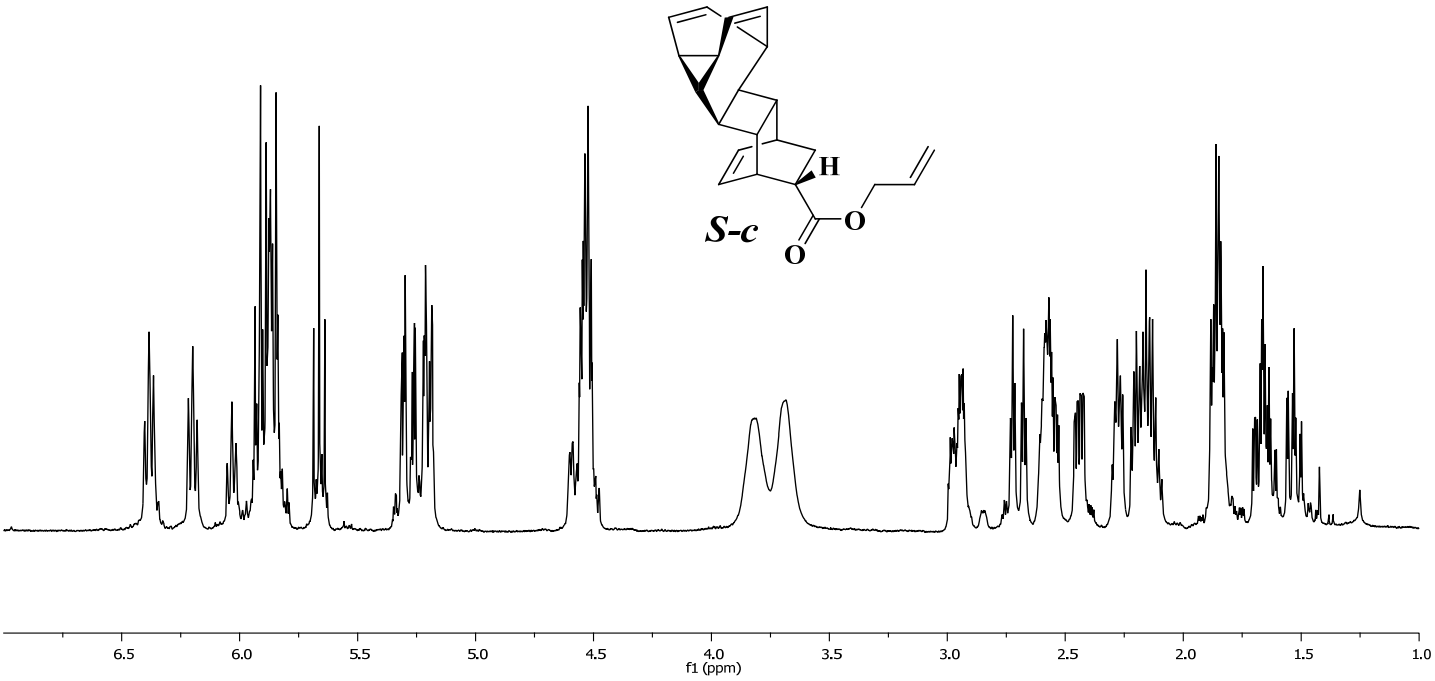
^{1}H NMR (400 MHz, $CDCl_3$):



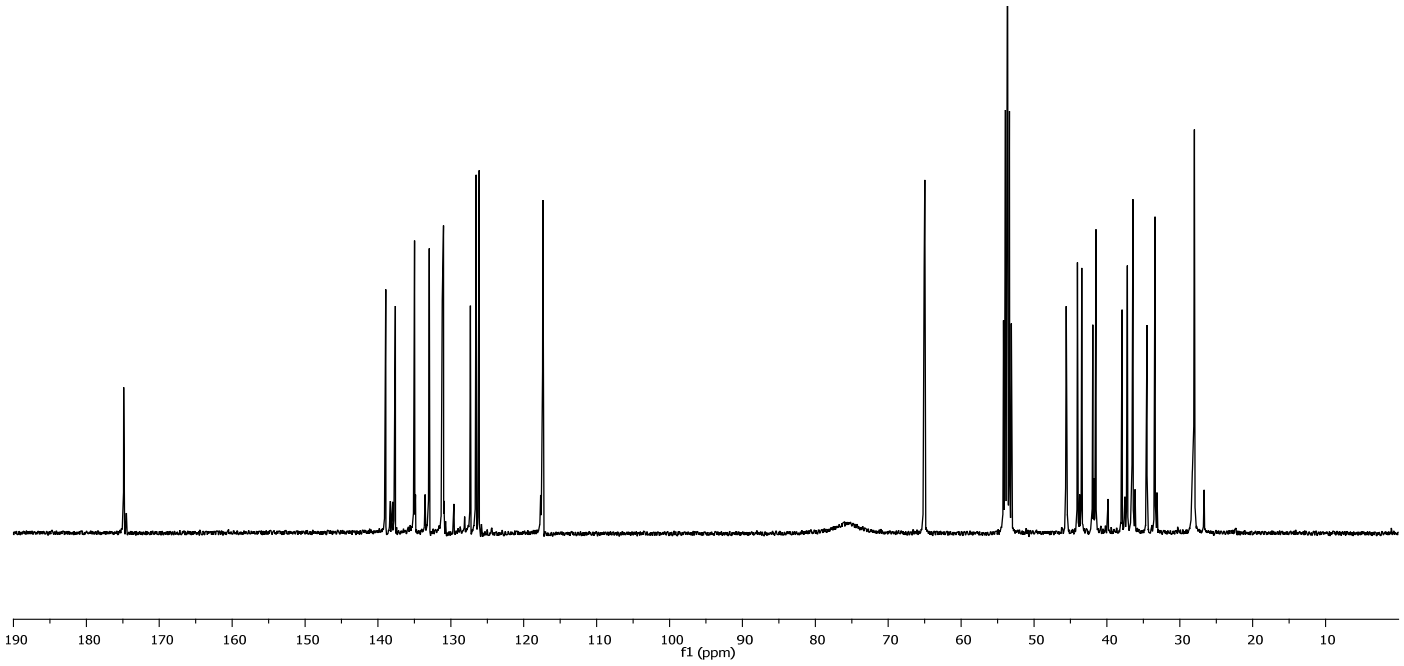
COSY (400 MHz, $CDCl_3$):



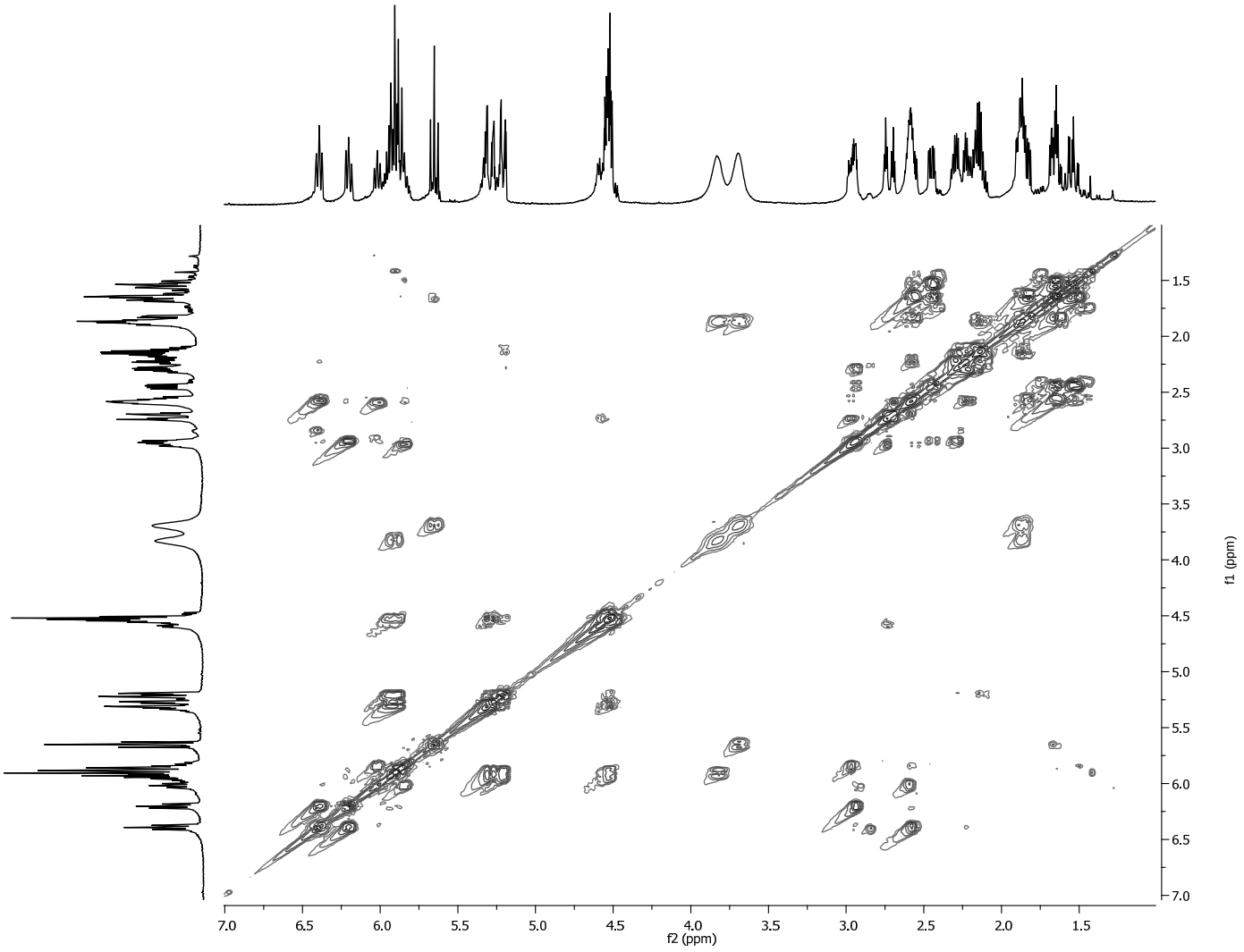
^{1}H NMR (400 MHz, $CDCl_3$):



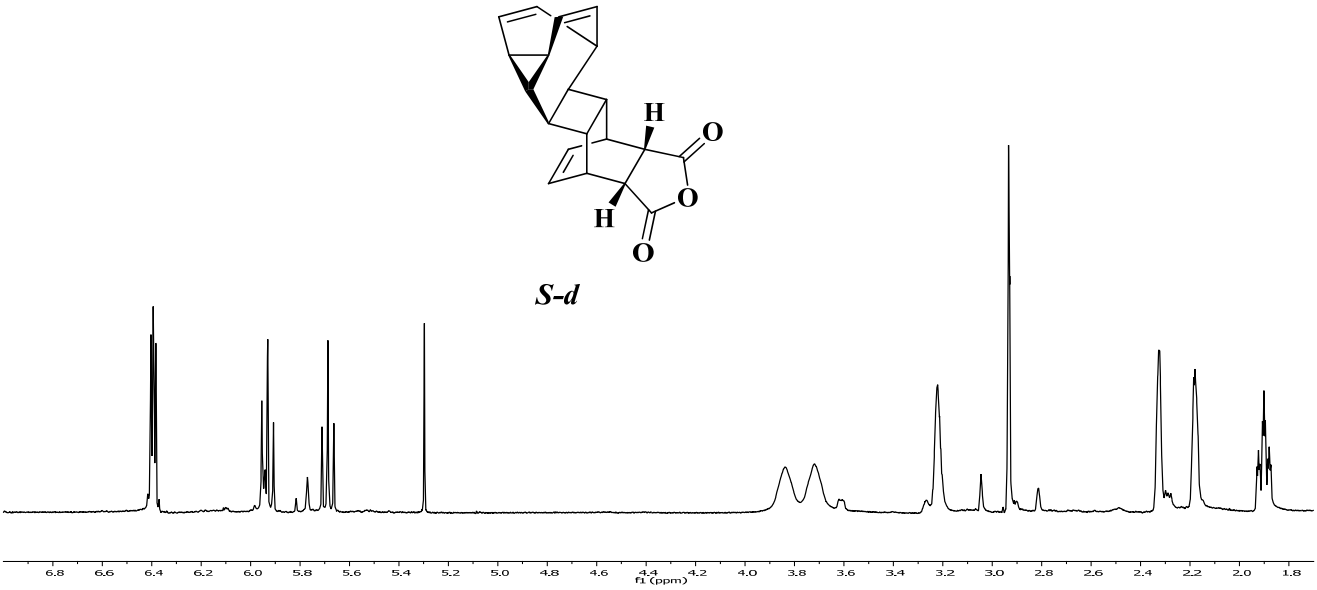
^{13}C NMR (400 MHz, CD_2Cl_2):



COSY (400 MHz, $CDCl_3$):

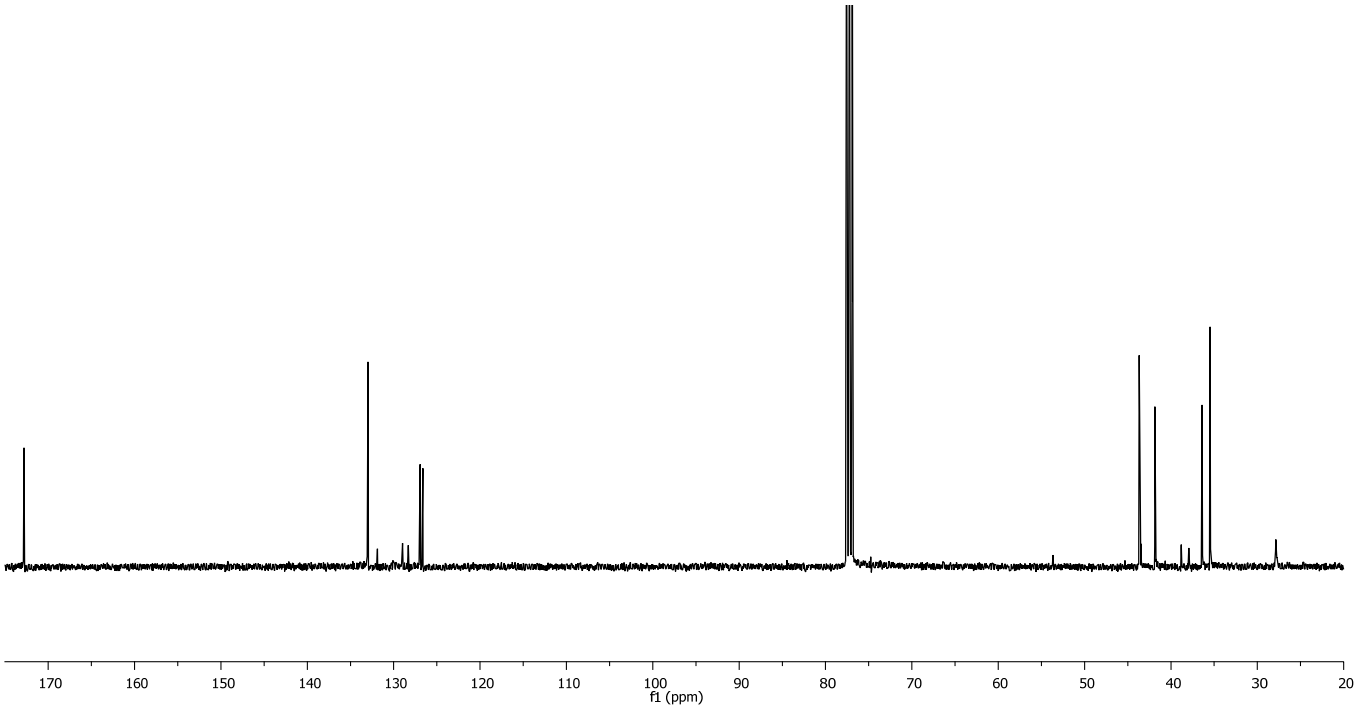


^{1}H NMR (400 MHz, $CDCl_3$):

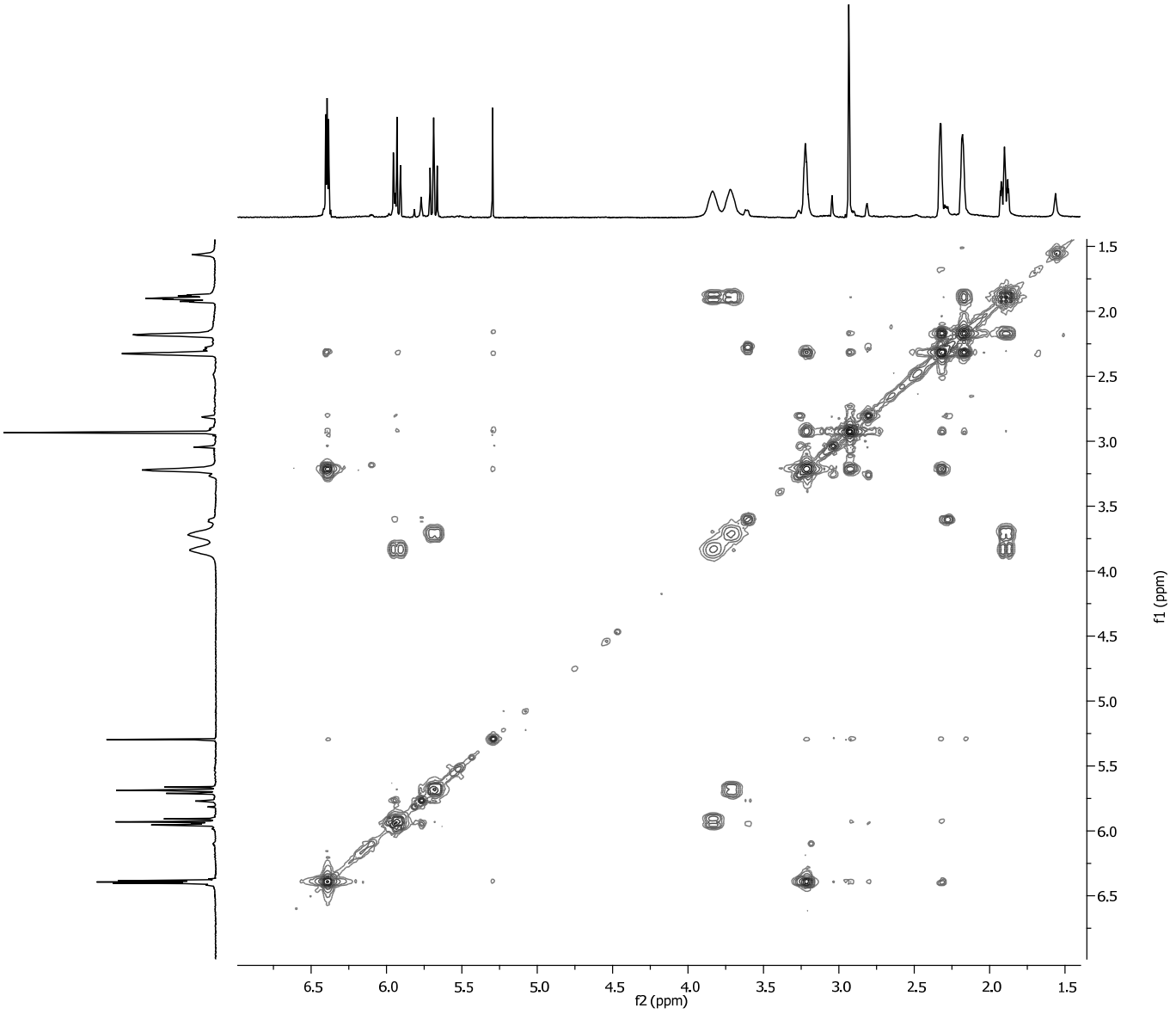


S-d

^{13}C NMR (400 MHz, $CDCl_3$):



COSY (400 MHz, $CDCl_3$):



VT NMR EXPERIMENTS

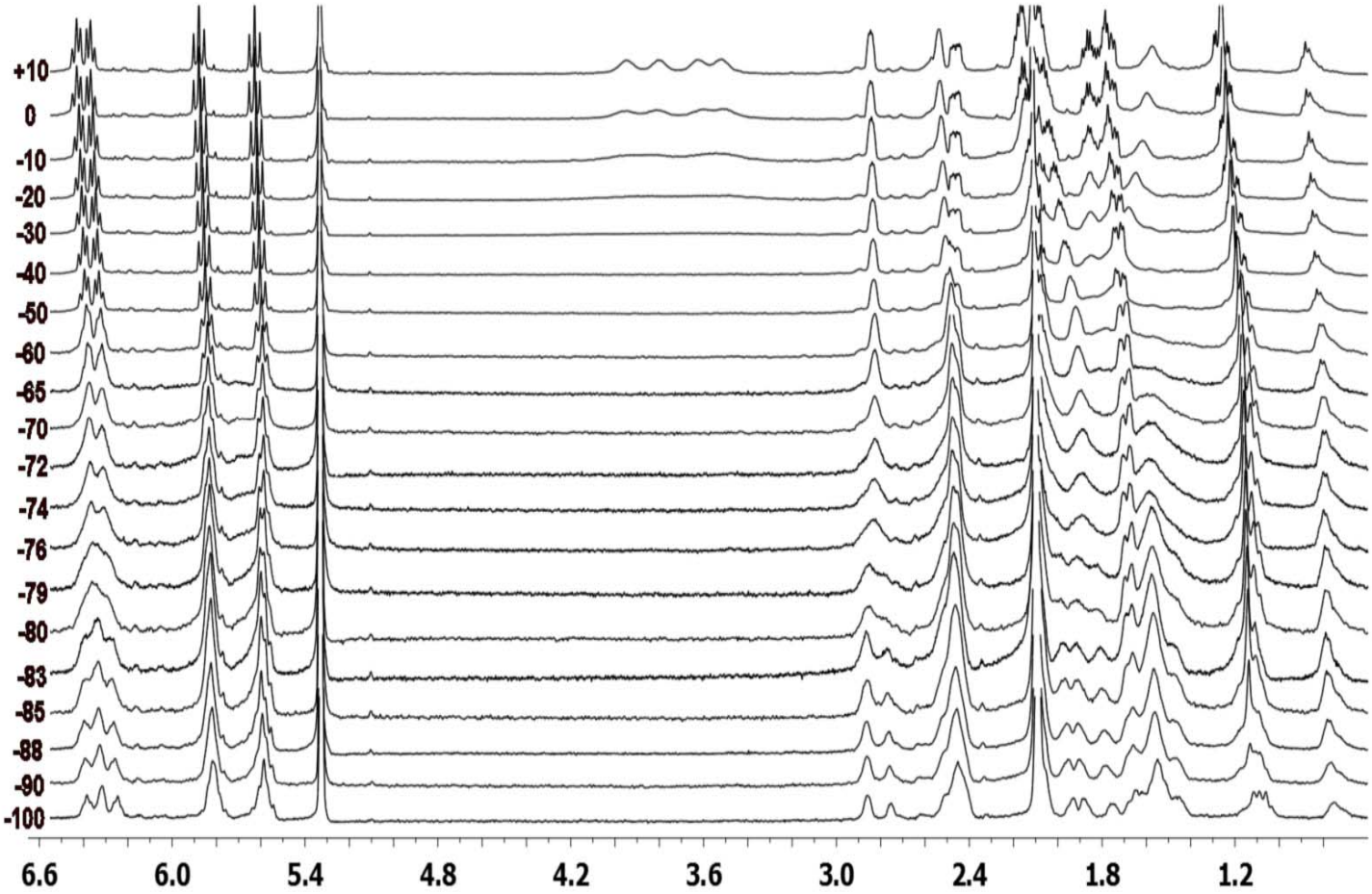


Figure S1. Low temperature VT NMR experiment with the endo adduct **6**

Low temperature VT NMR experiment with the oxetane **9**

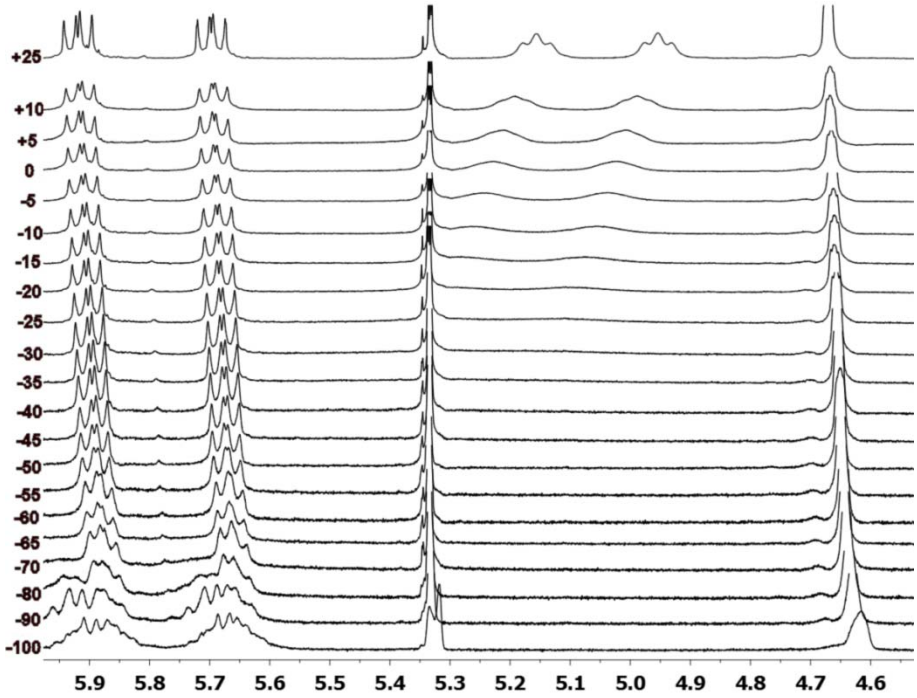


Figure S2. The low field portion of the spectrum

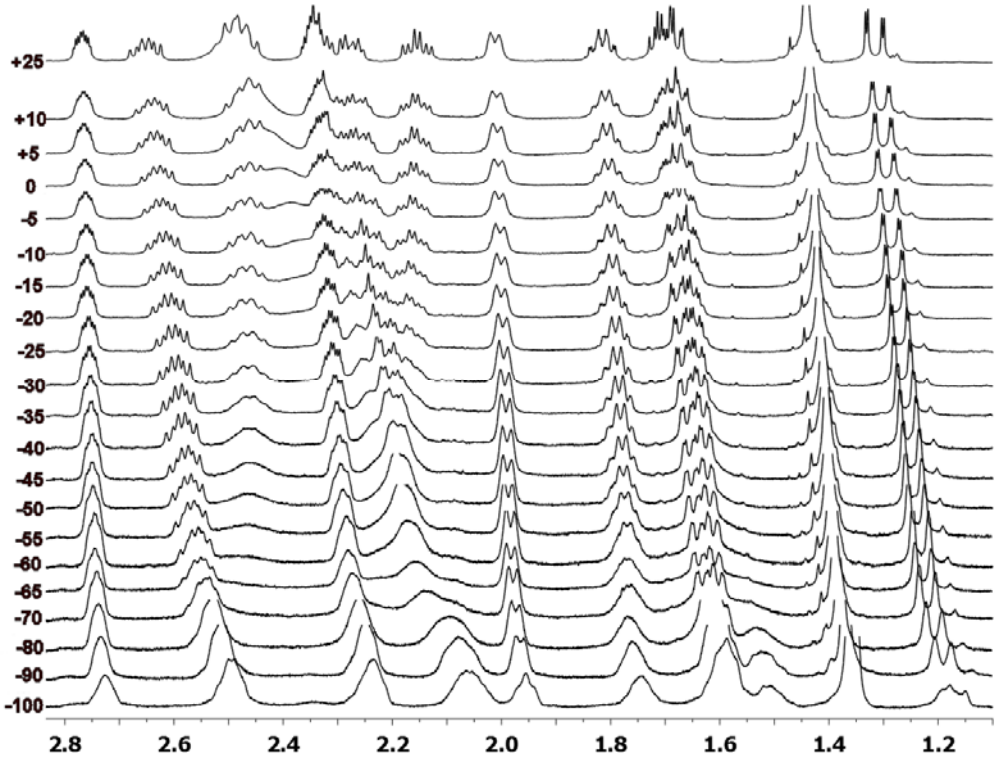


Figure S3. The high field portion of the spectrum

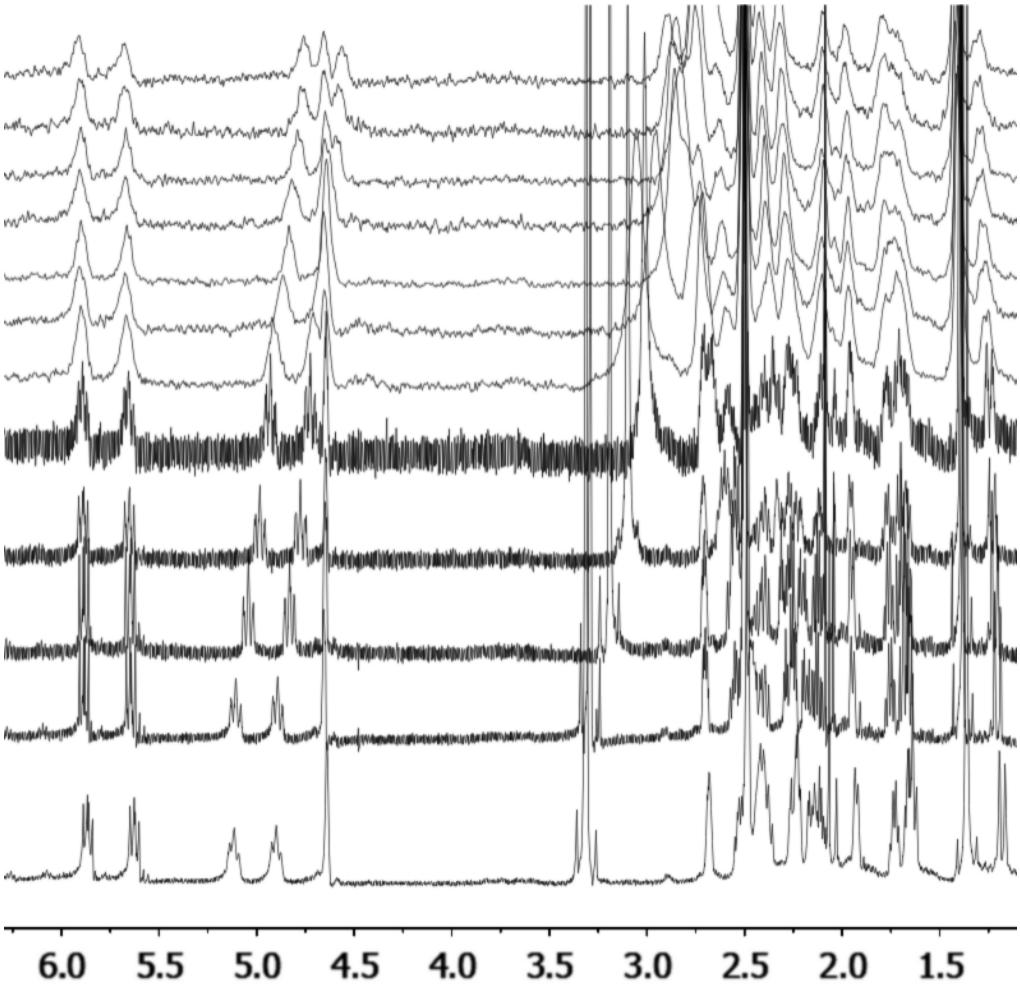
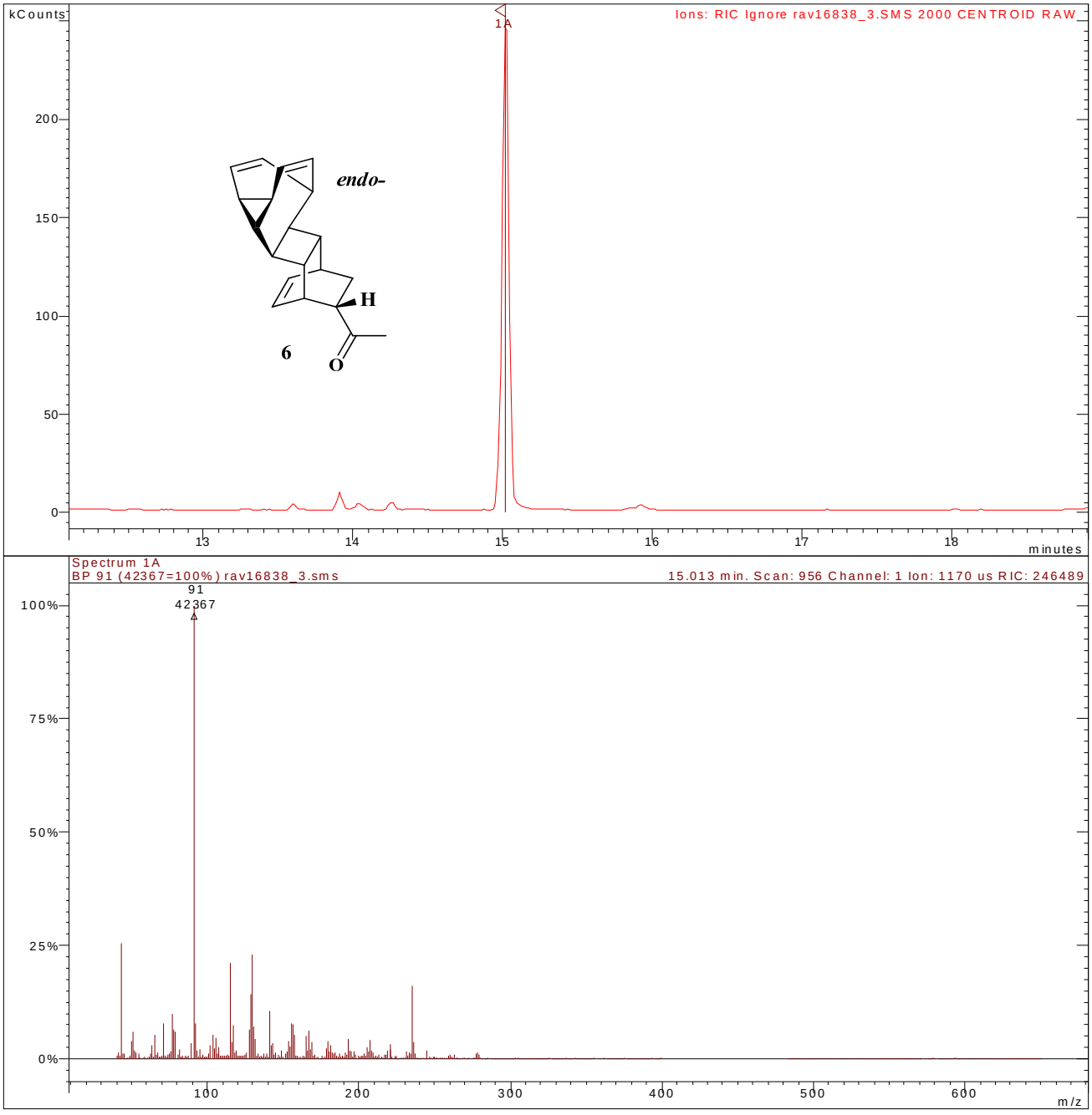


Figure S4. High temperature VT NMR experiment with oxetane **9** ($20^{o}C \rightarrow 160^{o}C$)

(The values of the changing chemical shift of the partially-averaged alkenyl proton at 5.2ppm was used in Figure 3, main text)

GCMS chromatograms.

MS Data Review All Plots - 1/24/2009 1:51 PM



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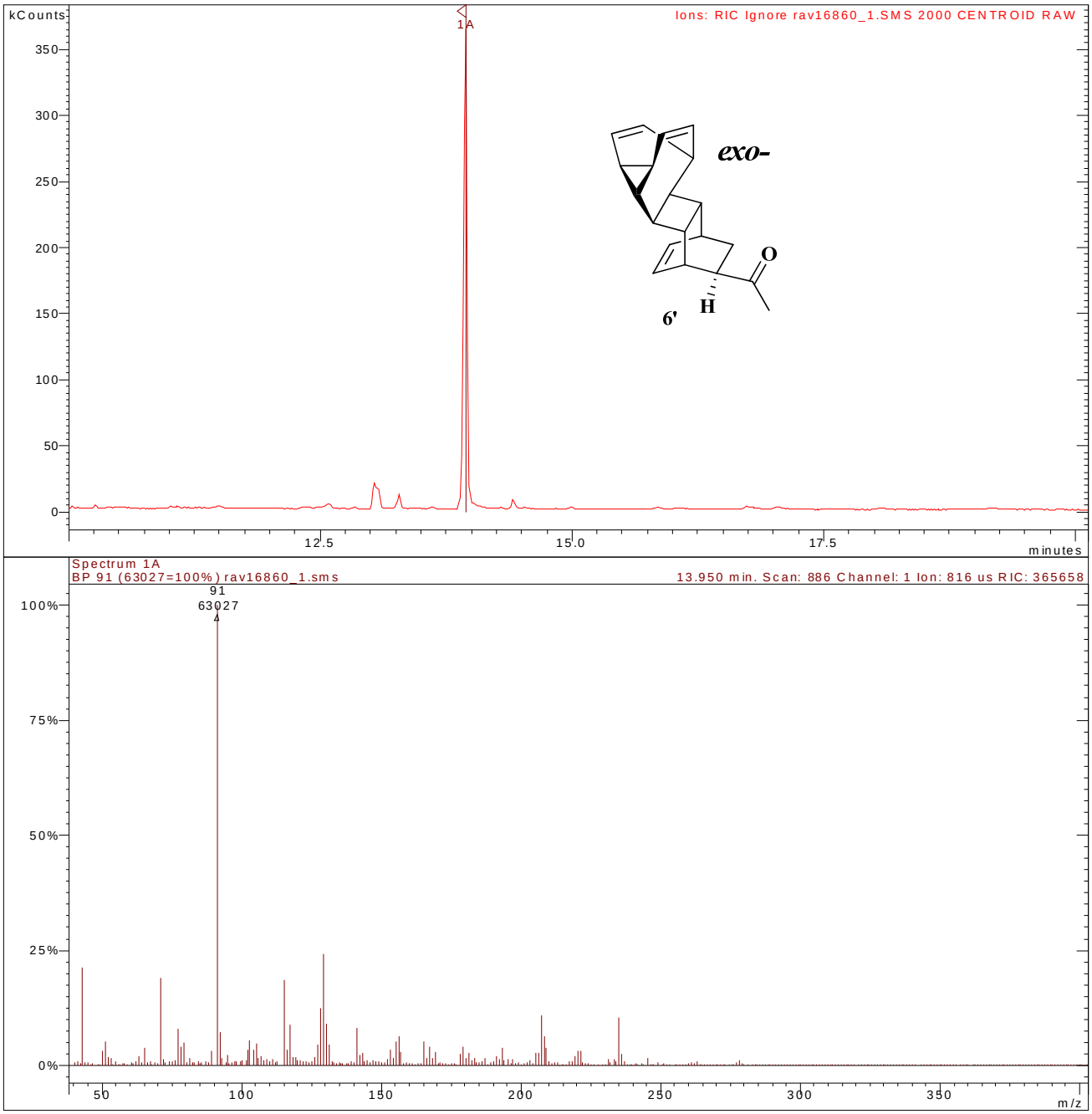

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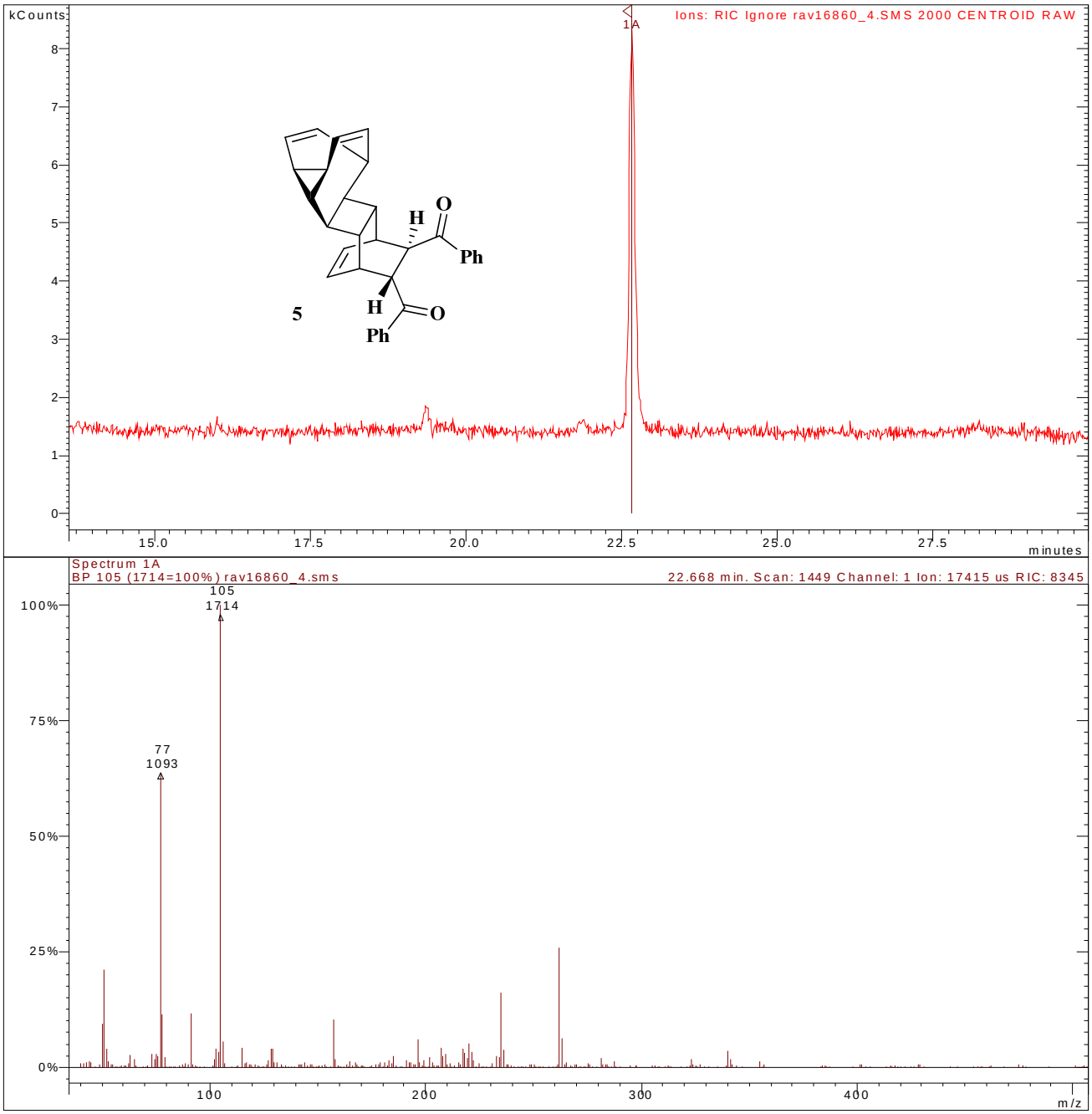

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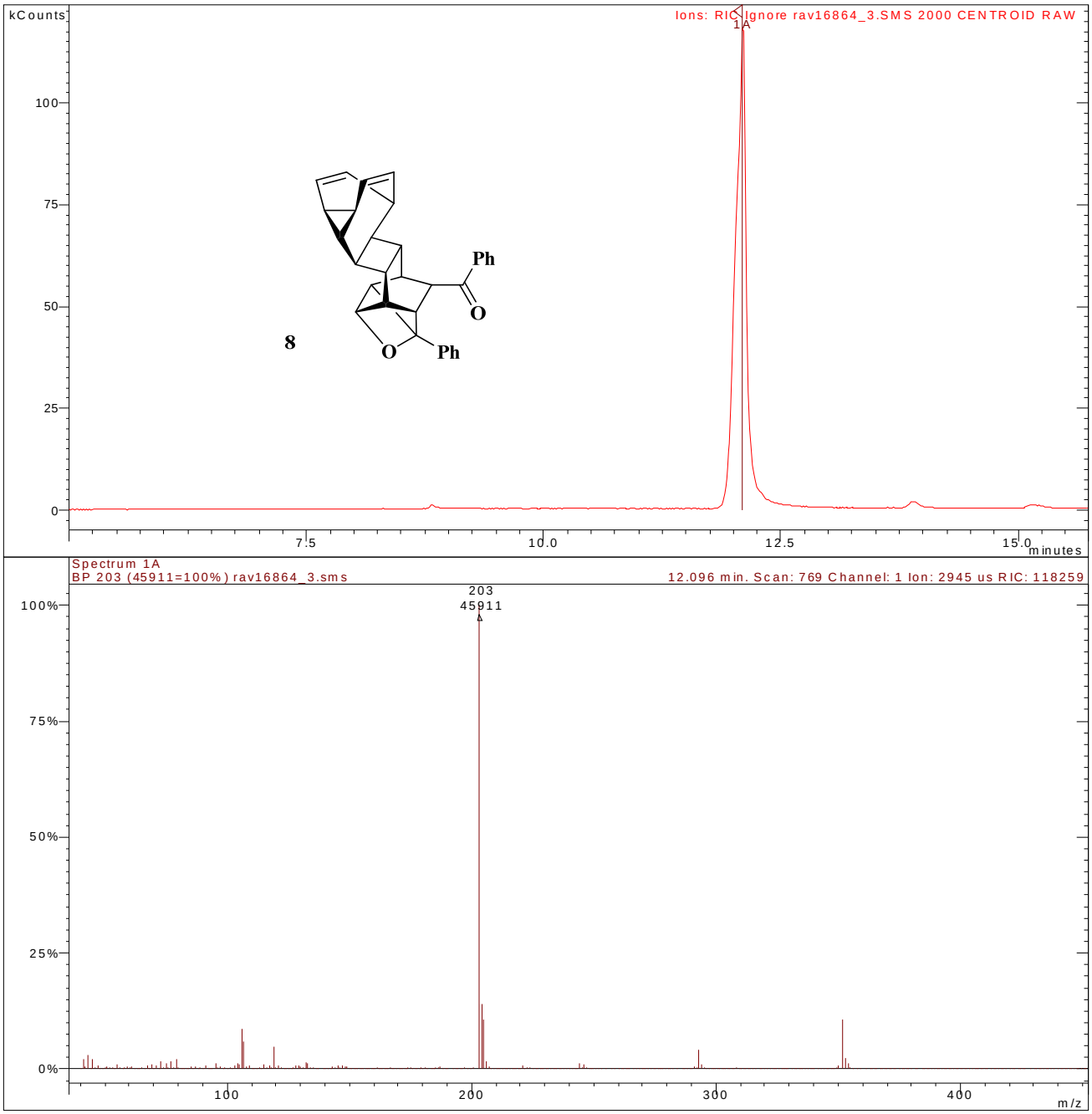


XRay Data for D.-A. adduct 5

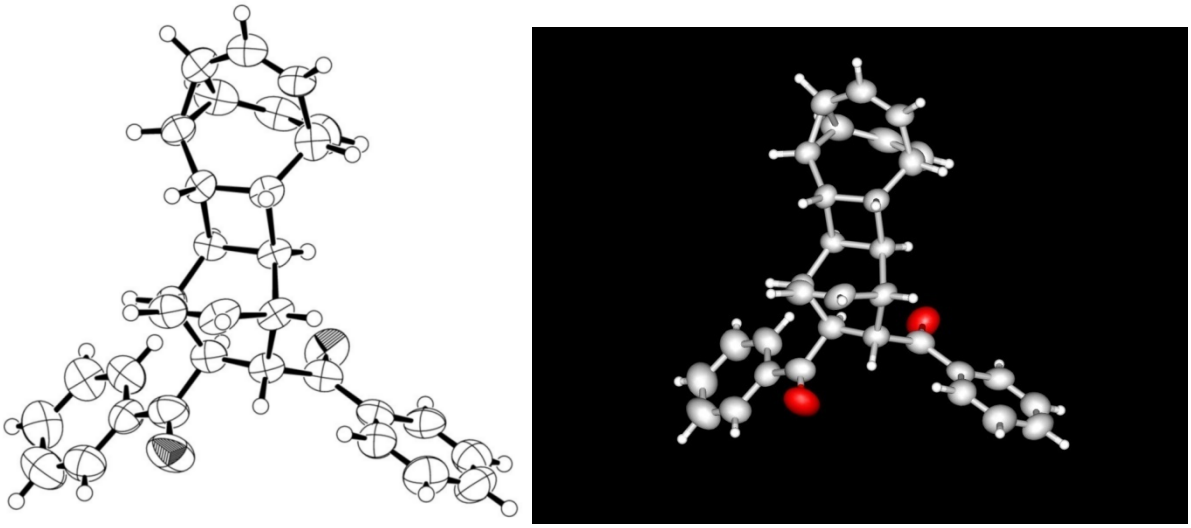


Figure S5. Ortep drawing of **5.**

Data Collection

A colorless plate crystal of $C_{32}H_{28}O_2$ having approximate dimensions of 0.32 x 0.24 x 0.07 mm was mounted on a glass fiber. All measurements were made on a Rigaku Mercury2 CCD area detector with graphite monochromated Mo-Kα radiation.

Indexing was performed from 4 images that were exposed for 20 seconds. The crystal-to-detector distance was 50.10 mm.

Cell constants and an orientation matrix for data collection corresponded to a primitive monoclinic cell with dimensions:

a = 15.99(4) Å
b = 13.390(17) Å β = 102.28(7)^o
c = 11.462(15) Å
V = 2397.9(74) Å^3

For Z = 4 and F.W. = 444.57, the calculated density is 1.231 g/cm^3. The systematic absences of:

h0l: l ± 2n
0k0: k ± 2n

uniquely determine the space group to be:

$P2_1/c$ (#14)

The data were collected at a temperature of -50 ± 1^{o}C to a maximum 2θ value of 55.0^o. A total of 360 oscillation images were collected. A sweep of data was done using ω scans from -120.0 to 60.0^o in 1.0^o step, at χ=54.0^o and ϕ = 0.0^o. The exposure rate was 70.0 [sec./^{o}]. The detector swing angle was -29.60^o. A second sweep was performed using ω scans from -120.0 to 60.0^o in 1.0^o step, at χ=54.0^o and ϕ = 120.0^o. The exposure rate was 70.0 [sec./^{o}]. The detector swing angle was -29.60^o. The crystal-to-detector distance was 50.10 mm. Readout was performed in the 0.146 mm pixel mode.

Data Reduction

Of the 16014 reflections that were collected, 5409 were unique (R_{int} = 0.076). Data were collected and processed using CrystalClear (Rigaku). Net intensities and sigmas were derived as follows:

$$F^2 = [\Sigma(P_i - mB_{ave})] \cdot Lp^{-1}$$

where P_i is the value in counts of the i^{th} pixel
m is the number of pixels in the integration area
B_{ave} is the background average
Lp is the Lorentz and polarization factor

$$B_{ave} = \Sigma(B_j)/n$$

where n is the number of pixels in the background area
B_j is the value of the j^{th} pixel in counts

$$\sigma^2(F^2_{hkl}) = [(\Sigma P_i) + m((\Sigma(B_{ave} - B_j)^2)/(n-1))] \cdot Lp \cdot errmul + (erradd \cdot F^2)^2$$

where erradd = 0.00
errmul = 1.00

The linear absorption coefficient, μ, for Mo-Kα radiation is 0.750 cm^{-1}. The data were corrected for Lorentz and polarization effects.

Structure Solution and Refinement

The structure was solved by and expanded using Fourier techniques[3]. The non-hydrogen atoms were refined anisotropically. Hydrogen atoms were included but not refined. The final cycle of full-matrix least-squares refinement[4] on F^2 was based on 5409 observed reflections and 320 variable parameters and converged (largest parameter shift was 0.01 times its esd) with unweighted and weighted agreement factors of:

$$R1 = \Sigma \, ||Fo| - |Fc|| \, / \, \Sigma \, |Fo| = 0.0691$$

$$wR2 = [\Sigma (w (Fo^2 - Fc^2)^2)/ \Sigma \, w(Fo^2)^2]^{1/2} = 0.1825$$

The standard deviation of an observation of unit weight[5] was 1.01. Unit weights were used. The maximum and minimum peaks on the final difference Fourier map corresponded to 0.18 and -0.18 $e^-/Å^3$, respectively.

Neutral atom scattering factors were taken from Cromer and Waber[6]. Anomalous dispersion effects were included in Fcalc[7]; the values for $\Delta f'$ and $\Delta f''$ were those of Creagh and McAuley[8]. The values for the mass attenuation coefficients are those of Creagh and Hubbell[9]. All calculations were performed using the CrystalStructure[10] crystallographic software package except for refinement, which was performed using SHELXL-97[11].

References

(1) CrystalClear: Rigaku Corporation, 1999. CrystalClear Software User's Guide, Molecular Structure Corporation, (c) 2000.J.W.Pflugrath (1999) Acta Cryst. D55, 1718-1725.

(3) DIRDIF99: Beurskens, P.T., Admiraal, G., Beurskens, G., Bosman, W.P., de Gelder, R., Israel, R. and Smits, J.M.M.(1999). The DIRDIF-99 program system, Technical Report of the Crystallography Laboratory, University of Nijmegen, The Netherlands.

(4) Least Squares function minimized: (SHELXL97)

$\Sigma w(F_o^2-F_c^2)^2$ where w = Least Squares weights.

(5) Standard deviation of an observation of unit weight:

$[\Sigma w(F_o^2-F_c^2)^2/(N_o-N_v)]^{1/2}$

where N_o = number of observations
N_v = number of variables

(6) Cromer, D. T. & Waber, J. T.; "International Tables for X-ray Crystallography", Vol. IV, The Kynoch Press, Birmingham, England, Table 2.2 A (1974).

(7) Ibers, J. A. & Hamilton, W. C.; Acta Crystallogr., 17, 781 (1964).

(8) Creagh, D. C. & McAuley, W.J .; "International Tables for Crystallography", Vol C, (A.J.C. Wilson, ed.), Kluwer Academic Publishers, Boston, Table 4.2.6.8, pages 219-222 (1992).

(9) Creagh, D. C. & Hubbell, J.H..; "International Tables for Crystallography", Vol C, (A.J.C. Wilson, ed.), Kluwer Academic Publishers, Boston, Table 4.2.4.3, pages 200-206 (1992).

(10) CrystalStructure 3.8: Crystal Structure Analysis Package, Rigaku and Rigaku Americas (2000-2007). 9009 New Trails Dr. The Woodlands TX 77381 USA.

(11) SHELX97: Sheldrick, G.M. (1997).

EXPERIMENTAL DETAILS

A. Crystal Data

Empirical Formula	$C_{32}H_{28}O_2$
Formula Weight	444.57
Crystal Color, Habit	colorless, plate
Crystal Dimensions	0.32 X 0.24 X 0.07 mm
Crystal System	monoclinic
Lattice Type	Primitive
Indexing Images	4 images @ 20 seconds
Detector Position	50.10 mm
Pixel Size	0.146 mm
Lattice Parameters	a = 15.99(4) Å b = 13.390(17) Å c = 11.462(15) Å β = 102.28(7) ^{o} V = 2397.9(74) Å^3
Space Group	$P2_1/c$ (#14)
Z value	4
D_{calc}	1.231 g/cm^3

F_{000}	944.00
μ(MoKα)	0.750 cm^{-1}

B. Intensity Measurements

Diffractometer	Rigaku SCXmini
Radiation	MoKα (λ = 0.71075 Å) graphite monochromated
Detector Aperture	75 mm round
Data Images	360 exposures
ω oscillation Range (χ=54.0, ϕ=0.0)	-120.0 - 60.0^o
Exposure Rate	70.0 sec./^{o}
Detector Swing Angle	-29.60^o
ω oscillation Range (χ=54.0, ϕ=120.0)	-120.0 - 60.0^o
Pixel Size	0.146 mm
$2\theta_{max}$	55.0^o
No. of Reflections Measured	Total: 16014 Unique: 5409 (R_{int} = 0.076)
Corrections	Lorentz-polarization

C. Structure Solution and Refinement

Structure Solution	Direct Methods
Refinement	Full-matrix least-squares on F^2
Function Minimized	Σ w $(Fo^2 - Fc^2)^2$
Least Squares Weights	$w = 1/ [\sigma^2(Fo^2) + (0.0628 \cdot P)^2 + 0.6234 \cdot P]$ where $P = (Max(Fo^2,0) + 2Fc^2)/3$
$2\theta_{max}$ cutoff	55.0^o
Anomalous Dispersion	All non-hydrogen atoms
No. Observations (All reflections)	5409
No. Variables	320
Reflection/Parameter Ratio	16.90
Residuals: R1 (I>2.00σ(I))	0.0691
Residuals: R (All reflections)	0.1367
Residuals: wR2 (All reflections)	0.1825
Goodness of Fit Indicator	1.015
Max Shift/Error in Final Cycle	0.009
Maximum peak in Final Diff. Map	0.18 $e^-/Å^3$
Minimum peak in Final Diff. Map	-0.18 $e^-/Å^3$

Table S1. Atomic coordinates and B_{iso}/B_{eq} and occupancy

atom	x	y	z	B_{eq}	occ
O(1A)	0.11938(16)	-0.48761(18)	0.2256(2)	6.55(6)	0.893(2)
O(2A)	0.24421(14)	-0.71521(16)	0.03154(17)	4.88(4)	0.893(2)
C(1A)	0.15024(17)	-0.39125(15)	0.0649(2)	3.88(5)	0.893(2)
C(2A)	0.19839(13)	-0.37777(17)	-0.0215(2)	4.38(6)	0.893(2)
C(3A)	0.17992(19)	-0.2991(2)	-0.1020(2)	5.21(7)	0.893(2)
C(4A)	0.1133(2)	-0.23395(18)	-0.0961(2)	5.88(8)	0.893(2)
C(5A)	0.06514(17)	-0.2474(2)	-0.0096(3)	6.58(9)	0.893(2)
C(6A)	0.08361(17)	-0.3261(2)	0.0709(2)	5.46(7)	0.893(2)
C(7A)	0.16784(19)	-0.4740(2)	0.1569(2)	4.20(6)	0.893(2)
C(8A)	0.17140(12)	-0.81506(12)	0.1494(2)	3.51(5)	0.893(2)
C(9A)	0.14980(14)	-0.88385(19)	0.05711(14)	4.15(6)	0.893(2)
C(10A)	0.10527(17)	-0.97011(17)	0.0733(2)	5.01(7)	0.893(2)
C(11A)	0.08234(17)	-0.98758(14)	0.1819(2)	5.68(8)	0.893(2)
C(12A)	0.10394(16)	-0.9188(2)	0.27426(18)	5.53(7)	0.893(2)
C(13A)	0.14847(13)	-0.83254(15)	0.25801(16)	4.22(6)	0.893(2)
C(14A)	0.22033(17)	-0.7232(2)	0.1262(2)	3.46(5)	0.893(2)
O(1B)	0.2523(10)	-0.5602(13)	-0.0104(14)	5.3(4)	0.107(2)
O(2B)	0.1146(12)	-0.6417(13)	0.2901(19)	6.5(5)	0.107(2)
C(1B)	0.1775(14)	-0.4118(11)	0.017(2)	3.88(5)	0.107(2)
C(2B)	0.1959(13)	-0.358(2)	-0.077(2)	4.38(6)	0.107(2)
C(3B)	0.1515(18)	-0.270(2)	-0.1144(19)	5.21(7)	0.107(2)
C(4B)	0.0888(19)	-0.2366(17)	-0.056(2)	5.88(8)	0.107(2)
C(5B)	0.0704(15)	-0.291(2)	0.038(2)	6.58(9)	0.107(2)
C(6B)	0.1148(16)	-0.3784(18)	0.0754(19)	5.46(7)	0.107(2)
C(7B)	0.2236(14)	-0.5075(13)	0.0592(19)	4.20(6)	0.107(2)
C(8B)	0.1378(13)	-0.7980(9)	0.2078(17)	3.51(5)	0.107(2)
C(9B)	0.1533(14)	-0.8352(14)	0.1012(16)	4.15(6)	0.107(2)
C(10B)	0.1299(17)	-0.9325(16)	0.0664(17)	5.01(7)	0.107(2)
C(11B)	0.0909(17)	-0.9926(11)	0.138(2)	5.68(8)	0.107(2)
C(12B)	0.0754(15)	-0.9554(15)	0.245(2)	5.53(7)	0.107(2)
C(13B)	0.0988(14)	-0.8581(15)	0.2796(14)	4.22(6)	0.107(2)
C(14B)	0.1624(12)	-0.6917(12)	0.2421(17)	3.46(5)	0.107(2)
C(15)	0.24759(16)	-0.53786(18)	0.1669(2)	3.85(4)	
C(16)	0.32895(16)	-0.48248(19)	0.2401(2)	3.89(5)	
C(17)	0.33185(17)	-0.4941(2)	0.3714(2)	4.82(6)	
C(18)	0.33222(16)	-0.5872(2)	0.4089(2)	4.62(6)	
C(19)	0.32624(15)	-0.66612(19)	0.3124(2)	3.77(4)	
C(20)	0.24051(15)	-0.64248(18)	0.2192(2)	3.51(4)	
C(21)	0.40611(15)	-0.54062(17)	0.2107(2)	3.24(4)	
C(22)	0.40121(15)	-0.65179(17)	0.2466(2)	3.24(4)	
C(23)	0.49721(15)	-0.53136(17)	0.2941(2)	3.43(4)	
C(24)	0.49438(15)	-0.64539(17)	0.3219(2)	3.44(4)	
C(25)	0.56005(16)	-0.71385(19)	0.2824(2)	3.96(5)	
C(26)	0.65065(17)	-0.6919(2)	0.3468(2)	4.27(5)	
C(27)	0.69210(16)	-0.6075(2)	0.3378(2)	4.09(5)	
C(28)	0.65969(17)	-0.5192(2)	0.2652(2)	4.29(5)	
C(29)	0.56697(16)	-0.4856(2)	0.2408(2)	4.09(5)	
C(30)	0.60002(18)	-0.5312(2)	0.1387(2)	4.97(6)	
C(31)	0.57512(18)	-0.6307(2)	0.0903(2)	5.22(6)	
C(32)	0.55701(17)	-0.7101(2)	0.1482(2)	4.83(6)	

$B_{eq} = 8/3\ \pi^2(U_{11}(aa^*)^2 + U_{22}(bb^*)^2 + U_{33}(cc^*)^2 + 2U_{12}(aa^*bb^*)\cos\gamma + 2U_{13}(aa^*cc^*)\cos\beta + 2U_{23}(bb^*cc^*)\cos\alpha)$

Table S2. Atomic coordinates and B $_{iso}$ involving hydrogens/B_{eq} and occupancy

atom	x	y	z	B_{eq}	occ
H(2A)	0.2435	-0.4218	-0.0255	5.694	0.893
H(3A)	0.2125	-0.2900	-0.1605	6.769	0.893
H(4A)	0.1008	-0.1808	-0.1505	7.643	0.893
H(5A)	0.0201	-0.2034	-0.0056	8.558	0.893
H(6A)	0.0510	-0.3352	0.1294	7.102	0.893
H(9A)	0.1653	-0.8720	-0.0163	5.396	0.893
H(10A)	0.0907	-1.0166	0.0109	6.515	0.893
H(11A)	0.0522	-1.0459	0.1929	7.389	0.893
H(12A)	0.0884	-0.9306	0.3477	7.186	0.893
H(13A)	0.1631	-0.7860	0.3205	5.484	0.893
H(2B)	0.2383	-0.3802	-0.1167	5.694	0.107
H(3B)	0.1640	-0.2333	-0.1786	6.769	0.107
H(4B)	0.0588	-0.1773	-0.0814	7.643	0.107
H(5B)	0.0280	-0.2682	0.0777	8.558	0.107
H(6B)	0.1024	-0.4151	0.1395	7.102	0.107
H(9B)	0.1797	-0.7946	0.0525	5.396	0.107
H(10B)	0.1404	-0.9577	-0.0057	6.515	0.107
H(11B)	0.0750	-1.0584	0.1148	7.389	0.107
H(12B)	0.0490	-0.9960	0.2935	7.186	0.107
H(13B)	0.0883	-0.8330	0.3517	5.484	0.107
H(15A)	0.2568	-0.5473	0.0848	5.003	0.893
H(15B)	0.2036	-0.5037	0.2014	5.003	0.107
H(16)	0.3298	-0.4113	0.2170	5.054	
H(17)	0.3333	-0.4392	0.4228	6.267	
H(18)	0.3359	-0.6035	0.4896	6.009	
H(19)	0.3258	-0.7344	0.3455	4.903	
H(20A)	0.1935	-0.6408	0.2631	4.568	0.893
H(20B)	0.2498	-0.6837	0.1514	4.568	0.107
H(21)	0.4086	-0.5337	0.1255	4.212	
H(22)	0.3966	-0.6973	0.1775	4.209	
H(23)	0.4924	-0.4931	0.3663	4.457	
H(24)	0.4949	-0.6559	0.4076	4.474	
H(25)	0.5468	-0.7832	0.3023	5.150	
H(26)	0.6799	-0.7419	0.3970	5.547	
H(27)	0.7485	-0.6034	0.3828	5.311	
H(28)	0.7015	-0.4639	0.2710	5.571	
H(29)	0.5614	-0.4121	0.2336	5.311	
H(30)	0.6109	-0.4824	0.0789	6.463	
H(31)	0.5716	-0.6388	0.0080	6.783	
H(32)	0.5411	-0.7687	0.1038	6.277	

$B_{eq} = 8/3\ \pi^2(U_{11}(aa^*)^2 + U_{22}(bb^*)^2 + U_{33}(cc^*)^2 + 2U_{12}(aa^*bb^*)\cos\gamma + 2U_{13}(aa^*cc^*)\cos\beta + 2U_{23}(bb^*cc^*)\cos\alpha)$

Table S3. Anisotropic displacement parameters

atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
O(1A)	0.0829(16)	0.0774(16)	0.1075(19)	0.0185(13)	0.0628(15)	0.0187(14)
O(2A)	0.0836(15)	0.0666(13)	0.0410(11)	-0.0106(11)	0.0261(10)	-0.0079(10)
C(1A)	0.0410(16)	0.0498(16)	0.0563(18)	0.0005(14)	0.0097(13)	-0.0030(15)
C(2A)	0.0592(18)	0.0506(18)	0.059(2)	0.0066(15)	0.0180(16)	0.0042(16)
C(3A)	0.081(2)	0.056(2)	0.0611(19)	0.0089(18)	0.0158(18)	0.0063(16)
C(4A)	0.087(2)	0.064(2)	0.067(2)	0.017(2)	0.0040(19)	0.0095(18)
C(5A)	0.078(2)	0.069(2)	0.102(3)	0.030(2)	0.015(2)	0.008(2)
C(6A)	0.057(2)	0.069(2)	0.083(2)	0.0162(18)	0.0179(17)	0.0003(19)
C(7A)	0.0509(16)	0.0507(16)	0.0637(19)	-0.0029(14)	0.0254(14)	-0.0083(14)
C(8A)	0.0434(17)	0.0466(15)	0.0427(15)	0.0038(13)	0.0076(13)	-0.0015(13)
C(9A)	0.0467(16)	0.0473(18)	0.0610(19)	-0.0016(14)	0.0054(14)	-0.0089(15)
C(10A)	0.0493(19)	0.052(2)	0.085(2)	-0.0022(15)	0.0043(17)	-0.0084(19)
C(11A)	0.0602(19)	0.0483(17)	0.109(3)	-0.0032(15)	0.023(2)	0.006(2)
C(12A)	0.073(2)	0.059(2)	0.082(2)	-0.0009(19)	0.025(2)	0.0138(19)
C(13A)	0.0561(19)	0.0495(17)	0.0552(18)	-0.0016(15)	0.0131(15)	0.0058(14)
C(14A)	0.0454(15)	0.0498(16)	0.0367(14)	0.0035(13)	0.0097(11)	-0.0012(12)
O(1B)	0.064(11)	0.079(12)	0.053(10)	0.015(9)	0.002(8)	-0.001(9)
O(2B)	0.075(13)	0.070(12)	0.115(16)	-0.011(10)	0.047(11)	-0.038(11)
C(1B)	0.0410(16)	0.0498(16)	0.0563(18)	0.0005(14)	0.0097(13)	-0.0030(15)
C(2B)	0.0592(18)	0.0506(18)	0.059(2)	0.0066(15)	0.0180(16)	0.0042(16)
C(3B)	0.081(2)	0.056(2)	0.0611(19)	0.0089(18)	0.0158(18)	0.0063(16)
C(4B)	0.087(2)	0.064(2)	0.067(2)	0.017(2)	0.0040(19)	0.0095(18)
C(5B)	0.078(2)	0.069(2)	0.102(3)	0.030(2)	0.015(2)	0.008(2)
C(6B)	0.057(2)	0.069(2)	0.083(2)	0.0162(18)	0.0179(17)	0.0003(19)
C(7B)	0.0509(16)	0.0507(16)	0.0637(19)	-0.0029(14)	0.0254(14)	-0.0083(14)
C(8B)	0.0434(17)	0.0466(15)	0.0427(15)	0.0038(13)	0.0076(13)	-0.0015(13)
C(9B)	0.0467(16)	0.0473(18)	0.0610(19)	-0.0016(14)	0.0054(14)	-0.0089(15)
C(10B)	0.0493(19)	0.052(2)	0.085(2)	-0.0022(15)	0.0043(17)	-0.0084(19)
C(11B)	0.0602(19)	0.0483(17)	0.109(3)	-0.0032(15)	0.023(2)	0.006(2)
C(12B)	0.073(2)	0.059(2)	0.082(2)	-0.0009(19)	0.025(2)	0.0138(19)
C(13B)	0.0561(19)	0.0495(17)	0.0552(18)	-0.0016(15)	0.0131(15)	0.0058(14)
C(14B)	0.0454(15)	0.0498(16)	0.0367(14)	0.0035(13)	0.0097(11)	-0.0012(12)
C(15)	0.0534(15)	0.0462(14)	0.0490(14)	0.0009(12)	0.0164(11)	-0.0008(12)
C(16)	0.0514(15)	0.0427(13)	0.0568(15)	-0.0025(11)	0.0185(12)	-0.0078(12)
C(17)	0.0575(16)	0.073(2)	0.0598(17)	-0.0108(15)	0.0282(13)	-0.0273(16)
C(18)	0.0567(16)	0.090(2)	0.0333(13)	-0.0151(15)	0.0188(11)	-0.0122(14)
C(19)	0.0566(15)	0.0526(14)	0.0360(12)	-0.0079(12)	0.0142(11)	0.0060(11)
C(20)	0.0452(13)	0.0519(14)	0.0398(12)	-0.0027(11)	0.0168(10)	-0.0023(11)
C(21)	0.0494(14)	0.0435(13)	0.0327(11)	0.0014(11)	0.0143(10)	0.0006(10)
C(22)	0.0494(14)	0.0430(13)	0.0328(11)	-0.0007(11)	0.0137(10)	0.0005(10)
C(23)	0.0493(14)	0.0435(13)	0.0398(12)	-0.0031(11)	0.0145(10)	-0.0044(11)
C(24)	0.0494(14)	0.0490(14)	0.0324(12)	-0.0023(11)	0.0088(10)	0.0029(10)
C(25)	0.0521(15)	0.0440(13)	0.0527(15)	0.0034(12)	0.0071(12)	-0.0003(12)
C(26)	0.0546(16)	0.0587(16)	0.0480(15)	0.0053(14)	0.0091(12)	0.0013(13)
C(27)	0.0456(14)	0.0648(17)	0.0444(14)	-0.0013(13)	0.0085(11)	-0.0076(13)
C(28)	0.0514(15)	0.0582(16)	0.0556(16)	-0.0057(13)	0.0167(12)	0.0029(13)
C(29)	0.0529(15)	0.0478(14)	0.0587(16)	-0.0011(12)	0.0211(12)	0.0086(12)
C(30)	0.0628(17)	0.085(2)	0.0464(15)	0.0025(16)	0.0236(13)	0.0156(15)
C(31)	0.0636(18)	0.104(2)	0.0336(14)	0.0053(18)	0.0166(12)	-0.0114(16)
C(32)	0.0555(16)	0.0707(19)	0.0565(17)	0.0049(15)	0.0103(13)	-0.0265(16)

The general temperature factor expression: $\exp(-2\pi^2(a^{*2}U_{11}h^2 + b^{*2}U_{22}k^2 + c^{*2}U_{33}l^2 + 2a^*b^*U_{12}hk + 2a^*c^*U_{13}hl + 2b^*c^*U_{23}kl))$

Table S4. Bond lengths (Å)

atom	atom	distance	atom	atom	distance
O(1A)	C(7A)	1.230(4)	O(2A)	C(14A)	1.229(3)
C(1A)	C(2A)	1.390(3)	C(1A)	C(6A)	1.390(3)
C(1A)	C(7A)	1.514(3)	C(1A)	C(1B)	0.82(2)
C(1A)	C(5B)	1.83(2)	C(1A)	C(6B)	0.63(2)
C(2A)	C(3A)	1.390(3)	C(2A)	C(1B)	0.76(2)
C(2A)	C(2B)	0.69(2)	C(3A)	C(4A)	1.390(4)
C(3A)	C(2B)	0.85(2)	C(3A)	C(3B)	0.59(2)
C(4A)	C(5A)	1.390(5)	C(4A)	C(3B)	0.84(2)
C(4A)	C(4B)	0.66(3)	C(5A)	C(6A)	1.390(4)
C(5A)	C(4B)	0.73(3)	C(5A)	C(5B)	0.79(2)
C(6A)	C(5B)	0.61(2)	C(6A)	C(6B)	0.86(2)
C(7A)	C(1B)	1.84(2)	C(7A)	C(6B)	1.70(2)
C(7A)	C(7B)	1.64(2)	C(7A)	C(15)	1.519(3)
C(8A)	C(9A)	1.390(2)	C(8A)	C(13A)	1.390(3)
C(8A)	C(14A)	1.511(3)	C(8A)	C(8B)	0.97(2)
C(8A)	C(9B)	0.628(18)	C(9A)	C(10A)	1.390(3)
C(9A)	C(9B)	0.818(19)	C(9A)	C(10B)	0.74(2)
C(10A)	C(11A)	1.390(4)	C(10A)	C(10B)	0.65(2)
C(10A)	C(11B)	0.88(2)	C(11A)	C(12A)	1.390(3)
C(11A)	C(10B)	1.82(2)	C(11A)	C(11B)	0.55(3)
C(11A)	C(12B)	0.87(2)	C(12A)	C(13A)	1.390(3)
C(12A)	C(11B)	1.82(2)	C(12A)	C(12B)	0.70(2)
C(12A)	C(13B)	0.82(2)	C(13A)	C(8B)	0.730(17)
C(13A)	C(9B)	1.82(2)	C(13A)	C(13B)	0.94(2)
C(14A)	C(9B)	1.83(2)	C(14A)	C(14B)	1.82(2)
C(14A)	C(20)	1.504(3)	O(1B)	C(7B)	1.22(2)
O(2B)	C(14B)	1.23(2)	C(1B)	C(2B)	1.39(3)
C(1B)	C(6B)	1.39(3)	C(1B)	C(7B)	1.50(2)
C(2B)	C(3B)	1.39(3)	C(3B)	C(4B)	1.39(4)
C(4B)	C(5B)	1.39(4)	C(5B)	C(6B)	1.39(3)
C(7B)	C(15)	1.28(2)	C(8B)	C(9B)	1.39(2)
C(8B)	C(13B)	1.39(2)	C(8B)	C(14B)	1.51(2)
C(9B)	C(10B)	1.39(2)	C(10B)	C(11B)	1.39(3)
C(11B)	C(12B)	1.39(3)	C(12B)	C(13B)	1.39(2)
C(14B)	C(20)	1.48(2)	C(15)	C(16)	1.576(3)
C(15)	C(20)	1.538(3)	C(16)	C(17)	1.504(3)
C(16)	C(21)	1.555(3)	C(17)	C(18)	1.318(4)
C(18)	C(19)	1.518(3)	C(19)	C(20)	1.580(3)
C(19)	C(22)	1.558(3)	C(21)	C(22)	1.551(3)
C(21)	C(23)	1.568(3)	C(22)	C(24)	1.557(3)
C(23)	C(24)	1.563(3)	C(23)	C(29)	1.510(3)
C(24)	C(25)	1.533(3)	C(25)	C(26)	1.508(3)
C(25)	C(32)	1.529(3)	C(26)	C(27)	1.325(3)
C(27)	C(28)	1.475(3)	C(28)	C(29)	1.517(3)
C(28)	C(30)	1.564(3)	C(29)	C(30)	1.512(4)
C(30)	C(31)	1.465(4)	C(31)	C(32)	1.318(4)

Table S5. Bond lengths involving hydrogens (Å)

atom	atom	distance	atom	atom	distance
C(1A)	H(6B)	1.303(2)	C(2A)	H(2A)	0.940(2)
H(2A)	C(1B)	1.26(2)	H(2A)	C(2B)	1.22(2)
C(3A)	H(3A)	0.940(2)	C(3A)	H(3B)	1.231(2)
H(3A)	C(3B)	1.23(3)	C(4A)	H(4A)	0.940(2)
C(4A)	H(4B)	1.194(3)	C(5A)	H(5A)	0.940(2)
C(5A)	H(4B)	1.238(3)	C(5A)	H(5B)	1.298(3)

C(6A)	H(6A)	0.940(2)	C(6A)	H(5B)	1.195(2)
H(6A)	C(5B)	1.29(3)	C(7A)	H(6B)	1.292(2)
C(7A)	H(15B)	0.787(2)	C(8A)	H(9B)	1.178(2)
C(9A)	H(9A)	0.9401(18)	C(9A)	H(9B)	1.292(2)
C(9A)	H(10B)	1.213(2)	C(10A)	H(10A)	0.940(2)
C(10A)	H(10B)	1.175(2)	C(11A)	H(11A)	0.940(2)
C(11A)	H(11B)	1.211(2)	H(11A)	C(11B)	1.20(2)
C(12A)	H(12A)	0.940(2)	H(12A)	C(12B)	1.20(2)
H(12A)	C(13B)	1.28(2)	C(13A)	H(13A)	0.9400(18)
H(13A)	C(8B)	1.279(19)	C(14A)	H(20B)	0.727(2)
O(1B)	H(15A)	1.092(16)	C(2B)	H(2B)	0.94(2)
C(3B)	H(3B)	0.94(2)	C(4B)	H(4B)	0.94(2)
C(5B)	H(5B)	0.94(2)	C(6B)	H(6B)	0.94(2)
C(7B)	H(15A)	0.765(19)	C(9B)	H(9B)	0.94(2)
C(10B)	H(10B)	0.94(2)	C(11B)	H(11B)	0.940(16)
C(12B)	H(12B)	0.94(2)	C(13B)	H(13B)	0.940(18)
C(14B)	H(20A)	0.848(16)	C(15)	H(15A)	0.990(2)
C(15)	H(15B)	0.990(2)	C(16)	H(16)	0.990(2)
C(17)	H(17)	0.940(3)	C(18)	H(18)	0.940(2)
C(19)	H(19)	0.990(2)	C(20)	H(20A)	0.990(2)
C(20)	H(20B)	0.990(2)	C(21)	H(21)	0.990(2)
C(22)	H(22)	0.990(2)	C(23)	H(23)	0.990(2)
C(24)	H(24)	0.990(2)	C(25)	H(25)	0.990(2)
C(26)	H(26)	0.940(2)	C(27)	H(27)	0.940(2)
C(28)	H(28)	0.990(2)	C(29)	H(29)	0.990(2)
C(30)	H(30)	0.990(3)	C(31)	H(31)	0.940(2)
C(32)	H(32)	0.940(3)			

Table S6. Bond angles (^{O})

atom	atom	atom	angle	atom	atom	atom	angle
C(2A)	C(1A)	C(6A)	120.0(2)	C(2A)	C(1A)	C(7A)	122.8(2)
C(2A)	C(1A)	C(1B)	27.2(12)	C(2A)	C(1A)	C(5B)	105.0(9)
C(2A)	C(1A)	C(6B)	139(2)	C(6A)	C(1A)	C(7A)	117.1(2)
C(6A)	C(1A)	C(1B)	140.4(14)	C(6A)	C(1A)	C(5B)	15.1(9)
C(6A)	C(1A)	C(6B)	24(2)	C(7A)	C(1A)	C(1B)	99.9(13)
C(7A)	C(1A)	C(5B)	132.2(9)	C(7A)	C(1A)	C(6B)	96(2)
C(1B)	C(1A)	C(5B)	126.1(17)	C(1B)	C(1A)	C(6B)	149(2)
C(5B)	C(1A)	C(6B)	37(2)	C(1A)	C(2A)	C(3A)	120.0(2)
C(1A)	C(2A)	C(1B)	29.3(15)	C(1A)	C(2A)	C(2B)	141.6(18)
C(3A)	C(2A)	C(1B)	141.6(15)	C(3A)	C(2A)	C(2B)	29(2)
C(1B)	C(2A)	C(2B)	146(2)	C(2A)	C(3A)	C(4A)	120.0(2)
C(2A)	C(3A)	C(2B)	22.9(16)	C(2A)	C(3A)	C(3B)	135(2)
C(4A)	C(3A)	C(2B)	137.7(16)	C(4A)	C(3A)	C(3B)	17(2)
C(2B)	C(3A)	C(3B)	148(3)	C(3A)	C(4A)	C(5A)	120.0(2)
C(3A)	C(4A)	C(3B)	11.7(15)	C(3A)	C(4A)	C(4B)	125(2)
C(5A)	C(4A)	C(3B)	130.3(17)	C(5A)	C(4A)	C(4B)	5.0(19)
C(3B)	C(4A)	C(4B)	135(2)	C(4A)	C(5A)	C(6A)	120.0(2)
C(4A)	C(5A)	C(4B)	4.5(18)	C(4A)	C(5A)	C(5B)	127(2)
C(6A)	C(5A)	C(4B)	124.5(19)	C(6A)	C(5A)	C(5B)	7(2)
C(4B)	C(5A)	C(5B)	131(2)	C(1A)	C(6A)	C(5A)	120.0(2)
C(1A)	C(6A)	C(5B)	129(2)	C(1A)	C(6A)	C(6B)	17.3(17)
C(5A)	C(6A)	C(5B)	9(2)	C(5A)	C(6A)	C(6B)	134.4(16)
C(5B)	C(6A)	C(6B)	142(3)	O(1A)	C(7A)	C(1A)	120.3(2)
O(1A)	C(7A)	C(1B)	143.6(7)	O(1A)	C(7A)	C(6B)	98.9(9)
O(1A)	C(7A)	C(7B)	155.1(7)	O(1A)	C(7A)	C(15)	120.1(2)
C(1A)	C(7A)	C(1B)	25.9(6)	C(1A)	C(7A)	C(6B)	21.5(9)
C(1A)	C(7A)	C(7B)	76.8(6)	C(1A)	C(7A)	C(15)	119.5(2)
C(1B)	C(7A)	C(6B)	46.0(11)	C(1B)	C(7A)	C(7B)	50.9(9)

C(1B)	C(7A)	C(15)	95.5(6)	C(6B)	C(7A)	C(7B)	96.3(11)
C(6B)	C(7A)	C(15)	141.0(9)	C(7B)	C(7A)	C(15)	47.6(7)
C(9A)	C(8A)	C(13A)	119.99(17)	C(9A)	C(8A)	C(14A)	117.3(2)
C(9A)	C(8A)	C(8B)	126.6(10)	C(9A)	C(8A)	C(9B)	18.4(17)
C(13A)	C(8A)	C(14A)	122.67(18)	C(13A)	C(8A)	C(8B)	29.8(9)
C(13A)	C(8A)	C(9B)	124(2)	C(14A)	C(8A)	C(8B)	108.3(8)
C(14A)	C(8A)	C(9B)	110.7(19)	C(8B)	C(8A)	C(9B)	119(2)
C(8A)	C(9A)	C(10A)	120.01(19)	C(8A)	C(9A)	C(9B)	14.1(12)
C(8A)	C(9A)	C(10B)	121.1(15)	C(10A)	C(9A)	C(9B)	123.2(15)
C(10A)	C(9A)	C(10B)	5(2)	C(9B)	C(9A)	C(10B)	126(2)
C(9A)	C(10A)	C(11A)	120.0(2)	C(9A)	C(10A)	C(10B)	6(2)
C(9A)	C(10A)	C(11B)	129.2(13)	C(11A)	C(10A)	C(10B)	121.2(18)
C(11A)	C(10A)	C(11B)	10.4(11)	C(10B)	C(10A)	C(11B)	130(2)
C(10A)	C(11A)	C(12A)	120.0(2)	C(10A)	C(11A)	C(10B)	17.9(6)
C(10A)	C(11A)	C(11B)	16.7(16)	C(10A)	C(11A)	C(12B)	140.0(14)
C(12A)	C(11A)	C(10B)	102.2(6)	C(12A)	C(11A)	C(11B)	135(2)
C(12A)	C(11A)	C(12B)	24.9(16)	C(10B)	C(11A)	C(11B)	33.2(18)
C(10B)	C(11A)	C(12B)	123.5(16)	C(11B)	C(11A)	C(12B)	157(2)
C(11A)	C(12A)	C(13A)	120.0(2)	C(11A)	C(12A)	C(11B)	12.4(8)
C(11A)	C(12A)	C(12B)	31(2)	C(11A)	C(12A)	C(13B)	134.5(11)
C(13A)	C(12A)	C(11B)	107.8(8)	C(13A)	C(12A)	C(12B)	144(2)
C(13A)	C(12A)	C(13B)	41.3(16)	C(11B)	C(12A)	C(12B)	43(2)
C(11B)	C(12A)	C(13B)	127.4(12)	C(12B)	C(12A)	C(13B)	131(2)
C(8A)	C(13A)	C(12A)	120.01(17)	C(8A)	C(13A)	C(8B)	41.3(16)
C(8A)	C(13A)	C(9B)	16.7(6)	C(8A)	C(13A)	C(13B)	133.8(9)
C(12A)	C(13A)	C(8B)	126.2(13)	C(12A)	C(13A)	C(9B)	104.3(6)
C(12A)	C(13A)	C(13B)	35.0(13)	C(8B)	C(13A)	C(9B)	44.2(15)
C(8B)	C(13A)	C(13B)	112(2)	C(9B)	C(13A)	C(13B)	117.9(11)
O(2A)	C(14A)	C(8A)	119.8(2)	O(2A)	C(14A)	C(9B)	102.4(6)
O(2A)	C(14A)	C(14B)	157.5(5)	O(2A)	C(14A)	C(20)	120.2(2)
C(8A)	C(14A)	C(9B)	18.7(6)	C(8A)	C(14A)	C(14B)	72.4(5)
C(8A)	C(14A)	C(20)	120.1(2)	C(9B)	C(14A)	C(14B)	86.2(8)
C(9B)	C(14A)	C(20)	136.9(7)	C(14B)	C(14A)	C(20)	51.9(5)
C(1A)	C(1B)	C(2A)	123(2)	C(1A)	C(1B)	C(7A)	54.2(14)
C(1A)	C(1B)	C(2B)	125.4(19)	C(1A)	C(1B)	C(6B)	13.6(10)
C(1A)	C(1B)	C(7B)	112(2)	C(2A)	C(1B)	C(7A)	155(2)
C(2A)	C(1B)	C(2B)	15.9(11)	C(2A)	C(1B)	C(6B)	122(2)
C(2A)	C(1B)	C(7B)	117(2)	C(7A)	C(1B)	C(2B)	171.1(16)
C(7A)	C(1B)	C(6B)	61.8(13)	C(7A)	C(1B)	C(7B)	57.6(12)
C(2B)	C(1B)	C(6B)	120.0(18)	C(2B)	C(1B)	C(7B)	122(2)
C(6B)	C(1B)	C(7B)	118(2)	C(2A)	C(2B)	C(3A)	128(3)
C(2A)	C(2B)	C(1B)	17.7(13)	C(2A)	C(2B)	C(3B)	123(2)
C(3A)	C(2B)	C(1B)	130(2)	C(3A)	C(2B)	C(3B)	13.2(14)
C(1B)	C(2B)	C(3B)	120(2)	C(3A)	C(3B)	C(4A)	152(3)
C(3A)	C(3B)	C(2B)	19.2(19)	C(3A)	C(3B)	C(4B)	134(3)
C(4A)	C(3B)	C(2B)	140(2)	C(4A)	C(3B)	C(4B)	19.5(14)
C(2B)	C(3B)	C(4B)	120(2)	C(4A)	C(4B)	C(5A)	170(3)
C(4A)	C(4B)	C(3B)	25.2(17)	C(4A)	C(4B)	C(5B)	145(3)
C(5A)	C(4B)	C(3B)	145(2)	C(5A)	C(4B)	C(5B)	25.4(16)
C(3B)	C(4B)	C(5B)	120(2)	C(1A)	C(5B)	C(5A)	128(2)
C(1A)	C(5B)	C(6A)	36(2)	C(1A)	C(5B)	C(4B)	105(2)
C(1A)	C(5B)	C(6B)	15.9(11)	C(5A)	C(5B)	C(6A)	164(4)
C(5A)	C(5B)	C(4B)	23.4(16)	C(5A)	C(5B)	C(6B)	143(3)
C(6A)	C(5B)	C(4B)	141(3)	C(6A)	C(5B)	C(6B)	22(2)
C(4B)	C(5B)	C(6B)	120(2)	C(1A)	C(6B)	C(6A)	139(3)
C(1A)	C(6B)	C(7A)	62.2(18)	C(1A)	C(6B)	C(1B)	17.8(14)
C(1A)	C(6B)	C(5B)	127(3)	C(6A)	C(6B)	C(7A)	150(2)
C(6A)	C(6B)	C(1B)	135(2)	C(6A)	C(6B)	C(5B)	15.6(14)
C(7A)	C(6B)	C(1B)	72.2(14)	C(7A)	C(6B)	C(5B)	165(2)

C(1B)	C(6B)	C(5B)	120(2)	C(7A)	C(7B)	O(1B)	159.7(18)
C(7A)	C(7B)	C(1B)	71.5(14)	C(7A)	C(7B)	C(15)	61.4(10)
O(1B)	C(7B)	C(1B)	121(2)	O(1B)	C(7B)	C(15)	111.6(16)
C(1B)	C(7B)	C(15)	127.1(19)	C(8A)	C(8B)	C(13A)	108.9(19)
C(8A)	C(8B)	C(9B)	23.2(10)	C(8A)	C(8B)	C(13B)	131.0(14)
C(8A)	C(8B)	C(14B)	104.5(16)	C(13A)	C(8B)	C(9B)	114.3(18)
C(13A)	C(8B)	C(13B)	39.2(14)	C(13A)	C(8B)	C(14B)	112.8(18)
C(9B)	C(8B)	C(13B)	120.0(15)	C(9B)	C(8B)	C(14B)	118.9(17)
C(13B)	C(8B)	C(14B)	121.1(18)	C(8A)	C(9B)	C(9A)	148(2)
C(8A)	C(9B)	C(13A)	39.5(15)	C(8A)	C(9B)	C(14A)	50.6(15)
C(8A)	C(9B)	C(8B)	37.5(17)	C(8A)	C(9B)	C(10B)	134(2)
C(9A)	C(9B)	C(13A)	127.9(18)	C(9A)	C(9B)	C(14A)	135(2)
C(9A)	C(9B)	C(8B)	146(2)	C(9A)	C(9B)	C(10B)	25.7(12)
C(13A)	C(9B)	C(14A)	88.6(8)	C(13A)	C(9B)	C(8B)	21.5(6)
C(13A)	C(9B)	C(10B)	103.7(14)	C(14A)	C(9B)	C(8B)	77.1(11)
C(14A)	C(9B)	C(10B)	158(2)	C(8B)	C(9B)	C(10B)	120.0(19)
C(9A)	C(10B)	C(10A)	169(4)	C(9A)	C(10B)	C(11A)	136(2)
C(9A)	C(10B)	C(9B)	28.5(13)	C(9A)	C(10B)	C(11B)	148(2)
C(10A)	C(10B)	C(11A)	40.8(14)	C(10A)	C(10B)	C(9B)	145(3)
C(10A)	C(10B)	C(11B)	29.0(15)	C(11A)	C(10B)	C(9B)	107.5(15)
C(11A)	C(10B)	C(11B)	12.5(9)	C(9B)	C(10B)	C(11B)	120(2)
C(10A)	C(11B)	C(11A)	153(2)	C(10A)	C(11B)	C(12A)	122.5(14)
C(10A)	C(11B)	C(10B)	21.2(10)	C(10A)	C(11B)	C(12B)	138.7(17)
C(11A)	C(11B)	C(12A)	32.9(15)	C(11A)	C(11B)	C(10B)	134(2)
C(11A)	C(11B)	C(12B)	14.4(13)	C(12A)	C(11B)	C(10B)	102.1(13)
C(12A)	C(11B)	C(12B)	20.2(10)	C(10B)	C(11B)	C(12B)	120.0(17)
C(11A)	C(12B)	C(12A)	124(3)	C(11A)	C(12B)	C(11B)	9.1(10)
C(11A)	C(12B)	C(13B)	129(2)	C(12A)	C(12B)	C(11B)	117(3)
C(12A)	C(12B)	C(13B)	26.3(13)	C(11B)	C(12B)	C(13B)	120(2)
C(12A)	C(13B)	C(13A)	104(2)	C(12A)	C(13B)	C(8B)	118(2)
C(12A)	C(13B)	C(12B)	22.4(11)	C(13A)	C(13B)	C(8B)	29.2(9)
C(13A)	C(13B)	C(12B)	117(2)	C(8B)	C(13B)	C(12B)	120.0(18)
C(14A)	C(14B)	O(2B)	155.8(16)	C(14A)	C(14B)	C(8B)	74.7(12)
C(14A)	C(14B)	C(20)	52.9(7)	O(2B)	C(14B)	C(8B)	118.6(19)
O(2B)	C(14B)	C(20)	117.6(14)	C(8B)	C(14B)	C(20)	123.8(16)
C(7A)	C(15)	C(7B)	71.0(10)	C(7A)	C(15)	C(16)	111.1(2)
C(7A)	C(15)	C(20)	114.3(2)	C(7B)	C(15)	C(16)	114.1(9)
C(7B)	C(15)	C(20)	129.4(8)	C(16)	C(15)	C(20)	109.99(18)
C(15)	C(16)	C(17)	109.3(2)	C(15)	C(16)	C(21)	104.60(19)
C(17)	C(16)	C(21)	107.94(19)	C(16)	C(17)	C(18)	115.0(2)
C(17)	C(18)	C(19)	115.1(2)	C(18)	C(19)	C(20)	105.32(19)
C(18)	C(19)	C(22)	109.34(19)	C(20)	C(19)	C(22)	107.13(18)
C(14A)	C(20)	C(14B)	75.2(7)	C(14A)	C(20)	C(15)	113.6(2)
C(14A)	C(20)	C(19)	111.06(19)	C(14B)	C(20)	C(15)	127.4(6)
C(14B)	C(20)	C(19)	115.7(7)	C(15)	C(20)	C(19)	108.72(18)
C(16)	C(21)	C(22)	109.6(2)	C(16)	C(21)	C(23)	120.34(19)
C(22)	C(21)	C(23)	90.39(16)	C(19)	C(22)	C(21)	109.54(19)
C(19)	C(22)	C(24)	118.86(18)	C(21)	C(22)	C(24)	89.89(16)
C(21)	C(23)	C(24)	89.07(16)	C(21)	C(23)	C(29)	117.13(19)
C(24)	C(23)	C(29)	122.3(2)	C(22)	C(24)	C(23)	90.36(16)
C(22)	C(24)	C(25)	115.97(18)	C(23)	C(24)	C(25)	118.2(2)
C(24)	C(25)	C(26)	112.7(2)	C(24)	C(25)	C(32)	113.6(2)
C(26)	C(25)	C(32)	107.9(2)	C(25)	C(26)	C(27)	124.9(2)
C(26)	C(27)	C(28)	127.3(2)	C(27)	C(28)	C(29)	123.6(2)
C(27)	C(28)	C(30)	120.8(2)	C(29)	C(28)	C(30)	58.72(17)
C(23)	C(29)	C(28)	125.6(2)	C(23)	C(29)	C(30)	124.0(2)
C(28)	C(29)	C(30)	62.20(17)	C(28)	C(30)	C(29)	59.08(17)
C(28)	C(30)	C(31)	120.5(2)	C(29)	C(30)	C(31)	123.3(2)
C(30)	C(31)	C(32)	127.9(2)	C(25)	C(32)	C(31)	124.7(2)

Table S7. Torsion angles (°)

C(2A)	C(1A)	C(6A)	C(5A)	-0.0(3)	C(2A)	C(1A)	C(6A)	C(5B)	2(3)
C(2A)	C(1A)	C(6A)	C(6B)	149(4)	C(6A)	C(1A)	C(2A)	C(3A)	0.0(3)
C(6A)	C(1A)	C(2A)	C(1B)	-145(3)	C(6A)	C(1A)	C(2A)	C(2B)	-26(3)
C(2A)	C(1A)	C(7A)	O(1A)	-174.3(2)	C(2A)	C(1A)	C(7A)	C(1B)	-15.9(14)
C(2A)	C(1A)	C(7A)	C(6B)	-169(2)	C(2A)	C(1A)	C(7A)	C(7B)	-13.9(7)
C(2A)	C(1A)	C(7A)	C(15)	7.9(3)	C(7A)	C(1A)	C(2A)	C(3A)	-178.8(2)
C(7A)	C(1A)	C(2A)	C(1B)	36(3)	C(7A)	C(1A)	C(2A)	C(2B)	155(3)
C(2A)	C(1A)	C(1B)	C(7A)	150(2)	C(2A)	C(1A)	C(1B)	C(2B)	-19.2(15)
C(2A)	C(1A)	C(1B)	C(6B)	-90(5)	C(2A)	C(1A)	C(1B)	C(7B)	148(4)
C(1B)	C(1A)	C(2A)	C(3A)	145(3)	C(1B)	C(1A)	C(2A)	C(2B)	119(4)
C(2A)	C(1A)	C(5B)	C(5A)	-2(3)	C(2A)	C(1A)	C(5B)	C(6A)	-178(2)
C(2A)	C(1A)	C(5B)	C(4B)	-1.5(19)	C(2A)	C(1A)	C(5B)	C(6B)	161(3)
C(5B)	C(1A)	C(2A)	C(3A)	0.6(8)	C(5B)	C(1A)	C(2A)	C(1B)	-145(3)
C(5B)	C(1A)	C(2A)	C(2B)	-25(3)	C(2A)	C(1A)	C(6B)	C(6A)	-43(6)
C(2A)	C(1A)	C(6B)	C(7A)	165(2)	C(2A)	C(1A)	C(6B)	C(1B)	45(3)
C(2A)	C(1A)	C(6B)	C(5B)	-29(5)	C(6B)	C(1A)	C(2A)	C(3A)	18(3)
C(6B)	C(1A)	C(2A)	C(1B)	-127(4)	C(6B)	C(1A)	C(2A)	C(2B)	-7(4)
C(6A)	C(1A)	C(7A)	O(1A)	6.8(3)	C(6A)	C(1A)	C(7A)	C(1B)	165.3(14)
C(6A)	C(1A)	C(7A)	C(6B)	12(2)	C(6A)	C(1A)	C(7A)	C(7B)	167.3(7)
C(6A)	C(1A)	C(7A)	C(15)	-170.9(2)	C(7A)	C(1A)	C(6A)	C(5A)	178.9(2)
C(7A)	C(1A)	C(6A)	C(5B)	-178.9(8)	C(7A)	C(1A)	C(6A)	C(6B)	-32(4)
C(6A)	C(1A)	C(1B)	C(2A)	51(4)	C(6A)	C(1A)	C(1B)	C(7A)	-159.3(18)
C(6A)	C(1A)	C(1B)	C(2B)	32(3)	C(6A)	C(1A)	C(1B)	C(6B)	-39(4)
C(6A)	C(1A)	C(1B)	C(7B)	-161.5(10)	C(1B)	C(1A)	C(6A)	C(5A)	-24(2)
C(1B)	C(1A)	C(6A)	C(5B)	-22(3)	C(1B)	C(1A)	C(6A)	C(6B)	125(5)
C(6A)	C(1A)	C(5B)	C(5A)	176(6)	C(6A)	C(1A)	C(5B)	C(4B)	177(4)
C(6A)	C(1A)	C(5B)	C(6B)	-21(3)	C(5B)	C(1A)	C(6A)	C(5A)	-2(3)
C(5B)	C(1A)	C(6A)	C(6B)	147(5)	C(6A)	C(1A)	C(6B)	C(7A)	-152(4)
C(6A)	C(1A)	C(6B)	C(1B)	87(6)	C(6A)	C(1A)	C(6B)	C(5B)	13(2)
C(6B)	C(1A)	C(6A)	C(5A)	-149(4)	C(6B)	C(1A)	C(6A)	C(5B)	-147(5)
C(7A)	C(1A)	C(1B)	C(2A)	-150(2)	C(7A)	C(1A)	C(1B)	C(2B)	-169(2)
C(7A)	C(1A)	C(1B)	C(6B)	120(4)	C(7A)	C(1A)	C(1B)	C(7B)	-2.2(18)
C(1B)	C(1A)	C(7A)	O(1A)	-158.5(14)	C(1B)	C(1A)	C(7A)	C(6B)	-153(2)
C(1B)	C(1A)	C(7A)	C(7B)	2.0(15)	C(1B)	C(1A)	C(7A)	C(15)	23.8(14)
C(7A)	C(1A)	C(5B)	C(5A)	177(2)	C(7A)	C(1A)	C(5B)	C(6A)	1.3(9)
C(7A)	C(1A)	C(5B)	C(4B)	177.8(13)	C(7A)	C(1A)	C(5B)	C(6B)	-20(3)
C(5B)	C(1A)	C(7A)	O(1A)	6.5(11)	C(5B)	C(1A)	C(7A)	C(1B)	164.9(18)
C(5B)	C(1A)	C(7A)	C(6B)	12(2)	C(5B)	C(1A)	C(7A)	C(7B)	166.9(13)
C(5B)	C(1A)	C(7A)	C(15)	-171.3(11)	C(7A)	C(1A)	C(6B)	C(6A)	152(4)
C(7A)	C(1A)	C(6B)	C(1B)	-121(4)	C(7A)	C(1A)	C(6B)	C(5B)	165(2)
C(6B)	C(1A)	C(7A)	O(1A)	-6(2)	C(6B)	C(1A)	C(7A)	C(1B)	153(2)
C(6B)	C(1A)	C(7A)	C(7B)	155(2)	C(6B)	C(1A)	C(7A)	C(15)	177(2)
C(1B)	C(1A)	C(5B)	C(5A)	-21(4)	C(1B)	C(1A)	C(5B)	C(6A)	163(3)
C(1B)	C(1A)	C(5B)	C(4B)	-21(2)	C(1B)	C(1A)	C(5B)	C(6B)	142(3)
C(5B)	C(1A)	C(1B)	C(2A)	44(3)	C(5B)	C(1A)	C(1B)	C(7A)	-166.2(16)
C(5B)	C(1A)	C(1B)	C(2B)	25(3)	C(5B)	C(1A)	C(1B)	C(6B)	-46(4)
C(5B)	C(1A)	C(1B)	C(7B)	-168.5(13)	C(1B)	C(1A)	C(6B)	C(6A)	-87(6)
C(1B)	C(1A)	C(6B)	C(7A)	121(4)	C(1B)	C(1A)	C(6B)	C(5B)	-74(6)
C(6B)	C(1A)	C(1B)	C(2A)	90(5)	C(6B)	C(1A)	C(1B)	C(7A)	-120(4)
C(6B)	C(1A)	C(1B)	C(2B)	71(5)	C(6B)	C(1A)	C(1B)	C(7B)	-122(4)
C(5B)	C(1A)	C(6B)	C(6A)	-13(2)	C(5B)	C(1A)	C(6B)	C(7A)	-165(2)
C(5B)	C(1A)	C(6B)	C(1B)	74(6)	C(6B)	C(1A)	C(5B)	C(5A)	-163(5)
C(6B)	C(1A)	C(5B)	C(6A)	21(3)	C(6B)	C(1A)	C(5B)	C(4B)	-162(4)
C(1A)	C(2A)	C(3A)	C(4A)	-0.0(3)	C(1A)	C(2A)	C(3A)	C(2B)	-146(3)
C(1A)	C(2A)	C(3A)	C(3B)	-10(3)	C(1A)	C(2A)	C(1B)	C(7A)	-76(5)
C(1A)	C(2A)	C(1B)	C(2B)	102(5)	C(1A)	C(2A)	C(1B)	C(6B)	16.2(14)
C(1A)	C(2A)	C(1B)	C(7B)	-146(4)	C(1A)	C(2A)	C(2B)	C(3A)	51(5)

C(1A)	C(2A)	C(2B)	C(1B)	-50(3)	C(1A)	C(2A)	C(2B)	C(3B)	37(4)
C(3A)	C(2A)	C(1B)	C(1A)	-53(4)	C(3A)	C(2A)	C(1B)	C(7A)	-129(4)
C(3A)	C(2A)	C(1B)	C(2B)	49(4)	C(3A)	C(2A)	C(1B)	C(6B)	-37(4)
C(3A)	C(2A)	C(1B)	C(7B)	161.0(11)	C(1B)	C(2A)	C(3A)	C(4A)	27(2)
C(1B)	C(2A)	C(3A)	C(2B)	-119(4)	C(1B)	C(2A)	C(3A)	C(3B)	16(4)
C(3A)	C(2A)	C(2B)	C(1B)	-102(5)	C(3A)	C(2A)	C(2B)	C(3B)	-14.6(18)
C(2B)	C(2A)	C(3A)	C(4A)	146(3)	C(2B)	C(2A)	C(3A)	C(3B)	136(4)
C(1B)	C(2A)	C(2B)	C(3A)	102(5)	C(1B)	C(2A)	C(2B)	C(3B)	87(5)
C(2B)	C(2A)	C(1B)	C(1A)	-102(5)	C(2B)	C(2A)	C(1B)	C(7A)	-178(4)
C(2B)	C(2A)	C(1B)	C(6B)	-86(5)	C(2B)	C(2A)	C(1B)	C(7B)	112(4)
C(2A)	C(3A)	C(4A)	C(5A)	0.0(3)	C(2A)	C(3A)	C(4A)	C(3B)	-154(9)
C(2A)	C(3A)	C(4A)	C(4B)	1(2)	C(2A)	C(3A)	C(2B)	C(1B)	23(2)
C(2A)	C(3A)	C(2B)	C(3B)	69(6)	C(2A)	C(3A)	C(3B)	C(4A)	33(10)
C(2A)	C(3A)	C(3B)	C(2B)	-31(3)	C(2A)	C(3A)	C(3B)	C(4B)	19(6)
C(4A)	C(3A)	C(2B)	C(2A)	-46(4)	C(4A)	C(3A)	C(2B)	C(1B)	-23(3)
C(4A)	C(3A)	C(2B)	C(3B)	22(4)	C(2B)	C(3A)	C(4A)	C(5A)	19(2)
C(2B)	C(3A)	C(4A)	C(3B)	-135(9)	C(2B)	C(3A)	C(4A)	C(4B)	20(3)
C(4A)	C(3A)	C(3B)	C(2B)	-63(10)	C(4A)	C(3A)	C(3B)	C(4B)	-13(5)
C(3B)	C(3A)	C(4A)	C(5A)	154(9)	C(3B)	C(3A)	C(4A)	C(4B)	155(9)
C(2B)	C(3A)	C(3B)	C(4A)	63(10)	C(2B)	C(3A)	C(3B)	C(4B)	50(7)
C(3B)	C(3A)	C(2B)	C(2A)	-69(6)	C(3B)	C(3A)	C(2B)	C(1B)	-46(6)
C(3A)	C(4A)	C(5A)	C(6A)	-0.0(3)	C(3A)	C(4A)	C(5A)	C(4B)	172(29)
C(3A)	C(4A)	C(5A)	C(5B)	-2(2)	C(3A)	C(4A)	C(3B)	C(2B)	27(6)
C(3A)	C(4A)	C(3B)	C(4B)	30(11)	C(3A)	C(4A)	C(4B)	C(5A)	-9(30)
C(3A)	C(4A)	C(4B)	C(3B)	-7(2)	C(3A)	C(4A)	C(4B)	C(5B)	-4(7)
C(5A)	C(4A)	C(3B)	C(3A)	-30(10)	C(5A)	C(4A)	C(3B)	C(2B)	-3(5)
C(5A)	C(4A)	C(3B)	C(4B)	-0(3)	C(3B)	C(4A)	C(5A)	C(6A)	7(2)
C(3B)	C(4A)	C(5A)	C(4B)	178(29)	C(3B)	C(4A)	C(5A)	C(5B)	5(3)
C(5A)	C(4A)	C(4B)	C(3B)	2(31)	C(5A)	C(4A)	C(4B)	C(5B)	5(24)
C(4B)	C(4A)	C(5A)	C(6A)	-172(29)	C(4B)	C(4A)	C(5A)	C(5B)	-173(29)
C(3B)	C(4A)	C(4B)	C(5A)	-2(31)	C(3B)	C(4A)	C(4B)	C(5B)	4(5)
C(4B)	C(4A)	C(3B)	C(3A)	-30(11)	C(4B)	C(4A)	C(3B)	C(2B)	-3(5)
C(4A)	C(5A)	C(6A)	C(1A)	0.0(3)	C(4A)	C(5A)	C(6A)	C(5B)	-169(15)
C(4A)	C(5A)	C(6A)	C(6B)	-12(2)	C(4A)	C(5A)	C(4B)	C(3B)	-1(24)
C(4A)	C(5A)	C(4B)	C(5B)	-7(31)	C(4A)	C(5A)	C(5B)	C(1A)	3(4)
C(4A)	C(5A)	C(5B)	C(6A)	12(17)	C(4A)	C(5A)	C(5B)	C(4B)	1(2)
C(4A)	C(5A)	C(5B)	C(6B)	-5(5)	C(6A)	C(5A)	C(4B)	C(4A)	9(30)
C(6A)	C(5A)	C(4B)	C(3B)	7(6)	C(6A)	C(5A)	C(4B)	C(5B)	2(2)
C(4B)	C(5A)	C(6A)	C(1A)	-1(2)	C(4B)	C(5A)	C(6A)	C(5B)	-169(15)
C(4B)	C(5A)	C(6A)	C(6B)	-13(3)	C(6A)	C(5A)	C(5B)	C(1A)	-9(13)
C(6A)	C(5A)	C(5B)	C(4B)	-12(17)	C(6A)	C(5A)	C(5B)	C(6B)	-17(11)
C(5B)	C(5A)	C(6A)	C(1A)	169(15)	C(5B)	C(5A)	C(6A)	C(6B)	156(16)
C(4B)	C(5A)	C(5B)	C(1A)	2(4)	C(4B)	C(5A)	C(5B)	C(6A)	12(17)
C(4B)	C(5A)	C(5B)	C(6B)	-6(6)	C(5B)	C(5A)	C(4B)	C(4A)	7(31)
C(5B)	C(5A)	C(4B)	C(3B)	6(7)	C(1A)	C(6A)	C(5B)	C(5A)	-13(17)
C(1A)	C(6A)	C(5B)	C(4B)	-5(7)	C(1A)	C(6A)	C(5B)	C(6B)	15(2)
C(1A)	C(6A)	C(6B)	C(7A)	124(7)	C(1A)	C(6A)	C(6B)	C(1B)	-26(2)
C(1A)	C(6A)	C(6B)	C(5B)	-44(7)	C(5A)	C(6A)	C(5B)	C(1A)	13(17)
C(5A)	C(6A)	C(5B)	C(4B)	7(10)	C(5A)	C(6A)	C(5B)	C(6B)	28(18)
C(5A)	C(6A)	C(6B)	C(1A)	38(5)	C(5A)	C(6A)	C(6B)	C(7A)	162(3)
C(5A)	C(6A)	C(6B)	C(1B)	12(4)	C(5A)	C(6A)	C(6B)	C(5B)	-6(3)
C(5B)	C(6A)	C(6B)	C(1A)	44(7)	C(5B)	C(6A)	C(6B)	C(7A)	168(4)
C(5B)	C(6A)	C(6B)	C(1B)	18(6)	C(6B)	C(6A)	C(5B)	C(1A)	-15(2)
C(6B)	C(6A)	C(5B)	C(5A)	-28(18)	C(6B)	C(6A)	C(5B)	C(4B)	-21(8)
O(1A)	C(7A)	C(1B)	C(1A)	32(2)	O(1A)	C(7A)	C(1B)	C(2A)	126(4)
O(1A)	C(7A)	C(1B)	C(2B)	123(12)	O(1A)	C(7A)	C(1B)	C(6B)	18.9(17)
O(1A)	C(7A)	C(1B)	C(7B)	-150.2(10)	O(1A)	C(7A)	C(6B)	C(1A)	175.2(18)
O(1A)	C(7A)	C(6B)	C(6A)	33(4)	O(1A)	C(7A)	C(6B)	C(1B)	-168.8(10)
O(1A)	C(7A)	C(6B)	C(5B)	46(8)	O(1A)	C(7A)	C(7B)	O(1B)	5(6)

O(1A)	C(7A)	C(7B)	C(1B)	135.5(15)	O(1A)	C(7A)	C(7B)	C(15)	-69.3(19)
O(1A)	C(7A)	C(15)	C(7B)	152.9(9)	O(1A)	C(7A)	C(15)	C(16)	-97.8(3)
O(1A)	C(7A)	C(15)	C(20)	27.4(3)	C(1A)	C(7A)	C(1B)	C(2A)	93(5)
C(1A)	C(7A)	C(1B)	C(2B)	91(12)	C(1A)	C(7A)	C(1B)	C(6B)	-13.4(13)
C(1A)	C(7A)	C(1B)	C(7B)	177.5(19)	C(1A)	C(7A)	C(6B)	C(6A)	-142(6)
C(1A)	C(7A)	C(6B)	C(1B)	16.0(14)	C(1A)	C(7A)	C(6B)	C(5B)	-129(9)
C(1A)	C(7A)	C(7B)	O(1B)	-131(5)	C(1A)	C(7A)	C(7B)	C(1B)	-1.1(8)
C(1A)	C(7A)	C(7B)	C(15)	154.1(7)	C(1A)	C(7A)	C(15)	C(7B)	-29.3(9)
C(1A)	C(7A)	C(15)	C(16)	80.0(2)	C(1A)	C(7A)	C(15)	C(20)	-154.8(2)
C(1B)	C(7A)	C(6B)	C(1A)	-16.0(14)	C(1B)	C(7A)	C(6B)	C(6A)	-158(5)
C(1B)	C(7A)	C(6B)	C(5B)	-145(8)	C(6B)	C(7A)	C(1B)	C(1A)	13.4(13)
C(6B)	C(7A)	C(1B)	C(2A)	107(5)	C(6B)	C(7A)	C(1B)	C(2B)	104(12)
C(6B)	C(7A)	C(1B)	C(7B)	-169.1(17)	C(1B)	C(7A)	C(7B)	O(1B)	-130(5)
C(1B)	C(7A)	C(7B)	C(15)	155.2(14)	C(7B)	C(7A)	C(1B)	C(1A)	-177.5(19)
C(7B)	C(7A)	C(1B)	C(2A)	-84(5)	C(7B)	C(7A)	C(1B)	C(2B)	-87(12)
C(7B)	C(7A)	C(1B)	C(6B)	169.1(17)	C(1B)	C(7A)	C(15)	C(7B)	-19.1(10)
C(1B)	C(7A)	C(15)	C(16)	90.2(6)	C(1B)	C(7A)	C(15)	C(20)	-144.6(6)
C(15)	C(7A)	C(1B)	C(1A)	-159.4(12)	C(15)	C(7A)	C(1B)	C(2A)	-66(5)
C(15)	C(7A)	C(1B)	C(2B)	-69(12)	C(15)	C(7A)	C(1B)	C(6B)	-172.8(12)
C(15)	C(7A)	C(1B)	C(7B)	18.1(10)	C(6B)	C(7A)	C(7B)	O(1B)	-122(5)
C(6B)	C(7A)	C(7B)	C(1B)	7.9(12)	C(6B)	C(7A)	C(7B)	C(15)	163.1(9)
C(7B)	C(7A)	C(6B)	C(1A)	-25(2)	C(7B)	C(7A)	C(6B)	C(6A)	-166(4)
C(7B)	C(7A)	C(6B)	C(1B)	-8.5(13)	C(7B)	C(7A)	C(6B)	C(5B)	-154(8)
C(6B)	C(7A)	C(15)	C(7B)	-27.4(15)	C(6B)	C(7A)	C(15)	C(16)	81.9(12)
C(6B)	C(7A)	C(15)	C(20)	-152.9(12)	C(15)	C(7A)	C(6B)	C(1A)	-5(2)
C(15)	C(7A)	C(6B)	C(6A)	-146(3)	C(15)	C(7A)	C(6B)	C(1B)	11.5(18)
C(15)	C(7A)	C(6B)	C(5B)	-134(7)	C(7B)	C(7A)	C(15)	C(16)	109.3(9)
C(7B)	C(7A)	C(15)	C(20)	-125.5(9)	C(15)	C(7A)	C(7B)	O(1B)	75(4)
C(15)	C(7A)	C(7B)	C(1B)	-155.2(14)	C(9A)	C(8A)	C(13A)	C(12A)	-0.0(2)
C(9A)	C(8A)	C(13A)	C(8B)	-112(2)	C(9A)	C(8A)	C(13A)	C(9B)	-21(2)
C(9A)	C(8A)	C(13A)	C(13B)	-40.8(18)	C(13A)	C(8A)	C(9A)	C(10A)	0.0(2)
C(13A)	C(8A)	C(9A)	C(9B)	107(6)	C(13A)	C(8A)	C(9A)	C(10B)	-6(2)
C(9A)	C(8A)	C(14A)	O(2A)	-4.8(3)	C(9A)	C(8A)	C(14A)	C(9B)	19(2)
C(9A)	C(8A)	C(14A)	C(14B)	154.5(6)	C(9A)	C(8A)	C(14A)	C(20)	175.8(2)
C(14A)	C(8A)	C(9A)	C(10A)	179.6(2)	C(14A)	C(8A)	C(9A)	C(9B)	-73(6)
C(14A)	C(8A)	C(9A)	C(10B)	173(2)	C(9A)	C(8A)	C(8B)	C(13A)	87(2)
C(9A)	C(8A)	C(8B)	C(9B)	-20(2)	C(9A)	C(8A)	C(8B)	C(13B)	49(2)
C(9A)	C(8A)	C(8B)	C(14B)	-151.7(8)	C(8B)	C(8A)	C(9A)	C(10A)	-34.9(11)
C(8B)	C(8A)	C(9A)	C(9B)	72(7)	C(8B)	C(8A)	C(9A)	C(10B)	-41(2)
C(9A)	C(8A)	C(9B)	C(13A)	84(7)	C(9A)	C(8A)	C(9B)	C(14A)	-115(6)
C(9A)	C(8A)	C(9B)	C(8B)	119(6)	C(9A)	C(8A)	C(9B)	C(10B)	36(4)
C(9B)	C(8A)	C(9A)	C(10A)	-107(6)	C(9B)	C(8A)	C(9A)	C(10B)	-114(7)
C(13A)	C(8A)	C(14A)	O(2A)	174.8(2)	C(13A)	C(8A)	C(14A)	C(9B)	-162(2)
C(13A)	C(8A)	C(14A)	C(14B)	-25.9(6)	C(13A)	C(8A)	C(14A)	C(20)	-4.6(3)
C(14A)	C(8A)	C(13A)	C(12A)	-179.6(2)	C(14A)	C(8A)	C(13A)	C(8B)	68(2)
C(14A)	C(8A)	C(13A)	C(9B)	159(2)	C(14A)	C(8A)	C(13A)	C(13B)	139.6(18)
C(13A)	C(8A)	C(8B)	C(9B)	-108(2)	C(13A)	C(8A)	C(8B)	C(13B)	-38.0(13)
C(13A)	C(8A)	C(8B)	C(14B)	121(2)	C(8B)	C(8A)	C(13A)	C(12A)	112(2)
C(8B)	C(8A)	C(13A)	C(9B)	91(3)	C(8B)	C(8A)	C(13A)	C(13B)	71(2)
C(13A)	C(8A)	C(9B)	C(9A)	-84(7)	C(13A)	C(8A)	C(9B)	C(14A)	161(2)
C(13A)	C(8A)	C(9B)	C(8B)	34.7(12)	C(13A)	C(8A)	C(9B)	C(10B)	-48(4)
C(9B)	C(8A)	C(13A)	C(12A)	21(2)	C(9B)	C(8A)	C(13A)	C(8B)	-91(3)
C(9B)	C(8A)	C(13A)	C(13B)	-20(2)	C(14A)	C(8A)	C(8B)	C(13A)	-124.5(15)
C(14A)	C(8A)	C(8B)	C(9B)	128(2)	C(14A)	C(8A)	C(8B)	C(13B)	-162.6(19)
C(14A)	C(8A)	C(8B)	C(14B)	-3.8(15)	C(8B)	C(8A)	C(14A)	O(2A)	-156.1(11)
C(8B)	C(8A)	C(14A)	C(9B)	-132(2)	C(8B)	C(8A)	C(14A)	C(14B)	3.2(12)
C(8B)	C(8A)	C(14A)	C(20)	24.5(11)	C(14A)	C(8A)	C(9B)	C(9A)	115(6)
C(14A)	C(8A)	C(9B)	C(13A)	-161(2)	C(14A)	C(8A)	C(9B)	C(8B)	-126.6(17)
C(14A)	C(8A)	C(9B)	C(10B)	151(3)	C(9B)	C(8A)	C(14A)	O(2A)	-24(2)

C(9B)	C(8A)	C(14A)	C(14B)	136(2)
C(8B)	C(8A)	C(9B)	C(9A)	-119(6)
C(8B)	C(8A)	C(9B)	C(14A)	126.6(17)
C(9B)	C(8A)	C(8B)	C(13A)	108(2)
C(9B)	C(8A)	C(8B)	C(14B)	-132(2)
C(8A)	C(9A)	C(10A)	C(11B)	-6(2)
C(8A)	C(9A)	C(9B)	C(14A)	84(7)
C(8A)	C(9A)	C(9B)	C(10B)	-75(7)
C(8A)	C(9A)	C(10B)	C(11A)	12(4)
C(8A)	C(9A)	C(10B)	C(11B)	12(6)
C(10A)	C(9A)	C(9B)	C(13A)	28(2)
C(10A)	C(9A)	C(9B)	C(8B)	10(4)
C(9B)	C(9A)	C(10A)	C(11A)	-16.1(16)
C(9B)	C(9A)	C(10A)	C(11B)	-22(2)
C(10A)	C(9A)	C(10B)	C(9B)	-64(16)
C(10B)	C(9A)	C(10A)	C(11A)	103(16)
C(9B)	C(9A)	C(10B)	C(10A)	64(16)
C(9B)	C(9A)	C(10B)	C(11B)	-4(4)
C(10B)	C(9A)	C(9B)	C(13A)	22(3)
C(10B)	C(9A)	C(9B)	C(8B)	4(4)
C(9A)	C(10A)	C(11A)	C(10B)	-7(2)
C(9A)	C(10A)	C(11A)	C(12B)	20(2)
C(9A)	C(10A)	C(10B)	C(9B)	48(14)
C(9A)	C(10A)	C(11B)	C(11A)	29(10)
C(9A)	C(10A)	C(11B)	C(10B)	-8(2)
C(11A)	C(10A)	C(10B)	C(9A)	-80(16)
C(11A)	C(10A)	C(10B)	C(11B)	7(2)
C(10B)	C(10A)	C(11A)	C(11B)	-148(9)
C(11A)	C(10A)	C(11B)	C(12A)	-20(7)
C(11A)	C(10A)	C(11B)	C(12B)	-4(5)
C(11B)	C(10A)	C(11A)	C(10B)	148(9)
C(10B)	C(10A)	C(11B)	C(11A)	37(10)
C(10B)	C(10A)	C(11B)	C(12B)	33(5)
C(11B)	C(10A)	C(10B)	C(11A)	-7(2)
C(10A)	C(11A)	C(12A)	C(13A)	0.0(3)
C(10A)	C(11A)	C(12A)	C(12B)	149(3)
C(10A)	C(11A)	C(10B)	C(9A)	164(5)
C(10A)	C(11A)	C(10B)	C(11B)	-16(4)
C(10A)	C(11A)	C(11B)	C(10B)	18(5)
C(10A)	C(11A)	C(12B)	C(12A)	-44(4)
C(10A)	C(11A)	C(12B)	C(13B)	-12(4)
C(12A)	C(11A)	C(10B)	C(10A)	-174(2)
C(12A)	C(11A)	C(10B)	C(11B)	170(4)
C(10B)	C(11A)	C(12A)	C(11B)	-8(3)
C(10B)	C(11A)	C(12A)	C(13B)	52(2)
C(12A)	C(11A)	C(11B)	C(10B)	-14(6)
C(11B)	C(11A)	C(12A)	C(13A)	10(3)
C(11B)	C(11A)	C(12A)	C(13B)	60(4)
C(12A)	C(11A)	C(12B)	C(13B)	32(2)
C(12B)	C(11A)	C(12A)	C(11B)	-159(4)
C(10B)	C(11A)	C(11B)	C(10A)	-18(5)
C(10B)	C(11A)	C(11B)	C(12B)	-8(8)
C(11B)	C(11A)	C(10B)	C(10A)	16(4)
C(10B)	C(11A)	C(12B)	C(12A)	-34(4)
C(10B)	C(11A)	C(12B)	C(13B)	-2(2)
C(12B)	C(11A)	C(10B)	C(10A)	-160(2)
C(12B)	C(11A)	C(10B)	C(11B)	-176(4)
C(11B)	C(11A)	C(12B)	C(13B)	-7(8)
C(12B)	C(11A)	C(11B)	C(12A)	22(5)

C(9B)	C(8A)	C(14A)	C(20)	157(2)
C(8B)	C(8A)	C(9B)	C(13A)	-34.7(12)
C(8B)	C(8A)	C(9B)	C(10B)	-83(4)
C(9B)	C(8A)	C(8B)	C(13B)	70(3)
C(8A)	C(9A)	C(10A)	C(10B)	-103(16)
C(8A)	C(9A)	C(9B)	C(13A)	-53(5)
C(8A)	C(9A)	C(9B)	C(8B)	-71(5)
C(8A)	C(9A)	C(10B)	C(10A)	80(16)
C(8A)	C(9A)	C(10B)	C(9B)	15.9(17)
C(10A)	C(9A)	C(9B)	C(8A)	81(7)
C(10A)	C(9A)	C(9B)	C(14A)	165.5(13)
C(10A)	C(9A)	C(9B)	C(10B)	6(2)
C(9B)	C(9A)	C(10A)	C(10B)	-120(16)
C(10A)	C(9A)	C(10B)	C(11A)	-68(15)
C(10A)	C(9A)	C(10B)	C(11B)	-68(16)
C(10B)	C(9A)	C(10A)	C(11B)	98(16)
C(9B)	C(9A)	C(10B)	C(11A)	-4(4)
C(10B)	C(9A)	C(9B)	C(8A)	75(7)
C(10B)	C(9A)	C(9B)	C(14A)	160(2)
C(9A)	C(10A)	C(11A)	C(12A)	-0.0(3)
C(9A)	C(10A)	C(11A)	C(11B)	-154(9)
C(9A)	C(10A)	C(10B)	C(11A)	80(16)
C(9A)	C(10A)	C(10B)	C(11B)	87(16)
C(9A)	C(10A)	C(11B)	C(12A)	9(3)
C(9A)	C(10A)	C(11B)	C(12B)	25(5)
C(11A)	C(10A)	C(10B)	C(9B)	-32(5)
C(10B)	C(10A)	C(11A)	C(12A)	7(2)
C(10B)	C(10A)	C(11A)	C(12B)	27(3)
C(11A)	C(10A)	C(11B)	C(10B)	-37(10)
C(11B)	C(10A)	C(11A)	C(12A)	154(9)
C(11B)	C(10A)	C(11A)	C(12B)	174(9)
C(10B)	C(10A)	C(11B)	C(12A)	17(4)
C(11B)	C(10A)	C(10B)	C(9A)	-87(16)
C(11B)	C(10A)	C(10B)	C(9B)	-39(6)
C(10A)	C(11A)	C(12A)	C(11B)	-10(3)
C(10A)	C(11A)	C(12A)	C(13B)	50(2)
C(10A)	C(11A)	C(10B)	C(9B)	162(3)
C(10A)	C(11A)	C(11B)	C(12A)	32(11)
C(10A)	C(11A)	C(11B)	C(12B)	9(15)
C(10A)	C(11A)	C(12B)	C(11B)	-4(6)
C(12A)	C(11A)	C(10B)	C(9A)	-10(3)
C(12A)	C(11A)	C(10B)	C(9B)	-12.3(16)
C(10B)	C(11A)	C(12A)	C(13A)	2.2(8)
C(10B)	C(11A)	C(12A)	C(12B)	151(3)
C(12A)	C(11A)	C(11B)	C(10A)	-32(11)
C(12A)	C(11A)	C(11B)	C(12B)	-22(5)
C(11B)	C(11A)	C(12A)	C(12B)	159(4)
C(12A)	C(11A)	C(12B)	C(11B)	40(9)
C(12B)	C(11A)	C(12A)	C(13A)	-149(3)
C(12B)	C(11A)	C(12A)	C(13B)	-99(4)
C(10B)	C(11A)	C(11B)	C(12A)	14(6)
C(11B)	C(11A)	C(10B)	C(9A)	180(6)
C(11B)	C(11A)	C(10B)	C(9B)	178(3)
C(10B)	C(11A)	C(12B)	C(11B)	5(5)
C(12B)	C(11A)	C(10B)	C(9A)	4(4)
C(12B)	C(11A)	C(10B)	C(9B)	2(2)
C(11B)	C(11A)	C(12B)	C(12A)	-40(9)
C(12B)	C(11A)	C(11B)	C(10A)	-9(15)
C(12B)	C(11A)	C(11B)	C(10B)	8(8)

C(11A)	C(12A)	C(13A)	C(8A)	-0.0(3)
C(11A)	C(12A)	C(13A)	C(9B)	6.2(7)
C(11A)	C(12A)	C(11B)	C(10A)	164(5)
C(11A)	C(12A)	C(11B)	C(12B)	16(3)
C(11A)	C(12A)	C(12B)	C(13B)	-111(3)
C(11A)	C(12A)	C(13B)	C(8B)	-59(3)
C(13A)	C(12A)	C(11B)	C(10A)	-7(2)
C(13A)	C(12A)	C(11B)	C(10B)	-1.2(17)
C(11B)	C(12A)	C(13A)	C(8A)	2.3(8)
C(11B)	C(12A)	C(13A)	C(9B)	8.4(10)
C(13A)	C(12A)	C(12B)	C(11A)	50(5)
C(13A)	C(12A)	C(12B)	C(13B)	-61(2)
C(12B)	C(12A)	C(13A)	C(8B)	22(4)
C(12B)	C(12A)	C(13A)	C(13B)	97(3)
C(13A)	C(12A)	C(13B)	C(12B)	130(3)
C(13B)	C(12A)	C(13A)	C(8B)	-75(2)
C(11B)	C(12A)	C(12B)	C(11A)	6.5(14)
C(12B)	C(12A)	C(11B)	C(10A)	148(4)
C(12B)	C(12A)	C(11B)	C(10B)	154(3)
C(11B)	C(12A)	C(13B)	C(8B)	-46(3)
C(13B)	C(12A)	C(11B)	C(10A)	34(3)
C(13B)	C(12A)	C(11B)	C(10B)	40(2)
C(12B)	C(12A)	C(13B)	C(13A)	-130(3)
C(13B)	C(12A)	C(12B)	C(11A)	111(3)
C(8A)	C(13A)	C(8B)	C(9B)	24.3(11)
C(8A)	C(13A)	C(8B)	C(14B)	-116(3)
C(8A)	C(13A)	C(9B)	C(14A)	-14.3(15)
C(8A)	C(13A)	C(9B)	C(10B)	147(3)
C(8A)	C(13A)	C(13B)	C(8B)	-42.3(16)
C(12A)	C(13A)	C(8B)	C(8A)	-96(2)
C(12A)	C(13A)	C(8B)	C(13B)	36.6(15)
C(12A)	C(13A)	C(9B)	C(8A)	-161(2)
C(12A)	C(13A)	C(9B)	C(14A)	-175.4(5)
C(12A)	C(13A)	C(9B)	C(10B)	-14.1(16)
C(12A)	C(13A)	C(13B)	C(12B)	-19.2(12)
C(8B)	C(13A)	C(9B)	C(9A)	-151(3)
C(8B)	C(13A)	C(9B)	C(10B)	-142(3)
C(9B)	C(13A)	C(8B)	C(13B)	108(2)
C(8B)	C(13A)	C(13B)	C(12A)	122.9(18)
C(13B)	C(13A)	C(8B)	C(8A)	-132.7(19)
C(13B)	C(13A)	C(8B)	C(14B)	112(2)
C(9B)	C(13A)	C(13B)	C(8B)	-48.5(16)
C(13B)	C(13A)	C(9B)	C(8A)	164(2)
C(13B)	C(13A)	C(9B)	C(14A)	149.9(15)
C(13B)	C(13A)	C(9B)	C(10B)	-49(2)
O(2A)	C(14A)	C(9B)	C(9A)	23(2)
O(2A)	C(14A)	C(9B)	C(8B)	-170.8(9)
O(2A)	C(14A)	C(14B)	O(2B)	-2(3)
O(2A)	C(14A)	C(14B)	C(20)	-77.0(16)
O(2A)	C(14A)	C(20)	C(15)	29.7(3)
C(8A)	C(14A)	C(9B)	C(9A)	-136(4)
C(8A)	C(14A)	C(9B)	C(8B)	30.1(16)
C(8A)	C(14A)	C(14B)	O(2B)	-129(3)
C(8A)	C(14A)	C(14B)	C(20)	156.4(6)
C(8A)	C(14A)	C(20)	C(15)	-150.9(2)
C(9B)	C(14A)	C(14B)	O(2B)	-116(3)
C(9B)	C(14A)	C(14B)	C(20)	169.4(7)
C(14B)	C(14A)	C(9B)	C(9A)	-178(2)
C(14B)	C(14A)	C(9B)	C(8B)	-11.8(11)
C(11A)	C(12A)	C(13A)	C(8B)	49(2)
C(11A)	C(12A)	C(13A)	C(13B)	124.7(16)
C(11A)	C(12A)	C(11B)	C(10B)	170(4)
C(11A)	C(12A)	C(12B)	C(11B)	-6.5(14)
C(11A)	C(12A)	C(13B)	C(13A)	-87(2)
C(11A)	C(12A)	C(13B)	C(12B)	43(3)
C(13A)	C(12A)	C(11B)	C(11A)	-171(2)
C(13A)	C(12A)	C(11B)	C(12B)	-155(2)
C(11B)	C(12A)	C(13A)	C(8B)	52(2)
C(11B)	C(12A)	C(13A)	C(13B)	126.9(18)
C(13A)	C(12A)	C(12B)	C(11B)	43(4)
C(12B)	C(12A)	C(13A)	C(8A)	-27(3)
C(12B)	C(12A)	C(13A)	C(9B)	-21(3)
C(13A)	C(12A)	C(13B)	C(8B)	27.6(12)
C(13B)	C(12A)	C(13A)	C(8A)	-124.7(16)
C(13B)	C(12A)	C(13A)	C(9B)	-118.5(18)
C(11B)	C(12A)	C(12B)	C(13B)	-104(3)
C(12B)	C(12A)	C(11B)	C(11A)	-16(3)
C(11B)	C(12A)	C(13B)	C(13A)	-73(2)
C(11B)	C(12A)	C(13B)	C(12B)	56(3)
C(13B)	C(12A)	C(11B)	C(11A)	-129(3)
C(13B)	C(12A)	C(11B)	C(12B)	-113(3)
C(12B)	C(12A)	C(13B)	C(8B)	-102(3)
C(13B)	C(12A)	C(12B)	C(11B)	104(3)
C(8A)	C(13A)	C(8B)	C(13B)	132.7(19)
C(8A)	C(13A)	C(9B)	C(9A)	137(4)
C(8A)	C(13A)	C(9B)	C(8B)	-71(3)
C(8A)	C(13A)	C(13B)	C(12A)	81(2)
C(8A)	C(13A)	C(13B)	C(12B)	61(2)
C(12A)	C(13A)	C(8B)	C(9B)	-72(2)
C(12A)	C(13A)	C(8B)	C(14B)	148.4(11)
C(12A)	C(13A)	C(9B)	C(9A)	-24(2)
C(12A)	C(13A)	C(9B)	C(8B)	128(2)
C(12A)	C(13A)	C(13B)	C(8B)	-122.9(18)
C(8B)	C(13A)	C(9B)	C(8A)	71(3)
C(8B)	C(13A)	C(9B)	C(14A)	57(2)
C(9B)	C(13A)	C(8B)	C(8A)	-24.3(11)
C(9B)	C(13A)	C(8B)	C(14B)	-140(3)
C(8B)	C(13A)	C(13B)	C(12B)	104(2)
C(13B)	C(13A)	C(8B)	C(9B)	-108(2)
C(9B)	C(13A)	C(13B)	C(12A)	74.4(18)
C(9B)	C(13A)	C(13B)	C(12B)	55(2)
C(13B)	C(13A)	C(9B)	C(9A)	-58(3)
C(13B)	C(13A)	C(9B)	C(8B)	93(2)
O(2A)	C(14A)	C(9B)	C(8A)	159.1(19)
O(2A)	C(14A)	C(9B)	C(13A)	170.9(5)
O(2A)	C(14A)	C(9B)	C(10B)	46(4)
O(2A)	C(14A)	C(14B)	C(8B)	124.6(14)
O(2A)	C(14A)	C(20)	C(14B)	154.5(7)
O(2A)	C(14A)	C(20)	C(19)	-93.3(2)
C(8A)	C(14A)	C(9B)	C(13A)	11.8(14)
C(8A)	C(14A)	C(9B)	C(10B)	-113(4)
C(8A)	C(14A)	C(14B)	C(8B)	-2.0(8)
C(8A)	C(14A)	C(20)	C(14B)	-26.1(7)
C(8A)	C(14A)	C(20)	C(19)	86.1(2)
C(9B)	C(14A)	C(14B)	C(8B)	11.0(10)
C(14B)	C(14A)	C(9B)	C(8A)	-42(2)
C(14B)	C(14A)	C(9B)	C(13A)	-30.1(8)
C(14B)	C(14A)	C(9B)	C(10B)	-155(4)

C(9B)	C(14A)	C(20)	C(14B)	-15.5(11)	C(9B)	C(14A)	C(20)	C(15)	-140.3(9)
C(9B)	C(14A)	C(20)	C(19)	96.7(9)	C(20)	C(14A)	C(9B)	C(8A)	-30(2)
C(20)	C(14A)	C(9B)	C(9A)	-165.9(18)	C(20)	C(14A)	C(9B)	C(13A)	-18.0(13)
C(20)	C(14A)	C(9B)	C(8B)	0.4(12)	C(20)	C(14A)	C(9B)	C(10B)	-142(3)
C(14B)	C(14A)	C(20)	C(15)	-124.8(7)	C(14B)	C(14A)	C(20)	C(19)	112.2(7)
C(20)	C(14A)	C(14B)	O(2B)	75(3)	C(20)	C(14A)	C(14B)	C(8B)	-158.4(11)
C(1A)	C(1B)	C(2B)	C(2A)	89(5)	C(1A)	C(1B)	C(2B)	C(3A)	-4(4)
C(1A)	C(1B)	C(2B)	C(3B)	-15(3)	C(1A)	C(1B)	C(6B)	C(6A)	111(6)
C(1A)	C(1B)	C(6B)	C(7A)	-53(4)	C(1A)	C(1B)	C(6B)	C(5B)	117(5)
C(1A)	C(1B)	C(7B)	C(7A)	2.2(17)	C(1A)	C(1B)	C(7B)	O(1B)	164(2)
C(1A)	C(1B)	C(7B)	C(15)	-25(3)	C(2A)	C(1B)	C(2B)	C(3A)	-93(5)
C(2A)	C(1B)	C(2B)	C(3B)	-104(5)	C(2A)	C(1B)	C(6B)	C(1A)	-99(5)
C(2A)	C(1B)	C(6B)	C(6A)	13(4)	C(2A)	C(1B)	C(6B)	C(7A)	-152(2)
C(2A)	C(1B)	C(6B)	C(5B)	18(3)	C(2A)	C(1B)	C(7B)	C(7A)	152(2)
C(2A)	C(1B)	C(7B)	O(1B)	-46(3)	C(2A)	C(1B)	C(7B)	C(15)	125(2)
C(7A)	C(1B)	C(2B)	C(2A)	5(12)	C(7A)	C(1B)	C(2B)	C(3A)	-88(12)
C(7A)	C(1B)	C(2B)	C(3B)	-99(12)	C(7A)	C(1B)	C(6B)	C(1A)	53(4)
C(7A)	C(1B)	C(6B)	C(6A)	165(3)	C(7A)	C(1B)	C(6B)	C(5B)	170(2)
C(7A)	C(1B)	C(7B)	O(1B)	162(2)	C(7A)	C(1B)	C(7B)	C(15)	-27.5(16)
C(2B)	C(1B)	C(6B)	C(1A)	-117(5)	C(2B)	C(1B)	C(6B)	C(6A)	-6(4)
C(2B)	C(1B)	C(6B)	C(7A)	-170.0(19)	C(2B)	C(1B)	C(6B)	C(5B)	0(3)
C(6B)	C(1B)	C(2B)	C(2A)	104(5)	C(6B)	C(1B)	C(2B)	C(3A)	11(3)
C(6B)	C(1B)	C(2B)	C(3B)	-0(3)	C(2B)	C(1B)	C(7B)	C(7A)	170(2)
C(2B)	C(1B)	C(7B)	O(1B)	-28(3)	C(2B)	C(1B)	C(7B)	C(15)	142(2)
C(7B)	C(1B)	C(2B)	C(2A)	-77(5)	C(7B)	C(1B)	C(2B)	C(3A)	-170(2)
C(7B)	C(1B)	C(2B)	C(3B)	179.4(17)	C(6B)	C(1B)	C(7B)	C(7A)	-11.0(17)
C(6B)	C(1B)	C(7B)	O(1B)	151(2)	C(6B)	C(1B)	C(7B)	C(15)	-38(3)
C(7B)	C(1B)	C(6B)	C(1A)	64(5)	C(7B)	C(1B)	C(6B)	C(6A)	175(2)
C(7B)	C(1B)	C(6B)	C(7A)	10.5(17)	C(7B)	C(1B)	C(6B)	C(5B)	-179.5(17)
C(2A)	C(2B)	C(3B)	C(3A)	120(5)	C(2A)	C(2B)	C(3B)	C(4A)	-19(5)
C(2A)	C(2B)	C(3B)	C(4B)	-20(4)	C(3A)	C(2B)	C(3B)	C(4A)	-139(7)
C(3A)	C(2B)	C(3B)	C(4B)	-140(5)	C(1B)	C(2B)	C(3B)	C(3A)	140(5)
C(1B)	C(2B)	C(3B)	C(4A)	1(2)	C(1B)	C(2B)	C(3B)	C(4B)	0(3)
C(3A)	C(3B)	C(4B)	C(4A)	161(7)	C(3A)	C(3B)	C(4B)	C(5A)	-20(8)
C(3A)	C(3B)	C(4B)	C(5B)	-17(6)	C(4A)	C(3B)	C(4B)	C(5A)	179(8)
C(4A)	C(3B)	C(4B)	C(5B)	-178(3)	C(2B)	C(3B)	C(4B)	C(4A)	178(4)
C(2B)	C(3B)	C(4B)	C(5A)	-3(6)	C(2B)	C(3B)	C(4B)	C(5B)	-0(3)
C(4A)	C(4B)	C(5B)	C(1A)	4(6)	C(4A)	C(4B)	C(5B)	C(5A)	-178(8)
C(4A)	C(4B)	C(5B)	C(6A)	7(9)	C(4A)	C(4B)	C(5B)	C(6B)	-2(3)
C(5A)	C(4B)	C(5B)	C(1A)	-178(3)	C(5A)	C(4B)	C(5B)	C(6A)	-175(7)
C(5A)	C(4B)	C(5B)	C(6B)	176(4)	C(3B)	C(4B)	C(5B)	C(1A)	6(3)
C(3B)	C(4B)	C(5B)	C(5A)	-176(4)	C(3B)	C(4B)	C(5B)	C(6A)	9(6)
C(1A)	C(5B)	C(6B)	C(6A)	145(6)	C(1A)	C(5B)	C(6B)	C(7A)	121(10)
C(1A)	C(5B)	C(6B)	C(1B)	-20(2)	C(5A)	C(5B)	C(6B)	C(1A)	22(6)
C(5A)	C(5B)	C(6B)	C(6A)	168(8)	C(5A)	C(5B)	C(6B)	C(7A)	144(6)
C(5A)	C(5B)	C(6B)	C(1B)	3(5)	C(6A)	C(5B)	C(6B)	C(1A)	-145(6)
C(6A)	C(5B)	C(6B)	C(7A)	-24(9)	C(6A)	C(5B)	C(6B)	C(1B)	-165(5)
C(4B)	C(5B)	C(6B)	C(1A)	20(4)	C(4B)	C(5B)	C(6B)	C(6A)	165(6)
C(4B)	C(5B)	C(6B)	C(7A)	141(7)	C(7A)	C(7B)	C(15)	C(16)	-105.2(5)
C(7A)	C(7B)	C(15)	C(20)	106.3(8)	O(1B)	C(7B)	C(15)	C(7A)	-158.9(19)
O(1B)	C(7B)	C(15)	C(16)	95.8(16)	O(1B)	C(7B)	C(15)	C(20)	-53(2)
C(1B)	C(7B)	C(15)	C(7A)	30.0(18)	C(1B)	C(7B)	C(15)	C(16)	-75(2)
C(1B)	C(7B)	C(15)	C(20)	136.3(15)	C(8A)	C(8B)	C(9B)	C(9A)	123(4)
C(8A)	C(8B)	C(9B)	C(13A)	81(2)	C(8A)	C(8B)	C(9B)	C(14A)	-39.5(16)
C(8A)	C(8B)	C(9B)	C(10B)	125(3)	C(8A)	C(8B)	C(13B)	C(12A)	0(3)
C(8A)	C(8B)	C(13B)	C(13A)	67(2)	C(8A)	C(8B)	C(13B)	C(12B)	-25(3)
C(8A)	C(8B)	C(14B)	C(14A)	3.1(12)	C(8A)	C(8B)	C(14B)	O(2B)	161.1(18)
C(8A)	C(8B)	C(14B)	C(20)	-18(2)	C(13A)	C(8B)	C(9B)	C(8A)	-81(2)
C(13A)	C(8B)	C(9B)	C(9A)	42(5)	C(13A)	C(8B)	C(9B)	C(14A)	-121(2)

C(13A)	C(8B)	C(9B)	C(10B)	44(3)
C(13A)	C(8B)	C(13B)	C(12B)	-93(2)
C(13A)	C(8B)	C(14B)	O(2B)	-81(2)
C(9B)	C(8B)	C(13B)	C(12A)	25(3)
C(9B)	C(8B)	C(13B)	C(12B)	-0(3)
C(13B)	C(8B)	C(9B)	C(9A)	-2(3)
C(13B)	C(8B)	C(9B)	C(14A)	-164.7(17)
C(9B)	C(8B)	C(14B)	C(14A)	-16.6(16)
C(9B)	C(8B)	C(14B)	C(20)	-37(2)
C(14B)	C(8B)	C(9B)	C(9A)	179.2(18)
C(14B)	C(8B)	C(9B)	C(14A)	16.4(16)
C(13B)	C(8B)	C(14B)	C(14A)	164.5(18)
C(13B)	C(8B)	C(14B)	C(20)	143.8(17)
C(14B)	C(8B)	C(13B)	C(13A)	-89(2)
C(8A)	C(9B)	C(10B)	C(9A)	-133(5)
C(8A)	C(9B)	C(10B)	C(11A)	44(4)
C(9A)	C(9B)	C(10B)	C(10A)	-162(6)
C(9A)	C(9B)	C(10B)	C(11B)	177(2)
C(13A)	C(9B)	C(10B)	C(10A)	36(4)
C(13A)	C(9B)	C(10B)	C(11B)	15(2)
C(14A)	C(9B)	C(10B)	C(10A)	158(3)
C(14A)	C(9B)	C(10B)	C(11B)	137(3)
C(8B)	C(9B)	C(10B)	C(10A)	21(5)
C(8B)	C(9B)	C(10B)	C(11B)	0(3)
C(9A)	C(10B)	C(11B)	C(11A)	-0(8)
C(9A)	C(10B)	C(11B)	C(12B)	2(4)
C(10A)	C(10B)	C(11B)	C(12A)	-165(3)
C(11A)	C(10B)	C(11B)	C(10A)	158(6)
C(11A)	C(10B)	C(11B)	C(12B)	2(2)
C(9B)	C(10B)	C(11B)	C(11A)	-2(3)
C(9B)	C(10B)	C(11B)	C(12B)	-0(3)
C(10A)	C(11B)	C(12B)	C(12A)	-43(5)
C(11A)	C(11B)	C(12B)	C(12A)	143(8)
C(12A)	C(11B)	C(12B)	C(11A)	-143(8)
C(10B)	C(11B)	C(12B)	C(11A)	-173(7)
C(10B)	C(11B)	C(12B)	C(13B)	-0(3)
C(11A)	C(12B)	C(13B)	C(13A)	-32(3)
C(12A)	C(12B)	C(13B)	C(13A)	57(3)
C(11B)	C(12B)	C(13B)	C(12A)	-90(4)
C(11B)	C(12B)	C(13B)	C(8B)	0(3)
C(14A)	C(14B)	C(20)	C(19)	-106.6(4)
O(2B)	C(14B)	C(20)	C(15)	-45(2)
C(8B)	C(14B)	C(20)	C(14A)	25.2(14)
C(8B)	C(14B)	C(20)	C(19)	-81.3(16)
C(7A)	C(15)	C(16)	C(21)	-163.7(2)
C(7A)	C(15)	C(20)	C(14B)	10.3(9)
C(7B)	C(15)	C(16)	C(17)	158.8(10)
C(7B)	C(15)	C(20)	C(14A)	14.6(14)
C(7B)	C(15)	C(20)	C(19)	138.9(14)
C(16)	C(15)	C(20)	C(14B)	136.1(9)
C(20)	C(15)	C(16)	C(17)	-46.6(2)
C(15)	C(16)	C(17)	C(18)	57.1(2)
C(15)	C(16)	C(21)	C(23)	-160.9(2)
C(17)	C(16)	C(21)	C(23)	-44.6(2)
C(16)	C(17)	C(18)	C(19)	-2.2(3)
C(17)	C(18)	C(19)	C(22)	57.0(2)
C(18)	C(19)	C(20)	C(14B)	-89.4(8)
C(18)	C(19)	C(22)	C(21)	-49.0(2)
C(20)	C(19)	C(22)	C(21)	64.7(2)

C(13A)	C(8B)	C(13B)	C(12A)	-67(2)
C(13A)	C(8B)	C(14B)	C(14A)	121(2)
C(13A)	C(8B)	C(14B)	C(20)	101(2)
C(9B)	C(8B)	C(13B)	C(13A)	93(2)
C(13B)	C(8B)	C(9B)	C(8A)	-125(2)
C(13B)	C(8B)	C(9B)	C(13A)	-43.9(15)
C(13B)	C(8B)	C(9B)	C(10B)	0(3)
C(9B)	C(8B)	C(14B)	O(2B)	141(2)
C(14B)	C(8B)	C(9B)	C(8A)	56(2)
C(14B)	C(8B)	C(9B)	C(13A)	137(3)
C(14B)	C(8B)	C(9B)	C(10B)	-178.9(18)
C(13B)	C(8B)	C(14B)	O(2B)	-37(2)
C(14B)	C(8B)	C(13B)	C(12A)	-155.7(18)
C(14B)	C(8B)	C(13B)	C(12B)	178.8(18)
C(8A)	C(9B)	C(10B)	C(10A)	65(6)
C(8A)	C(9B)	C(10B)	C(11B)	44(5)
C(9A)	C(9B)	C(10B)	C(11A)	177(3)
C(13A)	C(9B)	C(10B)	C(9A)	-162(3)
C(13A)	C(9B)	C(10B)	C(11A)	14.6(18)
C(14A)	C(9B)	C(10B)	C(9A)	-40(4)
C(14A)	C(9B)	C(10B)	C(11A)	137(3)
C(8B)	C(9B)	C(10B)	C(9A)	-177(3)
C(8B)	C(9B)	C(10B)	C(11A)	-0.5(19)
C(9A)	C(10B)	C(11B)	C(10A)	158(7)
C(9A)	C(10B)	C(11B)	C(12A)	-8(6)
C(10A)	C(10B)	C(11B)	C(11A)	-158(6)
C(10A)	C(10B)	C(11B)	C(12B)	-155(4)
C(11A)	C(10B)	C(11B)	C(12A)	-8(3)
C(9B)	C(10B)	C(11B)	C(10A)	155(4)
C(9B)	C(10B)	C(11B)	C(12A)	-10(2)
C(10A)	C(11B)	C(12B)	C(11A)	174(10)
C(10A)	C(11B)	C(12B)	C(13B)	-13(5)
C(11A)	C(11B)	C(12B)	C(13B)	173(8)
C(12A)	C(11B)	C(12B)	C(13B)	29.8(16)
C(10B)	C(11B)	C(12B)	C(12A)	-30(3)
C(11A)	C(12B)	C(13B)	C(12A)	-89(4)
C(11A)	C(12B)	C(13B)	C(8B)	1(2)
C(12A)	C(12B)	C(13B)	C(8B)	90(3)
C(11B)	C(12B)	C(13B)	C(13A)	-33(3)
C(14A)	C(14B)	C(20)	C(15)	108.7(5)
O(2B)	C(14B)	C(20)	C(14A)	-153.5(18)
O(2B)	C(14B)	C(20)	C(19)	100.0(16)
C(8B)	C(14B)	C(20)	C(15)	133.9(12)
C(7A)	C(15)	C(16)	C(17)	80.9(2)
C(7A)	C(15)	C(20)	C(14A)	99.4(2)
C(7A)	C(15)	C(20)	C(19)	-136.4(2)
C(7B)	C(15)	C(16)	C(21)	-85.8(10)
C(7B)	C(15)	C(20)	C(14B)	-74.4(17)
C(16)	C(15)	C(20)	C(14A)	-134.8(2)
C(16)	C(15)	C(20)	C(19)	-10.6(2)
C(20)	C(15)	C(16)	C(21)	68.7(2)
C(15)	C(16)	C(21)	C(22)	-58.4(2)
C(17)	C(16)	C(21)	C(22)	57.9(2)
C(21)	C(16)	C(17)	C(18)	-56.1(2)
C(17)	C(18)	C(19)	C(20)	-57.8(2)
C(18)	C(19)	C(20)	C(14A)	-172.6(2)
C(18)	C(19)	C(20)	C(15)	61.7(2)
C(18)	C(19)	C(22)	C(24)	52.2(2)
C(20)	C(19)	C(22)	C(24)	165.84(19)

C(22)	C(19)	C(20)	C(14A)	71.1(2)	C(22)	C(19)	C(20)	C(14B)	154.3(8)
C(22)	C(19)	C(20)	C(15)	-54.6(2)	C(16)	C(21)	C(22)	C(19)	-5.9(2)
C(16)	C(21)	C(22)	C(24)	-126.66(18)	C(16)	C(21)	C(23)	C(24)	117.2(2)
C(16)	C(21)	C(23)	C(29)	-116.5(2)	C(22)	C(21)	C(23)	C(24)	4.06(18)
C(22)	C(21)	C(23)	C(29)	130.4(2)	C(23)	C(21)	C(22)	C(19)	116.69(18)
C(23)	C(21)	C(22)	C(24)	-4.07(18)	C(19)	C(22)	C(24)	C(23)	-108.3(2)
C(19)	C(22)	C(24)	C(25)	129.8(2)	C(21)	C(22)	C(24)	C(23)	4.08(18)
C(21)	C(22)	C(24)	C(25)	-117.8(2)	C(21)	C(23)	C(24)	C(22)	-4.04(18)
C(21)	C(23)	C(24)	C(25)	116.0(2)	C(21)	C(23)	C(29)	C(28)	-141.7(2)
C(21)	C(23)	C(29)	C(30)	-63.8(3)	C(24)	C(23)	C(29)	C(28)	-34.1(3)
C(24)	C(23)	C(29)	C(30)	43.9(3)	C(29)	C(23)	C(24)	C(22)	-126.0(2)
C(29)	C(23)	C(24)	C(25)	-6.0(2)	C(22)	C(24)	C(25)	C(26)	171.0(2)
C(22)	C(24)	C(25)	C(32)	47.8(2)	C(23)	C(24)	C(25)	C(26)	65.3(2)
C(23)	C(24)	C(25)	C(32)	-57.8(2)	C(24)	C(25)	C(26)	C(27)	-64.8(3)
C(24)	C(25)	C(32)	C(31)	64.5(3)	C(26)	C(25)	C(32)	C(31)	-61.2(3)
C(32)	C(25)	C(26)	C(27)	61.5(3)	C(25)	C(26)	C(27)	C(28)	0.0(4)
C(26)	C(27)	C(28)	C(29)	33.3(4)	C(26)	C(27)	C(28)	C(30)	-37.4(4)
C(27)	C(28)	C(29)	C(23)	5.1(3)	C(27)	C(28)	C(29)	C(30)	-108.4(2)
C(27)	C(28)	C(30)	C(29)	113.1(2)	C(27)	C(28)	C(30)	C(31)	0.1(3)
C(29)	C(28)	C(30)	C(31)	-113.0(3)	C(30)	C(28)	C(29)	C(23)	113.5(2)
C(23)	C(29)	C(30)	C(28)	-116.0(2)	C(23)	C(29)	C(30)	C(31)	-7.7(3)
C(28)	C(29)	C(30)	C(31)	108.3(2)	C(28)	C(30)	C(31)	C(32)	37.6(4)
C(29)	C(30)	C(31)	C(32)	-33.3(4)	C(30)	C(31)	C(32)	C(25)	-1.0(4)

The sign is positive if when looking from atom 2 to atom 3 a clock-wise motion of atom 1 would superimpose it on atom 4.

X-Ray Data for oxetane 8

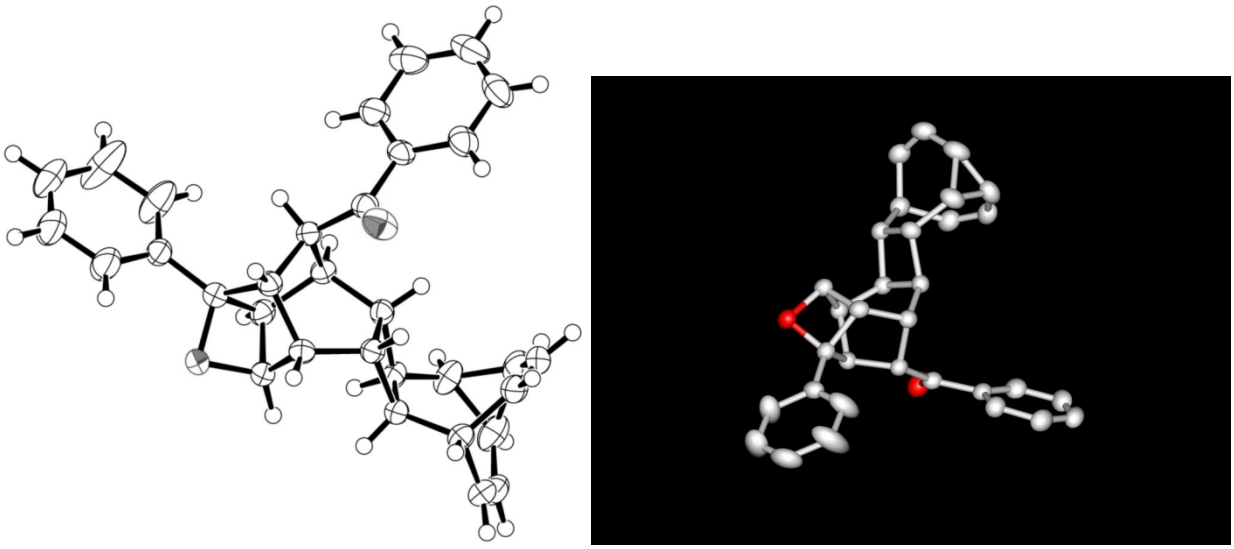


Figure S6. Ortep drawing of oxetane **8**.

Crystal data and structure refinement for oxetane **8**.

Identification code	shelxl
Empirical formula	C32 H28 O2
Formula weight	444.54
Temperature	223(2) K
Wavelength	0.71075 A
Crystal system, space group	Triclinic, P -1

Unit cell dimensions	a = 6.7012(4) A alpha = 106.6850(10) deg.
	b = 10.9484(6) A beta = 91.7060(10) deg.
	c = 16.1361(9) A gamma = 91.060(2) deg.
Volume	1133.07(11) A^3
Z, Calculated density	2, 1.303 Mg/m^3
Absorption coefficient	0.080 mm^-1
F(000)	472
Crystal size	0.40 x 0.15 x 0.10 mm
Theta range for data collection	3.04 to 27.47 deg.
Limiting indices	-8<=h<=8, -14<=k<=14, -20<=l<=20
Reflections collected / unique	11912 / 5162 [R(int) = 0.0225]
Completeness to theta = 27.47	99.3 %
Max. and min. transmission	0.9921 and 0.9689
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	5162 / 0 / 308
Goodness-of-fit on F^2	1.016
Final R indices [I>2sigma(I)]	R1 = 0.0504, wR2 = 0.1138
R indices (all data)	R1 = 0.0677, wR2 = 0.1251
Extinction coefficient	0.0086(17)
Largest diff. peak and hole	0.272 and -0.293 e.A^-3

Table S8. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for oxetane. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
O(1)	2625(2)	5818(1)	4925(1)	40(1)
O(2)	57(2)	9304(1)	7569(1)	48(1)
C(1)	3011(3)	9990(1)	8418(1)	34(1)
C(2)	1988(3)	10426(2)	9183(1)	45(1)
C(3)	2946(4)	11207(2)	9921(1)	55(1)
C(4)	4898(4)	11596(2)	9901(1)	59(1)
C(5)	5939(3)	11170(2)	9151(1)	55(1)
C(6)	5010(3)	10350(2)	8410(1)	43(1)
C(7)	1863(2)	9209(2)	7626(1)	33(1)
C(8)	4785(3)	7692(2)	5008(1)	35(1)
C(9)	6563(3)	8282(2)	5348(2)	65(1)
C(10)	7743(3)	8859(3)	4866(2)	87(1)
C(11)	7174(3)	8826(2)	4039(2)	62(1)
C(12)	5426(5)	8246(3)	3702(2)	80(1)
C(13)	4225(4)	7684(2)	4183(1)	70(1)
C(14)	3515(2)	7008(2)	5488(1)	33(1)
C(15)	1794(2)	7670(1)	6071(1)	30(1)
C(16)	3002(2)	8356(1)	6899(1)	29(1)
C(17)	4046(2)	7184(1)	7084(1)	29(1)
C(18)	4268(2)	6313(1)	6149(1)	32(1)

C(19)	2358(3)	5511(2)	5739(1)	34(1)
C(20)	730(2)	6418(2)	6167(1)	31(1)
C(21)	481(2)	6375(1)	7096(1)	29(1)
C(22)	2555(2)	6605(1)	7580(1)	29(1)
C(23)	2592(2)	5164(2)	7534(1)	32(1)
C(24)	356(2)	5012(2)	7205(1)	32(1)
C(25)	-1218(2)	4801(2)	7818(1)	35(1)
C(26)	-1094(3)	3483(2)	7934(1)	44(1)
C(27)	471(3)	3070(2)	8283(1)	48(1)
C(28)	2317(3)	3793(2)	8655(1)	50(1)
C(29)	3284(3)	4822(2)	8337(1)	42(1)
C(30)	2250(3)	5231(2)	9185(1)	47(1)
C(31)	364(3)	5902(2)	9292(1)	44(1)
C(32)	-1137(3)	5749(2)	8708(1)	40(1)

Table S9. Bond lengths [A] and angles [deg] for oxetane.

O(1)-C(19)	1.4609(19)
O(1)-C(14)	1.4612(18)
O(2)-C(7)	1.219(2)
C(1)-C(6)	1.391(2)
C(1)-C(2)	1.395(2)
C(1)-C(7)	1.499(2)
C(2)-C(3)	1.383(3)
C(3)-C(4)	1.372(3)
C(4)-C(5)	1.381(3)
C(5)-C(6)	1.393(3)
C(7)-C(16)	1.510(2)
C(8)-C(9)	1.366(3)
C(8)-C(13)	1.370(3)
C(8)-C(14)	1.494(2)
C(9)-C(10)	1.389(3)
C(10)-C(11)	1.368(4)
C(11)-C(12)	1.344(3)
C(12)-C(13)	1.386(3)
C(14)-C(18)	1.556(2)
C(14)-C(15)	1.564(2)
C(14)-C(19)	1.951(2)
C(15)-C(16)	1.530(2)
C(15)-C(20)	1.582(2)
C(16)-C(17)	1.570(2)
C(17)-C(22)	1.535(2)
C(17)-C(18)	1.548(2)
C(18)-C(19)	1.556(2)
C(19)-C(20)	1.531(2)
C(20)-C(21)	1.527(2)
C(21)-C(24)	1.553(2)
C(21)-C(22)	1.555(2)
C(22)-C(23)	1.559(2)
C(23)-C(29)	1.510(2)

C(23)-C(24)	1.565(2)
C(24)-C(25)	1.526(2)
C(25)-C(32)	1.510(2)
C(25)-C(26)	1.511(2)
C(26)-C(27)	1.323(3)
C(27)-C(28)	1.471(3)
C(28)-C(29)	1.510(2)
C(28)-C(30)	1.564(3)
C(29)-C(30)	1.507(3)
C(30)-C(31)	1.463(3)
C(31)-C(32)	1.332(3)
C(19)-O(1)-C(14)	83.75(10)
C(6)-C(1)-C(2)	119.03(16)
C(6)-C(1)-C(7)	122.88(15)
C(2)-C(1)-C(7)	118.00(16)
C(3)-C(2)-C(1)	120.4(2)
C(4)-C(3)-C(2)	120.3(2)
C(3)-C(4)-C(5)	120.09(18)
C(4)-C(5)-C(6)	120.2(2)
C(1)-C(6)-C(5)	119.88(19)
O(2)-C(7)-C(1)	119.84(14)
O(2)-C(7)-C(16)	121.62(14)
C(1)-C(7)-C(16)	118.50(14)
C(9)-C(8)-C(13)	117.92(17)
C(9)-C(8)-C(14)	122.15(16)
C(13)-C(8)-C(14)	119.85(16)
C(8)-C(9)-C(10)	120.4(2)
C(11)-C(10)-C(9)	120.9(2)
C(12)-C(11)-C(10)	118.9(2)
C(11)-C(12)-C(13)	120.6(2)
C(8)-C(13)-C(12)	121.3(2)
O(1)-C(14)-C(8)	112.55(12)
O(1)-C(14)-C(18)	91.04(11)
C(8)-C(14)-C(18)	126.27(14)
O(1)-C(14)-C(15)	105.33(12)
C(8)-C(14)-C(15)	122.47(13)
C(18)-C(14)-C(15)	93.40(12)
O(1)-C(14)-C(19)	48.12(8)
C(8)-C(14)-C(19)	155.12(13)
C(18)-C(14)-C(19)	51.19(9)
C(15)-C(14)-C(19)	81.37(10)
C(16)-C(15)-C(14)	100.03(12)
C(16)-C(15)-C(20)	110.63(12)
C(14)-C(15)-C(20)	97.39(11)
C(7)-C(16)-C(15)	116.68(13)
C(7)-C(16)-C(17)	117.09(13)
C(15)-C(16)-C(17)	99.65(11)
C(22)-C(17)-C(18)	111.52(12)
C(22)-C(17)-C(16)	106.33(12)
C(18)-C(17)-C(16)	100.68(12)
C(17)-C(18)-C(19)	114.77(12)
C(17)-C(18)-C(14)	109.83(12)

C(19)-C(18)-C(14)	77.61(11)
O(1)-C(19)-C(20)	103.01(13)
O(1)-C(19)-C(18)	91.07(11)
C(20)-C(19)-C(18)	100.65(12)
O(1)-C(19)-C(14)	48.13(8)
C(20)-C(19)-C(14)	84.60(10)
C(18)-C(19)-C(14)	51.20(9)
C(21)-C(20)-C(19)	110.22(13)
C(21)-C(20)-C(15)	115.36(12)
C(19)-C(20)-C(15)	95.76(12)
C(20)-C(21)-C(24)	114.74(12)
C(20)-C(21)-C(22)	109.01(12)
C(24)-C(21)-C(22)	89.98(11)
C(17)-C(22)-C(21)	110.29(12)
C(17)-C(22)-C(23)	121.02(12)
C(21)-C(22)-C(23)	89.55(11)
C(29)-C(23)-C(22)	117.80(14)
C(29)-C(23)-C(24)	122.23(13)
C(22)-C(23)-C(24)	89.38(11)
C(25)-C(24)-C(21)	115.54(13)
C(25)-C(24)-C(23)	118.05(13)
C(21)-C(24)-C(23)	89.42(11)
C(32)-C(25)-C(26)	107.60(14)
C(32)-C(25)-C(24)	115.38(13)
C(26)-C(25)-C(24)	111.08(14)
C(27)-C(26)-C(25)	124.21(16)
C(26)-C(27)-C(28)	127.45(17)
C(27)-C(28)-C(29)	125.20(17)
C(27)-C(28)-C(30)	120.64(16)
C(29)-C(28)-C(30)	58.67(12)
C(30)-C(29)-C(23)	123.77(15)
C(30)-C(29)-C(28)	62.46(13)
C(23)-C(29)-C(28)	124.25(16)
C(31)-C(30)-C(29)	123.09(16)
C(31)-C(30)-C(28)	120.82(16)
C(29)-C(30)-C(28)	58.87(12)
C(32)-C(31)-C(30)	126.98(17)
C(31)-C(32)-C(25)	125.47(16)

Table S10. Anisotropic displacement parameters (A^2 x 10^3) for oxetane.
The anisotropic displacement factor exponent takes the form:
-2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
O(1)	57(1)	32(1)	28(1)	5(1)	8(1)	-6(1)
O(2)	36(1)	45(1)	54(1)	1(1)	4(1)	8(1)
C(1)	44(1)	24(1)	34(1)	6(1)	0(1)	4(1)
C(2)	59(1)	34(1)	41(1)	8(1)	7(1)	10(1)
C(3)	88(2)	38(1)	35(1)	4(1)	3(1)	15(1)
C(4)	94(2)	33(1)	44(1)	4(1)	-23(1)	3(1)
C(5)	62(1)	42(1)	58(1)	13(1)	-19(1)	-9(1)
C(6)	48(1)	38(1)	41(1)	9(1)	-4(1)	-4(1)
C(7)	35(1)	28(1)	36(1)	9(1)	3(1)	1(1)
C(8)	42(1)	29(1)	35(1)	10(1)	10(1)	4(1)
C(9)	41(1)	98(2)	81(2)	66(2)	-8(1)	-11(1)
C(10)	43(1)	132(2)	126(2)	102(2)	-13(1)	-20(1)
C(11)	63(1)	61(1)	79(2)	47(1)	22(1)	4(1)
C(12)	116(2)	86(2)	43(1)	31(1)	-2(1)	-44(2)
C(13)	88(2)	85(2)	42(1)	27(1)	-11(1)	-45(1)
C(14)	38(1)	29(1)	30(1)	6(1)	3(1)	-2(1)
C(15)	31(1)	28(1)	30(1)	8(1)	1(1)	1(1)
C(16)	29(1)	27(1)	30(1)	8(1)	2(1)	-1(1)
C(17)	24(1)	31(1)	32(1)	10(1)	1(1)	0(1)
C(18)	31(1)	29(1)	36(1)	10(1)	9(1)	3(1)
C(19)	46(1)	27(1)	29(1)	6(1)	8(1)	-2(1)
C(20)	30(1)	31(1)	31(1)	7(1)	-1(1)	-4(1)
C(21)	26(1)	29(1)	30(1)	6(1)	4(1)	0(1)
C(22)	28(1)	32(1)	28(1)	8(1)	3(1)	1(1)
C(23)	30(1)	34(1)	36(1)	14(1)	10(1)	4(1)
C(24)	33(1)	30(1)	30(1)	6(1)	6(1)	-2(1)
C(25)	29(1)	38(1)	38(1)	10(1)	5(1)	-5(1)
C(26)	52(1)	38(1)	42(1)	11(1)	9(1)	-12(1)
C(27)	61(1)	37(1)	51(1)	20(1)	17(1)	1(1)
C(28)	47(1)	55(1)	61(1)	37(1)	9(1)	7(1)
C(29)	31(1)	54(1)	52(1)	30(1)	6(1)	3(1)
C(30)	46(1)	61(1)	39(1)	25(1)	-4(1)	-9(1)
C(31)	53(1)	43(1)	32(1)	6(1)	11(1)	-10(1)
C(32)	38(1)	38(1)	42(1)	6(1)	15(1)	-1(1)

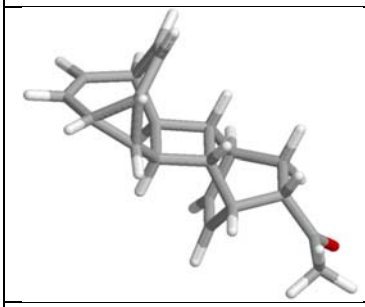
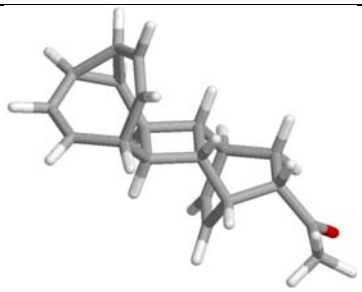
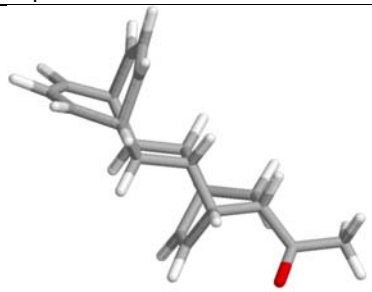
Table S11. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for oxetane.

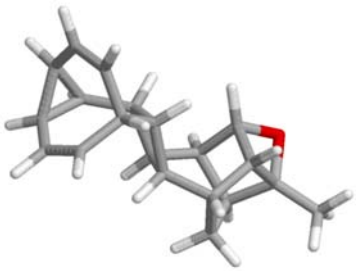
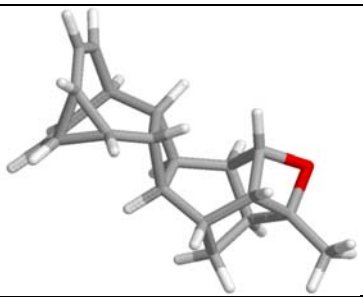
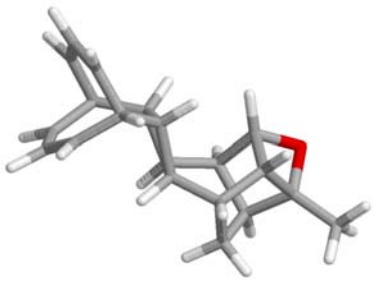
	x	y	z	U(eq)
H(2)	637	10187	9197	54
H(3)	2258	11474	10438	66
H(4)	5528	12152	10399	71
H(5)	7278	11434	9140	66
H(6)	5732	10042	7905	52
H(9)	6990	8297	5911	78
H(10)	8948	9278	5112	105
H(11)	7991	9202	3711	74
H(12)	5015	8221	3135	96
H(13)	3002	7290	3938	85
H(15)	942	8220	5827	36
H(16)	4050	8889	6741	35
H(17)	5348	7421	7401	34
H(18)	5553	5877	6026	38
H(19)	2256	4605	5731	41
H(20)	-549	6226	5826	37
H(21)	-560	6944	7404	35
H(22)	2455	7149	8184	35
H(23)	3429	4720	7050	39
H(24)	200	4362	6635	38
H(25)	-2545	4859	7548	42
H(26)	-2200	2920	7746	53
H(27)	394	2217	8295	57
H(28)	3280	3299	8897	60
H(29)	4757	4856	8415	51
H(30)	3167	5479	9702	56
H(31)	194	6506	9830	53
H(32)	-2239	6275	8863	48

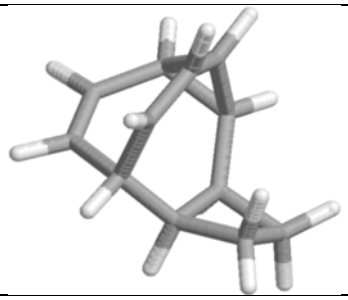
Computational Details

Gaussian 03, Revision E.01,
M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, J. A. Montgomery, Jr., T. Vreven, K. N. Kudin, J. C. Burant, J. M. Millam, S. S. Iyengar, J. Tomasi, V. Barone, B. Mennucci, M. Cossi, G. Scalmani, N. Rega, G. A. Petersson, H. Nakatsuji, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, M. Klene, X. Li, J. E. Knox, H. P. Hratchian, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, P. Y. Ayala, K. Morokuma, G. A. Voth, P. Salvador, J. J. Dannenberg, V. G. Zakrzewski, S. Dapprich, A. D. Daniels, M. C. Strain, O. Farkas, D. K. Malick, A. D. Rabuck, K. Raghavachari, J. B. Foresman, J. V. Ortiz, Q. Cui, A. G. Baboul, S. Clifford, J. Cioslowski, B. B. Stefanov, G. Liu, A. Liashenko, P. Piskorz, I. Komaromi, R. L. Martin, D. J. Fox, T. Keith, M. A. Al-Laham, C. Y. Peng, A. Nanayakkara, M. Challacombe, P. M. W. Gill, B. Johnson, W. Chen, M. W. Wong, C. Gonzalez, and J. A. Pople, Gaussian, Inc., Wallingford CT, 2004.

Table S12. Geometries calculated at B3LYP/6-311+G(d,p) level (for energies see Table 1 in the main text).

D.-A. adduct **6a**	D.-A. adduct **6b**	Cope Transition State **6ts**
		
C 1.2486 -0.9909 -0.3783	C 1.2456 -0.9454 -0.4511	C -1.2452 0.9492 -0.4506
C 0.9833 0.5080 -0.7554	C 0.9756 0.5784 -0.7017	C -1.0209 -0.5657 -0.7430
C -0.0223 -0.9894 0.5160	C -0.0080 -1.0051 0.4728	C 0.0445 0.9722 0.4188
C -0.2676 0.5091 0.1752	C -0.2751 0.5072 0.2184	C 0.2574 -0.5473 0.1428
C -1.2563 -1.8180 0.0905	C -1.2405 -1.8252 0.0276	C 1.2726 1.7606 -0.0911
C 2.0080 1.5863 -0.5054	C 2.0620 1.5977 -0.3393	C -2.0945 -1.5691 -0.3663
C -2.6810 0.2100 0.6559	C -2.6865 0.1621 0.6776	C 2.6673 -0.2728 0.5435
C -1.8167 -0.2497 -1.6313	C -1.8176 -0.1886 -1.6240	C 1.7645 0.0990 -1.7411
C -1.6694 0.6833 -0.4544	C -1.6774 0.6933 -0.4075	C 1.6400 -0.7702 -0.5140
C -2.4427 -1.2913 0.9485	C -2.4228 -1.3444 0.9173	C 2.4912 1.2720 0.7440
C -1.5957 -1.5339 -1.3514	C -1.5903 -1.4827 -1.3993	C 1.5594 1.3981 -1.5281
C -4.1291 0.5364 0.2891	C -4.1388 0.4746 0.3133	C 4.1054 -0.6492 0.2078
O -4.9845 -0.3137 0.1807	O -4.9821 -0.3855 0.1904	O 4.4173 -1.1509 -0.8496
C -4.4700 1.9999 0.0677	C -4.5003 1.9364 0.1159	C 5.1389 -0.4043 1.2916
C 2.5776 -1.3604 0.2914	C 2.5425 -1.4322 0.1448	C -2.5281 1.3990 0.2215
C 3.4902 1.4042 -0.7278	C 3.3203 1.3876 -1.1631	C -3.4814 -1.3772 -0.9017
C 2.9094 1.6738 0.7025	C 2.4599 1.6213 1.1252	C -2.6395 -1.6327 1.0289
C 4.1247 0.1138 -1.0553	C 4.0935 0.2987 -1.0944	C -4.2021 -0.1915 -0.9278
C 2.9975 0.6544 1.7609	C 3.0172 0.5966 1.7760	C -3.0040 -0.5645 1.8333
C 3.7564 -1.0987 -0.6289	C 3.8963 -0.8820 -0.2338	C -3.8367 1.0468 -0.4182
C 2.8492 -0.6647 1.6127	C 3.3342 -0.7295 1.2220	C -2.9914 0.7830 1.5077
H 1.1357 -1.6295 -1.2550	H 1.0853 -1.5087 -1.3719	H -1.1373 1.5380 -1.3625
H 0.6925 0.5788 -1.8045	H 0.7066 0.7449 -1.7451	H -0.7870 -0.7213 -1.7967
H 0.1908 -1.1738 1.5691	H 0.2362 -1.2436 1.5085	H -0.1435 1.2155 1.4652
H -0.1601 1.1809 1.0277	H -0.1875 1.1284 1.1101	H 0.1661 -1.1739 1.0305
H -1.1016 -2.8814 0.2710	H -1.0762 -2.8940 0.1619	H 1.1370 2.8342 0.0416
H 1.6478 2.5577 -0.8264	H 1.6597 2.5824 -0.5845	H -1.7340 -2.5587 -0.6460
H -2.4664 0.8103 1.5460	H -2.4902 0.7335 1.5909	H 2.4422 -0.7648 1.4955
H -2.0946 0.1106 -2.6125	H -2.0981 0.2114 -2.5890	H 2.0205 -0.3207 -2.7030
H -1.8465 1.7226 -0.7268	H -1.8640 1.7418 -0.6345	H 1.8161 -1.8194 -0.7424
H -3.3490 -1.8468 0.7179	H -3.3243 -1.9051 0.6801	H 3.3803 1.8105 0.4157
H -2.2231 -1.4415 2.0067	H -2.1870 -1.5269 1.9668	H 2.3433 1.5058 1.7993
H -1.6801 -2.3257 -2.0834	H -1.6725 -2.2432 -2.1640	H 1.6252 2.1507 -2.3021

H -5.5336 2.1499 0.2338	H -5.5666 2.0679 0.2799	H 5.0197 0.5763 1.7522
H -3.8899 2.6610 0.7112	H -3.9325 2.5948 0.7730	H 6.1390 -0.5068 0.8796
H -4.2473 2.2690 -0.9671	H -4.2771 2.2263 -0.9132	H 5.0038 -1.1474 2.0817
H 2.5369 -2.4331 0.4899	H 2.5416 -2.5098 0.2676	H -2.4703 2.4794 0.3531
H 3.9958 2.2586 -1.1558	H 3.6266 2.1952 -1.8166	H -3.9926 -2.2726 -1.2288
H 3.0903 2.6805 1.0528	H 2.3361 2.5583 1.6541	H -2.8395 -2.6260 1.4078
H 5.0112 0.1845 -1.6747	H 4.9943 0.2803 -1.6968	H -5.2232 -0.2706 -1.2822
H 3.2535 1.0310 2.7444	H 3.3181 0.7503 2.8059	H -3.4602 -0.8193 2.7827
H 4.3561 -1.9513 -0.9230	H 4.6830 -1.6186 -0.3176	H -4.5929 1.8203 -0.4111
H 2.9932 -1.2967 2.4803	H 3.8071 -1.3941 1.9316	H -3.4352 1.4662 2.2194
oxetane **8a**	oxetane **8b**	Cope Transition State **8ts**
		
C 0.8697 0.2037 0.7932	C 0.8785 -0.2237 -0.8153	C -0.8661 0.2559 -0.8015
C 0.9751 -0.9525 -0.2606	C 0.9679 0.9799 0.1885	C -0.9585 -0.9801 0.1474
C -0.1240 0.9504 -0.1389	C -0.1100 -0.9354 0.1570	C 0.1222 0.9318 0.1927
C -0.2135 -0.3123 -1.0494	C -0.2105 0.3674 1.0064	C 0.2155 -0.4015 0.9970
C -1.5296 1.3806 0.2989	C -1.5114 -1.4009 -0.2576	C 1.5273 1.4048 -0.2012
C 2.2494 -1.1545 -1.0425	C 2.2877 1.1923 0.9391	C -2.2584 -1.2283 0.8879
C -2.8046 0.0108 -1.1519	C -2.7984 0.0253 1.1267	C 2.8041 -0.0724 1.1385
C -1.9222 -1.1913 0.6218	C -1.9279 1.1491 -0.7032	C 1.9366 -1.1292 -0.7326
C -1.5872 -0.9680 -0.8671	C -1.5901 1.0007 0.7942	C 1.5938 -1.0312 0.7679
C -2.3312 1.4662 -1.0346	C -2.3108 -1.4293 1.0797	C 2.3215 1.3846 1.1396
C -2.2930 0.2593 1.0508	C -2.2855 -0.3239 -1.0617	C 2.3014 0.3537 -1.0385
C -3.5389 -0.1749 0.2142	C -3.5347 0.1386 -0.2460	C 3.5455 -0.1415 -0.2343
O -3.3250 -1.5627 0.5984	O -3.3341 1.5082 -0.6966	O 3.3412 -1.4940 -0.7325
C -4.9511 0.2981 0.3976	C -4.9418 -0.3570 -0.4072	C 4.9556 0.3528 -0.3714
C 2.1436 0.9277 1.2545	C 2.0971 -1.0036 -1.2467	C -2.1244 1.0237 -1.1723
C 3.5957 -1.2702 -0.3676	C 3.3803 1.6715 0.0007	C -3.4768 -1.5371 0.0743
C 3.2921 -0.1165 -1.3857	C 2.8198 -0.0113 1.6976	C -3.0140 -0.1363 1.5860
C 3.7949 -0.9799 1.0641	C 3.8698 0.9495 -1.0116	C -3.8853 -0.8678 -1.0712
C 3.3069 1.2902 -0.9531	C 3.2109 -1.1572 1.1322	C -3.2896 1.1414 1.1189
C 3.1784 -0.0445 1.7962	C 3.4826 -0.4207 -1.3949	C -3.3319 0.2682 -1.6450
C 2.8179 1.7729 0.1913	C 3.1654 -1.4960 -0.3002	C -2.9438 1.6840 -0.1062
H 0.3739 -0.1723 1.6887	H 0.3694 0.1004 -1.7244	H -0.3757 -0.0271 -1.7341
H 0.7275 -1.9249 0.1689	H 0.7241 1.9319 -0.2835	H -0.7154 -1.9165 -0.3565
H 0.3676 1.7808 -0.6435	H 0.3951 -1.7355 0.6963	H -0.3774 1.7173 0.7582
H -0.0028 -0.1442 -2.1058	H 0.0000 0.2483 2.0697	H -0.0012 -0.3231 2.0625
H -1.5188 2.3171 0.8557	H -1.4919 -2.3628 -0.7689	H 1.5134 2.3839 -0.6789
H 2.1083 -1.8743 -1.8416	H 2.1006 1.9813 1.6699	H -2.0806 -2.0363 1.5972
H -3.3867 -0.2316 -2.0378	H -3.3824 0.3044 2.0005	H 3.3833 -0.3837 2.0045
H -1.3109 -1.8634 1.2148	H -1.3228 1.7975 -1.3282	H 1.3313 -1.7527 -1.3820
H -1.6762 -1.9001 -1.4239	H -1.6877 1.9574 1.3060	H 1.6857 -2.0054 1.2468
H -3.1841 2.1429 -0.9629	H -3.1568 -2.1174 1.0427	H 3.1700 2.0706 1.1296
H -1.7156 1.8071 -1.8670	H -1.6905 -1.7225 1.9267	H 1.6987 1.6505 1.9937
H -2.4628 0.3839 2.1163	H -2.4546 -0.5009 -2.1199	H 2.4754 0.5664 -2.0893
H -5.2599 0.1939 1.4372	H -5.2557 -0.2890 -1.4483	H 5.2726 0.3263 -1.4134
H -5.6256 -0.2979 -0.2197	H -5.6219 0.2489 0.1942	H 5.6302 -0.2816 0.2063
H -5.0612 1.3435 0.1097	H -5.0372 -1.3944 -0.0869	H 5.0557 1.3753 -0.0077
H 1.8514 1.5955 2.0664	H 1.8592 -1.7248 -2.0204	H -1.8544 1.7694 -1.9192
H 4.2496 -2.0380 -0.7567	H 3.8088 2.6473 0.1937	H -4.1217 -2.3187 0.4521

H 3.7578 -0.2747 -2.3485 H 4.5563 -1.5783 1.5508 H 3.8219 1.9725 -1.6194 H 3.4671 0.0662 2.8341 H 2.9534 2.8252 0.4082	H 2.9533 0.1028 2.7662 H 4.6792 1.3753 -1.5930 H 3.6420 -1.9182 1.7724 H 4.0488 -0.8127 -2.2282 H 3.5597 -2.4758 -0.5308	H -3.4706 -0.4215 2.5243 H -4.8213 -1.2022 -1.5031 H -3.9472 1.7399 1.7383 H -3.8746 0.7153 -2.4672 H -3.3549 2.6524 -0.3574
Truncated cyclobutane-dehydrobullvalene moiety B Relaxed scan of dihedral a-b-c-d		
Φ_{abcd} = 0	Φ=1	Φ=2
C 1.089 0.758 -0.708 C 0.979 -0.805 -0.824 C 2.409 0.601 0.103 C 2.303 -0.946 -0.009 C -0.223 -1.559 -0.304 C -0.060 1.540 -0.059 C -1.647 -1.081 -0.472 C -0.996 -1.220 0.949 C -2.014 0.244 -1.011 C -0.759 -0.036 1.795 C -1.351 1.398 -0.849 C -0.348 1.171 1.387 H 1.262 1.197 -1.695 H 1.116 -1.114 -1.865 H 3.288 1.041 -0.374 H 2.349 0.973 1.127 H 3.120 -1.431 -0.548 H 2.175 -1.451 0.951 H -0.111 -2.631 -0.450 H 0.233 2.595 -0.075 H -2.369 -1.858 -0.695 H -1.354 -2.083 1.500 H -2.953 0.272 -1.559 H -0.993 -0.167 2.849 H -1.778 2.302 -1.274 H -0.267 1.963 2.124	C 1.091 0.757 -0.711 C 0.975 -0.805 -0.828 C 2.417 0.595 0.089 C 2.291 -0.952 -0.001 C -0.233 -1.556 -0.320 C -0.051 1.539 -0.046 C -1.655 -1.068 -0.481 C -1.003 -1.226 0.938 C -2.016 0.265 -1.004 C -0.754 -0.052 1.795 C -1.346 1.413 -0.832 C -0.335 1.156 1.397 H 1.253 1.201 -1.696 H 1.123 -1.113 -1.868 H 3.294 1.016 -0.406 H 2.376 0.984 1.109 H 3.107 -1.459 -0.522 H 2.145 -1.437 0.966 H -0.128 -2.628 -0.477 H 0.249 2.592 -0.053 H -2.382 -1.838 -0.712 H -1.366 -2.092 1.481 H -2.957 0.304 -1.547 H -0.986 -0.191 2.847 H -1.770 2.325 -1.243 H -0.245 1.940 2.142	C 1.092 0.756 -0.713 C 0.971 -0.805 -0.832 C 2.424 0.588 0.075 C 2.279 -0.958 0.006 C -0.245 -1.554 -0.338 C -0.040 1.537 -0.031 C -1.663 -1.052 -0.491 C -1.011 -1.233 0.925 C -2.019 0.290 -0.995 C -0.747 -0.071 1.794 C -1.341 1.431 -0.811 C -0.319 1.138 1.408 H 1.244 1.205 -1.698 H 1.129 -1.110 -1.871 H 3.300 0.989 -0.440 H 2.405 0.993 1.088 H 3.091 -1.487 -0.497 H 2.114 -1.424 0.980 H -0.149 -2.624 -0.509 H 0.267 2.588 -0.027 H -2.396 -1.815 -0.729 H -1.380 -2.101 1.459 H -2.963 0.341 -1.532 H -0.973 -0.221 2.846 H -1.761 2.350 -1.207 H -0.217 1.912 2.163
Φ=3	Φ=4	Φ=5
C 1.093 0.756 -0.716 C 0.966 -0.805 -0.836 C 2.432 0.581 0.060 C 2.266 -0.964 0.013 C -0.258 -1.551 -0.357 C -0.029 1.535 -0.016 C -1.672 -1.036 -0.501 C -1.019 -1.239 0.911 C -2.021 0.315 -0.986 C -0.740 -0.090 1.792 C -1.335 1.449 -0.789 C -0.302 1.119 1.420 H 1.235 1.210 -1.700 H 1.135 -1.108 -1.874 H 3.306 0.961 -0.473 H 2.433 1.002 1.067	C 1.094 0.755 -0.717 C 0.962 -0.805 -0.839 C 2.439 0.574 0.046 C 2.254 -0.969 0.020 C -0.269 -1.548 -0.374 C -0.019 1.533 -0.002 C -1.680 -1.021 -0.510 C -1.027 -1.245 0.899 C -2.023 0.337 -0.978 C -0.735 -0.108 1.791 C -1.329 1.464 -0.770 C -0.288 1.102 1.430 H 1.226 1.214 -1.701 H 1.142 -1.106 -1.876 H 3.310 0.934 -0.505 H 2.461 1.011 1.047	C 1.095 0.754 -0.718 C 0.959 -0.805 -0.841 C 2.446 0.567 0.033 C 2.243 -0.974 0.029 C -0.279 -1.545 -0.389 C -0.010 1.531 0.011 C -1.686 -1.007 -0.520 C -1.034 -1.250 0.886 C -2.023 0.358 -0.972 C -0.731 -0.124 1.789 C -1.323 1.479 -0.753 C -0.276 1.086 1.440 H 1.216 1.218 -1.701 H 1.149 -1.105 -1.877 H 3.314 0.908 -0.536 H 2.488 1.019 1.026

H 3.075 -1.514 -0.473	H 3.060 -1.539 -0.448	H 3.045 -1.562 -0.423
H 2.084 -1.410 0.993	H 2.057 -1.395 1.006	H 2.031 -1.379 1.020
H -0.170 -2.619 -0.542	H -0.190 -2.614 -0.572	H -0.207 -2.610 -0.599
H 0.286 2.583 0.000	H 0.303 2.579 0.025	H 0.319 2.574 0.048
H -2.410 -1.791 -0.747	H -2.422 -1.769 -0.764	H -2.433 -1.748 -0.781
H -1.394 -2.111 1.436	H -1.408 -2.119 1.415	H -1.421 -2.126 1.395
H -2.968 0.379 -1.517	H -2.971 0.414 -1.504	H -2.973 0.445 -1.493
H -0.960 -0.251 2.844	H -0.951 -0.279 2.842	H -0.945 -0.304 2.840
H -1.751 2.377 -1.170	H -1.741 2.400 -1.138	H -1.731 2.421 -1.108
H -0.188 1.882 2.184	H -0.164 1.855 2.203	H -0.143 1.829 2.220
Φ=6	Φ=7	Φ=8
C 1.096 0.754 -0.719	C 1.097 0.753 -0.720	C 1.098 0.752 -0.721
C 0.956 -0.806 -0.844	C 0.954 -0.806 -0.845	C 0.951 -0.806 -0.847
C 2.453 0.561 0.020	C 2.460 0.554 0.007	C 2.467 0.548 -0.006
C 2.232 -0.977 0.038	C 2.221 -0.981 0.047	C 2.210 -0.984 0.056
C -0.288 -1.542 -0.404	C -0.296 -1.539 -0.417	C -0.305 -1.536 -0.432
C -0.001 1.529 0.023	C 0.008 1.526 0.035	C 0.017 1.524 0.048
C -1.692 -0.994 -0.529	C -1.698 -0.982 -0.537	C -1.703 -0.969 -0.546
C -1.041 -1.254 0.875	C -1.049 -1.258 0.864	C -1.056 -1.262 0.852
C -2.023 0.377 -0.966	C -2.023 0.395 -0.960	C -2.022 0.414 -0.954
C -0.728 -0.139 1.787	C -0.726 -0.153 1.786	C -0.724 -0.168 1.783
C -1.317 1.492 -0.736	C -1.311 1.504 -0.720	C -1.304 1.517 -0.704
C -0.265 1.071 1.449	C -0.255 1.057 1.457	C -0.245 1.042 1.465
H 1.208 1.221 -1.701	H 1.200 1.225 -1.701	H 1.192 1.228 -1.701
H 1.157 -1.104 -1.877	H 1.165 -1.103 -1.877	H 1.173 -1.102 -1.877
H 3.317 0.882 -0.567	H 3.319 0.856 -0.597	H 3.320 0.828 -0.626
H 2.514 1.027 1.005	H 2.541 1.035 0.985	H 2.568 1.042 0.963
H 3.030 -1.584 -0.397	H 3.015 -1.605 -0.370	H 2.999 -1.625 -0.343
H 2.006 -1.363 1.034	H 1.981 -1.346 1.047	H 1.955 -1.328 1.060
H -0.223 -2.605 -0.624	H -0.239 -2.600 -0.648	H -0.254 -2.595 -0.672
H 0.335 2.570 0.070	H 0.350 2.565 0.090	H 0.365 2.560 0.112
H -2.443 -1.729 -0.797	H -2.453 -1.710 -0.812	H -2.462 -1.690 -0.828
H -1.434 -2.132 1.376	H -1.447 -2.137 1.358	H -1.460 -2.143 1.338
H -2.974 0.475 -1.484	H -2.974 0.503 -1.475	H -2.974 0.532 -1.465
H -0.940 -0.328 2.837	H -0.936 -0.351 2.833	H -0.933 -0.374 2.830
H -1.721 2.440 -1.079	H -1.711 2.458 -1.052	H -1.701 2.476 -1.024
H -0.124 1.805 2.236	H -0.107 1.783 2.251	H -0.089 1.758 2.266
Φ=9	Φ=10	Φ=11
C 1.099 0.752 -0.721	C 1.101 0.751 -0.720	C 1.103 0.750 -0.720
C 0.949 -0.806 -0.848	C 0.947 -0.806 -0.849	C 0.946 -0.806 -0.849
C 2.474 0.541 -0.018	C 2.481 0.534 -0.030	C 2.488 0.527 -0.042
C 2.199 -0.987 0.066	C 2.189 -0.989 0.076	C 2.179 -0.990 0.087
C -0.314 -1.532 -0.445	C -0.322 -1.529 -0.458	C -0.329 -1.526 -0.470
C 0.026 1.521 0.060	C 0.035 1.519 0.072	C 0.043 1.516 0.084
C -1.708 -0.956 -0.555	C -1.713 -0.944 -0.565	C -1.716 -0.932 -0.574
C -1.064 -1.266 0.840	C -1.072 -1.270 0.829	C -1.080 -1.273 0.817
C -2.021 0.433 -0.949	C -2.019 0.450 -0.945	C -2.016 0.467 -0.942
C -0.724 -0.182 1.781	C -0.725 -0.196 1.778	C -0.727 -0.209 1.776
C -1.297 1.529 -0.688	C -1.290 1.541 -0.674	C -1.282 1.552 -0.660
C -0.235 1.026 1.473	C -0.228 1.012 1.481	C -0.222 0.998 1.489
H 1.185 1.232 -1.699	H 1.178 1.235 -1.698	H 1.171 1.238 -1.696
H 1.181 -1.102 -1.876	H 1.190 -1.101 -1.875	H 1.199 -1.101 -1.872
H 3.322 0.800 -0.656	H 3.322 0.773 -0.684	H 3.322 0.745 -0.712
H 2.596 1.048 0.941	H 2.624 1.054 0.920	H 2.652 1.059 0.898
H 2.983 -1.645 -0.315	H 2.967 -1.664 -0.287	H 2.952 -1.681 -0.258
H 1.931 -1.309 1.073	H 1.908 -1.289 1.086	H 1.886 -1.269 1.100
H -0.269 -2.589 -0.697	H -0.283 -2.584 -0.719	H -0.296 -2.579 -0.740
H 0.380 2.554 0.134	H 0.394 2.549 0.154	H 0.408 2.543 0.175
H -2.471 -1.670 -0.845	H -2.479 -1.652 -0.861	H -2.485 -1.633 -0.878
H -1.474 -2.149 1.319	H -1.487 -2.154 1.300	H -1.501 -2.158 1.281

H -2.973 0.561 -1.457	H -2.971 0.588 -1.450	H -2.968 0.614 -1.445
H -0.932 -0.397 2.826	H -0.934 -0.418 2.822	H -0.937 -0.438 2.817
H -1.689 2.494 -0.997	H -1.678 2.510 -0.972	H -1.666 2.526 -0.948
H -0.073 1.734 2.281	H -0.060 1.711 2.295	H -0.049 1.689 2.308
Φ=12	Φ=13	Φ=14
C 1.104 0.749 -0.718	C 1.106 0.748 -0.717	C 1.108 0.747 -0.715
C 0.945 -0.807 -0.849	C 0.945 -0.807 -0.848	C 0.945 -0.808 -0.847
C 2.494 0.521 -0.053	C 2.501 0.514 -0.064	C 2.507 0.508 -0.075
C 2.170 -0.991 0.098	C 2.161 -0.992 0.110	C 2.152 -0.992 0.122
C -0.335 -1.523 -0.482	C -0.341 -1.520 -0.491	C -0.346 -1.517 -0.501
C 0.051 1.513 0.095	C 0.058 1.510 0.105	C 0.065 1.507 0.116
C -1.719 -0.921 -0.584	C -1.722 -0.911 -0.593	C -1.724 -0.900 -0.603
C -1.088 -1.276 0.806	C -1.096 -1.278 0.796	C -1.104 -1.280 0.786
C -2.013 0.482 -0.939	C -2.010 0.496 -0.938	C -2.006 0.510 -0.937
C -0.730 -0.221 1.773	C -0.734 -0.231 1.770	C -0.739 -0.241 1.768
C -1.275 1.561 -0.647	C -1.268 1.570 -0.636	C -1.260 1.579 -0.625
C -0.217 0.985 1.496	C -0.213 0.974 1.502	C -0.210 0.962 1.508
H 1.165 1.241 -1.693	H 1.159 1.243 -1.691	H 1.153 1.245 -1.688
H 1.209 -1.101 -1.869	H 1.219 -1.103 -1.865	H 1.230 -1.104 -1.861
H 3.321 0.719 -0.739	H 3.320 0.692 -0.764	H 3.318 0.666 -0.790
H 2.679 1.065 0.876	H 2.705 1.069 0.855	H 2.731 1.074 0.833
H 2.937 -1.697 -0.229	H 2.923 -1.712 -0.200	H 2.908 -1.725 -0.170
H 1.865 -1.249 1.113	H 1.845 -1.228 1.126	H 1.826 -1.207 1.140
H -0.307 -2.573 -0.760	H -0.318 -2.569 -0.776	H -0.327 -2.564 -0.794
H 0.421 2.538 0.194	H 0.434 2.533 0.211	H 0.446 2.527 0.229
H -2.491 -1.616 -0.895	H -2.496 -1.601 -0.910	H -2.500 -1.585 -0.927
H -1.515 -2.162 1.263	H -1.528 -2.164 1.246	H -1.542 -2.168 1.229
H -2.965 0.638 -1.441	H -2.960 0.659 -1.439	H -2.955 0.681 -1.437
H -0.943 -0.456 2.812	H -0.950 -0.472 2.808	H -0.958 -0.488 2.803
H -1.655 2.540 -0.926	H -1.644 2.553 -0.907	H -1.632 2.565 -0.888
H -0.040 1.669 2.321	H -0.034 1.651 2.332	H -0.029 1.633 2.343
Φ=15	Φ=16	Φ=17
C 1.109 0.746 -0.713	C 1.111 0.744 -0.711	C 1.113 0.743 -0.708
C 0.946 -0.808 -0.845	C 0.947 -0.809 -0.843	C 0.949 -0.810 -0.839
C 2.514 0.502 -0.085	C 2.520 0.496 -0.096	C 2.527 0.491 -0.105
C 2.144 -0.992 0.134	C 2.136 -0.991 0.147	C 2.129 -0.989 0.161
C -0.350 -1.514 -0.511	C -0.354 -1.512 -0.520	C -0.356 -1.510 -0.528
C 0.072 1.504 0.126	C 0.078 1.501 0.135	C 0.084 1.498 0.145
C -1.725 -0.891 -0.612	C -1.726 -0.882 -0.622	C -1.726 -0.874 -0.632
C -1.111 -1.282 0.776	C -1.119 -1.284 0.766	C -1.126 -1.287 0.756
C -2.002 0.524 -0.936	C -1.997 0.536 -0.937	C -1.992 0.546 -0.938
C -0.745 -0.251 1.765	C -0.752 -0.260 1.762	C -0.760 -0.268 1.758
C -1.253 1.587 -0.615	C -1.246 1.594 -0.606	C -1.239 1.601 -0.598
C -0.209 0.951 1.514	C -0.208 0.941 1.520	C -0.210 0.932 1.525
H 1.147 1.247 -1.685	H 1.142 1.248 -1.681	H 1.137 1.249 -1.677
H 1.241 -1.105 -1.856	H 1.252 -1.107 -1.850	H 1.264 -1.108 -1.844
H 3.316 0.639 -0.814	H 3.313 0.612 -0.838	H 3.309 0.587 -0.861
H 2.757 1.079 0.811	H 2.783 1.084 0.788	H 2.809 1.089 0.766
H 2.894 -1.737 -0.140	H 2.881 -1.748 -0.109	H 2.868 -1.758 -0.077
H 1.808 -1.185 1.153	H 1.791 -1.162 1.166	H 1.775 -1.139 1.181
H -0.336 -2.560 -0.810	H -0.344 -2.555 -0.825	H -0.349 -2.551 -0.839
H 0.457 2.521 0.247	H 0.468 2.516 0.264	H 0.477 2.511 0.279
H -2.503 -1.570 -0.944	H -2.505 -1.556 -0.961	H -2.505 -1.543 -0.978
H -1.555 -2.170 1.212	H -1.567 -2.173 1.195	H -1.579 -2.176 1.179
H -2.950 0.701 -1.436	H -2.944 0.720 -1.436	H -2.939 0.737 -1.437
H -0.968 -0.503 2.798	H -0.979 -0.517 2.793	H -0.993 -0.529 2.787
H -1.621 2.576 -0.869	H -1.611 2.587 -0.853	H -1.601 2.596 -0.837
H -0.026 1.616 2.354	H -0.025 1.600 2.364	H -0.028 1.585 2.373
Truncated cyclobutane-		

dehydrobullvalene moiety A Relaxed scan of dihedral a-b-c-d		
Φ = 0	Φ=1	Φ=2
C -0.978 -0.805 -0.824	C -0.983 -0.805 -0.820	C -0.987 -0.804 -0.816
C -1.089 0.758 -0.708	C -1.088 0.758 -0.706	C -1.088 0.759 -0.704
C -2.303 -0.946 -0.009	C -2.315 -0.939 -0.016	C -2.326 -0.932 -0.023
C -2.409 0.601 0.103	C -2.401 0.608 0.117	C -2.393 0.614 0.132
C 0.060 1.540 -0.059	C 0.070 1.542 -0.073	C 0.080 1.543 -0.087
C 0.223 -1.559 -0.304	C 0.210 -1.561 -0.287	C 0.199 -1.563 -0.270
C 1.351 1.398 -0.849	C 1.356 1.380 -0.868	C 1.360 1.364 -0.887
C 0.348 1.171 1.387	C 0.364 1.187 1.375	C 0.380 1.203 1.363
C 2.014 0.245 -1.011	C 2.012 0.221 -1.018	C 2.009 0.198 -1.026
C 0.759 -0.036 1.795	C 0.766 -0.019 1.795	C 0.774 -0.001 1.795
C 1.647 -1.081 -0.472	C 1.638 -1.096 -0.462	C 1.630 -1.109 -0.453
C 0.997 -1.220 0.949	C 0.989 -1.214 0.962	C 0.982 -1.208 0.974
H -1.116 -1.114 -1.865	H -1.111 -1.117 -1.861	H -1.105 -1.119 -1.857
H -1.262 1.197 -1.695	H -1.271 1.194 -1.693	H -1.281 1.190 -1.690
H -3.120 -1.431 -0.547	H -3.134 -1.402 -0.570	H -3.146 -1.373 -0.593
H -2.175 -1.451 0.951	H -2.205 -1.462 0.936	H -2.234 -1.473 0.922
H -3.288 1.041 -0.374	H -3.281 1.067 -0.340	H -3.273 1.090 -0.307
H -2.349 0.973 1.127	H -2.321 0.964 1.146	H -2.295 0.953 1.164
H -0.233 2.595 -0.075	H -0.215 2.598 -0.101	H -0.199 2.600 -0.125
H 0.111 -2.631 -0.450	H 0.090 -2.634 -0.420	H 0.071 -2.636 -0.390
H 1.777 2.302 -1.274	H 1.787 2.276 -1.305	H 1.795 2.251 -1.337
H 0.266 1.963 2.124	H 0.295 1.989 2.103	H 0.321 2.014 2.082
H 2.953 0.272 -1.559	H 2.949 0.236 -1.569	H 2.943 0.201 -1.581
H 0.993 -0.167 2.849	H 1.006 -0.139 2.848	H 1.018 -0.112 2.848
H 2.369 -1.858 -0.695	H 2.354 -1.880 -0.679	H 2.341 -1.901 -0.662
H 1.354 -2.083 1.500	H 1.341 -2.074 1.521	H 1.329 -2.064 1.540
Φ=3	Φ=4	Φ=5
C -0.991 -0.804 -0.812	C -0.996 -0.804 -0.807	C -1.001 -0.803 -0.803
C -1.087 0.759 -0.702	C -1.086 0.760 -0.699	C -1.085 0.760 -0.697
C -2.337 -0.925 -0.029	C -2.349 -0.916 -0.035	C -2.360 -0.908 -0.042
C -2.385 0.620 0.146	C -2.376 0.626 0.161	C -2.366 0.632 0.175
C 0.089 1.543 -0.101	C 0.100 1.544 -0.117	C 0.110 1.544 -0.133
C 0.188 -1.564 -0.253	C 0.175 -1.566 -0.233	C 0.162 -1.567 -0.216
C 1.364 1.346 -0.905	C 1.369 1.326 -0.926	C 1.373 1.307 -0.945
C 0.395 1.218 1.351	C 0.413 1.236 1.337	C 0.429 1.252 1.323
C 2.005 0.176 -1.033	C 2.001 0.149 -1.041	C 1.998 0.125 -1.047
C 0.781 0.016 1.795	C 0.789 0.036 1.794	C 0.796 0.054 1.793
C 1.621 -1.123 -0.443	C 1.612 -1.139 -0.432	C 1.602 -1.153 -0.421
C 0.975 -1.201 0.985	C 0.967 -1.192 0.998	C 0.960 -1.185 1.011
H -1.099 -1.122 -1.853	H -1.094 -1.125 -1.849	H -1.089 -1.128 -1.845
H -1.291 1.186 -1.688	H -1.301 1.182 -1.685	H -1.311 1.179 -1.682
H -3.158 -1.344 -0.614	H -3.171 -1.312 -0.636	H -3.182 -1.281 -0.657
H -2.262 -1.483 0.907	H -2.293 -1.491 0.892	H -2.322 -1.498 0.876
H -3.264 1.113 -0.273	H -3.254 1.138 -0.238	H -3.244 1.162 -0.203
H -2.268 0.942 1.182	H -2.239 0.931 1.200	H -2.210 0.918 1.217
H -0.183 2.602 -0.150	H -0.164 2.604 -0.179	H -0.147 2.605 -0.206
H 0.052 -2.638 -0.361	H 0.029 -2.640 -0.326	H 0.009 -2.641 -0.294
H 1.802 2.226 -1.369	H 1.810 2.196 -1.404	H 1.817 2.168 -1.436
H 0.347 2.038 2.061	H 0.377 2.066 2.036	H 0.405 2.091 2.013
H 2.937 0.166 -1.593	H 2.929 0.126 -1.606	H 2.923 0.089 -1.616
H 1.030 -0.085 2.848	H 1.045 -0.054 2.846	H 1.057 -0.026 2.845
H 2.327 -1.921 -0.645	H 2.312 -1.944 -0.624	H 2.297 -1.965 -0.606
H 1.317 -2.054 1.560	H 1.302 -2.042 1.583	H 1.289 -2.031 1.604
Φ=6	Φ=7	Φ=8
C -1.006 -0.803 -0.799	C -1.011 -0.802 -0.795	C -1.016 -0.801 -0.790
C -1.083 0.761 -0.695	C -1.082 0.762 -0.693	C -1.080 0.763 -0.690

C -2.372 -0.898 -0.048	C -2.383 -0.888 -0.054	C -2.394 -0.878 -0.060
C -2.356 0.639 0.190	C -2.347 0.645 0.205	C -2.337 0.650 0.219
C 0.120 1.544 -0.149	C 0.131 1.544 -0.164	C 0.140 1.543 -0.179
C 0.149 -1.567 -0.197	C 0.136 -1.568 -0.179	C 0.123 -1.568 -0.162
C 1.378 1.287 -0.965	C 1.381 1.267 -0.984	C 1.385 1.247 -1.002
C 0.446 1.269 1.309	C 0.463 1.285 1.295	C 0.480 1.299 1.281
C 1.994 0.099 -1.053	C 1.989 0.073 -1.060	C 1.985 0.049 -1.066
C 0.804 0.073 1.792	C 0.812 0.092 1.790	C 0.821 0.109 1.788
C 1.592 -1.169 -0.410	C 1.582 -1.183 -0.399	C 1.572 -1.197 -0.388
C 0.952 -1.176 1.023	C 0.944 -1.168 1.035	C 0.937 -1.161 1.047
H -1.084 -1.132 -1.840	H -1.080 -1.135 -1.835	H -1.076 -1.138 -1.830
H -1.321 1.175 -1.679	H -1.331 1.172 -1.676	H -1.341 1.169 -1.672
H -3.193 -1.246 -0.677	H -3.203 -1.212 -0.697	H -3.213 -1.177 -0.717
H -2.353 -1.505 0.861	H -2.384 -1.510 0.845	H -2.415 -1.515 0.828
H -3.232 1.186 -0.166	H -3.219 1.210 -0.130	H -3.206 1.232 -0.094
H -2.180 0.905 1.233	H -2.151 0.892 1.249	H -2.122 0.878 1.265
H -0.129 2.606 -0.235	H -0.111 2.607 -0.263	H -0.094 2.606 -0.289
H -0.014 -2.641 -0.261	H -0.035 -2.641 -0.228	H -0.056 -2.641 -0.198
H 1.826 2.137 -1.469	H 1.833 2.107 -1.502	H 1.840 2.079 -1.532
H 0.434 2.117 1.987	H 0.464 2.142 1.962	H 0.492 2.164 1.938
H 2.916 0.049 -1.626	H 2.909 0.010 -1.636	H 2.901 -0.027 -1.645
H 1.071 0.003 2.843	H 1.085 0.031 2.840	H 1.099 0.058 2.837
H 2.281 -1.988 -0.585	H 2.264 -2.009 -0.566	H 2.248 -2.029 -0.548
H 1.273 -2.019 1.626	H 1.260 -2.006 1.647	H 1.247 -1.995 1.666
Φ=9	Φ=10	Φ=11
C -1.021 -0.800 -0.785	C -1.027 -0.799 -0.780	C -1.032 -0.798 -0.775
C -1.079 0.764 -0.688	C -1.078 0.765 -0.684	C -1.077 0.766 -0.681
C -2.405 -0.867 -0.065	C -2.416 -0.857 -0.070	C -2.426 -0.846 -0.076
C -2.326 0.656 0.235	C -2.316 0.661 0.250	C -2.306 0.666 0.265
C 0.151 1.542 -0.194	C 0.160 1.541 -0.209	C 0.169 1.540 -0.223
C 0.110 -1.568 -0.143	C 0.097 -1.568 -0.125	C 0.084 -1.567 -0.107
C 1.388 1.226 -1.021	C 1.390 1.206 -1.039	C 1.392 1.186 -1.057
C 0.498 1.314 1.266	C 0.516 1.329 1.251	C 0.534 1.342 1.237
C 1.979 0.023 -1.072	C 1.973 -0.002 -1.079	C 1.967 -0.026 -1.085
C 0.830 0.127 1.785	C 0.841 0.144 1.782	C 0.851 0.161 1.779
C 1.561 -1.211 -0.378	C 1.550 -1.225 -0.367	C 1.539 -1.238 -0.358
C 0.930 -1.152 1.058	C 0.923 -1.144 1.070	C 0.917 -1.136 1.080
H -1.073 -1.141 -1.824	H -1.069 -1.144 -1.819	H -1.066 -1.146 -1.813
H -1.351 1.167 -1.667	H -1.362 1.165 -1.662	H -1.372 1.164 -1.657
H -3.222 -1.141 -0.736	H -3.230 -1.105 -0.755	H -3.237 -1.070 -0.772
H -2.447 -1.519 0.811	H -2.477 -1.521 0.795	H -2.507 -1.523 0.778
H -3.192 1.254 -0.057	H -3.178 1.275 -0.020	H -3.164 1.295 0.016
H -2.094 0.864 1.280	H -2.066 0.849 1.295	H -2.039 0.834 1.309
H -0.077 2.606 -0.316	H -0.060 2.605 -0.343	H -0.044 2.604 -0.368
H -0.078 -2.639 -0.165	H -0.100 -2.637 -0.133	H -0.121 -2.635 -0.102
H 1.846 2.048 -1.564	H 1.851 2.017 -1.595	H 1.856 1.988 -1.625
H 0.523 2.187 1.912	H 0.555 2.209 1.886	H 0.585 2.229 1.861
H 2.892 -0.066 -1.656	H 2.882 -0.105 -1.666	H 2.872 -0.141 -1.676
H 1.116 0.086 2.833	H 1.133 0.112 2.828	H 1.151 0.138 2.823
H 2.230 -2.050 -0.529	H 2.213 -2.070 -0.511	H 2.196 -2.089 -0.493
H 1.234 -1.982 1.687	H 1.222 -1.969 1.706	H 1.211 -1.957 1.724
Φ=12	Φ=13	Φ=14
C -1.037 -0.796 -0.771	C -1.042 -0.794 -0.766	C -1.047 -0.792 -0.762
C -1.076 0.768 -0.678	C -1.075 0.769 -0.675	C -1.073 0.771 -0.672
C -2.436 -0.835 -0.081	C -2.446 -0.823 -0.087	C -2.456 -0.810 -0.092
C -2.296 0.670 0.280	C -2.285 0.675 0.296	C -2.273 0.679 0.311
C 0.178 1.539 -0.237	C 0.188 1.538 -0.252	C 0.197 1.536 -0.266
C 0.071 -1.566 -0.090	C 0.058 -1.564 -0.072	C 0.045 -1.563 -0.055
C 1.394 1.167 -1.074	C 1.395 1.146 -1.091	C 1.397 1.125 -1.108
C 0.552 1.355 1.223	C 0.570 1.368 1.207	C 0.588 1.380 1.192

C 1.961 -0.049 -1.091	C 1.954 -0.075 -1.096	C 1.947 -0.099 -1.101
C 0.861 0.176 1.776	C 0.872 0.193 1.772	C 0.882 0.209 1.768
C 1.528 -1.251 -0.348	C 1.517 -1.264 -0.337	C 1.506 -1.277 -0.326
C 0.911 -1.128 1.090	C 0.905 -1.119 1.101	C 0.898 -1.110 1.111
H -1.063 -1.148 -1.807	H -1.059 -1.150 -1.801	H -1.056 -1.152 -1.796
H -1.383 1.163 -1.651	H -1.393 1.162 -1.645	H -1.404 1.162 -1.639
H -3.244 -1.034 -0.789	H -3.250 -0.998 -0.806	H -3.255 -0.960 -0.822
H -2.536 -1.524 0.761	H -2.566 -1.523 0.743	H -2.595 -1.522 0.725
H -3.148 1.314 0.052	H -3.132 1.333 0.090	H -3.114 1.352 0.127
H -2.013 0.818 1.323	H -1.986 0.801 1.337	H -1.958 0.784 1.350
H -0.028 2.602 -0.393	H -0.012 2.600 -0.419	H 0.004 2.598 -0.445
H -0.142 -2.632 -0.072	H -0.164 -2.629 -0.041	H -0.185 -2.625 -0.010
H 1.860 1.958 -1.654	H 1.863 1.926 -1.684	H 1.867 1.895 -1.712
H 0.615 2.249 1.836	H 0.647 2.269 1.809	H 0.678 2.287 1.782
H 2.862 -0.178 -1.685	H 2.850 -0.216 -1.694	H 2.839 -0.254 -1.702
H 1.169 0.162 2.818	H 1.187 0.187 2.812	H 1.204 0.212 2.806
H 2.179 -2.108 -0.476	H 2.162 -2.127 -0.458	H 2.144 -2.146 -0.439
H 1.199 -1.945 1.742	H 1.187 -1.932 1.761	H 1.174 -1.919 1.779
Φ=15	Φ=16	Φ=17
C -1.052 -0.790 -0.757	C -1.056 -0.788 -0.753	C -1.060 -0.786 -0.749
C -1.072 0.772 -0.669	C -1.071 0.774 -0.666	C -1.070 0.776 -0.663
C -2.465 -0.798 -0.098	C -2.474 -0.786 -0.104	C -2.482 -0.774 -0.111
C -2.262 0.683 0.326	C -2.251 0.685 0.341	C -2.239 0.688 0.355
C 0.206 1.534 -0.280	C 0.214 1.532 -0.292	C 0.223 1.531 -0.305
C 0.032 -1.561 -0.039	C 0.020 -1.559 -0.024	C 0.008 -1.557 -0.009
C 1.398 1.105 -1.124	C 1.399 1.087 -1.138	C 1.400 1.068 -1.153
C 0.605 1.392 1.177	C 0.621 1.402 1.164	C 0.637 1.412 1.150
C 1.940 -0.123 -1.106	C 1.934 -0.144 -1.110	C 1.927 -0.166 -1.114
C 0.891 0.224 1.764	C 0.900 0.237 1.761	C 0.908 0.251 1.757
C 1.495 -1.289 -0.316	C 1.484 -1.300 -0.307	C 1.474 -1.311 -0.297
C 0.892 -1.102 1.121	C 0.886 -1.095 1.129	C 0.880 -1.087 1.138
H -1.053 -1.154 -1.790	H -1.050 -1.155 -1.785	H -1.047 -1.156 -1.780
H -1.414 1.162 -1.633	H -1.423 1.163 -1.626	H -1.433 1.163 -1.620
H -3.259 -0.922 -0.838	H -3.262 -0.885 -0.854	H -3.264 -0.848 -0.870
H -2.624 -1.521 0.706	H -2.652 -1.518 0.687	H -2.680 -1.516 0.668
H -3.097 1.368 0.164	H -3.079 1.384 0.200	H -3.061 1.398 0.237
H -1.932 0.766 1.362	H -1.906 0.747 1.373	H -1.881 0.729 1.384
H 0.020 2.595 -0.469	H 0.034 2.593 -0.491	H 0.049 2.590 -0.514
H -0.206 -2.621 0.019	H -0.225 -2.616 0.045	H -0.244 -2.611 0.072
H 1.871 1.865 -1.739	H 1.874 1.837 -1.764	H 1.876 1.808 -1.789
H 0.707 2.304 1.757	H 0.734 2.319 1.733	H 0.761 2.334 1.709
H 2.828 -0.291 -1.710	H 2.818 -0.324 -1.716	H 2.807 -0.358 -1.723
H 1.219 0.234 2.800	H 1.233 0.255 2.795	H 1.248 0.275 2.789
H 2.127 -2.163 -0.421	H 2.111 -2.179 -0.405	H 2.095 -2.195 -0.388
H 1.163 -1.906 1.796	H 1.152 -1.894 1.812	H 1.142 -1.882 1.827

Table S13. Energies for the relaxed scans in cyclobutane-dihydrobullvalenes A and B and the distances from Ha and Hd to the cyclopropyl and the alkenyl termini of the fluxional Cope moiety

φ_{abcd}	B	A	E(B)	E(A)	Difference	Ha/d distances in B		Ha/d distances in A	
	(Hartrees)	(Hartrees)	(kcal/mol)	(kcal/mol)	(kcal/mol)	to cyclopr	to alkene	to cyclopr	to alkene
0	-465.7222293	-465.7222294	0.19539	0.195289	-0.0001	3.176	2.716	3.176	2.716
1	-465.7222734	-465.7221867	0.167705	0.222106	0.054401	3.151	2.728	3.202	2.703
2	-465.7223246	-465.7221414	0.135579	0.250527	0.114949	3.126	2.743	3.224	2.687
3	-465.7223844	-465.722093	0.098056	0.280924	0.182868	3.106	2.757	3.245	2.68
4	-465.7224446	-465.7220457	0.060247	0.310595	0.250348	3.085	2.776	3.271	2.67
5	-465.7224946	-465.7219994	0.028921	0.339631	0.31071	3.066	2.791	3.293	2.659
6	-465.722527	-465.7219576	0.008545	0.365843	0.357299	3.05	2.812	3.32	2.65
7	-465.7225406	-465.7219186	0	0.390339	0.390339	3.035	2.832	3.351	2.638
8	-465.7225371	-465.7218791	0.00221	0.415157	0.412947	3.016	2.857	3.373	2.63
9	-465.7225156	-465.7218359	0.015737	0.442243	0.426506	3.001	2.878	3.401	2.627
10	-465.7224721	-465.721784	0.042986	0.474787	0.431802	2.987	2.903	3.428	2.625
11	-465.7224016	-465.72172	0.087234	0.514937	0.427703	2.977	2.933	3.455	2.619
12	-465.7222972	-465.7216414	0.152797	0.564285	0.411488	2.968	2.958	3.482	2.617
13	-465.7221531	-465.7215478	0.243194	0.623005	0.379811	2.955	2.989	3.51	2.617
14	-465.7219666	-465.7214385	0.360219	0.691584	0.331365	2.946	3.015	3.533	2.618
15	-465.7217344	-465.7213118	0.505906	0.771129	0.265223	2.942	3.049	3.561	2.614
16	-465.7214535	-465.721162	0.682191	0.865118	0.182927	2.934	3.079	3.589	2.616
17	-465.7211213	-465.720982	0.890645	0.97807	0.087425	2.931	3.114	3.612	2.617
18	-465.7207338	-465.7207639	1.133821	1.114896	-0.01892	2.928	3.149	3.636	2.62
19	-465.7202882	-465.7205014	1.41344	1.27963	-0.13381	2.925	3.179	3.664	2.619

NMR CALCULATIONS

Geometries were obtained at B3LYP/6-311+G(d,p) level. Chemical shifts and spin-spin coupling constants were calculated with mPW1PW91/6-311+G(d,p) GIAO.

Table S14. Calculated chemical shifts for **9a** and **9b**, averaged by weighting at 20.6% of **9a** and 79.4% of **9b** and scaled as 29.086 – 0.908 δ_{calc}. The absolute error for most part was less then 0.1ppm, although one proton (the alpha proton in the oxetane moiety) deviated by 0.35 ppm (accented in red).

	Calculated (abs) δ		Averaged	Corrected/referenced	Experim. δ	Abs. Error
H ID#	**9a**	**9b**	20.6% **9a**	**29.086-0.908 δcalc**	**9**	**Δδ**
22	29.97	29.12	29.29	2.48	*2.5*	0.02
23	28.79	29.67	29.49	2.30	*2.4*	0.10
24	29.11	29.15	29.14	2.62	*2.5*	0.12
25	29.30	29.58	29.52	2.27	*2.35*	0.08
26	30.14	29.99	30.02	1.81	*1.82*	0.01
27	30.19	29.47	29.62	2.18	*2.17*	0.01
28	29.79	29.84	29.83	1.99	*2.06*	0.07
29	27.16	27.23	27.21	4.37	*4.72*	0.35
30	29.33	29.45	29.42	2.36	*2.3*	0.06
31	30.08	30.06	30.07	1.77	*1.68*	0.09
32	30.42	30.46	30.45	1.42	*1.33*	0.09
33	29.07	29.06	29.06	2.69	*2.81*	0.12
34	30.25	30.26	30.40	1.47	*1.48*	0.01
35	30.40	30.40	30.40	1.47	*1.48*	0.01
36	30.54	30.54	30.40	1.47	*1.48*	0.01
37	29.51	30.22	30.08	1.77	*1.7*	0.07
38	30.01	25.57	26.49	5.03	*5.0*	0.03
39	29.98	25.28	26.25	5.24	*5.19*	0.05
40	25.64	25.60	25.61	5.82	*5.72*	0.10
41	25.43	25.41	25.41	6.00	*5.94*	0.06
42	25.57	30.04	29.12	2.64	*2.5*	0.14
43	25.61	30.05	29.14	2.62	*2.66*	0.04

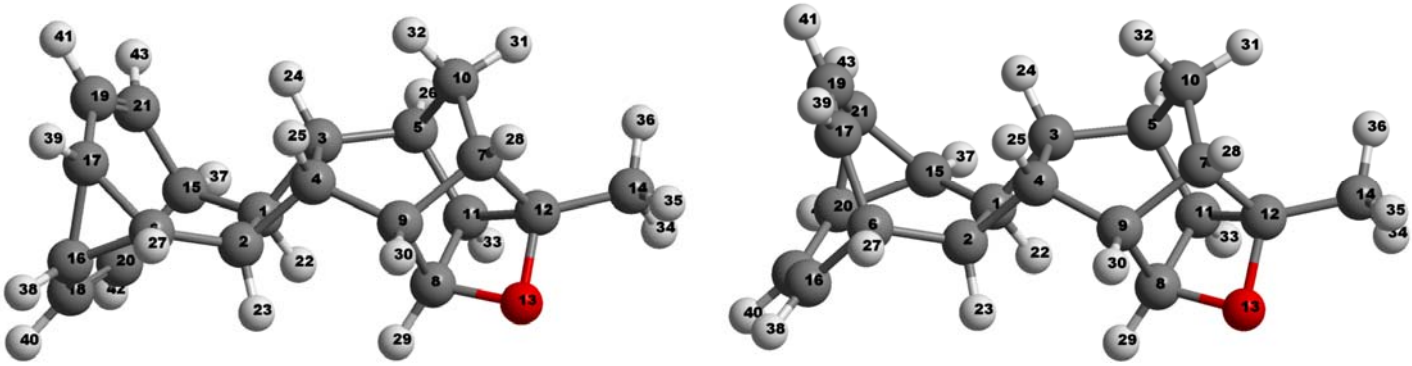


Figure S7. Labelling scheme for **9a** and **9b**

Table S15. Absolute values of the computed spin-spin coupling constants for **9a**

	22	23	24	25	26	27	28	29	30	31	32	33	34	35	36	37	38	39	40	41	42	43
22	0	9.5	6.7	1.4	0.3	0.2	0.2	0.4	0.1	0.1	0.2	0.4	0	0	0	6.4	0.1	0.2	0	0.1	0.3	0.4
23	9.5	0	1.4	2.7	0	3.7	0	0.3	0	0.2	0.1	0	0.1	0.1	0.1	0.5	0.3	0.2	0	0	0.1	0.4
24	6.7	1.4	0	9	4.8	0	0.1	0.2	0.1	0.2	0.2	0.2	0.1	0.1	0.1	0.3	0.1	0.1	0.1	0.1	0.1	0.3
25	1.4	2.7	9	0	0.4	0	0	0.7	4.2	0.1	0.4	0.1	0.1	0.1	0.1	0.1	0	0.2	0.1	0.1	0.1	0
26	0.3	0	4.8	0.4	0	0.1	1	0.2	0.2	6.4	0.3	5.4	0	0	0	0.2	0.1	0.1	0.1	0	0	0.1
27	0.2	3.7	0	0	0.1	0	0	0	0.1	0.1	0	0.1	0	0	0	0.1	8.6	8.5	0.1	0.2	0.3	0.3
28	0.2	0	0.1	0	1	0	0	0.4	5.8	1.9	1.8	0.9	0.3	0.3	0.3	0.1	0.1	0	0.1	0.1	0.1	0.1
29	0.4	0.3	0.2	0.7	0.2	0	0.4	0	1.8	0.1	0.2	3.1	0.3	0.3	0.3	0	0	0.1	0	0.1	0	0.1
30	0.1	0	0.1	4.2	0.2	0.1	5.8	1.8	0	0.2	0.4	1.2	0.1	0.1	0.1	0.1	0	0	0.1	0.1	0.1	0.1
31	0.1	0.2	0.2	0.1	6.4	0.1	1.9	0.1	0.2	0	12.5	0.3	0.1	0.1	0.1	0	0.1	0.1	0.1	0	0	0
32	0.2	0.1	0.2	0.4	0.3	0	1.8	0.2	0.4	12.5	0	0.1	0.1	0.1	0.1	0	0.1	0	0.1	0	0.1	0
33	0.4	0	0.2	0.1	5.4	0.1	0.9	3.1	1.2	0.3	0.1	0	0.4	0.4	0.4	0.1	0.1	0.1	0	0.1	0	0
34	0	0.1	0.1	0.1	0	0	0.3	0.3	0.1	0.1	0.1	0.4	0	0	0	0	0.1	0	0	0	0	0
35	0	0.1	0.1	0.1	0	0	0.3	0.3	0.1	0.1	0.1	0.4	0	0	0	0	0.1	0	0	0	0	0
36	0	0.1	0.1	0.1	0	0	0.3	0.3	0.1	0.1	0.1	0.4	0	0	0	0	0.1	0	0	0	0	0
37	6.4	0.5	0.3	0.1	0.2	0.1	0.1	0	0.1	0	0	0.1	0	0	0	0	0.3	0.3	0.2	0.4	8.1	8.3
38	0.1	0.3	0.1	0	0.1	8.6	0.1	0	0	0.1	0.1	0.1	0.1	0.1	0.1	0.3	0	7.8	7.6	0.2	0.4	0.3
39	0.2	0.2	0.1	0.2	0.1	8.5	0	0.1	0	0.1	0	0.1	0	0	0	0.3	7.8	0	0.1	7.7	0.2	0.4
40	0	0	0.1	0.1	0.1	0.1	0.1	0	0.1	0.1	0.1	0	0	0	0	0.2	7.6	0.1	0	0.1	11.4	0.3
41	0.1	0	0.1	0.1	0	0.2	0.1	0.1	0.1	0	0	0.1	0	0	0	0.4	0.2	7.7	0.1	0	0.3	11.1
42	0.3	0.1	0.1	0.1	0	0.3	0.1	0	0.1	0	0.1	0	0	0	0	8.1	0.4	0.2	11.4	0.3	0	0.3
43	0.4	0.4	0.3	0	0.1	0.3	0.1	0.1	0.1	0	0	0	0	0	0	8.3	0.3	0.4	0.3	11.1	0.3	0